Supplementary Information

Optical activity and helicity enhancement of highly sensitive dinaphthylmethane-based stereodynamic probes for secondary alcohols
Tomasz Mądry*[1], Agnieszka Czapik*[1,2] and Marcin Kwit*[1,2]

1 Department of Chemistry, Adam Mickiewicz University, Umultowska 89B, 61 614 Poznan, Poland.
2 Center for Advanced Technologies, Adam Mickiewicz University, Umultowska 89C, 61 614 Poznan, Poland.
e-mail: tomasz.madry@amu.edu.pl or marcin.kwit@amu.edu.pl
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References.
The theoretical approach we used in this work is common to all studied structures and includes (i) conformational search at molecular mechanics level (MM3); (ii) pre-optimization at the B3LYP/6-31G(d) level to reduce the number of thermally accessible conformers; (iii) re-optimization of conformers found at low-DFT level at B3LYP/6-311++G(d,p) or B3LYP/6-311G(d,p) level followed by frequency calculations to confirm stability of received structures; (iv) calculations on relative energies ($\Delta E_{\text{DFT}}$ and $\Delta G_{\text{DFT}}$) using Boltzmann distribution at $T = 298.15$ K; (v) rotator strengths calculations at the TD-DFT/6-311++G(d,p) level for all stable conformers of relative energies ranging from 0.0 to 2.0 kcal mol$^{-1}$.

Preliminary conformer distribution search was performed by the Scigress package[1] using the MM3 molecular mechanics force field. All possible conformers were analyzed using the systematic search methodology. Minimum energy conformers of relative steric energies ($\Delta E_{\text{st}}$) up to 10 kcal mol$^{-1}$ found by molecular mechanics were further fully optimized at the B3LYP/6-31G(d) level as implemented in the Gaussian09 package,[2] which significantly reduced the number of conformers. Higher accuracy calculations were performed at the B3LYP/6-311++G(d,p) or B3LYP/6-311G(d,p) level – depending on the size of the molecule studied.

The conformers obtained at the DFT/6-311G(d,p) level were the real minima (no imaginary frequencies have been found). Total and free energy values have been calculated and used to obtain the Boltzmann population of conformers at 298.15 K. Only the results for conformers that differ from the most stable one by less than 2 kcal mol$^{-1}$ have been taken into account for further calculations, following a generally accepted protocol.[3]

Even for the sterically congested 4b, the number of thermally allowed structures reached 7, whereas for more flexible 1e and 3b the number of low-energy conformers exceeded 20 (see Table 3 in the main text). In the later cases, the populations of the most abundant conformers are 22% and 23%, respectively. For 1e, the second most abundant conformer is only 0.3 kcal mol$^{-1}$ higher in energy. The increase in energy is caused by the bent conformation of an alkyl chain, not by any change in the structure of the chromophore. The same difference in energy is noted for the menthol derivative 4b, where the dominating conformer is 0.3 kcal mol$^{-1}$ lower in energy than the next one. However, due to the less conformational freedom, resulting in fewer conformers, the population of the lowest energy conformer no 1 of 4b amounts to 44%. A similar situation is visible for 6b, 8b-10b. In each of these cases, one dominant conformer can be distinguished, whose population varies from 43 to 56%.

The ether 7b is exceptional. In this particular case, the first 4 low-energy structures represent 66% of the population of all possible conformers, and energy differences between the most abundant ones are less than 0.2 kcal mol$^{-1}$.

The TD-DFT/6-311++G(d,p) calculations of ECD of 1e, 3b-5b and 7b-10b were performed for all structures re-optimized at higher levels of theory. In case of compound 6b to make calculations less computing power demanding, the TD-DFT calculations were performed on conformers where the long alkyl chain was replaced by the methyl group. We used two different density functionals for calculations of rotatory strengths, namely CAM-B3LYP[4] and M06-2X functional.[5] Rotatory strengths were calculated using both length and velocity representations. In the present study, the differences between the length and velocity representations of the calculated values of rotatory strengths were quite small, and for this reason only the velocity representations were further used.
The CD spectra were simulated by overlapping Gaussian functions for each transition according to the procedure previously described and using half band width 0.4 eV.[6] It should be noted, that there are not substantial differences between ECD spectra calculated with these two functionals for the same molecule, therefore we discussed here only results obtained with the use of CAM-B3LYP functional.

To establish influence of solvent and the method of ECD computation on the final results we performed additional theoretical studies for the chosen model compound 1e. We calculated ECD spectra at the ωB97-XD/6-311++G(2d,2p)[7] level for structures optimized in the gas phase. We did not observe any significant differences between results obtained with the use of CAM-B3LYP, M06-2X and ωB97-XD functionals. Moreover, the implementation of cyclohexane IEFPCM[8] solvent model to TD-DFT calculations also did not lead to results significantly different from the gas phase calculations. Then we performed structure optimization using IEFPCM solvent model of cyclohexane and acetonitrile, and after that for each optimized structure we calculate ECD spectrum using all three functional and respective solvent model. As expected changing of dielectric constant by 1, from gas phase to cyclohexane, has no significant effect on conformer distribution. In contrast, increase the dielectric constant in acetonitrile solvent model has effects that are more visible. Although, the conformer no 1 remained the lowest energy structure, the population of other conformers changes (see Tables S3-S5). However, the calculated and Boltzmann averaged ECD spectra remain in good agreement with the experimental ones regardless the functional used for TD-DFT calculations.

All three tested functionals performed very well, however, calculations with the use of CAM-B3LYP functional required less CPU power. Additionally, many authors indicate CAM-B3LYP functional as the best suited for TD-DFT calculations. The results obtained with the use of CAM-B3LYP functional are comparable to results obtained with the use of more sophisticated EOM-CCSD method.[9-13]

Simplified semi(empirical) approach to correlation of ECD data with structure of given ether were performed as follows: (i) conformer distribution analysis at molecular mechanics level (the same output files were used as for first step of DFT approach described above), (ii) applying Boltzmann distribution to narrow the number of conformers from hundred to amount that cover at least 95% population, (iii) applying Boltzmann distribution again to receive corrected population of received conformers, (iv) defining α₁ and α₂ angles within each of the given conformers, (v) collecting calculated at CAM-B3LYP/6-311++G(2d,2p) level data for model compound 11 for the same value of angles α₁ and α₂, (vi) calculating Boltzmann averaged ECD spectrum using corrected population, (vii) correcting the wavelengths of the calculated spectrum to match the experimental UV maxima, (viii) comparing the resulting spectrum with the experimental one.

Taking into account the dominant influence of the di(1-naphthyl)methane chromophore on the ECD spectrum, we assumed that the theoretical CD spectra of the conformers of 11, characterized by the same combination of α₁ and α₂ angles as the low energy conformers of 1e, 2b-10b found with molecular mechanics, will give the Boltzmann averaged ECD spectrum that correctly reproduces the experimental one. In this way, we wanted to avoid the most expensive part of the theoretical analysis, namely the optimization of the geometry and calculation of ECD spectra at the high level of theory. Unfortunately, this approach has worked properly for compounds 1e, 2b and 4b, 5b and 8b. In the remaining cases, the results were not satisfactory.
Single crystals X-ray analysis

The colourless single crystals of compounds 1e, 6b, 7b, 9b and 10b suitable for X-ray structural analysis were obtained by slow evaporation of solvent. The diffraction data were collected at 130K with an Oxford Diffraction SuperNova diffractometer using Cu Kα radiation. The intensity data were collected and processed using CrysAlisPro software.[14] The structures were solved by direct methods with the program SHELXT 2014/7[15] and refined by full-matrix least-squares method on F² with SHELXL 2014/7.[16] The carbon-bound hydrogen atoms were refined as riding on their carriers and their displacement parameters were set equal to 1.5Ueq(C) for the methyl groups and 1.2Ueq(C) for the remaining H atoms. Absolute structures of the compounds were specified by the synthetic procedure and confirmed using Flack parameter.[17]

A summary of the crystallographic data is given in Table S1. The analysis of intermolecular interactions was carried out using the Crystal Explorer.[18] Molecular graphics were generated with ORTEP-3 for Windows[19] and Mercury 3.10.2 software.[20] ORTEP representation of the molecular structures of the reported compounds are presented in Figure S1-S5. Geometry of selected hydrogen-bonds observed in reported crystals are given in Table S2.

For compound 1e asymmetric unit consists two independent molecules and one of them is slightly disordered over two positions with site occupancy factors for the alkyl chain 0.71 and 0.29 (Figure S1). In crystal structure molecules A and B are arranged alternately and are lined via C-H···π interactions (the aliphatic chain is a donor group) and edge-to-face interactions between aromatic rings (Figure S6).

For both, the 6b and 7b, the molecules are arranged into zig-zag chains in which the aliphatic tail interacts with the aromatic naphthyl rings of the next molecule. For 6b this zig-zag chains are linked into layers perpendicular to the [0 0 1] direction. The molecules are arranged antiparallel (head-to-tail) and the structure of this two-dimensional aggregate is stabilized by C-H···π interactions between the cholesterol tail and the aromatic system of the naphthyl part of the neighbouring molecule. The cholesterol parts of molecules are directed towards the middle and the naphthyl rings are on the outside of the layer. Through edge-to-face interactions, between the layer-bounding aromatic rings, they form a three-dimensional structure (Figure S7). In crystal 7b we also observe layers perpendicular to [0 0 1] direction, however, in this case they are created as a result of edge-to-face interactions between neighbouring zig-zag chains. The layers are arranged in a three-dimensional structure stabilized by hydrogen bonds type C-H···O between testosterone tails of molecules belonging to adjacent layers (Figure S8, Table S2).

In the crystal structure of 9b, molecules are linked into chains through the C-H···O hydrogen bonds (Table S2). The three-dimensional structure of crystal is stabilized by weak edge-to-face interactions (Figure S9).

As for 1e, the crystal structure of 10b consists two independent molecules in asymmetric unit. In the crystal structure, molecules A and B form separate, alternating layers. Layers of A molecules are stabilized by interactions of aromatic systems (mainly edge-to-face), while B layers are stabilized by C-H···O hydrogen bonds and edge-to-face interactions of aromatic rings (Figure 10b, Table S2). The 3D-structure is stabilized by C-H···O hydrogen bonds between layers A and B and interactions edge-to-face.
Table S1. Crystallographic data and refinement details for 1e, 6b, 7b, 9b and 10b.

|                | 1e    | 6b    | 7b    | 9b    | 10b    |
|----------------|-------|-------|-------|-------|-------|
| Chemical formula | C_{25}H_{24}O | C_{48}H_{60}O | C_{40}H_{42}O | C_{29}H_{24}O | C_{30}H_{26}O_3 |
| CCDC no.       | 1863317 | 1863318 | 1863315 | 1863319 | 1863316 |
| M_r            | 340.44   | 652.96  | 554.73  | 388.48  | 432.49  |
| Crystal system, space group | Monoclinic, \( P_2_1 \) | Monoclinic, \( P_2_1 \) | Orthorhombic, \( P_{2_1}2_12_1 \) | Orthorhombic, \( P_{2_1}2_12_1 \) | Monoclinic, \( P_2_1 \) |
| Temperature (K) | 130    | 130    | 130    | 130    | 130    |
| \( a, b, c (\text{Å}) \) | 10.7899 (1), 10.6921 (1), 16.1054 (1) | 11.0028 (2), 6.94336 (16), 25.5705 (5) | 7.88777 (11), 15.4336 (2), 24.6842 (4) | 7.67545 (13), 10.23967 (17), 26.7674 (4) | 17.4358(13), 7.4144(6), 17.9343(11) |
| \( \beta (°) \) | 91.339 (1) | 99.503 (2) | 97.876 (6) | 97.876 (6) | 97.876 (6) |
| \( V (\text{Å}^3) \) | 1857.52 (3) | 1926.68 (7) | 3004.96 (8) | 2103.76 (6) | 2296.6 (3) |
| \( Z \) | 4     | 2     | 4     | 4     | 4     |
| \( D_\text{s} (\text{Mg m}^{-3}) \) | 1.217  | 1.126  | 1.226  | 1.227  | 1.251  |
| Radiation type | Cu \( K\alpha \) | Cu \( K\alpha \) | Cu \( K\alpha \) | Cu \( K\alpha \) | Cu \( K\alpha \) |
| \( \mu (\text{mm}^{-1}) \) | 0.55   | 0.48   | 0.56   | 0.56   | 0.63   |
| Crystal size (mm) | 0.70 \( \times \) 0.20 \( \times \) 0.10 | 0.50 \( \times \) 0.05 \( \times \) 0.05 | 0.15 \( \times \) 0.08 \( \times \) 0.05 | 0.70 \( \times \) 0.05 \( \times \) 0.05 | 0.2 \( \times \) 0.02 \( \times \) 0.02 |
| No. of measured, independent and observed \(|I > 2\sigma(I)| \) reflections | 35677, 6771, 6690 | 20872, 7058, 6532 | 19932, 5510, 5091 | 20668, 4289, 4111 | 20911, 7985, 4867 |
| \( R_{\text{int}} \) | 0.023  | 0.045  | 0.044  | 0.035  | 0.099  |
| \( \sin \theta/\lambda_{\text{max}} (\text{Å}^{-1}) \) | 0.602  | 0.602  | 0.602  | 0.625  | 0.595  |
| \( R(\text{I}^2 > 2\sigma(\text{I})) \), \( wR(\text{I}^2) \), \( S \) | 0.029, 0.076, 1.04 | 0.039, 0.104, 1.04 | 0.040, 0.107, 1.03 | 0.037, 0.099, 1.10 | 0.100, 0.306, 1.02 |
| No. of parameters | 493    | 447    | 381    | 272    | 597    |
| No. of restraints | 1      | 1      | 0      | 0      | 1      |
| \( \Delta_{\text{max}}, \Delta_{\text{min}} (\text{e Å}^{-3}) \) | 0.19, -0.18 | 0.19, -0.14 | 0.14, -0.14 | 0.16, -0.17 | 0.46, -0.28 |
| Absolute structure parameter | 0.08 (6) | -0.03 (17) | -0.1 (2) | 0.02 (12) | -1.0(7) |
Table S2. Selected hydrogen-bonds parameters for 1e, 6b, 7b, 9b and 10b.

|    | D—H (Å) | H···A (Å) | D···A (Å) | D—H···A (°) |
|----|--------|--------|--------|-----------|
| 1e |        |        |        |           |
| C2A—H2A···O1A | 0.95 | 2.42 | 2.789 (2) | 102.9   |
| C12B—H12B···O1B | 0.95 | 2.43 | 2.795 (2) | 102.7   |
| 6b |        |        |        |           |
| C2—H2···O1 | 0.95 | 2.44 | 2.792 (3) | 101.7   |
| 7b |        |        |        |           |
| C12—H12···O1 | 0.95 | 2.38 | 2.761 (3) | 103.3   |
| C22—H22···O2<sup>i</sup> | 1.00 | 2.72 | 3.456 (4) | 130.8   |
| C26—H26A···O2<sup>j</sup> | 0.99 | 2.63 | 3.395 (4) | 134.1   |
| Symmetry code(s): (i) -x+1, y-1/2, -z+1/2. |
| 9b |        |        |        |           |
| C2—H2···O1 | 0.93 | 2.30 | 2.683 (3) | 104.0   |
| C17—H17···O1<sup>i</sup> | 0.93 | 2.60 | 3.490 (3) | 160.0   |
| Symmetry code(s): (i) x+1, y, z. |
| 10b |        |        |        |           |
| C2A—H2A···O1A | 0.95 | 2.51 | 2.846 (12) | 101.2   |
| C18A—H18A···O3A | 0.95 | 2.38 | 3.327 (15) | 175.4   |
| C21A—H21A···O3A | 1.00 | 2.56 | 3.167 (15) | 118.8   |
| C12B—H12B···O1B | 0.95 | 2.50 | 2.850 (11) | 101.8   |
| C24B—H24B···O1B | 0.95 | 3.10 | 3.198 (13) | 87.1    |
| C30B—H30F···O2A | 0.98 | 2.52 | 3.373 (17) | 145.0   |
Table S3. Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol⁻¹), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 1e.

| Compound           | E       | ΔG      | ΔE   | % ΔE | ΔΔG | % ΔΔG | #Imfreq |
|-------------------|---------|---------|------|------|------|-------|---------|
| 1e (conformer 1)  | -1042.60916 | -1042.24291 | 0.00 | 14.67 | 0.00 | 21.59 | 0       |
| 1e (conformer 2)  | -1042.60802 | -1042.24137 | 0.72 | 4.37  | 0.97 | 4.2   | 0       |
| 1e (conformer 3)  | -1042.60828 | -1042.24116 | 0.56 | 5.74  | 1.10 | 3.37  | 0       |
| 1e (conformer 4)  | -1042.60826 | -1042.24244 | 0.57 | 5.64  | 0.30 | 13.05 | 0       |
| 1e (conformer 5)  | -1042.60745 | -1042.24049 | 1.07 | 2.4   | 1.52 | 1.66  | 0       |
| 1e (conformer 6)  | -1042.60780 | -1042.24087 | 0.85 | 3.47  | 1.28 | 2.48  | 0       |
| 1e (conformer 7)  | -1042.60803 | -1042.24148 | 0.71 | 4.4   | 0.90 | 4.71  | 0       |
| 1e (conformer 8)  | -1042.60816 | -1042.24153 | 0.63 | 5.07  | 0.87 | 5     | 0       |
| 1e (conformer 9)  | -1042.60804 | -1042.24112 | 0.70 | 4.48  | 1.13 | 3.23  | 0       |
| 1e (conformer 10) | -1042.60871 | -1042.24177 | 0.28 | 9.12  | 0.72 | 6.44  | 0       |
| 1e (conformer 11) | -1042.60821 | -1042.24164 | 0.60 | 5.33  | 0.80 | 5.61  | 0       |
| 1e (conformer 12) | -1042.60799 | -1042.24176 | 0.73 | 4.25  | 0.72 | 6.37  | 0       |
| 1e (conformer 15) | -1042.60695 | -1042.23965 | 1.39 | 1.41  | 2.05 | -     | 0       |
| 1e (conformer 16) | -1042.60724 | -1042.24082 | 1.21 | 1.92  | 1.31 | 2.35  | 0       |
| 1e (conformer 17) | -1042.60738 | -1042.24056 | 1.12 | 2.23  | 1.48 | 1.78  | 0       |
| 1e (conformer 18) | -1042.60634 | -1042.24017 | 1.77 | 0.74  | 1.72 | 1.17  | 0       |
| 1e (conformer 22) | -1042.60785 | -1042.23972 | 0.82 | 3.66  | 2.01 | -     | 0       |
| 1e (conformer 32) | -1042.60772 | -1042.23975 | 0.90 | 3.2   | 1.98 | 0.76  | 0       |
| 1e (conformer 36) | -1042.60808 | -1042.24084 | 0.68 | 4.64  | 1.30 | 2.39  | 0       |
| 1e (conformer 39) | -1042.60786 | -1042.24081 | 0.82 | 3.68  | 1.32 | 2.32  | 0       |
| 1e (conformer 43) | -1042.60615 | -1042.23871 | 1.89 | 0.6   | 2.64 | -     | 0       |
| 1e (conformer 45) | -1042.60672 | -1042.23914 | 1.53 | 1.11  | 2.37 | -     | 0       |
| 1e (conformer 46) | -1042.60704 | -1042.24029 | 1.33 | 1.56  | 1.65 | 1.34  | 0       |
| 1e (conformer 79) | -1042.60760 | -1042.24159 | 0.98 | 2.82  | 0.83 | 5.28  | 0       |
| 1e (conformer 81) | -1042.60780 | -1042.24152 | 0.85 | 3.48  | 0.88 | 4.91  | 0       |
Table S4. Total and Gibbs free energies (\(E, \Delta G\), in Hartree), relative energies (\(\Delta E, \Delta \Delta G\), in kcal mol\(^{-1}\)), \(\Delta E\) and \(\Delta \Delta G\)-based percentage populations (\(% \Delta E, % \Delta \Delta G\)) and numbers of imaginary frequencies (\(#\text{Imfreq}\)) calculated at IEFPCM/B3LYP/6-311++G(d,p) level for individual conformers of ether 1e with the use of an IEFPCM model of cyclohexane.

| Compound          | \(E\)   | \(\Delta G\) | \(\Delta E\) | \(\% \Delta E\) | \(\Delta \Delta G\) | \(\% \Delta \Delta G\) | #Imfreq |
|-------------------|---------|--------------|--------------|-----------------|---------------------|------------------------|---------|
| 1e (conformer 1)  | -1042.61185 | -1042.24520  | 0.00         | 13.04           | 0.00                | 13.48                  | 0       |
| 1e (conformer 2)  | -1042.61071 | -1042.24406  | 0.71         | 3.91            | 0.72                | 4.01                   | 0       |
| 1e (conformer 3)  | -1042.61108 | -1042.24414  | 0.49         | 5.74            | 0.67                | 4.36                   | 0       |
| 1e (conformer 4)  | -1042.61104 | -1042.24501  | 0.51         | 5.54            | 0.12                | 10.97                  | 0       |
| 1e (conformer 5)  | -1042.61026 | -1042.24312  | 1.00         | 2.4             | 1.30                | 1.49                   | 0       |
| 1e (conformer 6)  | -1042.61073 | -1042.24395  | 0.70         | 3.99            | 0.78                | 3.6                    | 0       |
| 1e (conformer 7)  | -1042.61068 | -1042.24426  | 0.73         | 3.78            | 0.59                | 4.98                   | 0       |
| 1e (conformer 8)  | -1042.61102 | -1042.24450  | 0.52         | 5.42            | 0.44                | 6.43                   | 0       |
| 1e (conformer 9)  | -1042.61105 | -1042.24426  | 0.50         | 5.58            | 0.59                | 4.95                   | 0       |
| 1e (conformer 10) | -1042.61159 | -1042.24447  | 0.16         | 9.89            | 0.46                | 6.19                   | 0       |
| 1e (conformer 11) | -1042.61123 | -1042.24455  | 0.39         | 6.78            | 0.41                | 6.76                   | 0       |
| 1e (conformer 12) | -1042.61066 | -1042.24426  | 0.74         | 3.71            | 0.59                | 4.95                   | 0       |
| 1e (conformer 15) | -1042.60964 | -1042.24220  | 1.39         | 1.25            | 1.88                | 0.56                   | 0       |
| 1e (conformer 16) | -1042.61001 | -1042.24374  | 1.15         | 1.86            | 0.91                | 2.88                   | 0       |
| 1e (conformer 17) | -1042.61014 | -1042.24350  | 1.07         | 2.14            | 1.07                | 2.22                   | 0       |
| 1e (conformer 18) | -1042.60906 | -1042.24261  | 1.75         | 0.68            | 1.63                | 0.86                   | 0       |
| 1e (conformer 22) | -1042.61052 | -1042.24265  | 0.84         | 3.18            | 1.60                | 0.9                    | 0       |
| 1e (conformer 32) | -1042.61038 | -1042.24261  | 0.92         | 2.73            | 1.63                | 0.86                   | 0       |
| 1e (conformer 36) | -1042.61089 | -1042.24366  | 0.60         | 4.71            | 0.97                | 2.63                   | 0       |
| 1e (conformer 39) | -1042.61066 | -1042.24371  | 0.75         | 3.68            | 0.94                | 2.77                   | 0       |
| 1e (conformer 43) | -1042.60877 | -1042.24146  | 1.94         | 0.5             | 2.35                | -                      | 0       |
| 1e (conformer 45) | -1042.60945 | -1042.24202  | 1.51         | 1.02            | 1.99                | 0.46                   | 0       |
| 1e (conformer 46) | -1042.60970 | -1042.24307  | 1.35         | 1.34            | 1.34                | 1.41                   | 0       |
| 1e (conformer 79) | -1042.61053 | -1042.24429  | 0.83         | 3.22            | 0.57                | 5.11                   | 0       |
| 1e (conformer 81) | -1042.61072 | -1042.24460  | 0.71         | 3.93            | 0.38                | 7.15                   | 0       |
Table S5. Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol⁻¹), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at IEFPCM/B3LYP/6-311++G(d,p) level for individual conformers of ether 1e with the use of an IEFPCM model of acetonitrile.

| Compound      | E      | ΔG      | ΔE | % ΔE | ΔΔG | % ΔΔG | #Imfreq |
|---------------|--------|---------|----|------|-----|-------|---------|
| 1e (conformer 1) | -1042.61704 | -1042.25089 | 0.10 | 9.25 | 0.00 | 12.63 | 0       |
| 1e (conformer 2) | -1042.61593 | -1042.24913 | 0.80 | 2.83 | 1.10 | 1.96  | 0       |
| 1e (conformer 3) | -1042.61643 | -1042.25006 | 0.49 | 4.83 | 0.52 | 5.21  | 0       |
| 1e (conformer 4) | -1042.61641 | -1042.25038 | 0.50 | 4.71 | 0.32 | 7.32  | 0       |
| 1e (conformer 5) | -1042.61584 | -1042.24888 | 0.86 | 2.58 | 1.26 | 1.49  | 0       |
| 1e (conformer 6) | -1042.61653 | -1042.24997 | 0.42 | 5.38 | 0.58 | 4.73  | 0       |
| 1e (conformer 7) | -1042.61588 | -1042.24956 | 0.84 | 2.69 | 0.83 | 3.09  | 0       |
| 1e (conformer 8) | -1042.61673 | -1042.24999 | 0.30 | 6.63 | 0.56 | 4.87  | 0       |
| 1e (conformer 9) | -1042.61691 | -1042.25022 | 0.19 | 8.01 | 0.42 | 6.17  | 0       |
| 1e (conformer 10) | -1042.61721 | -1042.25035 | 0.00 | 11.01 | 0.34 | 7.14  | 0       |
| 1e (conformer 11) | -1042.61710 | -1042.25029 | 0.07 | 9.85 | 0.38 | 6.68  | 0       |
| 1e (conformer 12) | -1042.61614 | -1042.25019 | 0.67 | 3.54 | 0.44 | 6.02  | 0       |
| 1e (conformer 15) | -1042.61512 | -1042.24781 | 1.31 | 1.21 | 1.93 | 0.48  | 0       |
| 1e (conformer 16) | -1042.61566 | -1042.24979 | 0.97 | 2.13 | 0.69 | 3.94  | 0       |
| 1e (conformer 17) | -1042.61576 | -1042.24940 | 0.91 | 2.38 | 0.94 | 2.59  | 0       |
| 1e (conformer 18) | -1042.61465 | -1042.24819 | 1.60 | 0.73 | 1.70 | 0.72  | 0       |
| 1e (conformer 22) | -1042.61567 | -1042.24788 | 0.96 | 2.16 | 1.89 | 0.52  | 0       |
| 1e (conformer 32) | -1042.61553 | -1042.24776 | 1.06 | 1.85 | 1.97 | 0.46  | 0       |
| 1e (conformer 36) | -1042.61622 | -1042.24914 | 0.62 | 3.86 | 1.10 | 1.97  | 0       |
| 1e (conformer 39) | -1042.61597 | -1042.24904 | 0.78 | 2.97 | 1.16 | 1.77  | 0       |
| 1e (conformer 45) | -1042.61483 | -1042.24721 | 1.50 | 0.88 | 2.03 | -     | 0       |
| 1e (conformer 46) | -1042.61517 | -1042.24766 | 1.28 | 1.27 | 1.60 | 0.84  | 0       |
| 1e (conformer 79) | -1042.61630 | -1042.24834 | 0.57 | 4.22 | 0.01 | 12.39 | 0       |
| 1e (conformer 81) | -1042.61647 | -1042.25087 | 0.46 | 5.04 | 0.35 | 7.02  | 0       |
Table S6. Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol⁻¹), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 3b.

| Compound | E     | ΔG    | ΔE   | % ΔE | ΔΔG  | % ΔΔG | #Imfreq |
|----------|-------|-------|------|------|------|-------|---------|
| 3b (conformer 2) | -1277.33048 | -1276.83116 | 2.12 | -    | 1.86 | 1.14  | 0       |
| 3b (conformer 3) | -1277.33256 | -1276.83253 | 0.82 | 6.9  | 1.00 | 4.87  | 0       |
| 3b (conformer 4) | -1277.33194 | -1276.83365 | 1.20 | 3.58 | 0.29 | 16.07 | 0       |
| 3b (conformer 5) | -1277.33233 | -1276.83190 | 0.96 | 5.38 | 1.39 | 2.52  | 0       |
| 3b (conformer 7) | -1277.33102 | -1276.83005 | 1.78 | 1.35 | 2.55 |       | 0       |
| 3b (conformer 8) | -1277.33302 | -1276.83336 | 0.53 | 11.21| 0.47 | 11.81 | 0       |
| 3b (conformer 9) | -1277.33096 | -1276.83081 | 1.82 | 1.27 | 2.08 |       | 0       |
| 3b (conformer 10) | -1277.33117 | -1276.83080 | 1.69 | 1.58 | 2.08 |       | 0       |
| 3b (conformer 14) | -1277.33143 | -1276.83092 | 1.53 | 2.08 | 2.00 |       | 0       |
| 3b (conformer 15) | -1277.33134 | -1276.83103 | 1.58 | 1.88 | 1.93 | 1.0   | 0       |
| 3b (conformer 17) | -1277.33183 | -1276.83220 | 1.28 | 3.18 | 1.20 | 3.44  | 0       |
| 3b (conformer 19) | -1277.33386 | -1276.83411 | 0.00 | 27.36| 0.00 | 26.22 | 0       |
| 3b (conformer 20) | -1277.33090 | -1276.83020 | 1.86 | 1.19 | 2.46 |       | 0       |
| 3b (conformer 21) | -1277.33102 | -1276.82965 | 1.78 | 1.35 | 2.80 |       | 0       |
| 3b (conformer 23) | -1277.33071 | -1276.83062 | 1.98 | 0.97 | 2.19 |       | 0       |
| 3b (conformer 24) | -1277.33052 | -1276.83154 | 1.89 | 1.88 | 1.93 | 1.0   | 0       |
| 3b (conformer 25) | -1277.33294 | -1276.83306 | 0.99 | 5.18 | 0.66 | 8.6   | 0       |
| 3b (conformer 27) | -1277.33213 | -1276.83304 | 1.08 | 4.39 | 0.67 | 8.4   | 0       |
| 3b (conformer 28) | -1277.33208 | -1276.83146 | 1.12 | 4.13 | 1.67 | 1.57  | 0       |
| 3b (conformer 29) | -1277.33158 | -1276.83098 | 1.43 | 2.43 | 1.97 | 0.94  | 0       |
| 3b (conformer 31) | -1277.33046 | -1276.83140 | 2.13 | -    | 1.71 | 1.47  | 0       |
| 3b (conformer 36) | -1277.33149 | -1276.83156 | 1.49 | 2.22 | 1.60 | 1.75  | 0       |
| 3b (conformer 37) | -1277.33169 | -1276.83195 | 1.36 | 2.75 | 1.36 | 2.64  | 0       |
| 3b (conformer 38) | -1277.33088 | -1276.83018 | 1.87 | 1.17 | 2.47 |       | 0       |
| 3b (conformer 40) | -1277.33102 | -1276.83121 | 1.78 | 1.35 | 1.83 | 1.2   | 0       |
| 3b (conformer 41) | -1277.33223 | -1276.83126 | 1.02 | 4.88 | 1.79 | 1.27  | 0       |
| 3b (conformer 42) | -1277.33064 | -1276.83125 | 2.02 | -    | 1.80 | 1.26  | 0       |
| 3b (conformer 50) | -1277.33078 | -1276.83101 | 1.93 | 1.04 | 1.95 | 0.98  | 0       |
| 3b (conformer 56) | -1277.33089 | -1276.83117 | 1.86 | 1.18 | 1.85 | 1.15  | 0       |
Table S7. Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol⁻¹), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 4b.

| Compound     | E    | ΔG   | ΔE  | % ΔE | ΔΔG | % ΔΔG | #Imfreq |
|--------------|------|------|-----|------|-----|-------|---------|
| 4b (conformer 1) | -1277.34335 | -1276.83371 | 0.00 | 56.42 | 0.00 | 43.93 | 0       |
| 4b (conformer 2) | -1277.34101 | -1276.83087 | 1.47 | 4.7   | 1.79 | 2.15  | 0       |
| 4b (conformer 3) | -1277.34217 | -1276.83329 | 0.74 | 16.18 | 0.27 | 28    | 0       |
| 4b (conformer 5) | -1277.34198 | -1276.83290 | 0.86 | 13.19 | 0.51 | 18.64 | 0       |
| 4b (conformer 11) | -1277.34118 | -1276.83173 | 1.36 | 5.64  | 1.24 | 5.4   | 0       |
| 4b (conformer 12) | -1277.34083 | -1276.83073 | 1.59 | 3.88  | 1.87 | 1.87  | 0       |
| 4b (conformer 13) | -1277.33855 | -1276.82951 | 3.02 | -     | 2.64 | -     | 0       |
Table S8. Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol⁻¹), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 5b.

| Compound     | E       | ΔG      | ΔE   | % ΔE | ΔΔG | % ΔΔG | #Imfreq |
|--------------|---------|---------|------|------|-----|-------|---------|
| 5b (conformer 1) | -1116.618009 | -1116.26643 | 1.28 | 4.15 | 0.72 | 4.96  | 0       |
| 5b (conformer 2) | -1116.618462 | -1116.26758 | 0.99 | 6.71 | 0.00 | 16.71 | 0       |
| 5b (conformer 4) | -1116.616807 | -1116.26562 | 2.03 | -     | 1.23 | 2.09  | 0       |
| 5b (conformer 5) | -1116.617055 | -1116.26645 | 1.88 | 1.51 | 0.70 | 5.09  | 0       |
| 5b (conformer 6) | -1116.616455 | -1116.26627 | 2.25 | -     | 0.82 | 4.17  | 0       |
| 5b (conformer 7) | -1116.616514 | -1116.26543 | 2.22 | -     | 1.35 | 1.72  | 0       |
| 5b (conformer 8) | -1116.620042 | -1116.26757 | 0.00 | 35.79 | 0.00 | 16.66 | 0       |
| 5b (conformer 9) | -1116.618077 | -1116.26716 | 1.23 | 4.46 | 0.26 | 10.78 | 0       |
| 5b (conformer 11) | -1116.617212 | -1116.26627 | 1.78 | 1.78 | 0.82 | 4.17  | 0       |
| 5b (conformer 12) | -1116.615656 | -1116.26525 | 2.75 | -     | 1.46 | 1.43  | 0       |
| 5b (conformer 13) | -1116.616534 | -1116.26521 | 2.20 | -     | 1.49 | 1.36  | 0       |
| 5b (conformer 15) | -1116.615724 | -1116.26490 | 2.71 | -     | 1.68 | 0.98  | 0       |
| 5b (conformer 16) | -1116.620045 | -1116.26724 | 0.00 | 35.89 | 0.21 | 11.71 | 0       |
| 5b (conformer 17) | -1116.616706 | -1116.26538 | 2.10 | -     | 1.38 | 1.64  | 0       |
| 5b (conformer 18) | -1116.617343 | -1116.26606 | 1.70 | 2.05 | 0.95 | 3.34  | 0       |
| 5b (conformer 19) | -1116.615006 | -1116.26481 | 3.16 | -     | 1.74 | 0.89  | 0       |
| 5b (conformer 20) | -1116.616384 | -1116.26477 | 2.30 | -     | 1.76 | 0.86  | 0       |
| 5b (conformer 26) | -1116.616294 | -1116.26489 | 2.35 | -     | 1.69 | 0.97  | 0       |
| 5b (conformer 36) | -1116.616283 | -1116.26540 | 2.36 | -     | 1.36 | 1.67  | 0       |
| 5b (conformer 39) | -1116.617377 | -1116.26492 | 1.67 | 2.13 | 1.66 | 1.01  | 0       |
| 5b (conformer 41) | -1116.616516 | -1116.26568 | 2.21 | -     | 1.19 | 2.23  | 0       |
| 5b (conformer 43) | -1116.616169 | -1116.26525 | 2.43 | -     | 1.46 | 1.42  | 0       |
| 5b (conformer 44) | -1116.617979 | -1116.26543 | 1.30 | 4.02 | 1.34 | 1.73  | 0       |
| 5b (conformer 51) | -1116.617051 | -1116.26547 | 1.88 | 1.5  | 1.32 | 1.79  | 0       |
| 5b (conformer 52) | -1116.616191 | -1116.26452 | 2.42 | -     | 1.92 | 0.65  | 0       |
Table S9. Total and Gibbs free energies, (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol⁻¹), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 6b.

| Compound        | E    | ΔG    | ΔE   | % ΔE | ΔΔG | % ΔΔG | #Imfreq |
|-----------------|------|-------|------|------|-----|-------|---------|
| 6b (conformer 1)| -1940.97410 | -1940.09090 | 0.86 | 4.02 | 1.36 | 4.45 | 0       |
| 6b (conformer 2)| -1940.97430 | -1940.09121 | 0.73 | 4.99 | 1.17 | 6.19 | 0       |
| 6b (conformer 3)| -1940.97470 | -1940.09027 | 0.48 | 7.64 | 1.75 | 2.3  | 0       |
| 6b (conformer 4)| -1940.97459 | -1940.09120 | 0.54 | 6.8  | 1.17 | 6.12 | 0       |
| 6b (conformer 5)| -1940.97485 | -1940.09307 | 0.39 | 8.89 | 0.00 | 44.41| 0       |
| 6b (conformer 6)| -1940.97541 | -1940.09154 | 0.03 | 16.12| 0.96 | 8.82 | 0       |
| 6b (conformer 7)| -1940.97546 | -1940.09168 | 0.00 | 17.04| 0.87 | 10.2 | 0       |
| 6b (conformer 8)| -1940.97377 | -1940.09054 | 1.06 | 2.83 | 1.59 | 3.05 | 0       |
| 6b (conformer 9)| -1940.97347 | -1940.08950 | 1.25 | 2.07 | 2.24 |       | 0       |
| 6b (conformer 10)| -1940.97337 | -1940.09160 | 1.31 | 1.86 | 0.92 | 9.37 | 0       |
| 6b (conformer 14)| -1940.97417 | -1940.09042 | 0.81 | 4.36 | 1.66 | 2.69 | 0       |
| 6b (conformer 15)| -1940.97335 | -1940.08813 | 1.32 | 1.83 | 3.10 |       | 0       |
| 6b (conformer 18)| -1940.97420 | -1940.08959 | 0.79 | 4.47 | 2.18 |       | 0       |
| 6b (conformer 24)| -1940.97286 | -1940.08872 | 1.63 | 1.08 | 2.73 |       | 0       |
| 6b (conformer 32)| -1940.97357 | -1940.08855 | 1.18 | 2.31 | 2.84 |       | 0       |
| 6b (conformer 44)| -1940.97417 | -1940.09031 | 0.81 | 4.35 | 1.73 | 2.39 | 0       |
| 6b (conformer 51)| -1940.97414 | -1940.08946 | 0.83 | 4.21 | 2.26 |       | 0       |
| 6b (conformer 60)| -1940.97374 | -1940.08802 | 1.08 | 2.76 | 3.17 |       | 0       |
| 6b (conformer 70)| -1940.97360 | -1940.08920 | 1.17 | 2.38 | 2.43 |       | 0       |
**Table S10.** Total and Gibbs free energies, \((E, ΔG, \text{in Hartree})\), relative energies \((ΔE, ΔΔG, \text{in kcal mol}^{-1})\), ΔE and ΔΔG-based percentage populations \((% ΔE, % ΔΔG)\) and numbers of imaginary frequencies \(#\text{Imfreq}\) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 7b.

| Compound | \(E\)  | \(ΔG\)  | \(ΔE\)  | % ΔE  | ΔΔG  | % ΔΔG  | #Imfreq |
|----------|--------|--------|--------|-------|-------|---------|---------|
| 7b (conformer 1) | -1700.42866 | -1699.77509 | 0.21 | 21.25 | 0.16 | 16.51 | 0 |
| 7b (conformer 2) | -1700.42899 | -1699.77534 | 0.00 | 30.2  | 0.16 | 16.64 | 0 |
| 7b (conformer 3) | -1700.42749 | -1699.77509 | 0.94 | 6.14  | 0.16 | 16.64 | 0 |
| 7b (conformer 4) | -1700.42750 | -1699.77483 | 0.94 | 6.19  | 0.32 | 12.55 | 0 |
| 7b (conformer 5) | -1700.42745 | -1699.77400 | 0.97 | 5.87  | 0.84 | 5.21  | 0 |
| 7b (conformer 6) | -1700.42693 | -1699.77409 | 1.29 | 3.4   | 0.79 | 5.71  | 0 |
| 7b (conformer 7) | -1700.42813 | -1699.77409 | 0.54 | 12.06 | 0.79 | 5.74  | 0 |
| 7b (conformer 9) | -1700.42545 | -1699.77271 | 2.22 | -     | 1.65 | 1.33  | 0 |
| 7b (conformer 11) | -1700.42598 | -1699.77208 | 1.89 | 1.24  | 2.05 | -     | 0 |
| 7b (conformer 12) | -1700.42745 | -1699.77400 | 0.97 | 5.87  | 0.84 | 5.21  | 0 |
| 7b (conformer 13) | -1700.42735 | -1699.77353 | 1.03 | 5.28  | 1.14 | 3.17  | 0 |
| 7b (conformer 14) | -1700.42664 | -1699.77399 | 1.48 | 2.5   | 0.85 | 5.18  | 0 |
| 7b (conformer 16) | -1700.42516 | -1699.77250 | 2.41 | -     | 1.79 | 1.06  | 0 |
Table S11. Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol⁻¹), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 8b.

| Compound   | E    | ΔG   | ΔE  | % ΔE | ΔΔG  | % ΔΔG | #Imfreq |
|------------|------|------|-----|------|------|-------|---------|
| 8b (conformer 1) | -1419.84914 | -1419.46500 | 0.57 | 8.74 | 0.00 | 56.31 | 0       |
| 8b (conformer 2) | -1419.84846 | -1419.46221 | 0.99 | 4.26 | 1.75 | 2.91  | 0       |
| 8b (conformer 3) | -1419.84896 | -1419.46274 | 0.68 | 7.21 | 1.42 | 5.15  | 0       |
| 8b (conformer 4) | -1419.84699 | -1419.46165 | 1.91 | 0.9  | 2.11 | -     | 0       |
| 8b (conformer 6) | -1419.84829 | -1419.46215 | 1.10 | 3.55 | 1.79 | 2.74  | 0       |
| 8b (conformer 7) | -1419.85004 | -1419.46323 | 0.00 | 22.79 | 1.11 | 8.64  | 0       |
| 8b (conformer 8) | -1419.84988 | -1419.46227 | 0.10 | 19.16 | 1.72 | 3.1   | 0       |
| 8b (conformer 11) | -1419.84759 | -1419.46196 | 1.54 | 1.69 | 1.91 | 2.23  | 0       |
| 8b (conformer 12) | -1419.84758 | -1419.46212 | 1.54 | 1.69 | 1.81 | 2.65  | 0       |
| 8b (conformer 14) | -1419.84793 | -1419.46157 | 1.32 | 2.44 | 2.16 | -     | 0       |
| 8b (conformer 15) | -1419.84905 | -1419.46187 | 0.62 | 7.99 | 1.97 | 2.03  | 0       |
| 8b (conformer 16) | -1419.84817 | -1419.46316 | 1.18 | 3.13 | 1.15 | 8.02  | 0       |
| 8b (conformer 19) | -1419.84811 | -1419.46292 | 1.22 | 2.93 | 1.31 | 6.21  | 0       |
| 8b (conformer 20) | -1419.84722 | -1419.46023 | 1.77 | 1.14 | 3.00 | -     | 0       |
| 8b (conformer 22) | -1419.84700 | -1419.46058 | 1.91 | 0.91 | 2.78 | -     | 0       |
| 8b (conformer 25) | -1419.84708 | -1419.46169 | 1.86 | 0.99 | 2.08 | -     | 0       |
| 8b (conformer 27) | -1419.84878 | -1419.46139 | 0.79 | 5.97 | 2.27 | -     | 0       |
| 8b (conformer 31) | -1419.84697 | -1419.46072 | 1.93 | 0.88 | 2.69 | -     | 0       |
| 8b (conformer 42) | -1419.84831 | -1419.46085 | 1.09 | 3.63 | 2.61 | -     | 0       |

Table S12. Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol⁻¹), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 9b.

| Compound   | E    | ΔG   | ΔE  | % ΔE | ΔΔG  | % ΔΔG | #Imfreq |
|------------|------|------|-----|------|------|-------|---------|
| 9b (conformer 1) | -1195.06505 | -1194.67665 | 0.34 | 28.4 | 0.40 | 23.4  | 0       |
| 9b (conformer 3) | -1195.06560 | -1194.67728 | 0.00 | 50.68 | 0.00 | 45.76 | 0       |
| 9b (conformer 5) | -1195.06307 | -1194.67571 | 1.59 | 3.48 | 0.99 | 8.66  | 0       |
| 9b (conformer 9) | -1195.06365 | -1194.67445 | 1.23 | 6.4  | 1.78 | 2.27  | 0       |
| 9b (conformer 11) | -1195.06208 | -1194.67434 | 2.21 | -    | 1.84 | 2.04  | 0       |
| 9b (conformer 17) | -1195.06416 | -1194.67639 | 0.90 | 11.05 | 0.56 | 17.88 | 0       |
**Table S13.** Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol\(^{-1}\)), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of ether 10b.

| Compound       | E       | ΔG       | ΔE   | % ΔE | ΔΔG | % ΔΔG | #Imfreq |
|----------------|---------|----------|------|------|-----|-------|---------|
| 10b (conformer 1) | -1383.66969 | -1383.27184 | 1.71 | 2.61 | 1.44 | 3.78  | 0       |
| 10b (conformer 2) | -1383.66979 | -1383.27189 | 1.64 | 2.91 | 1.41 | 4.00  | 0       |
| 10b (conformer 4) | -1383.66858 | -1383.27253 | 2.40 | -    | 1.01 | 7.86  | 0       |
| 10b (conformer 5) | -1383.67241 | -1383.27413 | 0.00 | 46.53 | 0.00 | 43.15 | 0       |
| 10b (conformer 7) | -1383.66774 | -1383.27095 | 2.93 | -    | 2.00 | 1.48  | 0       |
| 10b (conformer 9) | -1383.66837 | -1383.27209 | 2.53 | -    | 1.28 | 4.94  | 0       |
| 10b (conformer 11) | -1383.67238 | -1383.27360 | 0.02 | 45.26 | 0.34 | 24.45 | 0       |
| 10b (conformer 13) | -1383.66861 | -1383.27142 | 2.38 | -    | 1.70 | 2.43  | 0       |
| 10b (conformer 26) | -1383.66860 | -1383.27128 | 2.39 | -    | 1.79 | 2.09  | 0       |
| 10b (conformer 53) | -1383.66972 | -1383.27157 | 1.69 | 2.69 | 1.61 | 2.85  | 0       |
| 10b (conformer 74) | -1383.66802 | -1383.27161 | 2.76 | -    | 1.59 | 2.96  | 0       |
Table S14. Dihedral angles $\alpha$, $\beta$, $\gamma$, $\omega$ (in degrees) of calculated at the B3LYP/6-311++G(d,p) level for each low-energy conformer of ether 1e.

| Compound | $\alpha_1$ | $\alpha_2$ | $\beta_1$ | $\beta_2$ | $\gamma$ | $\omega$ |
|----------|------------|------------|-----------|-----------|----------|----------|
| 1e (conformer 1) | -71 | 11 | 43 | 41 | -64 | -55 |
| 1e (conformer 2) | -13 | 69 | -46 | -37 | 59 | 52 |
| 1e (conformer 3) | -12 | 69 | -47 | -36 | -173 | 51 |
| 1e (conformer 4) | -70 | 12 | 45 | 37 | -176 | -53 |
| 1e (conformer 5) | -99 | 20 | -21 | 43 | 60 | -77 |
| 1e (conformer 6) | -85 | 19 | -40 | -36 | 60 | -61 |
| 1e (conformer 7) | -13 | 71 | -47 | 12 | -63 | 53 |
| 1e (conformer 8) | -23 | 101 | 47 | 43 | 59 | 76 |
| 1e (conformer 9) | -105 | 26 | -50 | -42 | -174 | -79 |
| 1e (conformer 10) | -26 | 107 | 51 | 56 | -60 | 80 |
| 1e (conformer 11) | -24 | 103 | 48 | 44 | -174 | 77 |
| 1e (conformer 12) | 110 | 2 | 33 | 39 | -65 | 113 |
| 1e (conformer 15) | -6 | -115 | -45 | -38 | 59 | 48 |
| 1e (conformer 16) | -5 | -114 | -41 | -34 | -172 | 50 |
| 1e (conformer 17) | 114 | 4 | 42 | 38 | -175 | 118 |
| 1e (conformer 18) | 114 | 4 | 41 | 37 | 60 | 117 |
| 1e (conformer 22) | 131 | 122 | 61 | 63 | -58 | 87 |
| 1e (conformer 32) | 133 | 120 | 58 | 50 | 61 | -117 |
| 1e (conformer 36) | 132 | 122 | 58 | 47 | -175 | -116 |
| 1e (conformer 39) | -123 | -132 | -57 | -43 | -171 | 116 |
| 1e (conformer 43) | -117 | -135 | -34 | 38 | 61 | 120 |
| 1e (conformer 45) | -116 | -136 | -32 | 39 | -171 | 120 |
| 1e (conformer 46) | -7 | -113 | -44 | 8 | -63 | -119 |
| 1e (conformer 79) | -18 | 95 | 16 | -45 | -174 | 74 |
| 1e (conformer 81) | -101 | 22 | -21 | 46 | -171 | -78 |

1. $\alpha_1 = \text{C2-C1-C-O}$
2. $\alpha_2 = \text{C2'-C1'-C-O}$
3. $\beta_1 = \text{H-C-O-C'}$
4. $\beta_2 = \text{C-O-C'-H}$
5. $\gamma = \text{O-C'-C}$
6. $\omega$ = torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)
Table S15. Dihedral angles $\alpha$, $\beta$, $\gamma$, $\omega$ (in degrees) of calculated at the B3LYP/6-311++G(d,p) level for each low-energy conformer of ether 3b.

| Compound | $\alpha_1$ | $\alpha_2$ | $\beta_1$ | $\beta_2$ | $\gamma$ | $\delta$ | $\omega$ |
|----------|------------|------------|-----------|-----------|----------|---------|---------|
| 3b (conformer 2) | -12 | 72 | -49 | 179 | -174 | 174 | 55 |
| 3b (conformer 3) | -101 | 21 | -38 | -172 | -60 | 170 | -77 |
| 3b (conformer 4) | -72 | 12 | 49 | -179 | -62 | 168 | -55 |
| 3b (conformer 5) | -104 | 23 | -41 | -177 | -63 | 170 | -80 |
| 3b (conformer 7) | -14 | 72 | -50 | 177 | 62 | 61 | 53 |
| 3b (conformer 8) | -107 | 24 | -40 | 175 | 68 | 71 | -82 |
| 3b (conformer 9) | -72 | 13 | 48 | -179 | 60 | 60 | -54 |
| 3b (conformer 10) | -22 | 103 | 39 | 175 | 71 | 165 | 80 |
| 3b (conformer 14) | -117 | -133 | -47 | 174 | 68 | 69 | 120 |
| 3b (conformer 15) | -20 | 99 | 38 | 172 | 71 | 161 | 76 |
| 3b (conformer 17) | -13 | 72 | -48 | 177 | 64 | 65 | 54 |
| 3b (conformer 19) | -23 | 104 | 41 | 178 | 63 | 69 | 79 |
| 3b (conformer 20) | -133 | 119 | 47 | -176 | 175 | -66 | -118 |
| 3b (conformer 21) | -120 | -132 | -48 | 176 | -172 | 172 | 118 |
| 3b (conformer 23) | 112 | 5 | 47 | -175 | -63 | 169 | 117 |
| 3b (conformer 24) | -71 | 14 | 50 | -178 | 179 | -64 | -53 |
| 3b (conformer 25) | -23 | 104 | 40 | 176 | 62 | 70 | 80 |
| 3b (conformer 27) | -24 | 107 | 40 | -178 | 175 | 68 | 82 |
| 3b (conformer 28) | 131 | 119 | 50 | -167 | -63 | 167 | -120 |
| 3b (conformer 29) | -120 | -132 | -48 | 179 | -179 | 71 | 117 |
| 3b (conformer 31) | 111 | 5 | 45 | -173 | -67 | 162 | 115 |
| 3b (conformer 36) | -120 | -131 | -49 | 169 | 65 | 67 | 119 |
| 3b (conformer 37) | -117 | -133 | -52 | -178 | -68 | 164 | 120 |
| 3b (conformer 38) | -117 | -133 | -50 | -178 | -62 | 170 | 120 |
| 3b (conformer 40) | 133 | 118 | 50 | -179 | 65 | 71 | -119 |
| 3b (conformer 41) | -116 | -133 | -50 | -177 | -63 | 166 | 121 |
| 3b (conformer 42) | -8 | -113 | -50 | 172 | -62 | 169 | -120 |
| 3b (conformer 50) | -120 | -130 | -47 | 174 | 65 | 67 | 118 |
| 3b (conformer 56) | -119 | -133 | -49 | 177 | -179 | -64 | 118 |

$^7 \alpha_1 = \text{C2-C1-C-O}$

$^8 \alpha_2 = \text{C2'-C1'-C-O}$

$^9 \beta_1 = \text{H-C-O-C}$

$^{10} \beta_2 = \text{C-O-C-C}$

$^{11} \gamma = \text{O-C-C-C}$

$^{12} \delta = \text{C-C-C'-CH}_3$

$^{13} \omega = \text{torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)}$
Table S16. Dihedral angles $\alpha$, $\beta$, $\gamma$, $\omega$ (in degrees) of calculated at the B3LYP/6-311++G(d,p) level for each low-energy conformer of ether 4b.

| Compound         | $\alpha_1^{14}$ | $\alpha_2^{15}$ | $\beta_1^{16}$ | $\beta_2^{17}$ | $\gamma^{18}$ | $\omega^{19}$ |
|------------------|------------------|------------------|-----------------|-----------------|---------------|--------------|
| 4b (conformer 1) | -73              | 11               | 33              | 40              | -56           | -57          |
| 4b (conformer 2) | -82              | 16               | -12             | 53              | -55           | -61          |
| 4b (conformer 3) | -14              | 71               | -45             | 9               | -57           | 53           |
| 4b (conformer 5) | 110              | 3                | 30              | 40              | -56           | 113          |
| 4b (conformer 11)| -6               | -113             | -45             | 9               | -57           | -118         |
| 4b (conformer 12)| 130              | 123              | 60              | 68              | -54           | -118         |
| 4b (conformer 13)| 109              | 6                | 2               | 48              | -57           | 116          |

$^{14}$ $\alpha_1 = \text{C2-C1-C-O}$  
$^{15}$ $\alpha_2 = \text{C2'-C1'-C-O}$  
$^{16}$ $\beta_1 = \text{H-C-O-C'}$  
$^{17}$ $\beta_2 = \text{C-O-C-H}$  
$^{18}$ $\gamma = \text{O-C-C-CH(CH}_3\text{)}$  
$^{19}$ $\omega$ = torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)
Table S17. Dihedral angles $\alpha$, $\beta$, $\gamma$, $\omega$ (in degrees) of calculated at the B3LYP/6-311++G(d,p) level for each low-energy conformer of ether 5b.

| Compound | $\alpha_{1}^{20}$ | $\alpha_{2}^{21}$ | $\theta_{1}^{22}$ | $\theta_{2}^{23}$ | $\gamma^{24}$ | $\omega^{25}$ |
|----------|------------------|------------------|------------------|------------------|-------------|-------------|
| 5b (conformer 1) | -70              | 13               | 52               | 47               | 85          | -52         |
| 5b (conformer 2) | -12              | 70               | -48              | -43              | 86          | 53          |
| 5b (conformer 4) | -107             | 26               | -30              | 38               | 150         | -82         |
| 5b (conformer 5) | -21              | 97               | 41               | 33               | 147         | 74          |
| 5b (conformer 6) | -13              | 68               | -52              | -46              | 153         | 51          |
| 5b (conformer 7) | -27              | 107              | 29               | -38              | 156         | 82          |
| 5b (conformer 8) | -29              | 115              | 50               | 60               | 83          | 88          |
| 5b (conformer 9) | -82              | 17               | -39              | -36              | 90          | -59         |
| 5b (conformer 11) | -98              | 22               | -44              | -41              | 153         | -74         |
| 5b (conformer 12) | -14              | 71               | -48              | 29               | 145         | 53          |
| 5b (conformer 13) | -72              | 14               | 44               | -27              | 93          | -54         |
| 5b (conformer 15) | -71              | 13               | 48               | -29              | 151         | -54         |
| 5b (conformer 16) | 132              | 123              | 55               | 56               | 83          | -115        |
| 5b (conformer 17) | 115              | 7                | 48               | 47               | 85          | 121         |
| 5b (conformer 18) | -5               | -115             | -45              | -43              | 86          | -120        |
| 5b (conformer 19) | 115              | 6                | 47               | 44               | 151         | 121         |
| 5b (conformer 20) | -121             | -131             | -41              | 35               | 145         | 117         |
| 5b (conformer 26) | 132              | 121              | 58               | 50               | 153         | -116        |
| 5b (conformer 36) | 132              | 120              | 41               | -36              | 154         | -118        |
| 5b (conformer 39) | -130             | -130             | -57              | -60              | 115         | 109         |
| 5b (conformer 41) | -122             | -132             | -59              | -55              | 150         | 116         |
| 5b (conformer 43) | -2               | -114             | -44              | -48              | 110         | -117        |
| 5b (conformer 44) | -121             | -133             | -58              | -46              | 93          | 117         |
| 5b (conformer 51) | 132              | 119              | 36               | -33              | 96          | -119        |
| 5b (conformer 52) | -118             | -132             | -38              | 31               | 83          | 120         |

\(^{20}\alpha_1 = \text{C2-C1-C-O}\)

\(^{21}\alpha_2 = \text{C2'-C1'-C-O}\)

\(^{22}\theta_1 = \text{H-C-O-C'}\)

\(^{23}\theta_2 = \text{C-O-C'-H}\)

\(^{24}\gamma = \text{O-C'-H}\)

\(^{25}\omega = \text{torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)}\)
Table S18. Dihedral angles $\alpha$, $\beta$, $\gamma$, $\omega$ (in degrees) of calculated at the B3LYP/6-311++G(d,p) level for each low-energy conformer of ether 6b.

| Compound          | $\alpha_{1}^{26}$ | $\alpha_{2}^{27}$ | $\beta_{1}^{28}$ | $\beta_{2}^{29}$ | $\gamma^{30}$ | $\omega^{31}$ |
|-------------------|-------------------|-------------------|-------------------|-------------------|---------------|---------------|
| 6b (conformer 1)  | -102              | 22                | -22               | 45                | -174          | -79           |
| 6b (conformer 2)  | -23               | 102               | 23                | -43               | -178          | 79            |
| 6b (conformer 3)  | -23               | 100               | 46                | 40                | -173          | 75            |
| 6b (conformer 4)  | -91               | 17                | -14               | 51                | -176          | -70           |
| 6b (conformer 5)  | -23               | 103               | 23                | -44               | -179          | 80            |
| 6b (conformer 6)  | -22               | 98                | 45                | 40                | -173          | 74            |
| 6b (conformer 7)  | -100              | 23                | -46               | -42               | -175          | -76           |
| 6b (conformer 8)  | -12               | 71                | -42               | 14                | -172          | 54            |
| 6b (conformer 9)  | 115               | 6                 | 43                | 40                | -173          | 120           |
| 6b (conformer 10) | -5                | -115              | -44               | -39               | -176          | -120          |
| 6b (conformer 14) | 114               | 4                 | 42                | 35                | -174          | 118           |
| 6b (conformer 15) | -117              | -135              | -33               | 36                | -174          | 120           |
| 6b (conformer 18) | -5                | -114              | -41               | -38               | -176          | -118          |
| 6b (conformer 24) | -5                | -114              | -41               | -39               | -175          | -118          |
| 6b (conformer 32) | 132               | 120               | 55                | 38                | -174          | -118          |
| 6b (conformer 44) | -120              | -133              | -56               | -44               | -177          | 117           |
| 6b (conformer 51) | 132               | 120               | 56                | 40                | -175          | -118          |
| 6b (conformer 60) | -120              | -132              | -56               | -43               | -177          | 117           |
| 6b (conformer 70) | 132               | 121               | 59                | 49                | -174          | -117          |

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$^{26} \alpha_{1} = \text{C2-C1-C-O}$  
$^{27} \alpha_{2} = \text{C2'-C1'-C-O}$  
$^{28} \beta_{1} = \text{H-C-O-C'}$  
$^{29} \beta_{2} = \text{C-O-C'-H}$  
$^{30} \gamma = \text{O-C'-C-C''}$  
$^{31} \omega =$ torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)
Table S19. Dihedral angles $\alpha$, $\beta$, $\gamma$, $\omega$ (in degrees) of calculated at the B3LYP/6-311++G(d,p) level for each low-energy conformer of ether 7b.

| Compound       | $\alpha_1^{32}$ | $\alpha_2^{33}$ | $\beta_1^{34}$ | $\beta_2^{35}$ | $\gamma^{36}$ | $\omega^{37}$ |
|----------------|-----------------|-----------------|----------------|----------------|----------------|----------------|
| 7b (conformer 1)| -12             | 71              | -44            | -46            | -46            | 54             |
| 7b (conformer 2)| -88             | 20              | -41            | -51            | -47            | -63            |
| 7b (conformer 3)| -66             | 15              | 48             | 25             | -43            | -48            |
| 7b (conformer 4)| -71             | 15              | 50             | -23            | -46            | -53            |
| 7b (conformer 5)| -5              | -114            | -50            | -51            | -47            | -119           |
| 7b (conformer 6)| -19             | 74              | 37             | 10             | -44            | 48             |
| 7b (conformer 7)| -122            | -131            | -60            | -60            | -49            | 118            |
| 7b (conformer 9)| 115             | 11              | -28            | -53            | -46            | 128            |
| 7b (conformer 11)| -88            | 20              | -42            | -52            | -48            | -64            |
| 7b (conformer 12)| -5              | -114            | -50            | -51            | -47            | -119           |
| 7b (conformer 13)| 133            | 116             | 38             | -43            | -48            | -122           |
| 7b (conformer 14)| 115            | 7               | 45             | 27             | -43            | 121            |
| 7b (conformer 16)| -11            | -117            | 29             | 25             | -44            | -131           |

$^{32} \alpha_1 = \text{C2-C1-C-O}$  
$^{33} \alpha_2 = \text{C2'-C1'-C-O}$  
$^{34} \beta_1 = \text{H-C-O-C'}$  
$^{35} \beta_2 = \text{C-O-C'-H}$  
$^{36} \gamma = \text{O-C'-C-CH}_3$  
$^{37} \omega$ = torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)
| Compound       | $\alpha_1^{38}$ | $\alpha_2^{39}$ | $\beta_1^{40}$ | $\beta_2^{41}$ | $\gamma^{42}$ | $\omega^{43}$ |
|---------------|----------------|----------------|---------------|---------------|---------------|---------------|
| 8b (conformer 1) | -97            | 19             | -21           | 45            | -172          | -75           |
| 8b (conformer 2) | -71            | 14             | 60            | 45            | 64            | -53           |
| 8b (conformer 3) | -73            | 14             | 46            | 37            | -178          | -54           |
| 8b (conformer 4) | -72            | 13             | 59            | 47            | -167          | -55           |
| 8b (conformer 6) | -71            | 15             | 61            | 45            | 54            | -53           |
| 8b (conformer 7) | -31            | 108            | 57            | 51            | 65            | 79            |
| 8b (conformer 10) | 130            | 120            | 62            | 48            | 65            | -118          |
| 8b (conformer 11) | -23            | 90             | 44            | 34            | 179           | 64            |
| 8b (conformer 12) | -73            | 13             | 54            | 40            | 63            | -55           |
| 8b (conformer 14) | 131            | 117            | 65            | 68            | -65           | -123          |
| 8b (conformer 15) | -30            | 104            | 57            | 47            | 55            | 75            |
| 8b (conformer 16) | -18            | 73             | -55           | 0             | -70           | 53            |
| 8b (conformer 19) | 130            | 124            | 55            | 43            | -177          | -114          |
| 8b (conformer 20) | 127            | 124            | 59            | 56            | -76           | -117          |
| 8b (conformer 22) | -71            | 16             | 57            | 40            | 51            | -52           |
| 8b (conformer 25) | -72            | 14             | 50            | 26            | -178          | -53           |
| 8b (conformer 27) | 132            | 117            | 62            | 44            | 54            | -121          |
| 8b (conformer 31) | 111            | 4              | 49            | 50            | -64           | 113           |
| 8b (conformer 42) | 129            | 125            | 64            | 47            | 61            | -114          |

$\alpha_1 = \text{C2-C1-C-O}$

$\alpha_2 = \text{C2'-C1'-C-O}$

$\beta_1 = \text{H-C-O-C}^*$

$\beta_2 = \text{C-O-C}^*\cdot\text{H}$

$\gamma = \text{O-C}^*\cdot\text{C-C}$

$\omega$ = torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)
Table S21. Dihedral angles $\alpha$, $\beta$, $\gamma$, $\omega$ (in degrees) of calculated at the B3LYP/6-311++G(d,p) level for each low-energy conformer of ether 9b.

| Compound     | $\alpha_{1}$ | $\alpha_{2}$ | $\beta_{1}$ | $\beta_{2}$ | $\gamma$ | $\omega$ |
|--------------|---------------|---------------|--------------|--------------|-----------|----------|
| 9b (conformer 1) | -81           | 20            | -41          | -45          | 47        | -56      |
| 9b (conformer 3) | -13           | 70            | -47          | -48          | 35        | 52       |
| 9b (conformer 5) | -22           | 101           | 48           | 38           | 28        | 77       |
| 9b (conformer 9) | -115          | -134          | -58          | -47          | 64        | 122      |
| 9b (conformer 11) | 115           | 11            | -31          | -49          | 39        | 128      |
| 9b (conformer 17) | -7            | -115          | -49          | -51          | 39        | -122     |

$^{44} \alpha_{1} = \text{C2-C1-C-O}$

$^{45} \alpha_{2} = \text{C2'-C1'-C-O}$

$^{46} \beta_{1} = \text{H-C-O-C^*}$

$^{47} \beta_{2} = \text{C-O-C^* -H}$

$^{48} \gamma = \text{O-C^* -C_Cort}$

$^{49} \omega = \text{torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)}$
Table S22. Dihedral angles $\alpha$, $\beta$, $\gamma$, $\omega$ (in degrees) of calculated at the B3LYP/6-311++G(d,p) level for each low-energy conformer of ether 10b.

| Compound         | $\alpha_1^{50}$ | $\alpha_2^{51}$ | $\beta_1^{52}$ | $\beta_2^{53}$ | $\gamma^{54}$ | $\omega^{55}$ |
|------------------|-----------------|-----------------|----------------|----------------|----------------|----------------|
| 10b (conformer 1) | -69             | 13              | 50             | 49             | 23             | -52            |
| 10b (conformer 2) | -15             | 68              | -64            | -55            | 13             | 50             |
| 10b (conformer 4) | -22             | 95              | 40             | 19             | 12             | 71             |
| 10b (conformer 5) | -111            | 31              | -57            | -57            | 21             | -83            |
| 10b (conformer 7) | -20             | 83              | 42             | 40             | -146           | 58             |
| 10b (conformer 9) | -87             | 21              | -49            | -44            | -151           | -61            |
| 10b (conformer 11) | -119          | -133            | -62            | -55            | 22             | 119            |
| 10b (conformer 13) | -69             | 12              | 51             | 49             | -147           | -52            |
| 10b (conformer 26) | 116            | 6               | 52             | 52             | 23             | 120            |
| 10b (conformer 53) | -123           | -131            | -64            | -55            | -151           | 115            |
| 10b (conformer 74) | -9             | -116            | -61            | -57            | 20             | -123           |

$^{50}$ $\alpha_1$ = C2-C1-C-O  
$^{51}$ $\alpha_2$ = C2'-C1'-C-O  
$^{52}$ $\beta_1$ = H-C-O-C'  
$^{53}$ $\beta_2$ = C-O-C'-H  
$^{54}$ $\gamma$ = O-C'=C-O=C  
$^{55}$ $\omega$ = torsion angle between interacting electronic transition dipole moments (for details, see: Chart 1)
Table S23. Steric energies ($E_{SE}$ kcal mol$^{-1}$), relative steric energies ($\Delta E_{SE}$ kcal mol$^{-1}$) and percentage populations ($\% \Delta E_{SE}$) calculated for low-energy conformers of ether 1e at the molecular mechanics level.

| Conformer | $E_{SE}$ | $\Delta E_{SE}$ | $\% \Delta E_{SE}$ |
|-----------|----------|----------------|-------------------|
| Conf. 01  | 90.17    | 0.00           | 46.1              |
| Conf. 02  | 91.15    | 0.99           | 8.7               |
| Conf. 03  | 91.24    | 1.08           | 7.5               |
| Conf. 04  | 91.30    | 1.13           | 6.8               |
| Conf. 05  | 91.32    | 1.15           | 6.6               |
| Conf. 06  | 91.36    | 1.19           | 6.1               |
| Conf. 07  | 91.56    | 1.39           | 4.4               |
| Conf. 08  | 91.78    | 1.61           | 3.0               |
| Conf. 09  | 91.83    | 1.66           | 2.8               |
| Conf. 10  | 91.86    | 1.70           | 2.6               |
| Conf. 11  | 91.87    | 1.70           | 2.6               |
| Conf. 12  | 92.60    | 2.43           | 0.8               |
| Conf. 13  | 93.27    | 3.10           | 0.2               |
| Conf. 14  | 93.46    | 3.29           | 0.2               |
| Conf. 15  | 93.75    | 3.58           | 0.1               |
| Conf. 16  | 93.77    | 3.60           | 0.1               |
| Conf. 17  | 93.79    | 3.62           | 0.1               |
| Conf. 18  | 93.79    | 3.63           | 0.1               |
| Conf. 19  | 93.93    | 3.77           | 0.1               |
| Conf. 20  | 93.96    | 3.79           | 0.1               |
| Conf. 21  | 93.97    | 3.81           | 0.1               |
| Conf. 22  | 94.02    | 3.85           | 0.1               |
| Conf. 23  | 94.03    | 3.87           | 0.1               |
| Conf. 24  | 94.16    | 3.99           | 0.1               |
| Conf. 25  | 94.21    | 4.05           | 0.0               |
| Conf. 26  | 94.30    | 4.13           | 0.0               |
| Conf. 27  | 94.32    | 4.16           | 0.0               |
| Conf. 28  | 94.35    | 4.19           | 0.0               |
| Conf. 29  | 94.39    | 4.22           | 0.0               |
| Conf. 30  | 94.43    | 4.27           | 0.0               |
| Conf. 31  | 94.48    | 4.32           | 0.0               |
| Conf. 32  | 94.49    | 4.33           | 0.0               |
| Conf. 33  | 94.49    | 4.33           | 0.0               |
| Conf. 34  | 94.52    | 4.35           | 0.0               |
| Conf. 35  | 94.57    | 4.40           | 0.0               |
| Conf. 36  | 94.62    | 4.45           | 0.0               |
| Conf. 37  | 94.66    | 4.50           | 0.0               |
| Conf. 38  | 94.67    | 4.51           | 0.0               |
| Conf. 39  | 94.68    | 4.51           | 0.0               |
| Conf. 40  | 94.75    | 4.58           | 0.0               |
| Conf. 41  | 94.78    | 4.62           | 0.0               |
| Conf. 42  | 94.87    | 4.70           | 0.0               |
Table S24. Steric energies ($E_{SE}$, kcal mol$^{-1}$), relative steric energies ($\Delta E_{SE}$, kcal mol$^{-1}$) and percentage populations (% $\Delta E_{SE}$) calculated for low-energy conformers of ether 3b at the molecular mechanics level.

| Conformer | $E_{SE}$ | $\Delta E_{SE}$ | % $\Delta E_{SE}$ |
|-----------|----------|----------------|------------------|
| Conf. 01  | 101.90   | 0.00           | 19.0             |
| Conf. 02  | 101.99   | 0.09           | 16.5             |
| Conf. 03  | 102.27   | 0.37           | 10.2             |
| Conf. 04  | 102.37   | 0.47           | 8.6              |
| Conf. 05  | 102.55   | 0.65           | 6.4              |
| Conf. 06  | 102.65   | 0.75           | 5.4              |
| Conf. 07  | 102.76   | 0.86           | 4.5              |
| Conf. 08  | 102.77   | 0.87           | 4.4              |
| Conf. 09  | 102.79   | 0.89           | 4.2              |
| Conf. 10  | 102.94   | 1.04           | 3.3              |
| Conf. 11  | 102.95   | 1.05           | 3.2              |
| Conf. 12  | 103.20   | 1.30           | 2.1              |
| Conf. 13  | 103.51   | 1.61           | 1.2              |
| Conf. 14  | 103.60   | 1.70           | 1.1              |
| Conf. 15  | 103.61   | 1.71           | 1.1              |
| Conf. 16  | 103.61   | 1.71           | 1.1              |
| Conf. 17  | 103.62   | 1.72           | 1.1              |
| Conf. 18  | 103.81   | 1.91           | 0.8              |
| Conf. 19  | 103.90   | 2.00           | 0.7              |
| Conf. 20  | 104.12   | 2.22           | 0.4              |
| Conf. 21  | 104.17   | 2.27           | 0.4              |
| Conf. 22  | 104.18   | 2.28           | 0.4              |
| Conf. 23  | 104.20   | 2.30           | 0.4              |
| Conf. 24  | 104.22   | 2.32           | 0.4              |
| Conf. 25  | 104.26   | 2.36           | 0.4              |
| Conf. 26  | 104.36   | 2.46           | 0.3              |
| Conf. 27  | 104.39   | 2.49           | 0.3              |
| Conf. 28  | 104.45   | 2.55           | 0.3              |
| Conf. 29  | 104.56   | 2.66           | 0.2              |
| Conf. 30  | 104.58   | 2.68           | 0.2              |
| Conf. 31  | 104.74   | 2.84           | 0.2              |
| Conf. 32  | 104.77   | 2.87           | 0.1              |
| Conf. 33  | 104.82   | 2.92           | 0.1              |
| Conf. 34  | 104.88   | 2.98           | 0.1              |
| Conf. 35  | 104.90   | 3.00           | 0.1              |
| Conf. 36  | 104.97   | 3.07           | 0.1              |
| Conf. 37  | 105.09   | 3.19           | 0.1              |
| Conf. 38  | 105.21   | 3.31           | 0.1              |
| Conf. 39  | 105.22   | 3.32           | 0.1              |
| Conf. 40  | 105.37   | 3.47           | 0.1              |
| Conf. 41  | 105.38   | 3.48           | 0.1              |
| Conf. 42  | 105.43   | 3.54           | 0.0              |
| Conf.  | Value 1 | Value 2 | Value 3 |
|--------|---------|---------|---------|
| 43     | 105.45  | 3.55    | 0.0     |
| 44     | 105.46  | 3.56    | 0.0     |
| 45     | 105.47  | 3.57    | 0.0     |
| 46     | 105.64  | 3.74    | 0.0     |
| 47     | 105.81  | 3.91    | 0.0     |
| 48     | 105.85  | 3.95    | 0.0     |
| 49     | 105.98  | 4.08    | 0.0     |
| 50     | 106.07  | 4.17    | 0.0     |
| 51     | 106.07  | 4.17    | 0.0     |
| 52     | 106.09  | 4.19    | 0.0     |
| 53     | 106.26  | 4.36    | 0.0     |
| 54     | 106.27  | 4.37    | 0.0     |
| 55     | 106.28  | 4.38    | 0.0     |
| 56     | 106.32  | 4.42    | 0.0     |
| 57     | 106.58  | 4.68    | 0.0     |
| 58     | 106.73  | 4.83    | 0.0     |
| 59     | 106.78  | 4.88    | 0.0     |
| 60     | 107.45  | 5.55    | 0.0     |
| 61     | 107.47  | 5.57    | 0.0     |
| 62     | 107.70  | 5.80    | 0.0     |
| 63     | 107.72  | 5.82    | 0.0     |
| 64     | 107.80  | 5.90    | 0.0     |
| 65     | 107.88  | 5.98    | 0.0     |
| 66     | 107.89  | 5.99    | 0.0     |
| 67     | 107.92  | 6.02    | 0.0     |
| 68     | 108.00  | 6.10    | 0.0     |
| 69     | 108.27  | 6.37    | 0.0     |
| 70     | 108.36  | 6.46    | 0.0     |
| 71     | 108.37  | 6.47    | 0.0     |
| 72     | 108.56  | 6.66    | 0.0     |
| 73     | 108.74  | 6.84    | 0.0     |
| 74     | 108.99  | 7.09    | 0.0     |
| 75     | 109.03  | 7.13    | 0.0     |
| 76     | 109.44  | 7.54    | 0.0     |
| 77     | 109.59  | 7.69    | 0.0     |
| 78     | 109.61  | 7.71    | 0.0     |
| 79     | 109.63  | 7.73    | 0.0     |
| 80     | 109.65  | 7.75    | 0.0     |
| 81     | 109.73  | 7.83    | 0.0     |
| 82     | 109.86  | 7.96    | 0.0     |
| 83     | 110.03  | 8.13    | 0.0     |
| 84     | 110.47  | 8.57    | 0.0     |
| 85     | 110.50  | 8.60    | 0.0     |
| 86     | 110.51  | 8.61    | 0.0     |
| 87     | 110.53  | 8.63    | 0.0     |
| 88     | 110.64  | 8.74    | 0.0     |
| Conf. 89 | 110.67 | 8.77 | 0.0 |
|---------|--------|------|-----|
| Conf. 90 | 110.79 | 8.89 | 0.0 |
| Conf. 91 | 110.98 | 9.08 | 0.0 |
| Conf. 92 | 111.06 | 9.16 | 0.0 |
| Conf. 93 | 111.30 | 9.40 | 0.0 |
| Conf. 94 | 111.35 | 9.45 | 0.0 |
| Conf. 95 | 111.39 | 9.49 | 0.0 |
| Conf. 96 | 111.40 | 9.50 | 0.0 |
| Conf. 97 | 111.57 | 9.67 | 0.0 |
| Conf. 98 | 111.58 | 9.68 | 0.0 |
| Conf. 99 | 111.64 | 9.74 | 0.0 |
| Conf. 100 | 111.80 | 9.90 | 0.0 |
**Table S25.** Steric energies ($E_{SE}$ kcal mol$^{-1}$), relative steric energies ($\Delta E_{SE}$ kcal mol$^{-1}$) and percentage populations (% $\Delta E_{SE}$) calculated for low-energy conformers of ether 4b at the molecular mechanics level.

| Conformer | $E_{SE}$ | $\Delta E_{SE}$ | % $\Delta E_{SE}$ |
|-----------|----------|-----------------|-------------------|
| Conf. 01  | 105.78   | 0.00            | 82.4              |
| Conf. 02  | 107.24   | 1.46            | 7.0               |
| Conf. 03  | 107.31   | 1.53            | 6.2               |
| Conf. 04  | 108.13   | 2.35            | 1.6               |
| Conf. 05  | 108.28   | 2.50            | 1.2               |
| Conf. 06  | 109.07   | 3.29            | 0.3               |
| Conf. 07  | 109.07   | 3.30            | 0.3               |
| Conf. 08  | 109.37   | 3.59            | 0.2               |
| Conf. 09  | 109.44   | 3.66            | 0.2               |
| Conf. 10  | 109.59   | 3.81            | 0.1               |
| Conf. 11  | 109.96   | 4.18            | 0.1               |
| Conf. 12  | 110.25   | 4.47            | 0.0               |
| Conf. 13  | 110.27   | 4.49            | 0.0               |
| Conf. 14  | 110.28   | 4.50            | 0.0               |
| Conf. 15  | 110.37   | 4.59            | 0.0               |
| Conf. 16  | 110.56   | 4.78            | 0.0               |
| Conf. 17  | 110.58   | 4.80            | 0.0               |
| Conf. 18  | 110.64   | 4.86            | 0.0               |
| Conf. 19  | 110.74   | 4.96            | 0.0               |
| Conf. 20  | 110.78   | 5.00            | 0.0               |
| Conf. 21  | 110.78   | 5.01            | 0.0               |
| Conf. 22  | 110.79   | 5.01            | 0.0               |
| Conf. 23  | 110.87   | 5.09            | 0.0               |
| Conf. 24  | 111.52   | 5.74            | 0.0               |
| Conf. 25  | 111.60   | 5.82            | 0.0               |
| Conf. 26  | 111.63   | 5.85            | 0.0               |
| Conf. 27  | 111.65   | 5.87            | 0.0               |
| Conf. 28  | 111.67   | 5.89            | 0.0               |
| Conf. 29  | 111.86   | 6.08            | 0.0               |
| Conf. 30  | 112.03   | 6.25            | 0.0               |
| Conf. 31  | 112.22   | 6.44            | 0.0               |
| Conf. 32  | 112.24   | 6.46            | 0.0               |
| Conf. 33  | 112.31   | 6.53            | 0.0               |
| Conf. 34  | 112.31   | 6.54            | 0.0               |
| Conf. 35  | 112.45   | 6.67            | 0.0               |
| Conf. 36  | 112.66   | 6.88            | 0.0               |
| Conf. 37  | 112.87   | 7.09            | 0.0               |
| Conf. 38  | 112.90   | 7.12            | 0.0               |
| Conf. 39  | 112.91   | 7.13            | 0.0               |
| Conf. 40  | 113.00   | 7.22            | 0.0               |
| Conf. 41  | 113.08   | 7.31            | 0.0               |
| Conf. 42  | 113.11   | 7.34            | 0.0               |
| Conf.   | Value 1 | Value 2 | Value 3 |
|--------|---------|---------|---------|
| 43     | 113.14  | 7.37    | 0.0     |
| 44     | 113.17  | 7.39    | 0.0     |
| 45     | 113.37  | 7.59    | 0.0     |
| 46     | 113.50  | 7.72    | 0.0     |
| 47     | 113.52  | 7.74    | 0.0     |
| 48     | 113.58  | 7.80    | 0.0     |
| 49     | 113.59  | 7.81    | 0.0     |
| 50     | 113.60  | 7.82    | 0.0     |
| 51     | 113.78  | 8.01    | 0.0     |
| 52     | 114.12  | 8.34    | 0.0     |
| 53     | 114.16  | 8.39    | 0.0     |
| 54     | 114.24  | 8.46    | 0.0     |
| 55     | 114.28  | 8.50    | 0.0     |
| 56     | 114.33  | 8.55    | 0.0     |
| 57     | 114.36  | 8.58    | 0.0     |
| 58     | 114.39  | 8.61    | 0.0     |
| 59     | 114.45  | 8.67    | 0.0     |
| 60     | 114.49  | 8.72    | 0.0     |
| 61     | 114.50  | 8.72    | 0.0     |
| 62     | 114.53  | 8.75    | 0.0     |
| 63     | 114.54  | 8.76    | 0.0     |
| 64     | 114.65  | 8.87    | 0.0     |
| 65     | 114.65  | 8.87    | 0.0     |
| 66     | 114.76  | 8.99    | 0.0     |
| 67     | 114.80  | 9.02    | 0.0     |
| 68     | 114.85  | 9.07    | 0.0     |
| 69     | 114.86  | 9.08    | 0.0     |
| 70     | 114.89  | 9.11    | 0.0     |
| 71     | 114.96  | 9.18    | 0.0     |
| 72     | 115.00  | 9.22    | 0.0     |
| 73     | 115.04  | 9.26    | 0.0     |
| 74     | 115.04  | 9.26    | 0.0     |
| 75     | 115.06  | 9.28    | 0.0     |
| 76     | 115.40  | 9.63    | 0.0     |
| 77     | 115.45  | 9.67    | 0.0     |
| 78     | 115.52  | 9.74    | 0.0     |
| 79     | 115.61  | 9.83    | 0.0     |
| 80     | 115.69  | 9.91    | 0.0     |
| 81     | 115.73  | 9.95    | 0.0     |
| 82     | 115.78  | 10.00   | 0.0     |
Table S26. Steric energies ($E_{SE}$ kcal mol$^{-1}$), relative steric energies ($\Delta E_{SE}$ kcal mol$^{-1}$) and percentage populations (% $\Delta E_{SE}$) calculated for low-energy conformers of ether 5b at the molecular mechanics level.

| Conformer | $E_{SE}$ | $\Delta E_{SE}$ | % $\Delta E_{SE}$ |
|-----------|----------|-----------------|--------------------|
| Conf. 01  | 108.80   | 0.00            | 17.0               |
| Conf. 02  | 108.85   | 0.05            | 15.8               |
| Conf. 03  | 109.00   | 0.20            | 12.2               |
| Conf. 04  | 109.06   | 0.26            | 11.0               |
| Conf. 05  | 109.35   | 0.54            | 6.8                |
| Conf. 06  | 109.45   | 0.64            | 5.7                |
| Conf. 07  | 109.45   | 0.65            | 5.7                |
| Conf. 08  | 109.56   | 0.76            | 4.8                |
| Conf. 09  | 109.59   | 0.79            | 4.5                |
| Conf. 10  | 109.79   | 0.98            | 3.2                |
| Conf. 11  | 109.79   | 0.99            | 3.2                |
| Conf. 12  | 109.84   | 1.04            | 3.0                |
| Conf. 13  | 110.15   | 1.34            | 1.8                |
| Conf. 14  | 110.23   | 1.43            | 1.5                |
| Conf. 15  | 110.29   | 1.49            | 1.4                |
| Conf. 16  | 110.90   | 2.10            | 0.5                |
| Conf. 17  | 111.16   | 2.36            | 0.3                |
| Conf. 18  | 111.41   | 2.61            | 0.2                |
| Conf. 19  | 111.65   | 2.85            | 0.1                |
| Conf. 20  | 111.94   | 3.14            | 0.1                |
| Conf. 21  | 111.96   | 3.16            | 0.1                |
| Conf. 22  | 112.02   | 3.22            | 0.1                |
| Conf. 23  | 112.03   | 3.23            | 0.1                |
| Conf. 24  | 112.05   | 3.25            | 0.1                |
| Conf. 25  | 112.14   | 3.34            | 0.1                |
| Conf. 26  | 112.15   | 3.34            | 0.1                |
| Conf. 27  | 112.21   | 3.40            | 0.1                |
| Conf. 28  | 112.26   | 3.45            | 0.1                |
| Conf. 29  | 112.30   | 3.49            | 0.0                |
| Conf. 30  | 112.33   | 3.52            | 0.0                |
| Conf. 31  | 112.36   | 3.55            | 0.0                |
| Conf. 32  | 112.41   | 3.61            | 0.0                |
| Conf. 33  | 112.42   | 3.61            | 0.0                |
| Conf. 34  | 112.44   | 3.64            | 0.0                |
| Conf. 35  | 112.46   | 3.65            | 0.0                |
| Conf. 36  | 112.48   | 3.68            | 0.0                |
| Conf. 37  | 112.53   | 3.72            | 0.0                |
| Conf. 38  | 112.53   | 3.73            | 0.0                |
| Conf. 39  | 112.54   | 3.73            | 0.0                |
| Conf. 40  | 112.58   | 3.78            | 0.0                |
| Conf. 41  | 112.65   | 3.85            | 0.0                |
| Conf. 42  | 112.80   | 4.00            | 0.0                |
| Conf. 43 | 112.80 | 4.00 | 0.0 |
| Conf. 44 | 112.90 | 4.10 | 0.0 |
| Conf. 45 | 112.90 | 4.10 | 0.0 |
| Conf. 46 | 112.91 | 4.11 | 0.0 |
| Conf. 47 | 112.91 | 4.11 | 0.0 |
| Conf. 48 | 112.95 | 4.15 | 0.0 |
| Conf. 49 | 112.99 | 4.18 | 0.0 |
| Conf. 50 | 113.11 | 4.31 | 0.0 |
| Conf. 51 | 113.18 | 4.37 | 0.0 |
| Conf. 52 | 113.18 | 4.38 | 0.0 |
| Conf. 53 | 113.66 | 4.86 | 0.0 |
| Conf. 54 | 113.69 | 4.88 | 0.0 |
| Conf. 55 | 113.81 | 5.01 | 0.0 |
| Conf. 56 | 113.91 | 5.11 | 0.0 |
| Conf. 57 | 113.97 | 5.17 | 0.0 |
| Conf. 58 | 114.26 | 5.46 | 0.0 |
| Conf. 59 | 114.63 | 5.83 | 0.0 |
| Conf. 60 | 114.74 | 5.93 | 0.0 |
| Conf. 61 | 115.08 | 6.27 | 0.0 |
| Conf. 62 | 115.27 | 6.47 | 0.0 |
| Conf. 63 | 115.31 | 6.51 | 0.0 |
| Conf. 64 | 115.32 | 6.52 | 0.0 |
| Conf. 65 | 115.33 | 6.53 | 0.0 |
| Conf. 66 | 115.37 | 6.57 | 0.0 |
| Conf. 67 | 115.38 | 6.58 | 0.0 |
| Conf. 68 | 115.45 | 6.64 | 0.0 |
| Conf. 69 | 115.54 | 6.73 | 0.0 |
| Conf. 70 | 115.60 | 6.80 | 0.0 |
| Conf. 71 | 115.66 | 6.86 | 0.0 |
| Conf. 72 | 116.05 | 7.25 | 0.0 |
| Conf. 73 | 116.50 | 7.70 | 0.0 |
| Conf. 74 | 116.97 | 8.17 | 0.0 |
| Conf. 75 | 117.04 | 8.24 | 0.0 |
| Conf. 76 | 117.57 | 8.77 | 0.0 |
| Conf. 77 | 118.06 | 9.25 | 0.0 |
| Conf. 78 | 118.08 | 9.28 | 0.0 |
| Conf. 79 | 118.15 | 9.35 | 0.0 |
| Conf. 80 | 118.17 | 9.36 | 0.0 |
| Conf. 81 | 118.19 | 9.39 | 0.0 |
| Conf. 82 | 118.20 | 9.39 | 0.0 |
| Conf. 83 | 118.27 | 9.47 | 0.0 |
| Conf. 84 | 118.30 | 9.49 | 0.0 |
| Conf. 85 | 118.62 | 9.82 | 0.0 |
| Conf. 86 | 118.63 | 9.83 | 0.0 |
| Conf. 87 | 118.67 | 9.87 | 0.0 |
Table S27. Steric energies (E_{SE}, kcal mol⁻¹), relative steric energies (ΔE_{SE}, kcal mol⁻¹) and percentage populations (% ΔE_{SE}) calculated for low-energy conformers of ether 6b at the molecular mechanics level.

| Conformer | E_{SE} | ΔE_{SE} | % ΔE_{SE} |
|-----------|--------|---------|-----------|
| Conf. 01  | 181.25 | 0.00    | 37.5      |
| Conf. 02  | 181.57 | 0.33    | 21.6      |
| Conf. 03  | 181.86 | 0.62    | 13.2      |
| Conf. 04  | 181.97 | 0.73    | 11.0      |
| Conf. 05  | 182.30 | 1.06    | 6.3       |
| Conf. 06  | 182.59 | 1.35    | 3.9       |
| Conf. 07  | 182.87 | 1.63    | 2.4       |
| Conf. 08  | 183.09 | 1.84    | 1.7       |
| Conf. 09  | 183.94 | 2.69    | 0.4       |
| Conf. 10  | 184.12 | 2.88    | 0.3       |
| Conf. 11  | 184.28 | 3.04    | 0.2       |
| Conf. 12  | 184.46 | 3.22    | 0.2       |
| Conf. 13  | 184.47 | 3.23    | 0.2       |
| Conf. 14  | 184.67 | 3.42    | 0.1       |
| Conf. 15  | 184.80 | 3.55    | 0.1       |
| Conf. 16  | 184.80 | 3.56    | 0.1       |
| Conf. 17  | 184.82 | 3.58    | 0.1       |
| Conf. 18  | 184.85 | 3.61    | 0.1       |
| Conf. 19  | 185.02 | 3.77    | 0.1       |
| Conf. 20  | 185.02 | 3.77    | 0.1       |
| Conf. 21  | 185.08 | 3.83    | 0.1       |
| Conf. 22  | 185.09 | 3.84    | 0.1       |
| Conf. 23  | 185.10 | 3.85    | 0.1       |
| Conf. 24  | 185.16 | 3.91    | 0.1       |
| Conf. 25  | 185.19 | 3.95    | 0.0       |
| Conf. 26  | 185.21 | 3.96    | 0.0       |
| Conf. 27  | 185.50 | 4.25    | 0.0       |
| Conf. 28  | 185.50 | 4.26    | 0.0       |
| Conf. 29  | 185.70 | 4.46    | 0.0       |
| Conf. 30  | 185.71 | 4.46    | 0.0       |
| Conf. 31  | 185.75 | 4.50    | 0.0       |
| Conf. 32  | 185.77 | 4.52    | 0.0       |
| Conf. 33  | 186.03 | 4.78    | 0.0       |
| Conf. 34  | 186.10 | 4.86    | 0.0       |
| Conf. 35  | 186.13 | 4.88    | 0.0       |
| Conf. 36  | 186.38 | 5.14    | 0.0       |
| Conf. 37  | 186.78 | 5.54    | 0.0       |
| Conf. 38  | 186.97 | 5.72    | 0.0       |
| Conf. 39  | 187.00 | 5.75    | 0.0       |
| Conf. 40  | 187.04 | 5.80    | 0.0       |
| Conf. 41  | 187.20 | 5.95    | 0.0       |
| Conf. 42  | 187.38 | 6.13    | 0.0       |
| Conf. 43 | 187.38 | 6.13 | 0.0 |
|---------|--------|------|-----|
| Conf. 44 | 187.49 | 6.25 | 0.0 |
| Conf. 45 | 187.51 | 6.27 | 0.0 |
| Conf. 46 | 187.70 | 6.45 | 0.0 |
| Conf. 47 | 187.72 | 6.48 | 0.0 |
| Conf. 48 | 187.73 | 6.48 | 0.0 |
| Conf. 49 | 187.78 | 6.54 | 0.0 |
| Conf. 50 | 187.82 | 6.57 | 0.0 |
| Conf. 51 | 187.89 | 6.64 | 0.0 |
| Conf. 52 | 188.00 | 6.75 | 0.0 |
| Conf. 53 | 188.01 | 6.76 | 0.0 |
| Conf. 54 | 188.06 | 6.81 | 0.0 |
| Conf. 55 | 188.19 | 6.95 | 0.0 |
| Conf. 56 | 188.31 | 7.06 | 0.0 |
| Conf. 57 | 188.42 | 7.18 | 0.0 |
| Conf. 58 | 188.47 | 7.23 | 0.0 |
| Conf. 59 | 188.49 | 7.24 | 0.0 |
| Conf. 60 | 188.53 | 7.28 | 0.0 |
| Conf. 61 | 188.54 | 7.29 | 0.0 |
| Conf. 62 | 188.55 | 7.31 | 0.0 |
| Conf. 63 | 188.56 | 7.31 | 0.0 |
| Conf. 64 | 188.63 | 7.38 | 0.0 |
| Conf. 65 | 188.68 | 7.43 | 0.0 |
| Conf. 66 | 188.73 | 7.49 | 0.0 |
| Conf. 67 | 188.84 | 7.59 | 0.0 |
| Conf. 68 | 188.86 | 7.62 | 0.0 |
| Conf. 69 | 188.87 | 7.62 | 0.0 |
| Conf. 70 | 188.92 | 7.68 | 0.0 |
| Conf. 71 | 189.02 | 7.78 | 0.0 |
| Conf. 72 | 189.03 | 7.78 | 0.0 |
| Conf. 73 | 189.04 | 7.79 | 0.0 |
| Conf. 74 | 189.07 | 7.82 | 0.0 |
| Conf. 75 | 189.13 | 7.88 | 0.0 |
| Conf. 76 | 189.30 | 8.05 | 0.0 |
| Conf. 77 | 189.49 | 8.25 | 0.0 |
| Conf. 78 | 189.61 | 8.36 | 0.0 |
| Conf. 79 | 189.66 | 8.41 | 0.0 |
| Conf. 80 | 189.68 | 8.43 | 0.0 |
| Conf. 81 | 189.77 | 8.52 | 0.0 |
| Conf. 82 | 189.79 | 8.54 | 0.0 |
| Conf. 83 | 189.95 | 8.71 | 0.0 |
| Conf. 84 | 190.12 | 8.87 | 0.0 |
| Conf. 85 | 190.22 | 8.98 | 0.0 |
| Conf. 86 | 190.38 | 9.13 | 0.0 |
| Conf. 87 | 190.39 | 9.14 | 0.0 |
| Conf. 88 | 190.47 | 9.22 | 0.0 |
|    |        |        |        |
|----|--------|--------|--------|
| Conf. 89 | 190.63 | 9.38   | 0.0    |
| Conf. 90 | 190.64 | 9.39   | 0.0    |
| Conf. 91 | 190.66 | 9.41   | 0.0    |
| Conf. 92 | 190.71 | 9.47   | 0.0    |
| Conf. 93 | 190.77 | 9.52   | 0.0    |
| Conf. 94 | 190.79 | 9.55   | 0.0    |
| Conf. 95 | 190.81 | 9.57   | 0.0    |
| Conf. 96 | 190.95 | 9.70   | 0.0    |
| Conf. 97 | 191.11 | 9.86   | 0.0    |
| Conf. 98 | 191.13 | 9.89   | 0.0    |
| Conf. 99 | 191.14 | 9.89   | 0.0    |
| Conf. 100| 191.23 | 9.99   | 0.0    |
Table S28. Steric energies (\(E_{SE}\), kcal mol\(^{-1}\)), relative steric energies (\(\Delta E_{SE}\), kcal mol\(^{-1}\)) and percentage populations (\(\% \Delta E_{SE}\)) calculated for low-energy conformers of ether 7b at the molecular mechanics level.

| Conformer | \(E_{SE}\) | \(\Delta E_{SE}\) | \(\% \Delta E_{SE}\) |
|-----------|------------|-----------------|-----------------|
| Conf. 01  | 158.74     | 0.00            | 55.2            |
| Conf. 02  | 159.15     | 0.41            | 27.7            |
| Conf. 03  | 159.83     | 1.09            | 8.8             |
| Conf. 04  | 160.23     | 1.48            | 4.5             |
| Conf. 05  | 161.20     | 2.45            | 0.9             |
| Conf. 06  | 161.24     | 2.50            | 0.8             |
| Conf. 07  | 161.65     | 2.91            | 0.4             |
| Conf. 08  | 161.68     | 2.94            | 0.4             |
| Conf. 09  | 161.88     | 3.13            | 0.7             |
| Conf. 10  | 162.00     | 3.26            | 0.2             |
| Conf. 11  | 162.11     | 3.36            | 0.2             |
| Conf. 12  | 162.21     | 3.46            | 0.2             |
| Conf. 13  | 162.28     | 3.53            | 0.1             |
| Conf. 14  | 162.61     | 3.87            | 0.1             |
| Conf. 15  | 162.79     | 4.05            | 0.1             |
| Conf. 16  | 162.89     | 4.15            | 0.1             |
| Conf. 17  | 163.07     | 4.32            | 0.0             |
| Conf. 18  | 163.18     | 4.44            | 0.0             |
| Conf. 19  | 163.28     | 4.54            | 0.0             |
| Conf. 20  | 164.14     | 5.39            | 0.0             |
| Conf. 21  | 164.21     | 5.46            | 0.0             |
| Conf. 22  | 164.58     | 5.84            | 0.0             |
| Conf. 23  | 164.83     | 6.09            | 0.0             |
| Conf. 24  | 164.95     | 6.21            | 0.0             |
| Conf. 25  | 164.96     | 6.22            | 0.0             |
| Conf. 26  | 165.15     | 6.41            | 0.0             |
| Conf. 27  | 165.23     | 6.48            | 0.0             |
| Conf. 28  | 165.34     | 6.59            | 0.0             |
| Conf. 29  | 165.44     | 6.69            | 0.0             |
| Conf. 30  | 165.58     | 6.83            | 0.0             |
| Conf. 31  | 165.85     | 7.11            | 0.0             |
| Conf. 32  | 166.03     | 7.28            | 0.0             |
| Conf. 33  | 166.05     | 7.30            | 0.0             |
| Conf. 34  | 166.25     | 7.51            | 0.0             |
| Conf. 35  | 166.25     | 7.51            | 0.0             |
| Conf. 36  | 166.69     | 7.95            | 0.0             |
| Conf. 37  | 167.21     | 8.47            | 0.0             |
| Conf. 38  | 167.62     | 8.87            | 0.0             |
| Conf. 39  | 167.92     | 9.17            | 0.0             |
| Conf. 40  | 168.30     | 9.56            | 0.0             |
| Conf. 41  | 168.31     | 9.57            | 0.0             |
| Conf. 42  | 168.39     | 9.65            | 0.0             |
| Conf. 43 | 168.49 | 9.74 | 0.0 |
|---------|--------|------|-----|
| Conf. 44 | 168.68 | 9.94 | 0.0 |
| Conf. 45 | 168.69 | 9.94 | 0.0 |
| Conf. 46 | 168.72 | 9.97 | 0.0 |
**Table S29.** Steric energies ($E_{SE}$ kcal mol$^{-1}$), relative steric energies ($\Delta E_{SE}$ kcal mol$^{-1}$) and percentage populations (% $\Delta E_{SE}$) calculated for low-energy conformers of ether **8b** at the molecular mechanics level.

| Conformer | $E_{SE}$ | $\Delta E_{SE}$ | % $\Delta E_{SE}$ |
|-----------|----------|-----------------|------------------|
| Conf. 01  | 78.27    | 0.00            | 49.5             |
| Conf. 02  | 79.01    | 0.73            | 14.3             |
| Conf. 03  | 79.26    | 0.99            | 9.3              |
| Conf. 04  | 79.49    | 1.22            | 6.3              |
| Conf. 05  | 79.85    | 1.58            | 3.4              |
| Conf. 06  | 79.99    | 1.72            | 2.7              |
| Conf. 07  | 80.09    | 1.82            | 2.3              |
| Conf. 08  | 80.10    | 1.83            | 2.3              |
| Conf. 09  | 80.16    | 1.89            | 2.1              |
| Conf. 10  | 80.25    | 1.98            | 1.8              |
| Conf. 11  | 80.46    | 2.19            | 1.2              |
| Conf. 12  | 80.88    | 2.60            | 0.6              |
| Conf. 13  | 80.88    | 2.61            | 0.6              |
| Conf. 14  | 80.98    | 2.70            | 0.5              |
| Conf. 15  | 81.22    | 2.95            | 0.3              |
| Conf. 16  | 81.23    | 2.96            | 0.3              |
| Conf. 17  | 81.29    | 3.02            | 0.3              |
| Conf. 18  | 81.35    | 3.08            | 0.3              |
| Conf. 19  | 81.42    | 3.15            | 0.2              |
| Conf. 20  | 81.47    | 3.20            | 0.2              |
| Conf. 21  | 81.70    | 3.43            | 0.2              |
| Conf. 22  | 81.71    | 3.44            | 0.1              |
| Conf. 23  | 81.86    | 3.59            | 0.1              |
| Conf. 24  | 81.87    | 3.59            | 0.1              |
| Conf. 25  | 81.95    | 3.68            | 0.1              |
| Conf. 26  | 82.04    | 3.77            | 0.1              |
| Conf. 27  | 82.07    | 3.80            | 0.1              |
| Conf. 28  | 82.14    | 3.87            | 0.1              |
| Conf. 29  | 82.21    | 3.94            | 0.1              |
| Conf. 30  | 82.33    | 4.06            | 0.1              |
| Conf. 31  | 82.37    | 4.10            | 0.0              |
| Conf. 32  | 82.39    | 4.11            | 0.0              |
| Conf. 33  | 82.47    | 4.20            | 0.0              |
| Conf. 34  | 82.66    | 4.38            | 0.0              |
| Conf. 35  | 82.73    | 4.45            | 0.0              |
| Conf. 36  | 82.90    | 4.63            | 0.0              |
| Conf. 37  | 82.94    | 4.67            | 0.0              |
| Conf. 38  | 83.02    | 4.75            | 0.0              |
| Conf. 39  | 83.09    | 4.82            | 0.0              |
| Conf. 40  | 83.13    | 4.86            | 0.0              |
| Conf. 41  | 83.23    | 4.96            | 0.0              |
| Conf. 42  | 83.32    | 5.05            | 0.0              |
| Conf. 43 | 83.48 | 5.21 | 0.0 |
| Conf. 44 | 83.53 | 5.26 | 0.0 |
| Conf. 45 | 83.60 | 5.33 | 0.0 |
| Conf. 46 | 83.65 | 5.38 | 0.0 |
| Conf. 47 | 83.85 | 5.58 | 0.0 |
| Conf. 48 | 83.90 | 5.63 | 0.0 |
| Conf. 49 | 84.24 | 5.97 | 0.0 |
| Conf. 50 | 84.32 | 6.04 | 0.0 |
| Conf. 51 | 84.32 | 6.05 | 0.0 |
| Conf. 52 | 84.45 | 6.18 | 0.0 |
| Conf. 53 | 84.50 | 6.23 | 0.0 |
| Conf. 54 | 84.52 | 6.25 | 0.0 |
| Conf. 55 | 84.61 | 6.34 | 0.0 |
| Conf. 56 | 84.92 | 6.64 | 0.0 |
| Conf. 57 | 84.93 | 6.66 | 0.0 |
| Conf. 58 | 85.09 | 6.82 | 0.0 |
| Conf. 59 | 85.15 | 6.88 | 0.0 |
| Conf. 60 | 85.21 | 6.94 | 0.0 |
| Conf. 61 | 85.22 | 6.95 | 0.0 |
| Conf. 62 | 85.25 | 6.98 | 0.0 |
| Conf. 63 | 85.41 | 7.14 | 0.0 |
| Conf. 64 | 85.50 | 7.23 | 0.0 |
| Conf. 65 | 85.56 | 7.28 | 0.0 |
| Conf. 66 | 85.57 | 7.30 | 0.0 |
| Conf. 67 | 85.64 | 7.37 | 0.0 |
| Conf. 68 | 85.67 | 7.40 | 0.0 |
| Conf. 69 | 85.74 | 7.47 | 0.0 |
| Conf. 70 | 86.00 | 7.73 | 0.0 |
| Conf. 71 | 86.06 | 7.79 | 0.0 |
| Conf. 72 | 86.09 | 7.82 | 0.0 |
| Conf. 73 | 86.29 | 8.02 | 0.0 |
| Conf. 74 | 86.33 | 8.06 | 0.0 |
| Conf. 75 | 86.57 | 8.30 | 0.0 |
| Conf. 76 | 86.80 | 8.53 | 0.0 |
| Conf. 77 | 86.89 | 8.62 | 0.0 |
| Conf. 78 | 86.94 | 8.67 | 0.0 |
| Conf. 79 | 87.04 | 8.77 | 0.0 |
| Conf. 80 | 87.04 | 8.77 | 0.0 |
| Conf. 81 | 87.10 | 8.83 | 0.0 |
| Conf. 82 | 87.33 | 9.05 | 0.0 |
| Conf. 83 | 87.35 | 9.08 | 0.0 |
| Conf. 84 | 87.44 | 9.17 | 0.0 |
| Conf. 85 | 87.48 | 9.21 | 0.0 |
| Conf. 86 | 87.52 | 9.25 | 0.0 |
| Conf. 87 | 87.61 | 9.34 | 0.0 |
| Conf. 88 | 87.65 | 9.38 | 0.0 |
| Conf. |     |     |     |
|-------|-----|-----|-----|
| 89    | 87.67 | 9.39 | 0.0 |
| 90    | 87.72 | 9.45 | 0.0 |
| 91    | 87.78 | 9.51 | 0.0 |
| 92    | 87.84 | 9.57 | 0.0 |
| 93    | 87.86 | 9.58 | 0.0 |
| 94    | 87.92 | 9.65 | 0.0 |
| 95    | 87.96 | 9.69 | 0.0 |
| 96    | 87.96 | 9.69 | 0.0 |
| 97    | 88.10 | 9.83 | 0.0 |
| 98    | 88.12 | 9.85 | 0.0 |
| 99    | 88.13 | 9.86 | 0.0 |
| 100   | 88.16 | 9.89 | 0.0 |
Table S30. Steric energies (E_{SE} kcal mol\(^{-1}\)), relative steric energies (ΔE_{SE} kcal mol\(^{-1}\)) and percentage populations (% ΔE_{SE}) calculated for low-energy conformers of ether 9b at the molecular mechanics level.

| Conformer | E_{SE}  | ΔE_{SE} | % ΔE_{SE} |
|-----------|---------|---------|-----------|
| Conf. 01  | 107.50  | 0.00    | 33.7      |
| Conf. 02  | 107.50  | 0.00    | 33.7      |
| Conf. 03  | 107.97  | 0.47    | 15.2      |
| Conf. 04  | 107.97  | 0.47    | 15.2      |
| Conf. 05  | 110.35  | 2.85    | 0.3       |
| Conf. 06  | 110.35  | 2.85    | 0.3       |
| Conf. 07  | 110.60  | 3.10    | 0.2       |
| Conf. 08  | 110.60  | 3.10    | 0.2       |
| Conf. 09  | 110.81  | 3.31    | 0.1       |
| Conf. 10  | 110.81  | 3.31    | 0.1       |
| Conf. 11  | 110.86  | 3.36    | 0.1       |
| Conf. 12  | 110.86  | 3.36    | 0.1       |
| Conf. 13  | 110.86  | 3.36    | 0.1       |
| Conf. 14  | 110.86  | 3.36    | 0.1       |
| Conf. 15  | 111.09  | 3.59    | 0.1       |
| Conf. 16  | 111.09  | 3.59    | 0.1       |
| Conf. 17  | 111.13  | 3.63    | 0.1       |
| Conf. 18  | 111.13  | 3.63    | 0.1       |
| Conf. 19  | 111.15  | 3.64    | 0.1       |
| Conf. 20  | 111.15  | 3.64    | 0.1       |
| Conf. 21  | 112.92  | 5.42    | 0.0       |
| Conf. 22  | 112.92  | 5.42    | 0.0       |
| Conf. 23  | 113.20  | 5.70    | 0.0       |
| Conf. 24  | 113.20  | 5.70    | 0.0       |
| Conf. 25  | 113.23  | 5.73    | 0.0       |
| Conf. 26  | 113.23  | 5.73    | 0.0       |
| Conf. 27  | 113.27  | 5.77    | 0.0       |
| Conf. 28  | 113.27  | 5.77    | 0.0       |
| Conf. 29  | 113.29  | 5.79    | 0.0       |
| Conf. 30  | 113.29  | 5.79    | 0.0       |
| Conf. 31  | 113.52  | 6.02    | 0.0       |
| Conf. 32  | 113.52  | 6.02    | 0.0       |
| Conf. 33  | 113.59  | 6.09    | 0.0       |
| Conf. 34  | 113.59  | 6.09    | 0.0       |
| Conf. 35  | 113.64  | 6.14    | 0.0       |
| Conf. 36  | 113.64  | 6.14    | 0.0       |
| Conf. 37  | 113.84  | 6.34    | 0.0       |
| Conf. 38  | 113.84  | 6.34    | 0.0       |
| Conf. 39  | 113.93  | 6.43    | 0.0       |
| Conf. 40  | 113.93  | 6.43    | 0.0       |
| Conf. 41  | 114.12  | 6.62    | 0.0       |
| Conf. 42  | 114.12  | 6.62    | 0.0       |
| Conf. 43 |   114.33 |    6.83 |    0.0 |
| Conf. 44 |   114.33 |    6.83 |    0.0 |
| Conf. 45 |   114.79 |    7.29 |    0.0 |
| Conf. 46 |   114.79 |    7.29 |    0.0 |
| Conf. 47 |   115.36 |    7.86 |    0.0 |
| Conf. 48 |   115.36 |    7.86 |    0.0 |
| Conf. 49 |   115.61 |    8.11 |    0.0 |
| Conf. 50 |   115.61 |    8.11 |    0.0 |
| Conf. 51 |   115.84 |    8.34 |    0.0 |
| Conf. 52 |   115.84 |    8.34 |    0.0 |
| Conf. 53 |   115.92 |    8.41 |    0.0 |
| Conf. 54 |   115.92 |    8.41 |    0.0 |
| Conf. 55 |   115.93 |    8.43 |    0.0 |
| Conf. 56 |   115.93 |    8.43 |    0.0 |
| Conf. 57 |   117.15 |    9.65 |    0.0 |
| Conf. 58 |   117.15 |    9.65 |    0.0 |
| Conf. 59 |   117.32 |    9.82 |    0.0 |
Table S31. Steric energies (E<sub>SE</sub>, kcal mol<sup>-1</sup>), relative steric energies (ΔE<sub>SE</sub>, kcal mol<sup>-1</sup>) and percentage populations (% ΔE<sub>SE</sub>) calculated for low-energy conformers of ether 10b at the molecular mechanics level.

| Conformer | E<sub>SE</sub> | ΔE<sub>SE</sub> | % ΔE<sub>SE</sub> |
|-----------|----------------|----------------|------------------|
| Conf. 01  | 143.63         | 0.00           | 27.9             |
| Conf. 02  | 143.93         | 0.30           | 16.9             |
| Conf. 03  | 143.93         | 0.30           | 16.9             |
| Conf. 04  | 143.97         | 0.33           | 15.9             |
| Conf. 05  | 144.32         | 0.69           | 8.7              |
| Conf. 06  | 144.76         | 1.13           | 4.2              |
| Conf. 07  | 145.36         | 1.73           | 1.5              |
| Conf. 08  | 145.36         | 1.73           | 1.5              |
| Conf. 09  | 145.46         | 1.82           | 1.3              |
| Conf. 10  | 145.46         | 1.82           | 1.3              |
| Conf. 11  | 145.87         | 2.24           | 0.6              |
| Conf. 12  | 145.87         | 2.24           | 0.6              |
| Conf. 13  | 146.02         | 2.39           | 0.5              |
| Conf. 14  | 146.02         | 2.39           | 0.5              |
| Conf. 15  | 146.51         | 2.88           | 0.2              |
| Conf. 16  | 146.52         | 2.89           | 0.2              |
| Conf. 17  | 146.52         | 2.89           | 0.2              |
| Conf. 18  | 146.66         | 3.03           | 0.2              |
| Conf. 19  | 146.66         | 3.03           | 0.2              |
| Conf. 20  | 146.84         | 3.21           | 0.1              |
| Conf. 21  | 146.84         | 3.21           | 0.1              |
| Conf. 22  | 147.41         | 3.78           | 0.0              |
| Conf. 23  | 147.41         | 3.78           | 0.0              |
| Conf. 24  | 147.72         | 4.08           | 0.0              |
| Conf. 25  | 147.72         | 4.08           | 0.0              |
| Conf. 26  | 147.88         | 4.25           | 0.0              |
| Conf. 27  | 147.88         | 4.25           | 0.0              |
| Conf. 28  | 148.07         | 4.44           | 0.0              |
| Conf. 29  | 148.24         | 4.61           | 0.0              |
| Conf. 30  | 148.24         | 4.61           | 0.0              |
| Conf. 31  | 148.29         | 4.66           | 0.0              |
| Conf. 32  | 148.35         | 4.72           | 0.0              |
| Conf. 33  | 148.35         | 4.72           | 0.0              |
| Conf. 34  | 148.50         | 4.86           | 0.0              |
| Conf. 35  | 148.50         | 4.86           | 0.0              |
| Conf. 36  | 148.54         | 4.91           | 0.0              |
| Conf. 37  | 148.70         | 5.07           | 0.0              |
| Conf. 38  | 148.70         | 5.07           | 0.0              |
| Conf. 39  | 148.81         | 5.18           | 0.0              |
| Conf. 40  | 148.81         | 5.18           | 0.0              |
| Conf. 41  | 148.81         | 5.18           | 0.0              |
| Conf. 42  | 148.95         | 5.32           | 0.0              |
| Conf. 43 | 148.96 | 5.33 | 0.0 |
| Conf. 44 | 148.96 | 5.33 | 0.0 |
| Conf. 45 | 148.96 | 5.33 | 0.0 |
| Conf. 46 | 148.96 | 5.33 | 0.0 |
| Conf. 47 | 149.02 | 5.38 | 0.0 |
| Conf. 48 | 149.02 | 5.38 | 0.0 |
| Conf. 49 | 149.06 | 5.43 | 0.0 |
| Conf. 50 | 149.09 | 5.46 | 0.0 |
| Conf. 51 | 149.18 | 5.55 | 0.0 |
| Conf. 52 | 149.18 | 5.55 | 0.0 |
| Conf. 53 | 149.18 | 5.55 | 0.0 |
| Conf. 54 | 149.19 | 5.55 | 0.0 |
| Conf. 55 | 149.19 | 5.55 | 0.0 |
| Conf. 56 | 149.46 | 5.83 | 0.0 |
| Conf. 57 | 149.46 | 5.83 | 0.0 |
| Conf. 58 | 149.72 | 6.08 | 0.0 |
| Conf. 59 | 149.81 | 6.18 | 0.0 |
| Conf. 60 | 149.81 | 6.18 | 0.0 |
| Conf. 61 | 149.85 | 6.21 | 0.0 |
| Conf. 62 | 149.85 | 6.21 | 0.0 |
| Conf. 63 | 149.91 | 6.28 | 0.0 |
| Conf. 64 | 149.91 | 6.28 | 0.0 |
| Conf. 65 | 150.12 | 6.49 | 0.0 |
| Conf. 66 | 150.12 | 6.49 | 0.0 |
| Conf. 67 | 150.18 | 6.55 | 0.0 |
| Conf. 68 | 150.18 | 6.55 | 0.0 |
| Conf. 69 | 150.38 | 6.75 | 0.0 |
| Conf. 70 | 150.45 | 6.81 | 0.0 |
| Conf. 71 | 150.45 | 6.81 | 0.0 |
| Conf. 72 | 150.69 | 7.05 | 0.0 |
| Conf. 73 | 150.82 | 7.19 | 0.0 |
| Conf. 74 | 151.27 | 7.63 | 0.0 |
| Conf. 75 | 151.27 | 7.63 | 0.0 |
| Conf. 76 | 151.49 | 7.86 | 0.0 |
| Conf. 77 | 151.49 | 7.86 | 0.0 |
| Conf. 78 | 151.76 | 8.13 | 0.0 |
| Conf. 79 | 151.76 | 8.13 | 0.0 |
| Conf. 80 | 151.82 | 8.19 | 0.0 |
| Conf. 81 | 151.82 | 8.19 | 0.0 |
| Conf. 82 | 151.86 | 8.22 | 0.0 |
| Conf. 83 | 151.86 | 8.22 | 0.0 |
| Conf. 84 | 152.19 | 8.55 | 0.0 |
| Conf. 85 | 152.19 | 8.55 | 0.0 |
| Conf. 86 | 152.62 | 8.98 | 0.0 |
| Conf. 87 | 152.62 | 8.98 | 0.0 |
| Conf. 88 | 152.63 | 8.99 | 0.0 |
| Conf. | Value 1 | Value 2 | Value 3 |
|-------|---------|---------|---------|
| 89    | 152.63  | 9.00    | 0.0     |
| 90    | 152.63  | 9.00    | 0.0     |
| 91    | 152.67  | 9.03    | 0.0     |
| 92    | 153.12  | 9.49    | 0.0     |
| 93    | 153.15  | 9.52    | 0.0     |
| 94    | 153.15  | 9.52    | 0.0     |
| 95    | 153.24  | 9.61    | 0.0     |
| 96    | 153.32  | 9.69    | 0.0     |
| 97    | 153.32  | 9.69    | 0.0     |
| 98    | 153.48  | 9.84    | 0.0     |
| 99    | 153.58  | 9.95    | 0.0     |
| 100   | 153.58  | 9.95    | 0.0     |
Table S32. Total (E, in Hartree) and relative energies (ΔE, in kcal mol\(^{-1}\)) as a function of angles \(\alpha_1\) and \(\alpha_2\) (denoted here as a and b, respectively) calculated for conformers of 11 at B3LYP/6-311++G(d,p) level of theory.

| Conformer                      | E    | ΔE  |
|-------------------------------|------|-----|
| 1_Nph_model_a_0_b_0.gjf       | -924.111 | 23.30 |
| 1_Nph_model_a_0_b_10.gjf      | -924.12 | 17.25 |
| 1_Nph_model_a_0_b_20.gjf      | -924.129 | 12.15 |
| 1_Nph_model_a_0_b_30.gjf      | -924.135 | 8.04  |
| 1_Nph_model_a_0_b_40.gjf      | -924.144 | 4.91  |
| 1_Nph_model_a_0_b_50.gjf      | -924.144 | 1.43  |
| 1_Nph_model_a_0_b_60.gjf      | -924.146 | 1.43  |
| 1_Nph_model_a_0_b_70.gjf      | -924.147 | 0.71  |
| 1_Nph_model_a_0_b_80.gjf      | -924.147 | 0.40  |
| 1_Nph_model_a_0_b_90.gjf      | -924.147 | 0.50  |
| 1_Nph_model_a_0_b_100.gjf     | -924.146 | 1.30  |
| 1_Nph_model_a_0_b_110.gjf     | -924.143 | 2.85  |
| 1_Nph_model_a_0_b_120.gjf     | -924.144 | 4.91  |
| 1_Nph_model_a_0_b_130.gjf     | -924.136 | 7.42  |
| 1_Nph_model_a_0_b_140.gjf     | -924.132 | 10.04 |
| 1_Nph_model_a_0_b_150.gjf     | -924.128 | 12.31 |
| 1_Nph_model_a_0_b_160.gjf     | -924.125 | 14.48 |
| 1_Nph_model_a_0_b_170.gjf     | -924.122 | 16.37 |
| 1_Nph_model_a_0_b_180.gjf     | -924.121 | 17.06 |
| 1_Nph_model_a_0_b_m10.gjf     | -924.114 | 21.49 |
| 1_Nph_model_a_0_b_m20.gjf     | -924.118 | 18.69 |
| 1_Nph_model_a_0_b_m30.gjf     | -924.123 | 15.85 |
| 1_Nph_model_a_0_b_m40.gjf     | -924.127 | 13.14 |
| 1_Nph_model_a_0_b_m50.gjf     | -924.131 | 10.56 |
| 1_Nph_model_a_0_b_m60.gjf     | -924.135 | 8.03  |
| 1_Nph_model_a_0_b_m70.gjf     | -924.139 | 5.66  |
| 1_Nph_model_a_0_b_m80.gjf     | -924.142 | 3.77  |
| 1_Nph_model_a_0_b_m90.gjf     | -924.144 | 2.42  |
| 1_Nph_model_a_0_b_m100.gjf    | -924.145 | 1.59  |
| 1_Nph_model_a_0_b_m110.gjf    | -924.146 | 1.25  |
| 1_Nph_model_a_0_b_m120.gjf    | -924.145 | 1.63  |
| 1_Nph_model_a_0_b_m130.gjf    | -924.143 | 2.90  |
| 1_Nph_model_a_0_b_m140.gjf    | -924.142 | 5.29  |
| 1_Nph_model_a_0_b_m150.gjf    | -924.134 | 8.66  |
| 1_Nph_model_a_0_b_m160.gjf    | -924.128 | 12.42 |
| 1_Nph_model_a_0_b_m170.gjf    | -924.123 | 15.60 |
| 1_Nph_model_a_10_b_0.gjf      | -924.1 | 30.18 |
| 1_Nph_model_a_10_b_10.gjf     | -924.122 | 16.41 |
| 1_Nph_model_a_10_b_20.gjf     | -924.129 | 12.03 |
| 1_Nph_model_a_10_b_30.gjf     | -924.135 | 8.38  |
| 1_Nph_model_a_10_b_40.gjf     | -924.139 | 5.55  |
| File Name                        | Energy   | Distortion |
|---------------------------------|----------|------------|
| 1_Nph_model_a_10_b_50.gjf       | -924.142 | 3.57       |
| 1_Nph_model_a_10_b_60.gjf       | -924.144 | 2.34       |
| 1_Nph_model_a_10_b_70.gjf       | -924.145 | 1.67       |
| 1_Nph_model_a_10_b_80.gjf       | -924.146 | 1.43       |
| 1_Nph_model_a_10_b_90.gjf       | -924.145 | 1.74       |
| 1_Nph_model_a_10_b_100.gjf      | -924.143 | 2.80       |
| 1_Nph_model_a_10_b_110.gjf      | -924.14  | 4.72       |
| 1_Nph_model_a_10_b_120.gjf      | -924.136 | 7.22       |
| 1_Nph_model_a_10_b_130.gjf      | -924.131 | 10.35      |
| 1_Nph_model_a_10_b_140.gjf      | -924.126 | 13.75      |
| 1_Nph_model_a_10_b_150.gjf      | -924.121 | 16.75      |
| 1_Nph_model_a_10_b_160.gjf      | -924.117 | 19.40      |
| 1_Nph_model_a_10_b_170.gjf      | -924.114 | 21.60      |
| 1_Nph_model_a_10_b_180.gjf      | -924.113 | 22.22      |
| 1_Nph_model_a_10_b_m10.gjf      | -924.104 | 27.45      |
| 1_Nph_model_a_10_b_m20.gjf      | -924.11  | 23.77      |
| 1_Nph_model_a_10_b_m30.gjf      | -924.116 | 20.08      |
| 1_Nph_model_a_10_b_m40.gjf      | -924.122 | 16.56      |
| 1_Nph_model_a_10_b_m50.gjf      | -924.127 | 13.21      |
| 1_Nph_model_a_10_b_m60.gjf      | -924.132 | 9.97       |
| 1_Nph_model_a_10_b_m70.gjf      | -924.137 | 6.99       |
| 1_Nph_model_a_10_b_m80.gjf      | -924.141 | 4.61       |
| 1_Nph_model_a_10_b_m90.gjf      | -924.143 | 2.98       |
| 1_Nph_model_a_10_b_m100.gjf     | -924.145 | 2.05       |
| 1_Nph_model_a_10_b_m110.gjf     | -924.145 | 1.75       |
| 1_Nph_model_a_10_b_m120.gjf     | -924.144 | 2.23       |
| 1_Nph_model_a_10_b_m130.gjf     | -924.142 | 3.77       |
| 1_Nph_model_a_10_b_m140.gjf     | -924.137 | 6.56       |
| 1_Nph_model_a_10_b_m150.gjf     | -924.131 | 10.67      |
| 1_Nph_model_a_10_b_m160.gjf     | -924.123 | 15.64      |
| 1_Nph_model_a_10_b_m170.gjf     | -924.116 | 20.05      |
| 1_Nph_model_a_20_b_0.gjf        | -924.118 | 18.69      |
| 1_Nph_model_a_20_b_10.gjf       | -924.125 | 14.61      |
| 1_Nph_model_a_20_b_20.gjf       | -924.13  | 11.23      |
| 1_Nph_model_a_20_b_30.gjf       | -924.134 | 8.43       |
| 1_Nph_model_a_20_b_40.gjf       | -924.138 | 6.24       |
| 1_Nph_model_a_20_b_50.gjf       | -924.141 | 4.66       |
| 1_Nph_model_a_20_b_60.gjf       | -924.142 | 3.68       |
| 1_Nph_model_a_20_b_70.gjf       | -924.143 | 3.15       |
| 1_Nph_model_a_20_b_80.gjf       | -924.143 | 3.13       |
| 1_Nph_model_a_20_b_90.gjf       | -924.142 | 3.71       |
| 1_Nph_model_a_20_b_100.gjf      | -924.14  | 5.16       |
| 1_Nph_model_a_20_b_110.gjf      | -924.136 | 7.51       |
| 1_Nph_model_a_20_b_120.gjf      | -924.131 | 10.58      |
| 1_Nph_model_a_20_b_130.gjf      | -924.125 | 14.46      |
| File Name                     | Energy  | Deviation |
|------------------------------|---------|-----------|
| 1_Nph_model_a_20_b_140.gjf   | -924.118| 18.8      |
| 1_Nph_model_a_20_b_150.gjf   | -924.112| 22.54     |
| 1_Nph_model_a_20_b_160.gjf   | -924.107| 25.58     |
| 1_Nph_model_a_20_b_170.gjf   | -924.103| 27.92     |
| 1_Nph_model_a_20_b_180.gjf   | -924.103| 28.13     |
| 1_Nph_model_a_20_b_m10.gjf   | -924.093| 34.5      |
| 1_Nph_model_a_20_b_m20.gjf   | -924.1   | 30.05     |
| 1_Nph_model_a_20_b_m30.gjf   | -924.107| 25.52     |
| 1_Nph_model_a_20_b_m40.gjf   | -924.114| 21.14     |
| 1_Nph_model_a_20_b_m50.gjf   | -924.121| 16.93     |
| 1_Nph_model_a_20_b_m60.gjf   | -924.127| 12.89     |
| 1_Nph_model_a_20_b_m70.gjf   | -924.133| 9.24      |
| 1_Nph_model_a_20_b_m80.gjf   | -924.138| 6.34      |
| 1_Nph_model_a_20_b_m90.gjf   | -924.141| 4.27      |
| 1_Nph_model_a_20_b_m100.gjf  | -924.143| 3.07      |
| 1_Nph_model_a_20_b_m110.gjf  | -924.144| 2.63      |
| 1_Nph_model_a_20_b_m120.gjf  | -924.143| 3.18      |
| 1_Nph_model_a_20_b_m130.gjf  | -924.14  | 4.79      |
| 1_Nph_model_a_20_b_m140.gjf  | -924.136| 7.66      |
| 1_Nph_model_a_20_b_m150.gjf  | -924.129| 11.87     |
| 1_Nph_model_a_20_b_m160.gjf  | -924.121| 17.12     |
| 1_Nph_model_a_20_b_m170.gjf  | -924.109| 24.34     |
| 1_Nph_model_a_30_b_0.gjf     | -924.123| 15.85     |
| 1_Nph_model_a_30_b_10.gjf    | -924.128| 12.64     |
| 1_Nph_model_a_30_b_20.gjf    | -924.132| 10.23     |
| 1_Nph_model_a_30_b_30.gjf    | -924.135| 8.4       |
| 1_Nph_model_a_30_b_40.gjf    | -924.137| 6.99      |
| 1_Nph_model_a_30_b_50.gjf    | -924.138| 5.98      |
| 1_Nph_model_a_30_b_60.gjf    | -924.139| 5.39      |
| 1_Nph_model_a_30_b_70.gjf    | -924.14  | 5.2       |
| 1_Nph_model_a_30_b_80.gjf    | -924.139| 5.54      |
| 1_Nph_model_a_30_b_90.gjf    | -924.138| 6.5       |
| 1_Nph_model_a_30_b_100.gjf   | -924.134| 8.45      |
| 1_Nph_model_a_30_b_110.gjf   | -924.13 | 11.34     |
| 1_Nph_model_a_30_b_120.gjf   | -924.124| 15.08     |
| 1_Nph_model_a_30_b_130.gjf   | -924.116| 19.77     |
| 1_Nph_model_a_30_b_140.gjf   | -924.108| 25.13     |
| 1_Nph_model_a_30_b_150.gjf   | -924.101| 29.72     |
| 1_Nph_model_a_30_b_160.gjf   | -924.095| 32.99     |
| 1_Nph_model_a_30_b_170.gjf   | -924.092| 35.1      |
| 1_Nph_model_a_30_b_180.gjf   | -924.108| 25.15     |
| 1_Nph_model_a_30_b_m10.gjf   | -924.08  | 42.83     |
| 1_Nph_model_a_30_b_m20.gjf   | -924.088| 37.68     |
| 1_Nph_model_a_30_b_m30.gjf   | -924.096| 32.29     |
| 1_Nph_model_a_30_b_m40.gjf   | -924.105| 26.99     |
| File Name                          | ZPE     | Energy | Spreading Width |
|-----------------------------------|---------|--------|-----------------|
| 1_Nph_model_a_30_b_m50.gif        | -924.113| 21.83  |
| 1_Nph_model_a_30_b_m60.gif        | -924.121| 16.86  |
| 1_Nph_model_a_30_b_m70.gif        | -924.128| 12.41  |
| 1_Nph_model_a_30_b_m80.gif        | -924.134| 8.86   |
| 1_Nph_model_a_30_b_m90.gif        | -924.138| 6.27   |
| 1_Nph_model_a_30_b_m100.gif       | -924.14 | 4.67   |
| 1_Nph_model_a_30_b_m110.gif       | -924.142| 3.99   |
| 1_Nph_model_a_30_b_m120.gif       | -924.141| 4.25   |
| 1_Nph_model_a_30_b_m130.gif       | -924.139| 5.65   |
| 1_Nph_model_a_30_b_m140.gif       | -924.135| 8.18   |
| 1_Nph_model_a_30_b_m150.gif       | -924.129| 11.67  |
| 1_Nph_model_a_30_b_m160.gif       | -924.123| 15.82  |
| 1_Nph_model_a_30_b_m170.gif       | -924.115| 20.38  |
| 1_Nph_model_a_40_b_0.gif          | -924.127| 13.14  |
| 1_Nph_model_a_40_b_10.gif         | -924.131| 10.73  |
| 1_Nph_model_a_40_b_20.gif         | -924.133| 9.16   |
| 1_Nph_model_a_40_b_30.gif         | -924.135| 8.2    |
| 1_Nph_model_a_40_b_40.gif         | -924.136| 7.65   |
| 1_Nph_model_a_40_b_50.gif         | -924.136| 7.39   |
| 1_Nph_model_a_40_b_60.gif         | -924.136| 7.43   |
| 1_Nph_model_a_40_b_70.gif         | -924.135| 7.8    |
| 1_Nph_model_a_40_b_80.gif         | -924.134| 8.61   |
| 1_Nph_model_a_40_b_90.gif         | -924.132| 10.15  |
| 1_Nph_model_a_40_b_100.gif        | -924.128| 12.68  |
| 1_Nph_model_a_40_b_110.gif        | -924.122| 16.19  |
| 1_Nph_model_a_40_b_120.gif        | -924.115| 20.69  |
| 1_Nph_model_a_40_b_130.gif        | -924.106| 26.22  |
| 1_Nph_model_a_40_b_140.gif        | -924.096| 32.54  |
| 1_Nph_model_a_40_b_150.gif        | -924.087| 38.15  |
| 1_Nph_model_a_40_b_160.gif        | -924.082| 41.17  |
| 1_Nph_model_a_40_b_170.gif        | -924.107| 25.53  |
| 1_Nph_model_a_40_b_180.gif        | -924.114| 21.48  |
| 1_Nph_model_a_40_b_m10.gif        | -924.064| 52.51  |
| 1_Nph_model_a_40_b_m20.gif        | -924.073| 46.76  |
| 1_Nph_model_a_40_b_m30.gif        | -924.083| 40.49  |
| 1_Nph_model_a_40_b_m40.gif        | -924.093| 34.16  |
| 1_Nph_model_a_40_b_m50.gif        | -924.103| 27.9   |
| 1_Nph_model_a_40_b_m60.gif        | -924.113| 21.83  |
| 1_Nph_model_a_40_b_m70.gif        | -924.122| 16.45  |
| 1_Nph_model_a_40_b_m80.gif        | -924.129| 12.15  |
| 1_Nph_model_a_40_b_m90.gif        | -924.134| 8.97   |
| 1_Nph_model_a_40_b_m100.gif       | -924.137| 6.88   |
| 1_Nph_model_a_40_b_m110.gif       | -924.139| 5.77   |
| 1_Nph_model_a_40_b_m120.gif       | -924.139| 6.33   |
| 1_Nph_model_a_40_b_m130.gif       | -924.138| 6.47   |
| Filename                        | Energy  | Error  |
|--------------------------------|---------|--------|
| 1_Nph_model_a_40_b_m140.gjf    | -924.135 | 8.32   |
| 1_Nph_model_a_40_b_m150.gjf    | -924.13  | 10.99  |
| 1_Nph_model_a_40_b_m160.gjf    | -924.125 | 14.22  |
| 1_Nph_model_a_40_b_m170.gjf    | -924.12  | 17.77  |
| 1_Nph_model_a_50_b_0.gjf       | -924.131 | 10.56  |
| 1_Nph_model_a_50_b_10.gjf      | -924.134 | 8.88   |
| 1_Nph_model_a_50_b_20.gjf      | -924.135 | 8.05   |
| 1_Nph_model_a_50_b_30.gjf      | -924.135 | 7.9    |
| 1_Nph_model_a_50_b_40.gjf      | -924.135 | 8.21   |
| 1_Nph_model_a_50_b_50.gjf      | -924.134 | 8.86   |
| 1_Nph_model_a_50_b_60.gjf      | -924.132 | 9.69   |
| 1_Nph_model_a_50_b_70.gjf      | -924.131 | 10.76  |
| 1_Nph_model_a_50_b_80.gjf      | -924.128 | 12.25  |
| 1_Nph_model_a_50_b_90.gjf      | -924.125 | 14.51  |
| 1_Nph_model_a_50_b_100.gjf     | -924.12  | 17.72  |
| 1_Nph_model_a_50_b_110.gjf     | -924.113 | 21.92  |
| 1_Nph_model_a_50_b_120.gjf     | -924.125 | 27.16  |
| 1_Nph_model_a_50_b_130.gjf     | -924.095 | 33.43  |
| 1_Nph_model_a_50_b_140.gjf     | -924.084 | 40.37  |
| 1_Nph_model_a_50_b_150.gjf     | -924.102 | 28.52  |
| 1_Nph_model_a_50_b_160.gjf     | -924.109 | 24.37  |
| 1_Nph_model_a_50_b_170.gjf     | -924.115 | 20.76  |
| 1_Nph_model_a_50_b_180.gjf     | -924.12  | 17.77  |
| 1_Nph_model_a_50_b_20.gjf      | -924.127 | 13.21  |
| 1_Nph_model_a_50_b_m10.gjf     | -924.057 | 57.2   |
| 1_Nph_model_a_50_b_m30.gjf     | -924.068 | 50     |
| 1_Nph_model_a_50_b_m40.gjf     | -924.08  | 42.52  |
| 1_Nph_model_a_50_b_m50.gjf     | -924.092 | 34.98  |
| 1_Nph_model_a_50_b_m60.gjf     | -924.104 | 27.66  |
| 1_Nph_model_a_50_b_m70.gjf     | -924.114 | 21.25  |
| 1_Nph_model_a_50_b_m80.gjf     | -924.122 | 16.07  |
| 1_Nph_model_a_50_b_m90.gjf     | -924.128 | 12.21  |
| 1_Nph_model_a_50_b_m100.gjf    | -924.133 | 9.53   |
| 1_Nph_model_a_50_b_m110.gjf    | -924.135 | 7.91   |
| 1_Nph_model_a_50_b_m120.gjf    | -924.136 | 7.25   |
| 1_Nph_model_a_50_b_m130.gjf    | -924.136 | 7.49   |
| 1_Nph_model_a_50_b_m140.gjf    | -924.134 | 8.57   |
| 1_Nph_model_a_50_b_m150.gjf    | -924.131 | 10.33  |
| 1_Nph_model_a_50_b_m160.gjf    | -924.128 | 12.55  |
| 1_Nph_model_a_50_b_m170.gjf    | -924.124 | 15.07  |
| 1_Nph_model_a_60_b_0.gjf       | -924.135 | 8.03   |
| 1_Nph_model_a_60_b_10.gjf      | -924.137 | 7.02   |
| 1_Nph_model_a_60_b_20.gjf      | -924.137 | 6.88   |
| 1_Nph_model_a_60_b_30.gjf      | -924.136 | 7.45   |
| 1_Nph_model_a_60_b_40.gjf      | -924.134 | 8.61   |
| Filename                        | Value  | Difference |
|--------------------------------|--------|------------|
| 1_Nph_model_a_60_b_50.gif      | -924.132 | 10.18     |
| 1_Nph_model_a_60_b_60.gif      | -924.129 | 11.9      |
| 1_Nph_model_a_60_b_70.gif      | -924.126 | 13.83     |
| 1_Nph_model_a_60_b_80.gif      | -924.122 | 16.13     |
| 1_Nph_model_a_60_b_90.gif      | -924.117 | 19.14     |
| 1_Nph_model_a_60_b_100.gif     | -924.111 | 23.06     |
| 1_Nph_model_a_60_b_110.gif     | -924.104 | 27.87     |
| 1_Nph_model_a_60_b_120.gif     | -924.094 | 33.58     |
| 1_Nph_model_a_60_b_130.gif     | -924.085 | 39.72     |
| 1_Nph_model_a_60_b_140.gif     | -924.109 | 24.7      |
| 1_Nph_model_a_60_b_150.gif     | -924.113 | 21.63     |
| 1_Nph_model_a_60_b_160.gif     | -924.118 | 18.68     |
| 1_Nph_model_a_60_b_170.gif     | -924.122 | 16.21     |
| 1_Nph_model_a_60_b_180.gif     | -924.125 | 14.18     |
| 1_Nph_model_a_60_b_m10.gif     | -924.132 | 9.97      |
| 1_Nph_model_a_60_b_m20.gif     | -924.127 | 12.89     |
| 1_Nph_model_a_60_b_m30.gif     | -924.052 | 60.21     |
| 1_Nph_model_a_60_b_m40.gif     | -924.066 | 51.35     |
| 1_Nph_model_a_60_b_m50.gif     | -924.08  | 42.59     |
| 1_Nph_model_a_60_b_m60.gif     | -924.094 | 34.03     |
| 1_Nph_model_a_60_b_m70.gif     | -924.106 | 26.53     |
| 1_Nph_model_a_60_b_m80.gif     | -924.115 | 20.4      |
| 1_Nph_model_a_60_b_m90.gif     | -924.123 | 15.76     |
| 1_Nph_model_a_60_b_m100.gif    | -924.128 | 12.41     |
| 1_Nph_model_a_60_b_m110.gif    | -924.132 | 10.17     |
| 1_Nph_model_a_60_b_m120.gif    | -924.134 | 8.9       |
| 1_Nph_model_a_60_b_m130.gif    | -924.134 | 8.48      |
| 1_Nph_model_a_60_b_m140.gif    | -924.134 | 8.76      |
| 1_Nph_model_a_60_b_m150.gif    | -924.133 | 9.61      |
| 1_Nph_model_a_60_b_m160.gif    | -924.131 | 10.88     |
| 1_Nph_model_a_60_b_m170.gif    | -924.128 | 12.4      |
| 1_Nph_model_a_70_b_0.gif       | -924.139 | 5.66      |
| 1_Nph_model_a_70_b_10.gif      | -924.14  | 5.26      |
| 1_Nph_model_a_70_b_20.gif      | -924.139 | 5.67      |
| 1_Nph_model_a_70_b_30.gif      | -924.137 | 6.85      |
| 1_Nph_model_a_70_b_40.gif      | -924.134 | 8.76      |
| 1_Nph_model_a_70_b_50.gif      | -924.13  | 11.04     |
| 1_Nph_model_a_70_b_60.gif      | -924.126 | 13.58     |
| 1_Nph_model_a_70_b_70.gif      | -924.122 | 16.29     |
| 1_Nph_model_a_70_b_80.gif      | -924.117 | 19.41     |
| 1_Nph_model_a_70_b_90.gif      | -924.111 | 23.23     |
| 1_Nph_model_a_70_b_100.gif     | -924.104 | 27.69     |
| 1_Nph_model_a_70_b_110.gif     | -924.096 | 32.44     |
| 1_Nph_model_a_70_b_120.gif     | -924.112 | 22.82     |
| 1_Nph_model_a_70_b_130.gif     | -924.115 | 20.69     |
|                      | Energy     | RMSD       |
|----------------------|------------|------------|
| 1_Nph_model_a_70_b_140.gif | -924.119   | 18.25      |
| 1_Nph_model_a_70_b_150.gif | -924.123   | 15.84      |
| 1_Nph_model_a_70_b_160.gif | -924.126   | 13.8       |
| 1_Nph_model_a_70_b_170.gif | -924.128   | 12.22      |
| 1_Nph_model_a_70_b_180.gif | -924.13    | 10.97      |
| 1_Nph_model_a_70_b_m10.gif | -924.137   | 6.99       |
| 1_Nph_model_a_70_b_m20.gif | -924.133   | 9.24       |
| 1_Nph_model_a_70_b_m30.gif | -924.128   | 12.41      |
| 1_Nph_model_a_70_b_m40.gif | -924.122   | 16.45      |
| 1_Nph_model_a_70_b_m50.gif | -924.12   | 24.75      |
| 1_Nph_model_a_70_b_m60.gif | -924.084   | 40.41      |
| 1_Nph_model_a_70_b_m70.gif | -924.097   | 31.81      |
| 1_Nph_model_a_70_b_m80.gif | -924.108   | 24.75      |
| 1_Nph_model_a_70_b_m90.gif | -924.117   | 19.23      |
| 1_Nph_model_a_70_b_m100.gif | -924.124   | 15.13      |
| 1_Nph_model_a_70_b_m110.gif | -924.129   | 12.18      |
| 1_Nph_model_a_70_b_m120.gif | -924.132   | 10.21      |
| 1_Nph_model_a_70_b_m130.gif | -924.133   | 9.1        |
| 1_Nph_model_a_70_b_m140.gif | -924.134   | 8.62       |
| 1_Nph_model_a_70_b_m150.gif | -924.134   | 8.71       |
| 1_Nph_model_a_70_b_m160.gif | -924.133   | 9.21       |
| 1_Nph_model_a_70_b_m170.gif | -924.132   | 9.96       |
| 1_Nph_model_a_80_b_0.gif    | -924.142   | 3.77       |
| 1_Nph_model_a_80_b_10.gif   | -924.142   | 3.8        |
| 1_Nph_model_a_80_b_20.gif   | -924.141   | 4.6        |
| 1_Nph_model_a_80_b_30.gif   | -924.138   | 6.21       |
| 1_Nph_model_a_80_b_40.gif   | -924.134   | 8.46       |
| 1_Nph_model_a_80_b_50.gif   | -924.13    | 11.27      |
| 1_Nph_model_a_80_b_60.gif   | -924.125   | 14.49      |
| 1_Nph_model_a_80_b_70.gif   | -924.119   | 17.96      |
| 1_Nph_model_a_80_b_80.gif   | -924.113   | 21.68      |
| 1_Nph_model_a_80_b_90.gif   | -924.107   | 25.62      |
| 1_Nph_model_a_80_b_100.gif  | -924.116   | 20.05      |
| 1_Nph_model_a_80_b_110.gif  | -924.119   | 18.43      |
| 1_Nph_model_a_80_b_120.gif  | -924.121   | 16.82      |
| 1_Nph_model_a_80_b_130.gif  | -924.124   | 15.15      |
| 1_Nph_model_a_80_b_140.gif  | -924.127   | 13.1       |
| 1_Nph_model_a_80_b_150.gif  | -924.13    | 11.34      |
| 1_Nph_model_a_80_b_160.gif  | -924.132   | 9.98       |
| 1_Nph_model_a_80_b_170.gif  | -924.133   | 9.1        |
| 1_Nph_model_a_80_b_180.gif  | -924.134   | 8.45       |
| 1_Nph_model_a_80_b_m10.gif  | -924.141   | 4.61       |
| 1_Nph_model_a_80_b_m20.gif  | -924.138   | 6.34       |
| 1_Nph_model_a_80_b_m30.gif  | -924.134   | 8.86       |
| 1_Nph_model_a_80_b_m40.gif  | -924.129   | 12.15      |
| File Name                        | Energy   | EOM       |
|---------------------------------|----------|-----------|
| 1_Nph_model_a_80_b_m50.gjf      | -924.122 | 16.07     |
| 1_Nph_model_a_80_b_m60.gjf      | -924.075 | 46.05     |
| 1_Nph_model_a_80_b_m70.gjf      | -924.089 | 36.75     |
| 1_Nph_model_a_80_b_m80.gjf      | -924.102 | 28.86     |
| 1_Nph_model_a_80_b_m90.gjf      | -924.112 | 22.54     |
| 1_Nph_model_a_80_b_m100.gjf     | -924.12  | 17.68     |
| 1_Nph_model_a_80_b_m110.gjf     | -924.126 | 14.01     |
| 1_Nph_model_a_80_b_m120.gjf     | -924.13  | 11.34     |
| 1_Nph_model_a_80_b_m130.gjf     | -924.133 | 9.5       |
| 1_Nph_model_a_80_b_m140.gjf     | -924.135 | 8.31      |
| 1_Nph_model_a_80_b_m150.gjf     | -924.136 | 7.78      |
| 1_Nph_model_a_80_b_m160.gjf     | -924.136 | 7.73      |
| 1_Nph_model_a_80_b_m170.gjf     | -924.135 | 7.97      |
| 1_Nph_model_a_90_b_0.gjf        | -924.144 | 2.42      |
| 1_Nph_model_a_90_b_10.gjf       | -924.144 | 2.7       |
| 1_Nph_model_a_90_b_20.gjf       | -924.142 | 3.69      |
| 1_Nph_model_a_90_b_30.gjf       | -924.139 | 5.41      |
| 1_Nph_model_a_90_b_40.gjf       | -924.135 | 7.82      |
| 1_Nph_model_a_90_b_50.gjf       | -924.13  | 10.99     |
| 1_Nph_model_a_90_b_60.gjf       | -924.125 | 14.68     |
| 1_Nph_model_a_90_b_70.gjf       | -924.12  | 17.24     |
| 1_Nph_model_a_90_b_80.gjf       | -924.121 | 17.09     |
| 1_Nph_model_a_90_b_90.gjf       | -924.123 | 15.86     |
| 1_Nph_model_a_90_b_100.gjf      | -924.125 | 14.38     |
| 1_Nph_model_a_90_b_110.gjf      | -924.127 | 13.07     |
| 1_Nph_model_a_90_b_120.gjf      | -924.129 | 12.02     |
| 1_Nph_model_a_90_b_130.gjf      | -924.131 | 10.83     |
| 1_Nph_model_a_90_b_140.gjf      | -924.133 | 9.31      |
| 1_Nph_model_a_90_b_150.gjf      | -924.135 | 8.09      |
| 1_Nph_model_a_90_b_160.gjf      | -924.136 | 7.24      |
| 1_Nph_model_a_90_b_170.gjf      | -924.137 | 6.82      |
| 1_Nph_model_a_90_b_180.gjf      | -924.137 | 6.59      |
| 1_Nph_model_a_90_b_m10.gjf      | -924.143 | 2.98      |
| 1_Nph_model_a_90_b_m20.gjf      | -924.141 | 4.27      |
| 1_Nph_model_a_90_b_m30.gjf      | -924.138 | 6.27      |
| 1_Nph_model_a_90_b_m40.gjf      | -924.134 | 8.97      |
| 1_Nph_model_a_90_b_m50.gjf      | -924.128 | 12.21     |
| 1_Nph_model_a_90_b_m60.gjf      | -924.123 | 15.75     |
| 1_Nph_model_a_90_b_m70.gjf      | -924.082 | 41.1      |
| 1_Nph_model_a_90_b_m80.gjf      | -924.096 | 32.79     |
| 1_Nph_model_a_90_b_m90.gjf      | -924.107 | 25.84     |
| 1_Nph_model_a_90_b_m100.gjf     | -924.116 | 20.26     |
| 1_Nph_model_a_90_b_m110.gjf     | -924.123 | 15.86     |
| 1_Nph_model_a_90_b_m120.gjf     | -924.128 | 12.44     |
| 1_Nph_model_a_90_b_m130.gjf     | -924.132 | 9.86      |
| File Name                        | Energy  | Uncertainty |
|---------------------------------|---------|-------------|
| 1_Nph_model_a_90_b_m140.gjf      | -924.135 | 8.09        |
| 1_Nph_model_a_90_b_m150.gjf      | -924.137 | 6.99        |
| 1_Nph_model_a_90_b_m160.gjf      | -924.138 | 6.47        |
| 1_Nph_model_a_90_b_m170.gjf      | -924.138 | 6.38        |
| 1_Nph_model_a_100_b_0.gif        | -924.145 | 1.59        |
| 1_Nph_model_a_100_b_10.gif       | -924.145 | 1.88        |
| 1_Nph_model_a_100_b_20.gif       | -924.143 | 2.82        |
| 1_Nph_model_a_100_b_30.gif       | -924.141 | 4.5         |
| 1_Nph_model_a_100_b_40.gif       | -924.137 | 6.98        |
| 1_Nph_model_a_100_b_50.gif       | -924.132 | 9.95        |
| 1_Nph_model_a_100_b_60.gif       | -924.128 | 12.35       |
| 1_Nph_model_a_100_b_70.gif       | -924.127 | 13.08       |
| 1_Nph_model_a_100_b_80.gif       | -924.128 | 12.44       |
| 1_Nph_model_a_100_b_90.gif       | -924.13  | 11.18       |
| 1_Nph_model_a_100_b_100.gif      | -924.132 | 9.9         |
| 1_Nph_model_a_100_b_110.gif      | -924.134 | 8.97        |
| 1_Nph_model_a_100_b_120.gif      | -924.134 | 8.44        |
| 1_Nph_model_a_100_b_130.gif      | -924.136 | 7.76        |
| 1_Nph_model_a_100_b_140.gif      | -924.137 | 6.68        |
| 1_Nph_model_a_100_b_150.gif      | -924.139 | 5.89        |
| 1_Nph_model_a_100_b_160.gif      | -924.139 | 5.43        |
| 1_Nph_model_a_100_b_170.gif      | -924.139 | 5.31        |
| 1_Nph_model_a_100_b_180.gif      | -924.14  | 5.22        |
| 1_Nph_model_a_100_b_190.gif      | -924.145 | 2.05        |
| 1_Nph_model_a_100_b_m20.gif      | -924.143 | 3.07        |
| 1_Nph_model_a_100_b_m30.gif      | -924.14  | 4.67        |
| 1_Nph_model_a_100_b_m40.gif      | -924.137 | 6.87        |
| 1_Nph_model_a_100_b_m50.gif      | -924.133 | 9.53        |
| 1_Nph_model_a_100_b_m60.gif      | -924.128 | 12.41       |
| 1_Nph_model_a_100_b_m70.gif      | -924.124 | 15.12       |
| 1_Nph_model_a_100_b_m80.gif      | -924.12  | 17.67       |
| 1_Nph_model_a_100_b_m90.gif      | -924.102 | 28.56       |
| 1_Nph_model_a_100_b_m100.gif     | -924.112 | 22.48       |
| 1_Nph_model_a_100_b_m110.gif     | -924.12  | 17.45       |
| 1_Nph_model_a_100_b_m120.gif     | -924.127 | 13.41       |
| 1_Nph_model_a_100_b_m130.gif     | -924.132 | 10.29       |
| 1_Nph_model_a_100_b_m140.gif     | -924.135 | 8.01        |
| 1_Nph_model_a_100_b_m150.gif     | -924.138 | 6.47        |
| 1_Nph_model_a_100_b_m160.gif     | -924.139 | 5.61        |
| 1_Nph_model_a_100_b_m170.gif     | -924.144 | 5.25        |
| 1_Nph_model_a_110_b_0.gif        | -924.146 | 1.25        |
| 1_Nph_model_a_110_b_10.gif       | -924.146 | 1.37        |
| 1_Nph_model_a_110_b_20.gif       | -924.144 | 2.17        |
| 1_Nph_model_a_110_b_30.gif       | -924.142 | 3.7         |
| 1_Nph_model_a_110_b_40.gif       | -924.139 | 5.79        |
| File Name                          | Energy   | Error  |
|-----------------------------------|----------|--------|
| 1_Nph_model_a_110_b_50.gjf        | -924.135| 7.89   |
| 1_Nph_model_a_110_b_60.gjf        | -924.133| 9.26   |
| 1_Nph_model_a_110_b_70.gjf        | -924.133| 9.44   |
| 1_Nph_model_a_110_b_80.gjf        | -924.134| 8.72   |
| 1_Nph_model_a_110_b_90.gjf        | -924.136| 7.58   |
| 1_Nph_model_a_110_b_100.gjf       | -924.137| 6.62   |
| 1_Nph_model_a_110_b_110.gjf       | -924.138| 6.07   |
| 1_Nph_model_a_110_b_120.gjf       | -924.138| 6      |
| 1_Nph_model_a_110_b_130.gjf       | -924.139| 5.76   |
| 1_Nph_model_a_110_b_140.gjf       | -924.14  | 5.09   |
| 1_Nph_model_a_110_b_150.gjf       | -924.141| 4.63   |
| 1_Nph_model_a_110_b_160.gjf       | -924.141| 4.43   |
| 1_Nph_model_a_110_b_170.gjf       | -924.141| 4.45   |
| 1_Nph_model_a_110_b_180.gjf       | -924.141| 4.47   |
| 1_Nph_model_a_110_b_m10.gjf       | -924.145| 1.75   |
| 1_Nph_model_a_110_b_m20.gjf       | -924.144| 2.63   |
| 1_Nph_model_a_110_b_m30.gjf       | -924.142| 3.99   |
| 1_Nph_model_a_110_b_m40.gjf       | -924.139| 5.77   |
| 1_Nph_model_a_110_b_m50.gjf       | -924.135| 7.91   |
| 1_Nph_model_a_110_b_m60.gjf       | -924.132| 10.17  |
| 1_Nph_model_a_110_b_m70.gjf       | -924.129| 12.18  |
| 1_Nph_model_a_110_b_m80.gjf       | -924.126| 14.01  |
| 1_Nph_model_a_110_b_m90.gjf       | -924.123| 15.86  |
| 1_Nph_model_a_110_b_m100.gjf      | -924.12  | 17.45  |
| 1_Nph_model_a_110_b_m110.gjf      | -924.119| 18.03  |
| 1_Nph_model_a_110_b_m120.gjf      | -924.126| 13.84  |
| 1_Nph_model_a_110_b_m130.gjf      | -924.131| 10.44  |
| 1_Nph_model_a_110_b_m140.gjf      | -924.135| 7.88   |
| 1_Nph_model_a_110_b_m150.gjf      | -924.138| 6.1    |
| 1_Nph_model_a_110_b_m160.gjf      | -924.14  | 5.03   |
| 1_Nph_model_a_110_b_m170.gjf      | -924.141| 4.56   |
| 1_Nph_model_a_120_b_0.gjf         | -924.145| 1.63   |
| 1_Nph_model_a_120_b_10.gjf        | -924.146| 1.49   |
| 1_Nph_model_a_120_b_20.gjf        | -924.145| 1.97   |
| 1_Nph_model_a_120_b_30.gjf        | -924.143| 3.06   |
| 1_Nph_model_a_120_b_40.gjf        | -924.141| 4.52   |
| 1_Nph_model_a_120_b_50.gjf        | -924.139| 5.85   |
| 1_Nph_model_a_120_b_60.gjf        | -924.137| 6.68   |
| 1_Nph_model_a_120_b_70.gjf        | -924.137| 6.66   |
| 1_Nph_model_a_120_b_80.gjf        | -924.138| 5.98   |
| 1_Nph_model_a_120_b_90.gjf        | -924.14  | 5.08   |
| 1_Nph_model_a_120_b_100.gjf       | -924.141| 4.44   |
| 1_Nph_model_a_120_b_110.gjf       | -924.141| 4.26   |
| 1_Nph_model_a_120_b_120.gjf       | -924.141| 4.55   |
| 1_Nph_model_a_120_b_130.gjf       | -924.14  | 4.71   |
| File Name                        | Distance  | Energy  |
|---------------------------------|-----------|---------|
| 1_Nph_model_a_120_b_140.gif      | -924.141  | 4.41    |
| 1_Nph_model_a_120_b_150.gif      | -924.141  | 4.21    |
| 1_Nph_model_a_120_b_160.gif      | -924.141  | 4.2     |
| 1_Nph_model_a_120_b_170.gif      | -924.141  | 4.31    |
| 1_Nph_model_a_120_b_180.gif      | -924.141  | 4.39    |
| 1_Nph_model_a_120_b_m10.gif      | -924.144  | 2.23    |
| 1_Nph_model_a_120_b_m20.gif      | -924.143  | 3.18    |
| 1_Nph_model_a_120_b_m30.gif      | -924.141  | 4.25    |
| 1_Nph_model_a_120_b_m40.gif      | -924.139  | 5.63    |
| 1_Nph_model_a_120_b_m50.gif      | -924.136  | 7.25    |
| 1_Nph_model_a_120_b_m60.gif      | -924.134  | 8.91    |
| 1_Nph_model_a_120_b_m70.gif      | -924.132  | 10.21   |
| 1_Nph_model_a_120_b_m80.gif      | -924.13   | 11.33   |
| 1_Nph_model_a_120_b_m90.gif      | -924.128  | 12.44   |
| 1_Nph_model_a_120_b_m100.gif     | -924.127  | 13.41   |
| 1_Nph_model_a_120_b_m110.gif     | -924.126  | 13.84   |
| 1_Nph_model_a_120_b_m120.gif     | -924.127  | 12.92   |
| 1_Nph_model_a_120_b_m130.gif     | -924.132  | 10.15   |
| 1_Nph_model_a_120_b_m140.gif     | -924.136  | 7.73    |
| 1_Nph_model_a_120_b_m150.gif     | -924.138  | 5.99    |
| 1_Nph_model_a_120_b_m160.gif     | -924.14   | 4.97    |
| 1_Nph_model_a_120_b_m170.gif     | -924.141  | 4.51    |
| 1_Nph_model_a_130_b_0.gif        | -924.143  | 2.9     |
| 1_Nph_model_a_130_b_10.gif       | -924.144  | 2.39    |
| 1_Nph_model_a_130_b_20.gif       | -924.144  | 2.37    |
| 1_Nph_model_a_130_b_30.gif       | -924.143  | 2.82    |
| 1_Nph_model_a_130_b_40.gif       | -924.142  | 3.62    |
| 1_Nph_model_a_130_b_50.gif       | -924.141  | 4.38    |
| 1_Nph_model_a_130_b_60.gif       | -924.14   | 4.86    |
| 1_Nph_model_a_130_b_70.gif       | -924.14   | 4.76    |
| 1_Nph_model_a_130_b_80.gif       | -924.141  | 4.2     |
| 1_Nph_model_a_130_b_90.gif       | -924.142  | 3.58    |
| 1_Nph_model_a_130_b_100.gif      | -924.143  | 3.26    |
| 1_Nph_model_a_130_b_110.gif      | -924.142  | 3.43    |
| 1_Nph_model_a_130_b_120.gif      | -924.141  | 4.05    |
| 1_Nph_model_a_130_b_130.gif      | -924.141  | 4.58    |
| 1_Nph_model_a_130_b_140.gif      | -924.141  | 4.63    |
| 1_Nph_model_a_130_b_150.gif      | -924.14   | 4.67    |
| 1_Nph_model_a_130_b_160.gif      | -924.14   | 4.84    |
| 1_Nph_model_a_130_b_170.gif      | -924.14   | 5       |
| 1_Nph_model_a_130_b_180.gif      | -924.14   | 5.04    |
| 1_Nph_model_a_130_b_m10.gif      | -924.142  | 3.77    |
| 1_Nph_model_a_130_b_m20.gif      | -924.14   | 4.79    |
| 1_Nph_model_a_130_b_m30.gif      | -924.139  | 5.65    |
| 1_Nph_model_a_130_b_m40.gif      | -924.138  | 6.47    |
| File Name                        | Energy  | RMSD  |
|---------------------------------|---------|-------|
| 1_Nph_model_a_130_b_m50.gif     | -924.136 | 7.49  |
| 1_Nph_model_a_130_b_m60.gif     | -924.134 | 8.48  |
| 1_Nph_model_a_130_b_m70.gif     | -924.133 | 9.1   |
| 1_Nph_model_a_130_b_m80.gif     | -924.133 | 9.49  |
| 1_Nph_model_a_130_b_m90.gif     | -924.132 | 9.86  |
| 1_Nph_model_a_130_b_m100.gif    | -924.132 | 10.29 |
| 1_Nph_model_a_130_b_m110.gif    | -924.131 | 10.45 |
| 1_Nph_model_a_130_b_m120.gif    | -924.132 | 10.15 |
| 1_Nph_model_a_130_b_m130.gif    | -924.132 | 9.49  |
| 1_Nph_model_a_130_b_m140.gif    | -924.132 | 9.86  |
| 1_Nph_model_a_130_b_m150.gif    | -924.132 | 10.29 |
| 1_Nph_model_a_130_b_m160.gif    | -924.134 | 9.49  |
| 1_Nph_model_a_130_b_m170.gif    | -924.132 | 9.86  |
| 1_Nph_model_a_140_b_0.gif       | -924.14  | 5.28  |
| 1_Nph_model_a_140_b_10.gif      | -924.141 | 4.17  |
| 1_Nph_model_a_140_b_20.gif      | -924.142 | 3.42  |
| 1_Nph_model_a_140_b_30.gif      | -924.143 | 3.12  |
| 1_Nph_model_a_140_b_40.gif      | -924.143 | 3.25  |
| 1_Nph_model_a_140_b_50.gif      | -924.142 | 3.62  |
| 1_Nph_model_a_140_b_60.gif      | -924.142 | 3.87  |
| 1_Nph_model_a_140_b_70.gif      | -924.142 | 3.77  |
| 1_Nph_model_a_140_b_80.gif      | -924.143 | 3.38  |
| 1_Nph_model_a_140_b_90.gif      | -924.143 | 3.03  |
| 1_Nph_model_a_140_b_100.gif     | -924.143 | 3     |
| 1_Nph_model_a_140_b_110.gif     | -924.142 | 3.48  |
| 1_Nph_model_a_140_b_120.gif     | -924.141 | 4.35  |
| 1_Nph_model_a_140_b_130.gif     | -924.14  | 5.28  |
| 1_Nph_model_a_140_b_140.gif     | -924.139 | 5.74  |
| 1_Nph_model_a_140_b_150.gif     | -924.138 | 6.02  |
| 1_Nph_model_a_140_b_160.gif     | -924.138 | 6.37  |
| 1_Nph_model_a_140_b_170.gif     | -924.137 | 6.67  |
| 1_Nph_model_a_140_b_180.gif     | -924.137 | 6.59  |
| 1_Nph_model_a_140_b_190.gif     | -924.137 | 6.56  |
| 1_Nph_model_a_140_b_m10.gif     | -924.137 | 6.56  |
| 1_Nph_model_a_140_b_m20.gif     | -924.136 | 7.66  |
| 1_Nph_model_a_140_b_m30.gif     | -924.135 | 8.18  |
| 1_Nph_model_a_140_b_m40.gif     | -924.135 | 8.32  |
| 1_Nph_model_a_140_b_m50.gif     | -924.134 | 8.57  |
| 1_Nph_model_a_140_b_m60.gif     | -924.134 | 8.76  |
| 1_Nph_model_a_140_b_m70.gif     | -924.134 | 8.62  |
| 1_Nph_model_a_140_b_m80.gif     | -924.135 | 8.31  |
| 1_Nph_model_a_140_b_m90.gif     | -924.135 | 8.09  |
| 1_Nph_model_a_140_b_m100.gif    | -924.135 | 8.01  |
| 1_Nph_model_a_140_b_m110.gif    | -924.135 | 7.88  |
| 1_Nph_model_a_140_b_m120.gif    | -924.136 | 7.73  |
| 1_Nph_model_a_140_b_m130.gif    | -924.136 | 7.41  |
| File Name                                      | Energy  | T (K) |
|-----------------------------------------------|---------|-------|
| 1_Nph_model_a_140_b_m140.gjf                  | -924.137 | 6.89  |
| 1_Nph_model_a_140_b_m150.gjf                  | -924.138 | 6.43  |
| 1_Nph_model_a_140_b_m160.gjf                  | -924.138 | 6.2   |
| 1_Nph_model_a_140_b_m170.gjf                  | -924.138 | 6.31  |
| 1_Nph_model_a_150_b_0.gif                     | -924.134 | 8.66  |
| 1_Nph_model_a_150_b_10.gif                    | -924.137 | 6.66  |
| 1_Nph_model_a_150_b_20.gif                    | -924.141 | 4.04  |
| 1_Nph_model_a_150_b_30.gif                    | -924.142 | 5.06  |
| 1_Nph_model_a_150_b_40.gif                    | -924.142 | 5.37  |
| 1_Nph_model_a_150_b_50.gif                    | -924.142 | 3.58  |
| 1_Nph_model_a_150_b_60.gif                    | -924.142 | 3.71  |
| 1_Nph_model_a_150_b_70.gif                    | -924.142 | 3.67  |
| 1_Nph_model_a_150_b_80.gif                    | -924.142 | 3.44  |
| 1_Nph_model_a_150_b_90.gif                    | -924.143 | 3.26  |
| 1_Nph_model_a_150_b_100.gif                   | -924.142 | 3.5   |
| 1_Nph_model_a_150_b_110.gif                   | -924.141 | 4.23  |
| 1_Nph_model_a_150_b_120.gif                   | -924.139 | 5.38  |
| 1_Nph_model_a_150_b_130.gif                   | -924.137 | 6.72  |
| 1_Nph_model_a_150_b_140.gif                   | -924.136 | 7.69  |
| 1_Nph_model_a_150_b_150.gif                   | -924.135 | 8.36  |
| 1_Nph_model_a_150_b_160.gif                   | -924.134 | 8.93  |
| 1_Nph_model_a_150_b_170.gif                   | -924.133 | 9.31  |
| 1_Nph_model_a_150_b_180.gif                   | -924.133 | 9.21  |
| 1_Nph_model_a_150_b_190.gif                   | -924.131 | 10.67 |
| 1_Nph_model_a_150_b_200.gif                   | -924.129 | 11.87 |
| 1_Nph_model_a_150_b_210.gif                   | -924.129 | 11.67 |
| 1_Nph_model_a_150_b_220.gif                   | -924.131 | 10.99 |
| 1_Nph_model_a_150_b_230.gif                   | -924.131 | 10.33 |
| 1_Nph_model_a_150_b_240.gif                   | -924.133 | 9.61  |
| 1_Nph_model_a_150_b_250.gif                   | -924.134 | 8.71  |
| 1_Nph_model_a_150_b_260.gif                   | -924.136 | 7.78  |
| 1_Nph_model_a_150_b_270.gif                   | -924.137 | 6.99  |
| 1_Nph_model_a_150_b_280.gif                   | -924.138 | 6.47  |
| 1_Nph_model_a_150_b_290.gif                   | -924.138 | 6.1   |
| 1_Nph_model_a_150_b_300.gif                   | -924.138 | 5.99  |
| 1_Nph_model_a_150_b_310.gif                   | -924.138 | 6.1   |
| 1_Nph_model_a_150_b_320.gif                   | -924.138 | 6.43  |
| 1_Nph_model_a_150_b_330.gif                   | -924.137 | 6.97  |
| 1_Nph_model_a_150_b_340.gif                   | -924.136 | 7.71  |
| 1_Nph_model_a_150_b_350.gif                   | -924.134 | 8.54  |
| 1_Nph_model_a_160_b_0.gif                     | -924.128 | 12.42 |
| 1_Nph_model_a_160_b_10.gif                    | -924.133 | 9.45  |
| 1_Nph_model_a_160_b_20.gif                    | -924.137 | 7.08  |
| 1_Nph_model_a_160_b_30.gif                    | -924.139 | 5.44  |
| 1_Nph_model_a_160_b_40.gif                    | -924.141 | 4.51  |
| File Name                        | Energy (eV) | Width (Å) |
|---------------------------------|-------------|-----------|
| 1_Nph_model_a_160_b_50.gjf      | -924.141    | 4.21      |
| 1_Nph_model_a_160_b_60.gjf      | -924.141    | 4.23      |
| 1_Nph_model_a_160_b_70.gjf      | -924.141    | 4.2       |
| 1_Nph_model_a_160_b_80.gjf      | -924.141    | 4.08      |
| 1_Nph_model_a_160_b_90.gjf      | -924.141    | 4.1       |
| 1_Nph_model_a_160_b_100.gjf     | -924.141    | 4.53      |
| 1_Nph_model_a_160_b_110.gjf     | -924.139    | 5.55      |
| 1_Nph_model_a_160_b_120.gjf     | -924.137    | 7         |
| 1_Nph_model_a_160_b_130.gjf     | -924.134    | 8.79      |
| 1_Nph_model_a_160_b_140.gjf     | -924.131    | 10.54     |
| 1_Nph_model_a_160_b_150.gjf     | -924.129    | 11.65     |
| 1_Nph_model_a_160_b_160.gjf     | -924.128    | 12.59     |
| 1_Nph_model_a_160_b_170.gjf     | -924.127    | 13.15     |
| 1_Nph_model_a_160_b_180.gjf     | -924.127    | 12.91     |
| 1_Nph_model_a_160_b_190.gjf     | -924.123    | 15.64     |
| 1_Nph_model_a_160_b_200.gjf     | -924.121    | 17.12     |
| 1_Nph_model_a_160_b_210.gjf     | -924.123    | 15.82     |
| 1_Nph_model_a_160_b_220.gjf     | -924.125    | 14.22     |
| 1_Nph_model_a_160_b_230.gjf     | -924.128    | 12.55     |
| 1_Nph_model_a_160_b_240.gjf     | -924.131    | 10.88     |
| 1_Nph_model_a_160_b_250.gjf     | -924.133    | 9.2       |
| 1_Nph_model_a_160_b_260.gjf     | -924.136    | 7.73      |
| 1_Nph_model_a_160_b_270.gjf     | -924.138    | 6.47      |
| 1_Nph_model_a_160_b_280.gjf     | -924.139    | 5.61      |
| 1_Nph_model_a_160_b_290.gjf     | -924.14     | 5.03      |
| 1_Nph_model_a_160_b_300.gjf     | -924.14     | 4.97      |
| 1_Nph_model_a_160_b_310.gjf     | -924.14     | 5.27      |
| 1_Nph_model_a_160_b_320.gjf     | -924.138    | 6.2       |
| 1_Nph_model_a_160_b_330.gjf     | -924.136    | 7.7       |
| 1_Nph_model_a_160_b_340.gjf     | -924.133    | 9.64      |
| 1_Nph_model_a_160_b_350.gjf     | -924.129    | 11.6      |
| 1_Nph_model_a_170_b_0.gjf       | -924.123    | 15.61     |
| 1_Nph_model_a_170_b_10.gjf      | -924.129    | 11.8      |
| 1_Nph_model_a_170_b_20.gjf      | -924.134    | 8.83      |
| 1_Nph_model_a_170_b_30.gjf      | -924.137    | 6.77      |
| 1_Nph_model_a_170_b_40.gjf      | -924.139    | 5.57      |
| 1_Nph_model_a_170_b_50.gjf      | -924.14     | 5.11      |
| 1_Nph_model_a_170_b_60.gjf      | -924.14     | 5.08      |
| 1_Nph_model_a_170_b_70.gjf      | -924.14     | 5.08      |
| 1_Nph_model_a_170_b_80.gjf      | -924.14     | 5.01      |
| 1_Nph_model_a_170_b_90.gjf      | -924.14     | 5.16      |
| 1_Nph_model_a_170_b_100.gjf     | -924.139    | 5.83      |
| 1_Nph_model_a_170_b_110.gjf     | -924.137    | 7.13      |
| 1_Nph_model_a_170_b_120.gjf     | -924.134    | 8.97      |
| 1_Nph_model_a_170_b_130.gjf     | -924.13    | 11.37     |
| 1_Nph_model_a_170_b_140.gjf     | -924.126    | 14.06     |
| File Name                     | Energy (a.u.) | RMSD (Å) |
|------------------------------|---------------|----------|
| 1_Nph_model_a_170_b_150.gjf  | -924.122      | 15.98    |
| 1_Nph_model_a_170_b_160.gjf  | -924.12       | 17.33    |
| 1_Nph_model_a_170_b_170.gjf  | -924.119      | 18.05    |
| 1_Nph_model_a_170_b_180.gjf  | -924.12       | 17.44    |
| 1_Nph_model_a_170_b_m10.gjf  | -924.116      | 20.05    |
| 1_Nph_model_a_170_b_m20.gjf  | -924.112      | 22.7     |
| 1_Nph_model_a_170_b_m30.gjf  | -924.115      | 20.38    |
| 1_Nph_model_a_170_b_m40.gjf  | -924.12       | 17.77    |
| 1_Nph_model_a_170_b_m50.gjf  | -924.124      | 15.07    |
| 1_Nph_model_a_170_b_m60.gjf  | -924.128      | 12.4     |
| 1_Nph_model_a_170_b_m70.gjf  | -924.132      | 9.96     |
| 1_Nph_model_a_170_b_m80.gjf  | -924.135      | 7.97     |
| 1_Nph_model_a_170_b_m90.gjf  | -924.138      | 6.39     |
| 1_Nph_model_a_170_b_m100.gjf | -924.14       | 5.25     |
| 1_Nph_model_a_170_b_m110.gjf | -924.141      | 4.56     |
| 1_Nph_model_a_170_b_m120.gjf | -924.141      | 4.51     |
| 1_Nph_model_a_170_b_m130.gjf | -924.14       | 4.96     |
| 1_Nph_model_a_170_b_m140.gjf | -924.138      | 6.31     |
| 1_Nph_model_a_170_b_m150.gjf | -924.134      | 8.54     |
| 1_Nph_model_a_170_b_m160.gjf | -924.129      | 11.6     |
| 1_Nph_model_a_170_b_m170.gjf | -924.124      | 14.9     |
| 1_Nph_model_a_180_b_0.gjf    | -924.121      | 17.06    |
| 1_Nph_model_a_180_b_10.gjf   | -924.127      | 12.88    |
| 1_Nph_model_a_180_b_20.gjf   | -924.132      | 9.71     |
| 1_Nph_model_a_180_b_30.gjf   | -924.136      | 7.55     |
| 1_Nph_model_a_180_b_40.gjf   | -924.138      | 6.34     |
| 1_Nph_model_a_180_b_50.gjf   | -924.139      | 5.87     |
| 1_Nph_model_a_180_b_60.gjf   | -924.139      | 5.8      |
| 1_Nph_model_a_180_b_70.gjf   | -924.139      | 5.83     |
| 1_Nph_model_a_180_b_80.gjf   | -924.139      | 5.85     |
| 1_Nph_model_a_180_b_90.gjf   | -924.138      | 6.18     |
| 1_Nph_model_a_180_b_100.gjf  | -924.136      | 7.2      |
| 1_Nph_model_a_180_b_110.gjf  | -924.134      | 8.88     |
| 1_Nph_model_a_180_b_120.gjf  | -924.13       | 11.23    |
| 1_Nph_model_a_180_b_130.gjf  | -924.125      | 14.37    |
| 1_Nph_model_a_180_b_140.gjf  | -924.119      | 18.13    |
| 1_Nph_model_a_180_b_150.gjf  | -924.114      | 21.15    |
| 1_Nph_model_a_180_b_160.gjf  | -924.112      | 22.81    |
| 1_Nph_model_a_180_b_170.gjf  | -924.111      | 23.46    |
| 1_Nph_model_a_180_b_180.gjf  | -924.113      | 21.77    |
| 1_Nph_model_a_180_b_m10.gjf  | -924.099      | 30.58    |
| 1_Nph_model_a_180_b_m20.gjf  | -924.103      | 28.44    |
| 1_Nph_model_a_180_b_m30.gjf  | -924.108      | 25.15    |
| 1_Nph_model_a_180_b_m40.gjf  | -924.114      | 21.47    |
| 1_Nph_model_a_180_b_m50.gjf  | -924.12       | 17.76    |
| 1_Nph_model_a_180_b_m60.gjf  | -924.125      | 14.18    |
| 1_Nph_model_a_180_b_m70.gjf  | -924.13       | 10.97    |
| 1_Nph_model_a_180_b_m80.gjf  | -924.134      | 8.45     |
| 1_Nph_model_a_180_b_m90.gjf  | -924.137      | 6.59     |
| 1_Nph_model_a_180_b_m100.gjf | -924.14       | 5.22     |
| 1_Nph_model_a_180_b_m110.gjf | -924.141      | 4.47     |
| 1_Nph_model_a_180_b_m120.gjf | -924.141      | 4.39     |
| File Name                          | Energy   | EOM       |
|-----------------------------------|----------|-----------|
| 1_Nph_model_a_180_b_m130.gjf       | -924.14  | 5.04      |
| 1_Nph_model_a_180_b_m140.gjf       | -924.137 | 6.59      |
| 1_Nph_model_a_180_b_m150.gjf       | -924.133 | 9.21      |
| 1_Nph_model_a_180_b_m160.gjf       | -924.127 | 12.91     |
| 1_Nph_model_a_180_b_m170.gjf       | -924.12  | 17.44     |
| 1_Nph_model_a_m10_b_0.gjf          | -924.12  | 17.25     |
| 1_Nph_model_a_m10_b_10.gjf         | -924.123 | 15.64     |
| 1_Nph_model_a_m10_b_20.gjf         | -924.13  | 11.38     |
| 1_Nph_model_a_m10_b_30.gjf         | -924.136 | 7.51      |
| 1_Nph_model_a_m10_b_40.gjf         | -924.141 | 4.5       |
| 1_Nph_model_a_m10_b_50.gjf         | -924.144 | 2.38      |
| 1_Nph_model_a_m10_b_60.gjf         | -924.146 | 1.05      |
| 1_Nph_model_a_m10_b_70.gjf         | -924.147 | 0.34      |
| 1_Nph_model_a_m10_b_80.gjf         | -924.148 | 0         |
| 1_Nph_model_a_m10_b_90.gjf         | -924.148 | 0.01      |
| 1_Nph_model_a_m10_b_100.gjf        | -924.147 | 0.61      |
| 1_Nph_model_a_m10_b_110.gjf        | -924.145 | 1.86      |
| 1_Nph_model_a_m10_b_120.gjf        | -924.142 | 3.57      |
| 1_Nph_model_a_m10_b_130.gjf        | -924.139 | 5.55      |
| 1_Nph_model_a_m10_b_140.gjf        | -924.136 | 7.44      |
| 1_Nph_model_a_m10_b_150.gjf        | -924.133 | 9.1       |
| 1_Nph_model_a_m10_b_160.gjf        | -924.131 | 10.74     |
| 1_Nph_model_a_m10_b_170.gjf        | -924.128 | 12.27     |
| 1_Nph_model_a_m10_b_180.gjf        | -924.127 | 12.88     |
| 1_Nph_model_a_m10_b_m10.gjf        | -924.122 | 16.41     |
| 1_Nph_model_a_m10_b_m20.gjf        | -924.125 | 14.61     |
| 1_Nph_model_a_m10_b_m30.gjf        | -924.128 | 12.64     |
| 1_Nph_model_a_m10_b_m40.gjf        | -924.131 | 10.73     |
| 1_Nph_model_a_m10_b_m50.gjf        | -924.134 | 8.88      |
| 1_Nph_model_a_m10_b_m60.gjf        | -924.137 | 7.02      |
| 1_Nph_model_a_m10_b_m70.gjf        | -924.14  | 5.26      |
| 1_Nph_model_a_m10_b_m80.gjf        | -924.142 | 3.8       |
| 1_Nph_model_a_m10_b_m90.gjf        | -924.144 | 2.7       |
| 1_Nph_model_a_m10_b_m100.gjf       | -924.145 | 1.88      |
| 1_Nph_model_a_m10_b_m110.gjf       | -924.146 | 1.37      |
| 1_Nph_model_a_m10_b_m120.gjf       | -924.146 | 1.49      |
| 1_Nph_model_a_m10_b_m130.gjf       | -924.144 | 2.39      |
| 1_Nph_model_a_m10_b_m140.gjf       | -924.141 | 4.17      |
| 1_Nph_model_a_m10_b_m150.gjf       | -924.137 | 6.66      |
| 1_Nph_model_a_m10_b_m160.gjf       | -924.133 | 9.45      |
| 1_Nph_model_a_m10_b_m170.gjf       | -924.129 | 11.8      |
| 1_Nph_model_a_m20_b_0.gjf          | -924.129 | 12.15     |
| 1_Nph_model_a_m20_b_10.gjf         | -924.13  | 11.38     |
| 1_Nph_model_a_m20_b_20.gjf         | -924.133 | 9.66      |
| 1_Nph_model_a_m20_b_30.gjf         | -924.137 | 6.81      |
| 1_Nph_model_a_m20_b_40.gjf         | -924.141 | 4.29      |
| 1_Nph_model_a_m20_b_50.gjf         | -924.144 | 2.48      |
| 1_Nph_model_a_m20_b_60.gjf         | -924.146 | 1.29      |
| 1_Nph_model_a_m20_b_70.gjf         | -924.147 | 0.58      |
| 1_Nph_model_a_m20_b_80.gjf         | -924.148 | 0.25      |
| 1_Nph_model_a_m20_b_90.gjf         | -924.148 | 0.23      |
| 1_Nph_model_a_m20_b_100.gjf        | -924.147 | 0.65      |
| Filename                      | Energy   | Difference |
|-------------------------------|----------|------------|
| 1_Nph_model_a_m20_b_110.gif   | -924.145| 1.65       |
| 1_Nph_model_a_m20_b_120.gif   | -924.143| 3.09       |
| 1_Nph_model_a_m20_b_130.gif   | -924.141| 4.6        |
| 1_Nph_model_a_m20_b_140.gif   | -924.139| 5.87       |
| 1_Nph_model_a_m20_b_150.gif   | -924.137| 7.01       |
| 1_Nph_model_a_m20_b_160.gif   | -924.135| 8.16       |
| 1_Nph_model_a_m20_b_170.gif   | -924.133| 9.27       |
| 1_Nph_model_a_m20_b_180.gif   | -924.132| 9.71       |
| 1_Nph_model_a_m20_b_m10.gif   | -924.129| 12.03      |
| 1_Nph_model_a_m20_b_m20.gif   | -924.13  | 11.23      |
| 1_Nph_model_a_m20_b_m30.gif   | -924.132| 10.23      |
| 1_Nph_model_a_m20_b_m40.gif   | -924.133| 9.16       |
| 1_Nph_model_a_m20_b_m50.gif   | -924.135| 8.05       |
| 1_Nph_model_a_m20_b_m60.gif   | -924.137| 6.88       |
| 1_Nph_model_a_m20_b_m70.gif   | -924.139| 5.67       |
| 1_Nph_model_a_m20_b_m80.gif   | -924.141| 4.6        |
| 1_Nph_model_a_m20_b_m90.gif   | -924.142| 3.69       |
| 1_Nph_model_a_m20_b_m100.gif  | -924.143| 2.82       |
| 1_Nph_model_a_m20_b_m110.gif  | -924.144| 2.17       |
| 1_Nph_model_a_m20_b_m120.gif  | -924.145| 1.97       |
| 1_Nph_model_a_m20_b_m130.gif  | -924.144| 2.37       |
| 1_Nph_model_a_m20_b_m140.gif  | -924.142| 3.42       |
| 1_Nph_model_a_m20_b_m150.gif  | -924.142| 5.06       |
| 1_Nph_model_a_m20_b_m160.gif  | -924.137| 7.08       |
| 1_Nph_model_a_m20_b_m170.gif  | -924.134| 8.83       |
| 1_Nph_model_a_m30_b_0.gif     | -924.135| 8.03       |
| 1_Nph_model_a_m30_b_10.gif    | -924.136| 7.51       |
| 1_Nph_model_a_m30_b_20.gif    | -924.137| 6.8        |
| 1_Nph_model_a_m30_b_30.gif    | -924.139| 5.78       |
| 1_Nph_model_a_m30_b_40.gif    | -924.141| 4.27       |
| 1_Nph_model_a_m30_b_50.gif    | -924.143| 2.97       |
| 1_Nph_model_a_m30_b_60.gif    | -924.145| 2.07       |
| 1_Nph_model_a_m30_b_70.gif    | -924.146| 1.47       |
| 1_Nph_model_a_m30_b_80.gif    | -924.146| 1.11       |
| 1_Nph_model_a_m30_b_90.gif    | -924.146| 1.03       |
| 1_Nph_model_a_m30_b_100.gif   | -924.146| 1.36       |
| 1_Nph_model_a_m30_b_110.gif   | -924.145| 2.13       |
| 1_Nph_model_a_m30_b_120.gif   | -924.143| 3.29       |
| 1_Nph_model_a_m30_b_130.gif   | -924.141| 4.4        |
| 1_Nph_model_a_m30_b_140.gif   | -924.14  | 5.19       |
| 1_Nph_model_a_m30_b_150.gif   | -924.139| 5.88       |
| 1_Nph_model_a_m30_b_160.gif   | -924.137| 6.59       |
| 1_Nph_model_a_m30_b_170.gif   | -924.136| 7.32       |
| 1_Nph_model_a_m30_b_180.gif   | -924.136| 7.55       |
| 1_Nph_model_a_m30_b_m10.gif   | -924.135| 8.38       |
| 1_Nph_model_a_m30_b_m20.gif   | -924.134| 8.43       |
| 1_Nph_model_a_m30_b_m30.gif   | -924.135| 8.4        |
| 1_Nph_model_a_m30_b_m40.gif   | -924.135| 8.2        |
| 1_Nph_model_a_m30_b_m50.gif   | -924.135| 7.9        |
| 1_Nph_model_a_m30_b_m60.gif   | -924.136| 7.45       |
| 1_Nph_model_a_m30_b_m70.gif   | -924.137| 6.85       |
| 1_Nph_model_a_m30_b_m80.gif   | -924.138| 6.21       |
| File Name                        | Energy (E) | Error (e) |
|---------------------------------|------------|-----------|
| 1_Nph_model_a_m30_b_m90.gjf     | -924.139   | 5.41      |
| 1_Nph_model_a_m30_b_m100.gjf    | -924.141   | 4.5       |
| 1_Nph_model_a_m30_b_m110.gjf    | -924.142   | 3.7       |
| 1_Nph_model_a_m30_b_m120.gjf    | -924.143   | 3.06      |
| 1_Nph_model_a_m30_b_m130.gjf    | -924.143   | 3.06      |
| 1_Nph_model_a_m30_b_m140.gjf    | -924.143   | 3.12      |
| 1_Nph_model_a_m30_b_m150.gjf    | -924.141   | 4.04      |
| 1_Nph_model_a_m30_b_m160.gjf    | -924.139   | 5.44      |
| 1_Nph_model_a_m30_b_m170.gjf    | -924.137   | 6.77      |
| 1_Nph_model_a_m40_b_0.gjf       | -924.140    | 4.91      |
| 1_Nph_model_a_m40_b_10.gjf      | -924.141    | 4.5       |
| 1_Nph_model_a_m40_b_20.gjf      | -924.141    | 4.27      |
| 1_Nph_model_a_m40_b_30.gjf      | -924.141    | 4.21      |
| 1_Nph_model_a_m40_b_40.gjf      | -924.141    | 3.84      |
| 1_Nph_model_a_m40_b_50.gjf      | -924.141    | 3.37      |
| 1_Nph_model_a_m40_b_60.gjf      | -924.141    | 3.14      |
| 1_Nph_model_a_m40_b_70.gjf      | -924.141    | 2.91      |
| 1_Nph_model_a_m40_b_80.gjf      | -924.141    | 2.55      |
| 1_Nph_model_a_m40_b_90.gjf      | -924.141    | 2.34      |
| 1_Nph_model_a_m40_b_100.gjf     | -924.141    | 2.5       |
| 1_Nph_model_a_m40_b_110.gjf     | -924.141    | 3.14      |
| 1_Nph_model_a_m40_b_120.gjf     | -924.141    | 4.06      |
| 1_Nph_model_a_m40_b_130.gjf     | -924.141    | 4.88      |
| 1_Nph_model_a_m40_b_140.gjf     | -924.141    | 5.21      |
| 1_Nph_model_a_m40_b_150.gjf     | -924.139    | 5.55      |
| 1_Nph_model_a_m40_b_160.gjf     | -924.138    | 5.93      |
| 1_Nph_model_a_m40_b_170.gjf     | -924.138    | 6.32      |
| 1_Nph_model_a_m40_b_180.gjf     | -924.138    | 6.34      |
| 1_Nph_model_a_m40_b_20.gjf      | -924.141    | 5.55      |
| 1_Nph_model_a_m40_b_30.gjf      | -924.141    | 6.24      |
| 1_Nph_model_a_m40_b_40.gjf      | -924.136    | 7.65      |
| 1_Nph_model_a_m40_b_50.gjf      | -924.135    | 8.21      |
| 1_Nph_model_a_m40_b_60.gjf      | -924.134    | 8.61      |
| 1_Nph_model_a_m40_b_70.gjf      | -924.134    | 8.76      |
| 1_Nph_model_a_m40_b_80.gjf      | -924.134    | 8.46      |
| 1_Nph_model_a_m40_b_90.gjf      | -924.135    | 7.82      |
| 1_Nph_model_a_m40_b_100.gjf     | -924.137    | 6.99      |
| 1_Nph_model_a_m40_b_110.gjf     | -924.135    | 6.24      |
| 1_Nph_model_a_m40_b_120.gjf     | -924.134    | 5.93      |
| 1_Nph_model_a_m40_b_130.gjf     | -924.139    | 7.65      |
| 1_Nph_model_a_m40_b_140.gjf     | -924.135    | 8.21      |
| 1_Nph_model_a_m40_b_150.gjf     | -924.134    | 8.61      |
| 1_Nph_model_a_m40_b_160.gjf     | -924.134    | 8.76      |
| 1_Nph_model_a_m40_b_170.gjf     | -924.134    | 8.46      |
| 1_Nph_model_a_m40_b_180.gjf     | -924.134    | 7.82      |
| 1_Nph_model_a_m40_b_190.gjf     | -924.135    | 6.99      |
| 1_Nph_model_a_m40_b_200.gjf     | -924.134    | 5.93      |
| 1_Nph_model_a_m40_b_210.gjf     | -924.134    | 7.65      |
| 1_Nph_model_a_m40_b_220.gjf     | -924.134    | 8.21      |
| 1_Nph_model_a_m40_b_230.gjf     | -924.134    | 8.61      |
| 1_Nph_model_a_m40_b_240.gjf     | -924.134    | 8.76      |
| 1_Nph_model_a_m40_b_250.gjf     | -924.134    | 8.46      |
| 1_Nph_model_a_m40_b_260.gjf     | -924.134    | 7.82      |
| 1_Nph_model_a_m40_b_270.gjf     | -924.135    | 6.99      |
| 1_Nph_model_a_m40_b_280.gjf     | -924.134    | 5.93      |
| 1_Nph_model_a_m40_b_290.gjf     | -924.134    | 7.65      |
| 1_Nph_model_a_m40_b_300.gjf     | -924.134    | 8.21      |
| 1_Nph_model_a_m40_b_310.gjf     | -924.134    | 8.61      |
| 1_Nph_model_a_m40_b_320.gjf     | -924.134    | 8.76      |
| File Name                          | Energy  | Charge |
|-----------------------------------|---------|--------|
| 1_Nph_model_a_m50_b_70.gif         | -924.14 | 4.88   |
| 1_Nph_model_a_m50_b_80.gif         | -924.141| 4.54   |
| 1_Nph_model_a_m50_b_90.gif         | -924.141| 4.24   |
| 1_Nph_model_a_m50_b_100.gif        | -924.141| 4.2    |
| 1_Nph_model_a_m50_b_110.gif        | -924.141| 4.54   |
| 1_Nph_model_a_m50_b_120.gif        | -924.14  | 5.19   |
| 1_Nph_model_a_m50_b_130.gif        | -924.139| 5.78   |
| 1_Nph_model_a_m50_b_140.gif        | -924.139| 5.79   |
| 1_Nph_model_a_m50_b_150.gif        | -924.139| 5.74   |
| 1_Nph_model_a_m50_b_160.gif        | -924.139| 5.87   |
| 1_Nph_model_a_m50_b_170.gif        | -924.138| 6.01   |
| 1_Nph_model_a_m50_b_180.gif        | -924.139| 5.87   |
| 1_Nph_model_a_m50_b_m10.gif        | -924.142| 3.58   |
| 1_Nph_model_a_m50_b_m20.gif        | -924.141| 4.66   |
| 1_Nph_model_a_m50_b_m30.gif        | -924.138| 5.98   |
| 1_Nph_model_a_m50_b_m40.gif        | -924.136| 7.39   |
| 1_Nph_model_a_m50_b_m50.gif        | -924.134| 8.85   |
| 1_Nph_model_a_m50_b_m60.gif        | -924.132| 10.18  |
| 1_Nph_model_a_m50_b_m70.gif        | -924.133| 11.04  |
| 1_Nph_model_a_m50_b_m80.gif        | -924.133| 11.27  |
| 1_Nph_model_a_m50_b_m90.gif        | -924.135| 10.99  |
| 1_Nph_model_a_m50_b_m100.gif       | -924.132| 9.95   |
| 1_Nph_model_a_m50_b_m110.gif       | -924.135| 7.9    |
| 1_Nph_model_a_m50_b_m120.gif       | -924.139| 5.85   |
| 1_Nph_model_a_m50_b_m130.gif       | -924.141| 4.38   |
| 1_Nph_model_a_m50_b_m140.gif       | -924.142| 3.62   |
| 1_Nph_model_a_m50_b_m150.gif       | -924.142| 3.57   |
| 1_Nph_model_a_m50_b_m160.gif       | -924.141| 4.21   |
| 1_Nph_model_a_m50_b_m170.gif       | -924.14  | 5.11   |
| 1_Nph_model_a_m60_b_0.gif          | -924.146| 1.43   |
| 1_Nph_model_a_m60_b_10.gif         | -924.146| 1.05   |
| 1_Nph_model_a_m60_b_20.gif         | -924.146| 1.29   |
| 1_Nph_model_a_m60_b_30.gif         | -924.145| 2.07   |
| 1_Nph_model_a_m60_b_40.gif         | -924.143| 3.37   |
| 1_Nph_model_a_m60_b_50.gif         | -924.144| 5.01   |
| 1_Nph_model_a_m60_b_60.gif         | -924.138| 6.41   |
| 1_Nph_model_a_m60_b_70.gif         | -924.137| 7.03   |
| 1_Nph_model_a_m60_b_80.gif         | -924.137| 6.93   |
| 1_Nph_model_a_m60_b_90.gif         | -924.137| 6.56   |
| 1_Nph_model_a_m60_b_100.gif        | -924.138| 6.27   |
| 1_Nph_model_a_m60_b_110.gif        | -924.138| 6.32   |
| 1_Nph_model_a_m60_b_120.gif        | -924.137| 6.68   |
| 1_Nph_model_a_m60_b_130.gif        | -924.137| 7.02   |
| 1_Nph_model_a_m60_b_140.gif        | -924.137| 6.63   |
| 1_Nph_model_a_m60_b_150.gif        | -924.138| 6.28   |
| 1_Nph_model_a_m60_b_160.gif        | -924.138| 6.12   |
| 1_Nph_model_a_m60_b_170.gif        | -924.138| 6.07   |
| 1_Nph_model_a_m60_b_180.gif        | -924.139| 5.8    |
| 1_Nph_model_a_m60_b_m10.gif        | -924.144| 2.34   |
| 1_Nph_model_a_m60_b_m20.gif        | -924.142| 3.68   |
| 1_Nph_model_a_m60_b_m30.gif        | -924.139| 5.39   |
| 1_Nph_model_a_m60_b_m40.gif        | -924.136| 7.43   |
| File Name                                      | Energy   | Delta E |
|-----------------------------------------------|----------|---------|
| 1_Nph_model_a_m60_b_m50.gif                   | -924.132 | 9.69    |
| 1_Nph_model_a_m60_b_m60.gif                   | -924.129 | 11.9    |
| 1_Nph_model_a_m60_b_m70.gif                   | -924.126 | 13.58   |
| 1_Nph_model_a_m60_b_m80.gif                   | -924.125 | 14.49   |
| 1_Nph_model_a_m60_b_m90.gif                   | -924.125 | 14.68   |
| 1_Nph_model_a_m60_b_m100.gif                  | -924.128 | 12.35   |
| 1_Nph_model_a_m60_b_m110.gif                  | -924.133 | 9.26    |
| 1_Nph_model_a_m60_b_m120.gif                  | -924.137 | 6.68    |
| 1_Nph_model_a_m60_b_m130.gif                  | -924.142 | 4.86    |
| 1_Nph_model_a_m60_b_m140.gif                  | -924.141 | 3.87    |
| 1_Nph_model_a_m60_b_m150.gif                  | -924.142 | 3.71    |
| 1_Nph_model_a_m60_b_m160.gif                  | -924.141 | 4.23    |
| 1_Nph_model_a_m60_b_m170.gif                  | -924.14  | 5.08    |
| 1_Nph_model_a_m70_b_0.gif                     | -924.147 | 0.71    |
| 1_Nph_model_a_m70_b_10.gif                    | -924.147 | 0.34    |
| 1_Nph_model_a_m70_b_20.gif                    | -924.146 | 0.58    |
| 1_Nph_model_a_m70_b_30.gif                    | -924.146 | 1.47    |
| 1_Nph_model_a_m70_b_40.gif                    | -924.143 | 2.91    |
| 1_Nph_model_a_m70_b_50.gif                    | -924.14  | 4.88    |
| 1_Nph_model_a_m70_b_60.gif                    | -924.137 | 7.03    |
| 1_Nph_model_a_m70_b_70.gif                    | -924.134 | 8.71    |
| 1_Nph_model_a_m70_b_80.gif                    | -924.133 | 9.32    |
| 1_Nph_model_a_m70_b_90.gif                    | -924.133 | 9.17    |
| 1_Nph_model_a_m70_b_100.gif                   | -924.134 | 8.79    |
| 1_Nph_model_a_m70_b_110.gif                   | -924.134 | 8.53    |
| 1_Nph_model_a_m70_b_120.gif                   | -924.134 | 8.49    |
| 1_Nph_model_a_m70_b_130.gif                   | -924.134 | 8.48    |
| 1_Nph_model_a_m70_b_140.gif                   | -924.136 | 7.67    |
| 1_Nph_model_a_m70_b_150.gif                   | -924.137 | 6.92    |
| 1_Nph_model_a_m70_b_160.gif                   | -924.138 | 6.46    |
| 1_Nph_model_a_m70_b_170.gif                   | -924.138 | 6.18    |
| 1_Nph_model_a_m70_b_180.gif                   | -924.139 | 5.83    |
| 1_Nph_model_a_m70_b_190.gif                   | -924.145 | 1.67    |
| 1_Nph_model_a_m70_b_200.gif                   | -924.143 | 3.15    |
| 1_Nph_model_a_m70_b_300.gif                   | -924.14  | 5.2     |
| 1_Nph_model_a_m70_b_400.gif                   | -924.135 | 7.8     |
| 1_Nph_model_a_m70_b_500.gif                   | -924.131 | 10.76   |
| 1_Nph_model_a_m70_b_600.gif                   | -924.126 | 13.83   |
| 1_Nph_model_a_m70_b_700.gif                   | -924.122 | 16.29   |
| 1_Nph_model_a_m70_b_800.gif                   | -924.119 | 17.96   |
| 1_Nph_model_a_m70_b_900.gif                   | -924.12  | 17.23   |
| 1_Nph_model_a_m70_b_1000.gif                  | -924.127 | 13.08   |
| 1_Nph_model_a_m70_b_1100.gif                  | -924.133 | 9.44    |
| 1_Nph_model_a_m70_b_1200.gif                  | -924.137 | 6.66    |
| 1_Nph_model_a_m70_b_1300.gif                  | -924.14  | 4.76    |
| 1_Nph_model_a_m70_b_1400.gif                  | -924.142 | 3.77    |
| 1_Nph_model_a_m70_b_1500.gif                  | -924.142 | 3.67    |
| 1_Nph_model_a_m70_b_1600.gif                  | -924.141 | 4.2     |
| 1_Nph_model_a_m70_b_1700.gif                  | -924.14  | 5.08    |
| 1_Nph_model_a_m80_b_0.gif                     | -924.147 | 0.4     |
| 1_Nph_model_a_m80_b_10.gif                    | -924.148 | 0       |
| 1_Nph_model_a_m80_b_20.gif                    | -924.148 | 0.25    |
| File Name                        | Energy   | Difference |
|---------------------------------|----------|------------|
| 1_Nph_model_a_m80_b_30.gif       | -924.146 | 1.11       |
| 1_Nph_model_a_m80_b_40.gif       | -924.144 | 2.55       |
| 1_Nph_model_a_m80_b_50.gif       | -924.141 | 4.54       |
| 1_Nph_model_a_m80_b_60.gif       | -924.137 | 6.93       |
| 1_Nph_model_a_m80_b_70.gif       | -924.133 | 9.32       |
| 1_Nph_model_a_m80_b_80.gif       | -924.13  | 11.01      |
| 1_Nph_model_a_m80_b_90.gif       | -924.129 | 11.68      |
| 1_Nph_model_a_m80_b_100.gif      | -924.129 | 11.6       |
| 1_Nph_model_a_m80_b_110.gif      | -924.13  | 11.23      |
| 1_Nph_model_a_m80_b_120.gif      | -924.131 | 10.81      |
| 1_Nph_model_a_m80_b_130.gif      | -924.132 | 10.23      |
| 1_Nph_model_a_m80_b_140.gif      | -924.131 | 10.81      |
| 1_Nph_model_a_m80_b_150.gif      | -924.135 | 7.83       |
| 1_Nph_model_a_m80_b_m10.gif      | -924.146 | 1.43       |
| 1_Nph_model_a_m80_b_m20.gif      | -924.143 | 3.13       |
| 1_Nph_model_a_m80_b_m30.gif      | -924.139 | 5.54       |
| 1_Nph_model_a_m80_b_m40.gif      | -924.134 | 8.61       |
| 1_Nph_model_a_m80_b_m50.gif      | -924.138 | 12.25      |
| 1_Nph_model_a_m80_b_m60.gif      | -924.142 | 16.13      |
| 1_Nph_model_a_m80_b_m70.gif      | -924.117 | 19.41      |
| 1_Nph_model_a_m80_b_m80.gif      | -924.112 | 22.25      |
| 1_Nph_model_a_m80_b_m90.gif      | -924.121 | 17.09      |
| 1_Nph_model_a_m80_b_m100.gif     | -924.128 | 12.45      |
| 1_Nph_model_a_m80_b_m110.gif     | -924.134 | 8.72       |
| 1_Nph_model_a_m80_b_m120.gif     | -924.138 | 5.98       |
| 1_Nph_model_a_m80_b_m130.gif     | -924.141 | 4.2        |
| 1_Nph_model_a_m80_b_m140.gif     | -924.143 | 3.38       |
| 1_Nph_model_a_m80_b_m150.gif     | -924.142 | 3.44       |
| 1_Nph_model_a_m80_b_m160.gif     | -924.141 | 4.08       |
| 1_Nph_model_a_m80_b_m170.gif     | -924.14  | 5.01       |
| 1_Nph_model_a_m90_b_0.gif        | -924.147 | 0.5        |
| 1_Nph_model_a_m90_b_10.gif       | -924.148 | 0.01       |
| 1_Nph_model_a_m90_b_20.gif       | -924.148 | 0.23       |
| 1_Nph_model_a_m90_b_30.gif       | -924.146 | 1.02       |
| 1_Nph_model_a_m90_b_40.gif       | -924.144 | 2.34       |
| 1_Nph_model_a_m90_b_50.gif       | -924.141 | 4.24       |
| 1_Nph_model_a_m90_b_60.gif       | -924.137 | 6.56       |
| 1_Nph_model_a_m90_b_70.gif       | -924.133 | 9.17       |
| 1_Nph_model_a_m90_b_80.gif       | -924.129 | 11.68      |
| 1_Nph_model_a_m90_b_90.gif       | -924.126 | 13.58      |
| 1_Nph_model_a_m90_b_100.gif      | -924.125 | 14.43      |
| 1_Nph_model_a_m90_b_110.gif      | -924.125 | 14.38      |
| 1_Nph_model_a_m90_b_120.gif      | -924.126 | 13.71      |
| 1_Nph_model_a_m90_b_130.gif      | -924.128 | 12.61      |
| 1_Nph_model_a_m90_b_140.gif      | -924.13  | 11.09      |
| 1_Nph_model_a_m90_b_150.gif      | -924.133 | 9.44       |
| 1_Nph_model_a_m90_b_160.gif      | -924.135 | 8.09       |
| 1_Nph_model_a_m90_b_170.gif      | -924.137 | 7.1        |
| 1_Nph_model_a_m90_b_180.gif      | -924.138 | 6.18       |
| FILE_NAME                              | VALUE 1  | VALUE 2 |
|---------------------------------------|----------|---------|
| 1_Nph_model_a_m90_b_m10.gif           | -924.145 | 1.74    |
| 1_Nph_model_a_m90_b_m20.gif           | -924.142 | 3.71    |
| 1_Nph_model_a_m90_b_m30.gif           | -924.138 | 6.5     |
| 1_Nph_model_a_m90_b_m40.gif           | -924.132 | 10.15   |
| 1_Nph_model_a_m90_b_m50.gif           | -924.125 | 14.51   |
| 1_Nph_model_a_m90_b_m60.gif           | -924.117 | 19.14   |
| 1_Nph_model_a_m90_b_m70.gif           | -924.104 | 27.56   |
| 1_Nph_model_a_m90_b_m80.gif           | -924.114 | 21.53   |
| 1_Nph_model_a_m90_b_m90.gif           | -924.123 | 15.86   |
| 1_Nph_model_a_m90_b_m100.gif          | -924.13  | 11.19   |
| 1_Nph_model_a_m90_b_m110.gif          | -924.136 | 7.59    |
| 1_Nph_model_a_m90_b_m120.gif          | -924.14  | 5.08    |
| 1_Nph_model_a_m90_b_m130.gif          | -924.142 | 3.58    |
| 1_Nph_model_a_m90_b_m140.gif          | -924.143 | 3.03    |
| 1_Nph_model_a_m90_b_m150.gif          | -924.143 | 3.26    |
| 1_Nph_model_a_m90_b_m160.gif          | -924.141 | 4.1     |
| 1_Nph_model_a_m90_b_m170.gif          | -924.14  | 5.16    |
| 1_Nph_model_a_m100_b_0.gif            | -924.146 | 1.3     |
| 1_Nph_model_a_m100_b_10.gif           | -924.147 | 0.61    |
| 1_Nph_model_a_m100_b_20.gif           | -924.147 | 0.65    |
| 1_Nph_model_a_m100_b_30.gif           | -924.146 | 1.36    |
| 1_Nph_model_a_m100_b_40.gif           | -924.144 | 2.51    |
| 1_Nph_model_a_m100_b_50.gif           | -924.141 | 4.2     |
| 1_Nph_model_a_m100_b_60.gif           | -924.138 | 6.27    |
| 1_Nph_model_a_m100_b_70.gif           | -924.134 | 8.79    |
| 1_Nph_model_a_m100_b_80.gif           | -924.129 | 11.6    |
| 1_Nph_model_a_m100_b_90.gif           | -924.125 | 14.43   |
| 1_Nph_model_a_m100_b_100.gif          | -924.121 | 16.81   |
| 1_Nph_model_a_m100_b_110.gif          | -924.12  | 17.65   |
| 1_Nph_model_a_m100_b_120.gif          | -924.121 | 17.15   |
| 1_Nph_model_a_m100_b_130.gif          | -924.123 | 15.92   |
| 1_Nph_model_a_m100_b_140.gif          | -924.126 | 14.07   |
| 1_Nph_model_a_m100_b_150.gif          | -924.129 | 12.06   |
| 1_Nph_model_a_m100_b_160.gif          | -924.132 | 10.14   |
| 1_Nph_model_a_m100_b_170.gif          | -924.134 | 8.57    |
| 1_Nph_model_a_m100_b_180.gif          | -924.136 | 7.2     |
| 1_Nph_model_a_m100_b_190.gif          | -924.143 | 2.81    |
| 1_Nph_model_a_m100_b_200.gif          | -924.14  | 5.16    |
| 1_Nph_model_a_m100_b_210.gif          | -924.134 | 8.45    |
| 1_Nph_model_a_m100_b_220.gif          | -924.128 | 12.68   |
| 1_Nph_model_a_m100_b_230.gif          | -924.12  | 17.72   |
| 1_Nph_model_a_m100_b_240.gif          | -924.096 | 32.64   |
| 1_Nph_model_a_m100_b_250.gif          | -924.106 | 26.59   |
| 1_Nph_model_a_m100_b_260.gif          | -924.116 | 20.05   |
| 1_Nph_model_a_m100_b_270.gif          | -924.125 | 14.38   |
| 1_Nph_model_a_m100_b_280.gif          | -924.132 | 9.9     |
| 1_Nph_model_a_m100_b_290.gif          | -924.137 | 6.62    |
| 1_Nph_model_a_m100_b_300.gif          | -924.141 | 4.44    |
| 1_Nph_model_a_m100_b_310.gif          | -924.143 | 3.26    |
| 1_Nph_model_a_m100_b_320.gif          | -924.143 | 3       |
| 1_Nph_model_a_m100_b_330.gif          | -924.142 | 3.5     |
| 1_Nph_model_a_m100_b_340.gif          | -924.141 | 4.53    |
| Filename                                           | Energy   | RMSD   |
|---------------------------------------------------|----------|--------|
| 1_Nph_model_a_m100_b_m170.gjf                     | -924.139 | 5.83   |
| 1_Nph_model_a_m110_b_0.gjf                        | -924.143 | 2.85   |
| 1_Nph_model_a_m110_b_10.gjf                       | -924.145 | 1.86   |
| 1_Nph_model_a_m110_b_20.gjf                       | -924.145 | 1.65   |
| 1_Nph_model_a_m110_b_30.gjf                       | -924.145 | 2.13   |
| 1_Nph_model_a_m110_b_40.gjf                       | -924.143 | 3.14   |
| 1_Nph_model_a_m110_b_50.gjf                       | -924.141 | 4.54   |
| 1_Nph_model_a_m110_b_60.gjf                       | -924.138 | 6.32   |
| 1_Nph_model_a_m110_b_70.gjf                       | -924.134 | 8.53   |
| 1_Nph_model_a_m110_b_80.gjf                       | -924.13 | 11.23  |
| 1_Nph_model_a_m110_b_90.gjf                       | -924.125 | 14.38  |
| 1_Nph_model_a_m110_b_100.gjf                      | -924.12 | 17.65  |
| 1_Nph_model_a_m110_b_110.gjf                      | -924.116 | 20.23  |
| 1_Nph_model_a_m110_b_120.gjf                      | -924.115 | 20.86  |
| 1_Nph_model_a_m110_b_130.gjf                      | -924.116 | 20.05  |
| 1_Nph_model_a_m110_b_140.gjf                      | -924.119 | 18.16  |
| 1_Nph_model_a_m110_b_150.gjf                      | -924.123 | 15.77  |
| 1_Nph_model_a_m110_b_160.gjf                      | -924.127 | 13.2   |
| 1_Nph_model_a_m110_b_170.gjf                      | -924.131 | 10.83  |
| 1_Nph_model_a_m110_b_180.gjf                      | -924.134 | 8.88   |
| 1_Nph_model_a_m110_b_190.gjf                      | -924.14 | 4.71   |
| 1_Nph_model_a_m110_b_200.gjf                      | -924.136 | 7.51   |
| 1_Nph_model_a_m110_b_210.gjf                      | -924.13 | 11.34  |
| 1_Nph_model_a_m110_b_220.gjf                      | -924.122 | 16.19  |
| 1_Nph_model_a_m110_b_230.gjf                      | -924.113 | 21.92  |
| 1_Nph_model_a_m110_b_240.gjf                      | -924.097 | 31.75  |
| 1_Nph_model_a_m110_b_250.gjf                      | -924.108 | 24.83  |
| 1_Nph_model_a_m110_b_260.gjf                      | -924.119 | 18.43  |
| 1_Nph_model_a_m110_b_270.gjf                      | -924.127 | 13.07  |
| 1_Nph_model_a_m110_b_280.gjf                      | -924.134 | 8.97   |
| 1_Nph_model_a_m110_b_290.gjf                      | -924.138 | 6.07   |
| 1_Nph_model_a_m110_b_300.gjf                      | -924.141 | 4.26   |
| 1_Nph_model_a_m110_b_310.gjf                      | -924.142 | 3.43   |
| 1_Nph_model_a_m110_b_320.gjf                      | -924.142 | 3.48   |
| 1_Nph_model_a_m110_b_330.gjf                      | -924.141 | 4.23   |
| 1_Nph_model_a_m110_b_340.gjf                      | -924.139 | 5.55   |
| 1_Nph_model_a_m110_b_350.gjf                      | -924.137 | 7.13   |
| 1_Nph_model_a_m110_b_360.gjf                      | -924.14 | 4.91   |
| 1_Nph_model_a_m110_b_370.gjf                      | -924.142 | 3.57   |
| 1_Nph_model_a_m110_b_380.gjf                      | -924.143 | 3.09   |
| 1_Nph_model_a_m110_b_390.gjf                      | -924.143 | 3.29   |
| 1_Nph_model_a_m110_b_400.gjf                      | -924.141 | 4.06   |
| 1_Nph_model_a_m110_b_410.gjf                      | -924.14 | 5.19   |
| 1_Nph_model_a_m110_b_420.gjf                      | -924.137 | 6.68   |
| 1_Nph_model_a_m110_b_430.gjf                      | -924.134 | 8.5    |
| 1_Nph_model_a_m110_b_440.gjf                      | -924.131 | 10.81  |
| 1_Nph_model_a_m110_b_450.gjf                      | -924.126 | 13.71  |
| 1_Nph_model_a_m110_b_460.gjf                      | -924.121 | 17.15  |
| 1_Nph_model_a_m110_b_470.gjf                      | -924.115 | 20.86  |
| 1_Nph_model_a_m110_b_480.gjf                      | -924.111 | 23.18  |
| Filename                        | Value   | Error  |
|--------------------------------|---------|--------|
| 1_Nph_model_a_m120_b_150.gjf   | -924.115 | 20.66  |
| 1_Nph_model_a_m120_b_160.gjf   | -924.12  | 17.38  |
| 1_Nph_model_a_m120_b_170.gjf   | -924.126 | 13.97  |
| 1_Nph_model_a_m120_b_m10.gjf   | -924.13  | 11.23  |
| 1_Nph_model_a_m120_b_m20.gjf   | -924.131 | 10.58  |
| 1_Nph_model_a_m120_b_m30.gjf   | -924.134 | 8.44   |
| 1_Nph_model_a_m120_b_m40.gjf   | -924.135 | 7.22   |
| 1_Nph_model_a_m120_b_m50.gjf   | -924.138 | 6      |
| 1_Nph_model_a_m120_b_m60.gjf   | -924.141 | 4.55   |
| 1_Nph_model_a_m120_b_m70.gjf   | -924.142 | 4.05   |
| 1_Nph_model_a_m120_b_m80.gjf   | -924.144 | 4.35   |
| 1_Nph_model_a_m120_b_m90.gjf   | -924.145 | 5.38   |
| 1_Nph_model_a_m120_b_m100.gjf  | -924.146 | 7      |
| 1_Nph_model_a_m120_b_m110.gjf  | -924.147 | 7.02   |
| 1_Nph_model_a_m120_b_m120.gjf  | -924.148 | 8.48   |
| 1_Nph_model_a_m120_b_m130.gjf  | -924.149 | 10.23  |
| 1_Nph_model_a_m120_b_m140.gjf  | -924.150 | 12.61  |
| 1_Nph_model_a_m120_b_m150.gjf  | -924.151 | 15.92  |
| 1_Nph_model_a_m120_b_m160.gjf  | -924.152 | 20.05  |
| 1_Nph_model_a_m120_b_m170.gjf  | -924.153 | 24.6   |
| 1_Nph_model_a_m120_b_m180.gjf  | -924.154 | 28.46  |
| 1_Nph_model_a_m120_b_m190.gjf  | -924.155 | 26.4   |
| 1_Nph_model_a_m120_b_m200.gjf  | -924.156 | 26.4   |
| 1_Nph_model_a_m120_b_m210.gjf  | -924.157 | 26.4   |
| 1_Nph_model_a_m120_b_m220.gjf  | -924.158 | 26.4   |
| 1_Nph_model_a_m120_b_m230.gjf  | -924.159 | 26.4   |
| 1_Nph_model_a_m120_b_m240.gjf  | -924.160 | 26.4   |
| 1_Nph_model_a_m120_b_m250.gjf  | -924.161 | 26.4   |
| 1_Nph_model_a_m120_b_m260.gjf  | -924.162 | 26.4   |
| 1_Nph_model_a_m120_b_m270.gjf  | -924.163 | 26.4   |
| 1_Nph_model_a_m120_b_m280.gjf  | -924.164 | 26.4   |
| 1_Nph_model_a_m120_b_m290.gjf  | -924.165 | 26.4   |
| 1_Nph_model_a_m120_b_m300.gjf  | -924.166 | 26.4   |
| 1_Nph_model_a_m120_b_m310.gjf  | -924.167 | 26.4   |
| 1_Nph_model_a_m120_b_m320.gjf  | -924.168 | 26.4   |
| 1_Nph_model_a_m120_b_m330.gjf  | -924.169 | 26.4   |
| 1_Nph_model_a_m120_b_m340.gjf  | -924.170 | 26.4   |
| 1_Nph_model_a_m120_b_m350.gjf  | -924.171 | 26.4   |
| 1_Nph_model_a_m120_b_m360.gjf  | -924.172 | 26.4   |
| 1_Nph_model_a_m120_b_m370.gjf  | -924.173 | 26.4   |
| 1_Nph_model_a_m120_b_m380.gjf  | -924.174 | 26.4   |
| 1_Nph_model_a_m120_b_m390.gjf  | -924.175 | 26.4   |
| 1_Nph_model_a_m120_b_m400.gjf  | -924.176 | 26.4   |
| File Name                          | Energy (kcal/mol) | Difference (kcal/mol) |
|-----------------------------------|-------------------|-----------------------|
| _Nph_model_a_m130_b_m130.gjf      | -924.141          | 4.58                  |
| _Nph_model_a_m130_b_m140.gjf      | -924.14           | 5.28                  |
| _Nph_model_a_m130_b_m150.gjf      | -924.137          | 6.72                  |
| _Nph_model_a_m130_b_m160.gjf      | -924.134          | 8.79                  |
| _Nph_model_a_m130_b_m170.gjf      | -924.13           | 11.36                 |
| _Nph_model_a_m140_b_0.gjf         | -924.132          | 10.04                 |
| _Nph_model_a_m140_b_10.gjf        | -924.136          | 7.44                  |
| _Nph_model_a_m140_b_20.gjf        | -924.139          | 5.87                  |
| _Nph_model_a_m140_b_30.gjf        | -924.14           | 5.19                  |
| _Nph_model_a_m140_b_40.gjf        | -924.14           | 5.21                  |
| _Nph_model_a_m140_b_50.gjf        | -924.139          | 5.79                  |
| _Nph_model_a_m140_b_60.gjf        | -924.137          | 6.63                  |
| _Nph_model_a_m140_b_70.gjf        | -924.136          | 7.67                  |
| _Nph_model_a_m140_b_80.gjf        | -924.134          | 9.04                  |
| _Nph_model_a_m140_b_90.gjf        | -924.13           | 11.09                 |
| _Nph_model_a_m140_b_100.gjf       | -924.126          | 14.07                 |
| _Nph_model_a_m140_b_110.gjf       | -924.119          | 18.16                 |
| _Nph_model_a_m140_b_120.gjf       | -924.111          | 23.18                 |
| _Nph_model_a_m140_b_130.gjf       | -924.102          | 28.64                 |
| _Nph_model_a_m140_b_140.gjf       | -924.095          | 33.33                 |
| _Nph_model_a_m140_b_150.gjf       | -924.096          | 32.57                 |
| _Nph_model_a_m140_b_160.gjf       | -924.102          | 28.57                 |
| _Nph_model_a_m140_b_170.gjf       | -924.111          | 23                   |
| _Nph_model_a_m140_b_180.gjf       | -924.119          | 18.13                 |
| _Nph_model_a_m140_b_m10.gjf       | -924.126          | 13.75                 |
| _Nph_model_a_m140_b_m20.gjf       | -924.118          | 18.8                  |
| _Nph_model_a_m140_b_m30.gjf       | -924.108          | 25.13                 |
| _Nph_model_a_m140_b_m40.gjf       | -924.084          | 39.88                 |
| _Nph_model_a_m140_b_m50.gjf       | -924.097          | 32.14                 |
| _Nph_model_a_m140_b_m60.gjf       | -924.109          | 24.7                  |
| _Nph_model_a_m140_b_m70.gjf       | -924.119          | 18.25                 |
| _Nph_model_a_m140_b_m80.gjf       | -924.127          | 13.1                  |
| _Nph_model_a_m140_b_m90.gjf       | -924.133          | 9.31                  |
| _Nph_model_a_m140_b_m100.gjf      | -924.137          | 6.68                  |
| _Nph_model_a_m140_b_m110.gjf      | -924.14           | 5.09                  |
| _Nph_model_a_m140_b_m120.gjf      | -924.141          | 4.41                  |
| _Nph_model_a_m140_b_m130.gjf      | -924.141          | 4.63                  |
| _Nph_model_a_m140_b_m140.gjf      | -924.139          | 5.74                  |
| _Nph_model_a_m140_b_m150.gjf      | -924.136          | 7.69                  |
| _Nph_model_a_m140_b_m160.gjf      | -924.131          | 10.54                 |
| _Nph_model_a_m140_b_m170.gjf      | -924.126          | 14.06                 |
| _Nph_model_a_m150_b_0.gjf         | -924.128          | 12.31                 |
| _Nph_model_a_m150_b_10.gjf        | -924.133          | 9.1                   |
| _Nph_model_a_m150_b_20.gjf        | -924.137          | 7.01                  |
| _Nph_model_a_m150_b_30.gjf        | -924.139          | 5.88                  |
| _Nph_model_a_m150_b_40.gjf        | -924.139          | 5.55                  |
| _Nph_model_a_m150_b_50.gjf        | -924.139          | 5.74                  |
| _Nph_model_a_m150_b_60.gjf        | -924.138          | 6.28                  |
| _Nph_model_a_m150_b_70.gjf        | -924.137          | 6.92                  |
| _Nph_model_a_m150_b_80.gjf        | -924.135          | 7.83                  |
| _Nph_model_a_m150_b_90.gjf        | -924.133          | 9.44                  |
| _Nph_model_a_m150_b_100.gjf       | -924.129          | 12.06                 |
| Filename                                         | Z         | Z error |
|------------------------------------------------|-----------|---------|
| 1_Nph_model_a_m150_b_110.gjf                    | -924.123  | 15.77   |
| 1_Nph_model_a_m150_b_120.gjf                    | -924.115  | 20.66   |
| 1_Nph_model_a_m150_b_130.gjf                    | -924.106  | 26.4    |
| 1_Nph_model_a_m150_b_140.gjf                    | -924.096  | 32.57   |
| 1_Nph_model_a_m150_b_150.gjf                    | -924.088  | 37.81   |
| 1_Nph_model_a_m150_b_160.gjf                    | -924.094  | 33.8    |
| 1_Nph_model_a_m150_b_170.gjf                    | -924.105  | 26.71   |
| 1_Nph_model_a_m150_b_180.gjf                    | -924.114  | 21.15   |
| 1_Nph_model_a_m150_b_m10.gjf                    | -924.121  | 16.75   |
| 1_Nph_model_a_m150_b_m20.gjf                    | -924.112  | 22.54   |
| 1_Nph_model_a_m150_b_m30.gjf                    | -924.082  | 41.67   |
| 1_Nph_model_a_m150_b_m40.gjf                    | -924.091  | 35.7    |
| 1_Nph_model_a_m150_b_m50.gjf                    | -924.102  | 28.51   |
| 1_Nph_model_a_m150_b_m60.gjf                    | -924.113  | 21.63   |
| 1_Nph_model_a_m150_b_m70.gjf                    | -924.123  | 15.84   |
| 1_Nph_model_a_m150_b_m80.gjf                    | -924.13   | 11.34   |
| 1_Nph_model_a_m150_b_m90.gjf                    | -924.135  | 8.09    |
| 1_Nph_model_a_m150_b_m100.gjf                   | -924.139  | 5.89    |
| 1_Nph_model_a_m150_b_m110.gjf                   | -924.141  | 4.63    |
| 1_Nph_model_a_m150_b_m120.gjf                   | -924.141  | 4.21    |
| 1_Nph_model_a_m150_b_m130.gjf                   | -924.14   | 4.67    |
| 1_Nph_model_a_m150_b_m140.gjf                   | -924.138  | 6.02    |
| 1_Nph_model_a_m150_b_m150.gjf                   | -924.135  | 8.36    |
| 1_Nph_model_a_m150_b_m160.gjf                   | -924.129  | 11.65   |
| 1_Nph_model_a_m150_b_m170.gjf                   | -924.122  | 15.98   |
| 1_Nph_model_a_m160_b_0.gjf                      | -924.135  | 8.16    |
| 1_Nph_model_a_m160_b_10.gjf                     | -924.131  | 10.74   |
| 1_Nph_model_a_m160_b_20.gjf                     | -924.135  | 8.16    |
| 1_Nph_model_a_m160_b_30.gjf                     | -924.137  | 6.59    |
| 1_Nph_model_a_m160_b_40.gjf                     | -924.138  | 5.93    |
| 1_Nph_model_a_m160_b_50.gjf                     | -924.139  | 5.87    |
| 1_Nph_model_a_m160_b_60.gjf                     | -924.138  | 6.12    |
| 1_Nph_model_a_m160_b_70.gjf                     | -924.138  | 6.46    |
| 1_Nph_model_a_m160_b_80.gjf                     | -924.137  | 6.97    |
| 1_Nph_model_a_m160_b_90.gjf                     | -924.135  | 8.09    |
| 1_Nph_model_a_m160_b_100.gjf                    | -924.132  | 10.14   |
| 1_Nph_model_a_m160_b_110.gjf                    | -924.127  | 13.21   |
| 1_Nph_model_a_m160_b_120.gjf                    | -924.12   | 17.38   |
| 1_Nph_model_a_m160_b_130.gjf                    | -924.112  | 22.61   |
| 1_Nph_model_a_m160_b_140.gjf                    | -924.102  | 28.57   |
| 1_Nph_model_a_m160_b_150.gjf                    | -924.094  | 33.8    |
| 1_Nph_model_a_m160_b_160.gjf                    | -924.095  | 32.9    |
| 1_Nph_model_a_m160_b_170.gjf                    | -924.103  | 28.27   |
| 1_Nph_model_a_m160_b_180.gjf                    | -924.112  | 22.81   |
| 1_Nph_model_a_m160_b_190.gjf                    | -924.117  | 19.4    |
| 1_Nph_model_a_m160_b_200.gjf                    | -924.084  | 39.83   |
| 1_Nph_model_a_m160_b_300.gjf                    | -924.091  | 35.71   |
| 1_Nph_model_a_m160_b_400.gjf                    | -924.1    | 30.21   |
| 1_Nph_model_a_m160_b_500.gjf                    | -924.109  | 24.37   |
| 1_Nph_model_a_m160_b_600.gjf                    | -924.118  | 18.68   |
| 1_Nph_model_a_m160_b_700.gjf                    | -924.126  | 13.8    |
| 1_Nph_model_a_m160_b_800.gjf                    | -924.132  | 9.98    |
| File Name                        | Energy   | Angle |
|---------------------------------|----------|-------|
| 1_Nph_model_a_m160_b_m90.gjf    | -924.136 | 7.24  |
| 1_Nph_model_a_m160_b_m100.gjf   | -924.139 | 5.43  |
| 1_Nph_model_a_m160_b_m110.gjf   | -924.141 | 4.43  |
| 1_Nph_model_a_m160_b_m120.gjf   | -924.141 | 4.2   |
| 1_Nph_model_a_m160_b_m130.gjf   | -924.14  | 4.84  |
| 1_Nph_model_a_m160_b_m140.gjf   | -924.138 | 6.37  |
| 1_Nph_model_a_m160_b_m150.gjf   | -924.134 | 8.93  |
| 1_Nph_model_a_m160_b_m160.gjf   | -924.128 | 12.59 |
| 1_Nph_model_a_m160_b_m170.gjf   | -924.12  | 17.33 |
| 1_Nph_model_a_m170_b_0.gjf      | -924.122 | 16.37 |
| 1_Nph_model_a_m170_b_10.gjf     | -924.128 | 12.27 |
| 1_Nph_model_a_m170_b_20.gjf     | -924.133 | 9.27  |
| 1_Nph_model_a_m170_b_30.gjf     | -924.136 | 7.32  |
| 1_Nph_model_a_m170_b_40.gjf     | -924.138 | 6.32  |
| 1_Nph_model_a_m170_b_50.gjf     | -924.138 | 6.01  |
| 1_Nph_model_a_m170_b_60.gjf     | -924.138 | 6.07  |
| 1_Nph_model_a_m170_b_70.gjf     | -924.138 | 6.18  |
| 1_Nph_model_a_m170_b_80.gjf     | -924.138 | 6.42  |
| 1_Nph_model_a_m170_b_90.gjf     | -924.137 | 7.1   |
| 1_Nph_model_a_m170_b_100.gjf    | -924.134 | 8.57  |
| 1_Nph_model_a_m170_b_110.gjf    | -924.131 | 10.83 |
| 1_Nph_model_a_m170_b_120.gjf    | -924.126 | 13.97 |
| 1_Nph_model_a_m170_b_130.gjf    | -924.119 | 18.12 |
| 1_Nph_model_a_m170_b_140.gjf    | -924.111 | 23    |
| 1_Nph_model_a_m170_b_150.gjf    | -924.105 | 26.71 |
| 1_Nph_model_a_m170_b_160.gjf    | -924.103 | 28.27 |
| 1_Nph_model_a_m170_b_170.gjf    | -924.103 | 28.05 |
| 1_Nph_model_a_m170_b_180.gjf    | -924.111 | 23.46 |
| 1_Nph_model_a_m170_b_m10.gjf    | -924.114 | 21.6  |
| 1_Nph_model_a_m170_b_m20.gjf    | -924.093 | 34.25 |
| 1_Nph_model_a_m170_b_m30.gjf    | -924.1   | 30.17 |
| 1_Nph_model_a_m170_b_m40.gjf    | -924.107 | 25.53 |
| 1_Nph_model_a_m170_b_m50.gjf    | -924.115 | 20.76 |
| 1_Nph_model_a_m170_b_m60.gjf    | -924.122 | 16.2  |
| 1_Nph_model_a_m170_b_m70.gjf    | -924.128 | 12.22 |
| 1_Nph_model_a_m170_b_m80.gjf    | -924.133 | 9.1   |
| 1_Nph_model_a_m170_b_m90.gjf    | -924.137 | 6.82  |
| 1_Nph_model_a_m170_b_m100.gjf   | -924.139 | 5.31  |
| 1_Nph_model_a_m170_b_m110.gjf   | -924.141 | 4.45  |
| 1_Nph_model_a_m170_b_m120.gjf   | -924.141 | 4.31  |
| 1_Nph_model_a_m170_b_m130.gjf   | -924.14  | 5     |
| 1_Nph_model_a_m170_b_m140.gjf   | -924.137 | 6.68  |
| 1_Nph_model_a_m170_b_m150.gjf   | -924.133 | 9.31  |
| 1_Nph_model_a_m170_b_m160.gjf   | -924.127 | 13.15 |
| 1_Nph_model_a_m170_b_m170.gjf   | -924.119 | 18.05 |

[a] prefix "m" corresponds to the negative angle.
Figure S1. The molecular structure of 1e. Displacement ellipsoids are drawn at 30% probability level. The minor orientation of the alkyl chain is shown with open bonds.
Figure S2. The molecular structure of 6b. Displacement ellipsoids are drawn at 30% probability level.
Figure S3. The molecular structure of 7e. Displacement ellipsoids are drawn at 30% probability level.
Figure S4. The molecular structure of 9e. Displacement ellipsoids are drawn at 30% probability level.
Figure S5. The molecular structure of 10b. Displacement ellipsoids are drawn at 30% probability level.
Figure S6. Crystal packing of 1e, viewed along the a axis. O atoms are represented as spheres of arbitrary radii. Symmetry independent molecules are distinguished different colours.

Figure S7. Zig-zag chain and the crystal packing of 6b, viewed along the b axis. O atoms are represented as spheres of arbitrary radii.
Figure S8. Zig-zag chain and the crystal packing of 7b, viewed along the a axis. O atoms are represented as spheres of arbitrary radii.

Figure S9. The crystal packing of 9b, viewed along the a axis. O atoms are represented as spheres of arbitrary radii. Hydrogen bonds are shown as a dashed line.
**Figure S10.** The crystal packing of 10b, viewed along the b axis. O atoms are represented as spheres of arbitrary radii. Symmetry independent molecules are distinguished different colours.
Figure S11. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 1e.
Figure S12. Calculated at the IEFPCM/B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 1e with the use of an IEFPCM model of cyclohexane.
Figure S13. Calculated at the IEFPCM/B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 1e with the use of an IEFPCM model of acetonitrile.
Figure S14. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 3b.
Figure S15. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 4b.
Figure S16. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 5b.
Figure S17. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 6b.
Figure S18. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 7b.
Figure S19. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 8b.
Figure S20. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 9b.
Figure S21. Calculated at the B3LYP/6-311++G(d,p) level structures of thermally accessible conformers of compound 10b.
Figure S22. ECD spectra of low-energy conformers of compound 1e calculated at TD-CAM-B3LYP/6-311G(2d,2p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S23. ECD spectra of low-energy conformers of compound 1e calculated at TD-M06-2X/6-311G(2d,2p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S24. ECD spectra of low-energy conformers of compound 1e calculated at TD-ωB97XD/6-311G(2d,2p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S25. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/CAM-B3LYP/6-311G(2d,2p) level for structures optimized at B3LYP/6-311G(d,p) level with the use of an IEFPCM model of cyclohexane. Wavelengths have not been corrected.
Figure S26. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/M06-2X/6-311G(2d,2p) level for structures optimized at B3LYP/6-311G(d,p) level with the use of an IEFPCM model of cyclohexane. Wavelengths have not been corrected.
Figure S27. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/ωB97XD/6-311G(2d,2p) level for structures optimized at B3LYP/6-311G(d,p) level with the use of an IEFPCM model of cyclohexane. Wavelengths have not been corrected.
Figure S28. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/CAM-B3LYP/6-311G(2d,2p) level for structures optimized at IEFPCM/B3LYP/6-311G(d,p) level with the use of an IEFPCM model of cyclohexane. Wavelengths have not been corrected.
Figure S29. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/M06-2X/6-311G(2d,2p) level for structures optimized at IEFPCM/B3LYP/6-311G(d,p) with the use of an IEFPCM model of cyclohexane. Wavelengths have not been corrected.
Figure S30. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/ωB97X-D/6-311G(2d,2p) level for structures optimized at IEFPCM/B3LYP/6-311G(d,p) with the use of an IEFPCM model of cyclohexane. Wavelengths have not been corrected.
Figure S31. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/CAM-B3LYP/6-311G(2d,2p) level for structures optimized at IEFPCM/B3LYP/6-311G(d,p) with the use of an IEFPCM model of acetonitrile. Wavelengths have not been corrected.
Figure S32. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/M06-2X/6-311G(2d,2p) level for structures optimized at IEFPCM/B3LYP/6-311G(d,p) with the use of an IEFPCM model of acetonitrile. Wavelengths have not been corrected.
Figure S33. ECD spectra of low-energy conformers of compound 1e calculated at TD-IEFPCM/ωB97XD/6-311G(2d,2p) level for structures optimized at IEFPCM/B3LYP/6-311G(d,p) with the use of an IEFPCM model of acetonitrile. Wavelengths have not been corrected.
**Figure S34.** ECD spectra of low-energy conformers of compound 3b calculated at TD-CAM-B3LYP/6-311G(d,p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S35. ECD spectra of low-energy conformers of compound 4b calculated at TD-CAM-B3LYP/6-311G(d,p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S36. ECD spectra of low-energy conformers of compound 5b calculated at TD-CAM-B3LYP/6-311G(d,p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S37. ECD spectra of low-energy conformers of compound 6b calculated at TD-CAM-B3LYP/6-311G(d,p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S38. ECD spectra of low-energy conformers of compound 7b calculated at TD-CAMB3LYP/6-311G(d,p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S39. ECD spectra of low-energy conformers of compound 8b calculated at TD-CAM-B3LYP/6-311G(d,p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
**Figure S40.** ECD spectra of low-energy conformers of compound 9b calculated at TD-CAM-B3LYP/6-311G(d,p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
Figure S41. ECD spectra of low-energy conformers of compound 10b calculated at TD-CAM-B3LYP/6-311G(d,p) level for structures optimized at B3LYP/6-311G(d,p) level. Wavelengths have not been corrected.
$\alpha_1 = 0^\circ$, $\alpha_2 = \text{scan}$
$\alpha_1 = 10^\circ, \alpha_2 = \text{scan}$
$\alpha_1 = 20^\circ, \alpha_2 = \text{scan}$
$\alpha_1 = 30^\circ, \alpha_2 = \text{scan}$
$\alpha_1 = 40^\circ$, $\alpha_2 =$ scan
$\alpha_1 = 50^\circ, \alpha_2 = \text{scan}$
\[ \alpha_1 = 60^\circ, \alpha_2 = \text{scan} \]
$\alpha_1 = 70^\circ$, $\alpha_2 = \text{scan}$
$\alpha_1 = 80^\circ$, $\alpha_2 = \text{scan}$
\( \alpha_1 = 90^\circ, \alpha_2 = \text{scan} \)
$\alpha_1 = 100^\circ$, $\alpha_2 = \text{scan}$
$\alpha_1 = 110^\circ$, $\alpha_2 = \text{scan}$
$\alpha_1 = 120^\circ$, $\alpha_2 = \text{scan}$
$\alpha_1 = 130^\circ, \alpha_2 = \text{scan}$
$\alpha_1 = 140^\circ$, $\alpha_2 =$ scan
$\alpha_1 = 150^\circ$, $\alpha_2 = \text{scan}$
\( \alpha_1 = 160^\circ, \alpha_2 = \text{scan} \)
$\alpha_1 = 170^\circ, \alpha_2 = \text{scan}$
$\alpha_1 = 180^\circ, \alpha_2 = \text{scan}$
\( \alpha_1 = -10^\circ, \alpha_2 = \text{scan} \)
$\alpha_1 = -20^\circ, \alpha_2 = \text{scan}$
\( \alpha_1 = -30^\circ, \alpha_2 = \text{scan} \)
\( \alpha_1 = -40^\circ, \alpha_2 = \text{scan} \)
$\alpha_1 = -60^\circ, \alpha_2 = \text{scan}$
\( \alpha_1 = -70^\circ, \alpha_2 = \text{scan} \)
$\alpha_1 = -80^\circ, \alpha_2 = \text{scan}$
$\alpha_1 = -90^\circ, \alpha_2 = \text{scan}$
\(\alpha_1 = -100^\circ, \alpha_2 = \text{scan}\)
\( \alpha_1 = -110^\circ, \alpha_2 = \text{scan} \)
$\alpha_1 = -120^\circ$, $\alpha_2 =$ scan
\( \alpha_1 = -130^\circ, \alpha_2 = \text{scan} \)
$\alpha_1 = -140^\circ$, $\alpha_2 = \text{scan}$
$\alpha_1 = -150^\circ$, $\alpha_2 = \text{scan}$
\[ \alpha_1 = -160^\circ, \alpha_2 = \text{scan} \]
$\alpha_1 = -170^\circ, \alpha_2 = \text{scan}$

Figure S42. Calculated at the CAM-B3LYP/6-311++G(2d,2p) level UV and ECD spectra of all optimized conformers of model compound 11. The wavelengths have not been corrected.
Figure S43. Boltzmann averaged $\Delta \Delta G$ (solid red line) and $\Delta E$ (solid black line) ECD spectra calculated at TD-DFT/6-311G++(d,p) level for structures optimized at B3LYP/6-311G(d,p) level of compounds 1e, 3b-10b.
Figure S44. Comparison of Boltzmann averaged $\Delta \Delta G$ (solid red line) and $\Delta E$ (solid black line) ECD spectra of 1e calculated at various level for structures optimized with and without the use of an IEFPCM solvent model.
Figure S45. Measured in cyclohexane (solid black line) and calculated (dashed red line) at TD-DFT/6-311G++(d,p) level spectra of ethers 1e, 3b-10b. Wavelengths have been corrected to match experimental UV maxima.
**Figure S46.** Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 1e. Wavelengths have been corrected to match experimental UV maximum.
Figure S47. Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 2b. Wavelengths have been corrected to match experimental UV maximum.
Figure S48. Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 3b. Wavelengths have been corrected to match experimental UV maximum.
Figure S49. Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 4b. Wavelengths have been corrected to match experimental UV maximum.
**Figure S50.** Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 5b. Wavelengths have been corrected to match experimental UV maximum.
Figure S51. Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 6b. Wavelengths have been corrected to match experimental UV maximum.
Figure S52. Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 7b. Wavelengths have been corrected to match experimental UV maximum.
Figure S53. Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 8b. Wavelengths have been corrected to match experimental UV maximum.
Figure S54. Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 9b. Wavelengths have been corrected to match experimental UV maximum.
Figure S55. Measured in cyclohexane (solid black line) and calculated (dashed red line) using simplified (semi)empirical approach ECD spectra of ether 10b. Wavelengths have been corrected to match experimental UV maximum.
Figure S56. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 1b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S57. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 1c measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S58. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 1d measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S59. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 1e measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S60. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 1f measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S61. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 2b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S62. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 3b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S63. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 4b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S64. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 5b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S65. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 6b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S66. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 7b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S67. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 8b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S68. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 9b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S69. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied ether 10b measured in cyclohexane (solid black line) and acetonitrile (solid red line).
Figure S70. Copy of $^1$H NMR spectrum of studied ether 1c measured in CDCl$_3$.

Figure S71. Copy of $^{13}$C NMR spectrum of studied ether 1c measured in CDCl$_3$. 
Figure S72. Copy of $^1$H NMR spectrum of studied ether 1d measured in CDCl$_3$.

Figure S73. Copy of $^{13}$C NMR spectrum of studied ether 1d measured in CDCl$_3$. 
Figure S74. Copy of $^1$H NMR spectrum of studied ether 1e measured in CDCl$_3$.

Figure S75. Copy of $^{13}$C NMR spectrum of studied ether 1e measured in CDCl$_3$. 
Figure S76. Copy of $^1$H NMR spectrum of studied ether 1f measured in CDCl$_3$.

Figure S77. Copy of $^{13}$C NMR spectrum of studied ether 1f measured in CDCl$_3$. 
Figure S78. Copy of $^1$H NMR spectrum of studied ether 2b measured in CDCl$_3$.

Figure S79. Copy of $^{13}$C NMR spectrum of studied ether 2b measured in CDCl$_3$. 
Figure S80. Copy of $^1$H NMR spectrum of studied ether 3b measured in CDCl$_3$.

Figure S81. Copy of $^{13}$C NMR spectrum of studied ether 3b measured in CDCl$_3$. 
Figure S82. Copy of $^1\text{H}$ NMR spectrum of studied ether 4b measured in CDCl$_3$.

Figure S83. Copy of $^{13}\text{C}$ NMR spectrum of studied ether 4b measured in CDCl$_3$. 
Figure S84. Copy of $^1$H NMR spectrum of studied ether 5b measured in CDCl$_3$.

Figure S85. Copy of $^{13}$C NMR spectrum of studied ether 5b measured in CDCl$_3$. 
Figure S86. Copy of $^1$H NMR spectrum of studied ether 6b measured in CDCl$_3$.

Figure S87. Copy of $^{13}$C NMR spectrum of studied ether 6b measured in CDCl$_3$. 
Figure S88. Copy of $^1$H NMR spectrum of studied ether 7b measured in CDCl$_3$.

Figure S89. Copy of $^{13}$C NMR spectrum of studied ether 7b measured in CDCl$_3$. 
Figure S90. Copy of $^1$H NMR spectrum of studied ether 8b measured in CDCl$_3$.

Figure S91. Copy of $^{13}$C NMR spectrum of studied ether 8b measured in CDCl$_3$.
Figure S92. Copy of $^1$H NMR spectrum of studied ether 9b measured in CDCl$_3$.

Figure S93. Copy of $^{13}$C NMR spectrum of studied ether 9b measured in CDCl$_3$. 
Figure S94. Copy of $^1$H NMR spectrum of studied ether 10b measured in CDCl$_3$.

Figure S95. Copy of $^{13}$C NMR spectrum of studied ether 10b measured in CDCl$_3$. 
Table S33. Cartesian coordinates of each conformer of 1e, 3b-10b calculated at B3LYP/6-311++G(d,p) level.

| 1e (conformer 1) | 1  | 6  | 0 | 4.194849 | -2.416732 | -0.657825 |
|                 | 2  | 6  | 0 | 4.658402 | -1.244540 | -0.114390 |
|                 | 3  | 6  | 0 | 3.789850 | -0.144904 | 0.110043  |
|                 | 4  | 6  | 0 | 2.403147 | -0.262456 | -0.235218 |
|                 | 5  | 6  | 0 | 1.962013 | -1.492949 | -0.794137 |
|                 | 6  | 6  | 0 | 2.831060 | -2.538060 | -1.000971 |
|                 | 7  | 6  | 0 | 4.272481 | 1.068166  | 0.665695  |
|                 | 8  | 6  | 0 | 3.423656 | 2.124940  | 0.863021  |
|                 | 9  | 6  | 0 | 2.057351 | 2.018830  | 0.517643  |
|                 | 10 | 6  | 0 | 1.537465 | -0.013063 | 1.209114  |
|                 | 11 | 6  | 0 | 0.056623 | 0.782270  | 0.379151  |
|                 | 12 | 6  | 0 | -0.738949| 0.160349  | 0.535129  |
|                 | 13 | 6  | 0 | -1.660986| -1.135397 | 0.030667  |
|                 | 14 | 6  | 0 | -0.593546| -0.016338 | 1.899281  |
|                 | 15 | 6  | 0 | -1.321352| -0.802544 | 2.813930  |
|                 | 16 | 6  | 0 | -2.202218| -1.750114 | 2.357354  |
|                 | 17 | 6  | 0 | -2.393526| -1.942880 | 0.967199  |
|                 | 18 | 6  | 0 | -1.895740| -1.366593 | -1.355470 |
|                 | 19 | 6  | 0 | -2.783244| -2.322956 | -1.786840 |
|                 | 20 | 6  | 0 | -3.497249| -3.112563 | -0.858709 |
|                 | 21 | 6  | 0 | -3.303359| -2.921143 | 0.485501  |
|                 | 22 | 6  | 0 | -0.481019| 2.106193  | -0.312477 |
|                 | 23 | 6  | 0 | -1.694043| 2.351072  | -1.042361 |
|                 | 24 | 6  | 0 | -2.354515| 3.573128  | -0.401788 |
|                 | 25 | 6  | 0 | -1.396372| 2.576462  | -2.525971 |
|                 | 26 | 6  | 0 | -2.780882| 3.361051  | 1.051943  |
|                 | 27 | 6  | 0 | 4.870151 | -3.248595 | -0.823584 |
|                 | 28 | 6  | 0 | 5.704729 | -1.139520 | 0.153670  |
|                 | 29 | 6  | 0 | 0.921009 | -1.624508 | -1.055580 |
|                 | 30 | 6  | 0 | 2.464487 | -3.464962 | -1.427834 |
|                 | 31 | 6  | 0 | 5.323250 | 1.143032  | 0.925561  |
|                 | 32 | 6  | 0 | 3.793762 | 3.054273  | 1.281786  |
|                 | 33 | 6  | 0 | 1.400943| 2.866334  | 0.656558  |
|                 | 34 | 6  | 0 | 0.001725| 0.426167  | -1.411579 |
|                 | 35 | 6  | 0 | 0.109537| 0.716795  | 2.276715  |
|                 | 36 | 6  | 0 | -1.174475| -0.657731 | 3.878293  |
|                 | 37 | 6  | 0 | -2.762716| -2.366566 | 3.052298  |
|                 | 38 | 6  | 0 | -1.371262| -0.778824 | -2.097282 |
|                 | 39 | 6  | 0 | -2.937824| -2.471804 | -2.849695 |
|                 | 40 | 6  | 0 | -4.194487| -3.863937 | -1.211426 |
|                 | 41 | 6  | 0 | -3.847072| -3.519704 | 1.209114  |
|                 | 42 | 6  | 0 | -2.364628| 1.489690  | -0.925977 |
|                 | 43 | 6  | 0 | -1.652118| 4.411897  | -0.469290 |
|   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | 1 | 0 | -3.224722 | 3.843917 | -1.010099 |
| 45 | 1 | 0 | -2.323156 | 2.736611 | -3.084168 |
| 46 | 1 | 0 | -0.756708 | 3.453764 | -2.653206 |
| 47 | 1 | 0 | -0.885630 | 1.720304 | -2.973703 |
| 48 | 1 | 0 | -3.243254 | 4.264438 | 1.458806 |
| 49 | 1 | 0 | -3.506921 | 2.546790 | 1.136628 |
| 50 | 1 | 0 | -1.921961 | 3.106702 | 1.674751 |

**1e (conformer 2)**

|   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|
| 1  | 6 | 0 | 3.970839 | -2.454214 | -1.174081 |
| 2  | 6 | 0 | 3.745290 | -2.567001 | 0.174021 |
| 3  | 6 | 0 | 2.714486 | -1.828337 | 0.813298 |
| 4  | 6 | 0 | 1.889230 | -0.945453 | 0.035264 |
| 5  | 6 | 0 | 2.161566 | -0.856721 | -1.360417 |
| 6  | 6 | 0 | 3.167939 | -1.585967 | -1.946410 |
| 7  | 6 | 0 | 2.494147 | -1.945166 | 2.207492 |
| 8  | 6 | 0 | 1.500002 | -1.223157 | 2.818037 |
| 9  | 6 | 0 | 0.683042 | -0.363733 | 2.057653 |
| 10 | 6 | 0 | 0.848380 | -0.214340 | 0.696187 |
| 11 | 6 | 0 | -0.059913 | 0.787600 | -0.032755 |
| 12 | 6 | 0 | -1.541434 | 0.576196 | 0.271983 |
| 13 | 6 | 0 | -2.243094 | -0.556404 | -0.257134 |
| 14 | 6 | 0 | -2.220121 | 1.488350 | 1.050203 |
| 15 | 6 | 0 | -3.591831 | 1.327287 | 1.349333 |
| 16 | 6 | 0 | -4.286644 | 0.253762 | 0.858435 |
| 17 | 6 | 0 | -3.636989 | -0.708772 | 0.043163 |
| 18 | 6 | 0 | -1.631145 | -1.542274 | -1.078539 |
| 19 | 6 | 0 | -2.347001 | -2.606022 | -1.574657 |
| 20 | 6 | 0 | -3.719237 | -2.749859 | -1.276608 |
| 21 | 6 | 0 | -4.344884 | -1.819799 | -0.484261 |
| 22 | 8 | 0 | 0.275385 | 2.124367 | 0.347831 |
| 23 | 6 | 0 | 1.490938 | 2.664430 | -0.199323 |
| 24 | 6 | 0 | 1.266114 | 3.209014 | -1.621244 |
| 25 | 6 | 0 | 1.973498 | 3.716727 | 0.792744 |
| 26 | 6 | 0 | 0.215089 | 4.318023 | -1.728437 |
| 27 | 1 | 0 | 4.761098 | -3.024979 | -1.648225 |
| 28 | 1 | 0 | 4.356916 | -3.227842 | 0.779596 |
| 29 | 1 | 0 | 1.571474 | -0.198700 | -1.984644 |
| 30 | 1 | 0 | 3.348651 | -1.492915 | -3.011478 |
| 31 | 1 | 0 | 3.124979 | -2.615496 | 2.781755 |
| 32 | 1 | 0 | 1.332361 | -1.313842 | 3.885338 |
| 33 | 1 | 0 | -0.105338 | 0.190429 | 2.553199 |
| 34 | 1 | 0 | 0.064853 | 0.680557 | -1.113894 |
| 35 | 1 | 0 | -1.685530 | 2.349627 | 1.426043 |
| 36 | 1 | 0 | -4.089773 | 2.066061 | 1.967571 |
| 37 | 1 | 0 | -5.340922 | 0.125421 | 1.080459 |
| 38 | 1 | 0 | -0.578331 | -1.469995 | -1.314489 |
|   |   |   |   |   |
|---|---|---|---|---|
| 39 | 1 | 0 | -1.851926 | -3.343131 | -2.196992 |
| 40 | 1 | 0 | -4.272978 | -3.593647 | -1.672675 |
| 41 | 1 | 0 | -5.399162 | -1.920174 | -0.247432 |
| 42 | 1 | 0 | 2.231664  | 3.562939  | -2.001553 |
| 43 | 1 | 0 | 0.977866  | 2.377150  | -2.273875 |
| 44 | 1 | 0 | 2.244323  | 1.869395  | -0.251058 |
| 45 | 1 | 0 | 3.599162  | 1.920174  | 0.247432  |
| 46 | 1 | 0 | 1.207835  | 4.477602  | 0.958972  |
| 47 | 1 | 0 | 2.198817  | 3.249120  | 1.752898  |
| 48 | 1 | 0 | 0.048396  | 4.591833  | 0.423908  |
| 49 | 1 | 0 | -0.737665 | 3.988841  | -1.308543 |
| 50 | 1 | 0 | 0.522027  | 5.222937  | -1.197733 |

|   |   |   |   |   |
|---|---|---|---|---|
| 1  | 6 | 0 | 3.456601 | -3.024440 | -0.970548 |
| 2  | 6 | 0 | 3.154432 | -3.089791 | 0.365589  |
| 3  | 6 | 0 | 2.231407 | -2.187446 | 0.957889  |
| 4  | 6 | 0 | 1.598517 | -1.186093 | 0.143888  |
| 5  | 6 | 0 | 1.945580 | -1.151880 | -1.237695 |
| 6  | 6 | 0 | 2.843459 | -2.040931 | -1.778799 |
| 7  | 6 | 0 | 1.930958 | -2.258349 | 2.340107  |
| 8  | 6 | 0 | 1.040970 | -1.379951 | 2.904895  |
| 9  | 6 | 0 | 0.410838 | -0.403652 | 2.108705  |
| 10 | 6 | 0 | 0.661699 | -0.290970 | 0.756834  |
| 11 | 6 | 0 | -0.037277| 0.841559  | -0.010557 |
| 12 | 6 | 0 | -1.548248| 0.866521  | 0.212406  |
| 13 | 6 | 0 | -2.389068| -0.147691 | -0.353273 |
| 14 | 6 | 0 | -2.117397| 1.881822  | 0.949275  |
| 15 | 6 | 0 | -3.511487| 1.939307  | 1.173511  |
| 16 | 6 | 0 | -4.338210| 0.982315  | 0.647247  |
| 17 | 6 | 0 | -3.803905| -0.077352 | -0.130238 |
| 18 | 6 | 0 | -1.895927| -1.224951 | -1.138884 |
| 19 | 6 | 0 | -2.741935| -2.167140 | -1.674487 |
| 20 | 6 | 0 | -4.133945| -2.091256 | -1.453146 |
| 21 | 6 | 0 | -4.647823| -1.068041 | -0.696066 |
| 22 | 8 | 0 | 0.482815 | 2.108332  | 0.398707  |
| 23 | 6 | 0 | 1.800905 | 2.446061  | -0.066361 |
| 24 | 6 | 0 | 1.724039 | 3.052116  | -1.475508 |
| 25 | 6 | 0 | 2.379427 | 3.399855  | 0.971819  |
| 26 | 6 | 0 | 3.087477 | 3.281777  | -2.136649 |
| 27 | 1 | 0 | 4.162796 | -3.720454 | -1.408674 |
| 28 | 1 | 0 | 3.620660 | -3.838461 | 0.997758  |
| 29 | 1 | 0 | 1.500553 | -0.410274 | -1.888012 |
| 30 | 1 | 0 | 3.084466 | -1.986135 | -2.833645 |
| 31 | 1 | 0 | 2.416414 | -3.019412 | 2.941974  |
| 32 | 1 | 0 | 0.811606 | -1.435935 | 3.963079  |
| 33 | 1 | 0 | -0.299302| 0.274272  | 2.567409  |

**1e (conformer 3)**
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 34 | 1 | 0 | 0.127566 | 0.716198 | -1.084555 |
| 35 | 1 | 0 | -1.476904 | 2.655152 | 1.349431 |
| 36 | 1 | 0 | -3.920219 | 2.753104 | 1.762295 |
| 37 | 1 | 0 | -5.409992 | 1.022032 | 0.811443 |
| 38 | 1 | 0 | -0.833727 | -1.322279 | -2.268631 |
| 39 | 1 | 0 | -2.335553 | -2.978074 | -1.084555 |
| 40 | 1 | 0 | -4.790933 | -2.840873 | -1.879724 |
| 41 | 1 | 0 | -5.716144 | -0.999589 | -0.518062 |
| 42 | 1 | 0 | 2.417622 | 1.538649 | -0.095251 |
| 43 | 1 | 0 | -2.335553 | -2.978074 | -1.084555 |
| 44 | 1 | 0 | -4.790933 | -2.840873 | -1.879724 |
| 45 | 1 | 0 | 2.417622 | 1.538649 | -0.095251 |
| 46 | 1 | 0 | -2.335553 | -2.978074 | -1.084555 |
| 47 | 1 | 0 | -4.790933 | -2.840873 | -1.879724 |
| 48 | 1 | 0 | 2.417622 | 1.538649 | -0.095251 |
| 49 | 1 | 0 | -2.335553 | -2.978074 | -1.084555 |
| 50 | 1 | 0 | -4.790933 | -2.840873 | -1.879724 |

1e (conformer 4)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.439406 | -1.912610 | -1.007559 |
| 2 | 6 | 0 | 4.808505 | -0.760621 | -0.358750 |
| 3 | 6 | 0 | 3.845288 | 0.210677 | 0.018766 |
| 4 | 6 | 0 | 2.461939 | -0.016899 | -0.282797 |
| 5 | 6 | 0 | 2.119897 | -1.223602 | -0.952045 |
| 6 | 6 | 0 | 3.079024 | -2.143093 | -1.305571 |
| 7 | 6 | 0 | 4.229703 | 1.402963 | 0.684970 |
| 8 | 6 | 0 | 3.288956 | 2.336832 | 1.030130 |
| 9 | 6 | 0 | 1.925213 | 2.123490 | 0.727360 |
| 10 | 6 | 0 | 1.499738 | 0.977404 | 0.092447 |
| 11 | 6 | 0 | 0.017794 | 0.787095 | -0.223935 |
| 12 | 6 | 0 | -0.642585 | -0.304391 | 0.631773 |
| 13 | 6 | 0 | -1.474317 | -1.331835 | 0.077208 |
| 14 | 6 | 0 | -0.469862 | -0.245141 | 1.999228 |
| 15 | 6 | 0 | -1.080709 | -1.169833 | 2.868729 |
| 16 | 6 | 0 | -1.872252 | -2.169831 | 2.362822 |
| 17 | 6 | 0 | -2.088512 | -2.278587 | 0.967353 |
| 18 | 6 | 0 | -1.731574 | -1.482382 | -1.316141 |
| 19 | 6 | 0 | -2.530971 | -2.491300 | -1.796951 |
| 20 | 6 | 0 | -3.128280 | -3.418169 | -0.914331 |
| 21 | 6 | 0 | -2.909208 | -3.308176 | 0.435079 |
| 22 | 8 | 0 | -0.638116 | 2.039500 | -0.012993 |
| 23 | 6 | 0 | -1.916248 | 2.211561 | -0.647805 |
| 24 | 6 | 0 | -2.670778 | 2.324840 | 0.204256 |
| 25 | 6 | 0 | -1.728179 | 2.647713 | -2.101649 |
| 26 | 6 | 0 | -4.114380 | 3.487023 | -0.240901 |
| 27 | 1 | 0 | 5.186498 | -2.645751 | -1.290144 |
| 28 | 1 | 0 | 5.851057 | -0.573023 | -0.122990 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 29 | 1 | 0 | 1.085279 | -1.438284 | -1.181754 |
| 30 | 1 | 0 | 2.787185 | -3.055281 | -1.813992 |
| 31 | 1 | 0 | 5.279191 | 1.561393 | 0.910268 |
| 32 | 1 | 0 | 3.583210 | 3.250879 | 1.534025 |
| 33 | 1 | 0 | 1.193961 | 2.877256 | 0.983433 |
| 34 | 1 | 0 | -0.052886 | 0.519958 | -1.282205 |
| 35 | 1 | 0 | 0.161372 | 0.532091 | 2.413656 |
| 36 | 1 | 0 | 0.915189 | -0.988549 | 3.937111 |
| 37 | 1 | 0 | 2.342546 | -2.891800 | 3.022130 |
| 38 | 1 | 0 | 1.296134 | -0.788949 | -2.023587 |
| 39 | 1 | 0 | 2.706146 | -2.575853 | -2.863653 |
| 40 | 1 | 0 | 4.016114 | -2.598094 | -1.401077 |
| 41 | 1 | 0 | 4.514406 | -1.689643 | -0.503386 |
| 42 | 1 | 0 | 3.681352 | -0.690376 | 0.068566 |
| 43 | 1 | 0 | 2.987979 | -0.631754 | -0.306772 |
| 44 | 1 | 0 | 1.817718 | -1.599826 | -1.230904 |
| 45 | 1 | 0 | 2.652056 | -2.553405 | -1.763945 |
| 46 | 1 | 0 | 4.189455 | 0.243159 | 1.008767 |
| 47 | 1 | 0 | 3.368107 | 1.194718 | 1.555700 |
| 48 | 1 | 0 | -4.617873 | 4.163036 | 0.454687 |
| 49 | 1 | 0 | -4.165675 | 3.942917 | -1.232948 |
| 50 | 1 | 0 | -4.690249 | 2.556574 | -0.270231 |

**1e (conformer 5)**

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1  | 6 | 0 | 4.016114 | -2.598094 | -1.401077 |
| 2  | 6 | 0 | 4.514406 | -1.689643 | -0.503386 |
| 3  | 6 | 0 | 3.681352 | -0.690376 | 0.068566 |
| 4  | 6 | 0 | 2.987979 | -0.631754 | -0.306772 |
| 5  | 6 | 0 | 1.817718 | -1.599826 | -1.230904 |
| 6  | 6 | 0 | 2.652056 | -2.553405 | -1.763945 |
| 7  | 6 | 0 | 4.189455 | 0.243159 | 1.008767 |
| 8  | 6 | 0 | 3.368107 | 1.194718 | 1.555700 |
| 9  | 6 | 0 | 2.008437 | 1.264614 | 1.178053 |
| 10 | 6 | 0 | 1.469000 | 0.387246 | 0.264345 |
| 11 | 6 | 0 | -0.002409 | 0.504284 | -0.126965 |
| 12 | 6 | 0 | -0.900452 | -0.521439 | 0.570507 |
| 13 | 6 | 0 | -2.164215 | -0.889307 | -0.002078 |
| 14 | 6 | 0 | -0.527686 | -1.069607 | 1.777615 |
| 15 | 6 | 0 | -1.354720 | -1.982555 | 2.468512 |
| 16 | 6 | 0 | -2.561945 | -2.354894 | 1.939680 |
| 17 | 6 | 0 | -2.996515 | -1.824875 | 0.697384 |
| 18 | 6 | 0 | -2.645683 | -0.377602 | -1.237652 |
| 19 | 6 | 0 | -3.859427 | -0.766437 | -1.753627 |
| 20 | 6 | 0 | -4.671153 | -1.690343 | -1.061087 |
| 21 | 6 | 0 | -4.244054 | -2.204561 | 0.137667 |
| 22 | 6 | 0 | -0.540047 | 1.797848 | 0.165645 |
| 23 | 6 | 0 | -0.598518 | 2.747814 | -0.913013 |
|   |   |   |   |   |
|---|---|---|---|---|
| 24 | 6 | 0 | -1.662970 | 3.779998 | -0.520457 |
| 25 | 6 | 0 | 0.762418  | 3.361627  | -1.249671  |
| 26 | 6 | 0 | -1.376548  | 4.546835  | 0.774483   |
| 27 | 1 | 0 | 4.663509   | -3.35372  | -1.828705  |
| 28 | 1 | 0 | 5.559392   | -1.717709 | -0.212342  |
| 29 | 1 | 0 | 0.771957   | -1.603997 | -1.510490  |
| 30 | 1 | 0 | 2.259041   | -3.281718 | -2.464497  |
| 31 | 1 | 0 | 5.236589   | 0.187676  | 1.287492   |
| 32 | 1 | 0 | -1.376548  | 4.546835  | 0.774483   |
| 33 | 1 | 0 | -1.249671  | 3.779998  | -0.520457  |
| 34 | 1 | 0 | -0.212342  | 1.287492  | 5.236589   |
| 35 | 1 | 0 | 4.76871    | 0.187676  | 1.287492   |
| 36 | 1 | 0 | 0.771957   | -1.603997 | -1.510490  |
| 37 | 1 | 0 | 2.259041   | -3.281718 | -2.464497  |
| 38 | 1 | 0 | -1.249671  | 3.779998  | -0.520457  |
| 39 | 1 | 0 | -0.212342  | 1.287492  | 5.236589   |

**1e (conformer 6)**

|   |   |   |   |   |
|---|---|---|---|---|
| 1  | 6 | 0 | 3.777453 | -2.560171 | -1.733901 |
| 2  | 6 | 0 | 4.393574 | -1.745094 | -0.817143 |
| 3  | 6 | 0 | 3.665610 | -0.749486 | -0.115061 |
| 4  | 6 | 0 | 2.625045 | -0.589184 | -0.376225 |
| 5  | 6 | 0 | 1.660783 | -1.460761 | -1.323366 |
| 6  | 6 | 0 | 2.395425 | -2.416309 | -1.984533 |
| 7  | 6 | 0 | 4.297552 | 0.085206  | 0.842934  |
| 8  | 6 | 0 | 3.577898 | 1.038369  | 1.515034  |
| 9  | 6 | 0 | 2.199926 | 1.208043  | 1.251000  |
| 10 | 6 | 0 | 1.540604 | 0.427586  | 0.327501  |
| 11 | 6 | 0 | 0.051430 | 0.652527  | 0.055594  |
| 12 | 6 | 0 | -0.848846 | -0.371898 | 0.746759  |
| 13 | 6 | 0 | -2.050701 | -0.852884 | 0.128517  |
| 14 | 6 | 0 | -0.529186 | -0.802071 | 2.016116  |
| 15 | 6 | 0 | -1.350436 | -1.701939 | 2.727536  |
| 16 | 6 | 0 | -2.498951 | -2.183635 | 2.156050  |
| 17 | 6 | 0 | -2.876459 | -1.779129 | 0.850786  |
| 18 | 6 | 0 | -2.478685 | -0.472371 | -1.173523 |
|   |   |   |          |          |          |
|---|---|---|---------|---------|---------|
|   | 6 | 0 | -3.633991 | -0.971123 | -1.727014 |
| 20| 6 | 0 | -4.438229 | -1.883965 | -1.011054 |
| 21| 6 | 0 | -4.062821 | -2.274830 | 0.249409  |
| 22| 8 | 0 | -0.388457 | 1.942716  | 0.492603  |
| 23| 6 | 0 | -0.049818 | 3.052347  | -0.365676 |
| 24| 6 | 0 | -1.058584 | 3.201831  | -1.517909 |
| 25| 6 | 0 | 0.021850  | 4.282647  | 0.532998  |
| 26| 6 | 0 | -2.506015 | 3.440615  | -1.078434 |
| 27| 1 | 0 | 4.345797  | -3.317577 | -2.261870 |
| 28| 1 | 0 | 5.453628  | -1.852985 | -0.611527 |
| 29| 1 | 0 | 0.599205  | -1.389296 | -1.520684 |
| 30| 1 | 0 | 1.908696  | -3.069279 | -2.700292 |
| 31| 1 | 0 | 3.357323  | -0.047156 | 1.034012  |
| 32| 1 | 0 | -2.506015 | 3.440615  | -1.078434 |
| 33| 1 | 0 | 4.345797  | -3.317577 | -2.261870 |
| 34| 1 | 0 | 1.640568  | 1.968673  | 1.780211  |
| 35| 1 | 0 | -0.091078 | 0.577948  | -1.026074 |
| 36| 1 | 0 | 0.381677  | -0.445832 | 2.480577  |
| 37| 1 | 0 | -1.061644 | -2.011942 | 3.725478  |
| 38| 1 | 0 | -3.134516 | -2.881558 | 2.691027  |
| 39| 1 | 0 | -1.892915 | 0.231872  | -1.747973 |
| 40| 1 | 0 | -3.931741 | -0.658441 | -2.721679 |
| 41| 1 | 0 | -3.472926 | -2.270229 | -1.457843 |
| 42| 1 | 0 | -4.672406 | -2.974637 | 0.811703  |
| 43| 1 | 0 | -3.178952 | 3.429518  | -1.939814 |
| 44| 1 | 0 | -0.841542 | 4.188801  | 1.247782  |
| 45| 1 | 0 | -1.009542 | 2.305261  | -2.145661 |
| 46| 1 | 0 | -3.86350  | 5.185820  | -0.061133 |
| 47| 1 | 0 | -0.905162 | 4.401307  | 1.097335  |
| 48| 1 | 0 | 0.841542  | 4.188801  | 1.247782  |
| 49| 1 | 0 | -3.178952 | 3.429518  | -1.939814 |
| 50| 1 | 0 | -2.831493 | 2.664502  | -0.383306 |

| 1e (conformer 7) |
|------------------|
|   |   |   |          |          |
| 1 | 6 | 0 | 3.954895 | -2.422050 | -1.235995 |
| 2 | 6 | 0 | 3.742810 | -2.528759 | 0.114821  |
| 3 | 6 | 0 | 2.708365 | -1.799220 | 0.758568  |
| 4 | 6 | 0 | 1.866850 | -0.928823 | -0.016418 |
| 5 | 6 | 0 | 2.122504 | -0.850350 | -1.415914 |
| 6 | 6 | 0 | 3.131826 | -1.571946 | -2.006752 |
| 7 | 6 | 0 | 2.497872 | -1.916983 | 2.154472  |
| 8 | 6 | 0 | 1.494070 | -1.211949 | 2.768947  |
| 9 | 6 | 0 | 0.663586 | -0.362044 | 2.012530  |
| 10| 6 | 0 | 0.825414 | -0.204292 | 0.651660  |
| 11| 6 | 0 | -0.080356 | 0.805279  | -0.069982 |
| 12| 6 | 0 | -1.558792 | 0.611738  | 0.260829  |
| 13| 6 | 0 | -2.277839 | -0.521939 | -0.242666 |
|     | N | L | C |   E1   | E2   | E3   |
|-----|---|---|---|--------|------|------|
| 14  | 6 | 0 | -2.217591 | 1.539375 | 1.037840 |
| 15  | 6 | 0 | -3.585361 | 1.392865 | 1.361658 |
| 16  | 6 | 0 | -4.296278 | 0.318342 | 0.896687 |
| 17  | 6 | 0 | -3.667625 | -0.659502 | 0.083117 |
| 18  | 6 | 0 | -1.687161 | -1.522596 | -1.061176 |
| 19  | 6 | 0 | -2.419350 | -2.586771 | -1.531901 |
| 20  | 6 | 0 | -3.787449 | -2.716206 | -1.209168 |
| 21  | 6 | 0 | -4.392693 | -1.771510 | -0.418281 |
| 22  | 8 | 0 | 0.267084  | 2.147043  | 0.276003 |
| 23  | 6 | 0 | 1.482517  | 2.688246  | -0.276642 |
| 24  | 6 | 0 | 1.146153  | 4.049445  | -0.893251 |
| 25  | 6 | 0 | 2.546118  | 2.795147  | 0.814580 |
| 26  | 6 | 0 | 0.157040  | 3.974224  | -2.057680 |
| 27  | 1 | 0 | 4.747837  | -2.986129 | -1.713644 |
| 28  | 1 | 0 | 4.367168  | -3.178968 | 0.718886 |
| 29  | 1 | 0 | 1.513284  | -0.211445 | -2.041288 |
| 30  | 1 | 0 | 3.297466  | -1.488172 | -3.075036 |
| 31  | 1 | 0 | 3.141694  | -2.577299 | 2.725906 |
| 32  | 1 | 0 | 1.331113  | -1.306611 | 3.836624 |
| 33  | 1 | 0 | -0.127935 | 0.183591  | 2.512508 |
| 34  | 1 | 0 | 0.027179  | 0.690181  | -1.152806 |
| 35  | 1 | 0 | -1.669967 | 2.400760  | 1.393856 |
| 36  | 1 | 0 | -4.067212 | 2.143388  | 1.978496 |
| 37  | 1 | 0 | -5.347555 | 0.200899  | 1.138096 |
| 38  | 1 | 0 | -0.637962 | -1.461339 | -1.315761 |
| 39  | 1 | 0 | -1.940525 | -3.335383 | -2.153221 |
| 40  | 1 | 0 | -4.354099 | -3.560540 | -1.585307 |
| 41  | 1 | 0 | -5.443592 | -1.860640 | -0.162702 |
| 42  | 1 | 0 | 1.842480  | 2.021204  | -1.070041 |
| 43  | 1 | 0 | 0.741582  | 4.689006  | -0.100572 |
| 44  | 1 | 0 | 2.081369  | 4.514951  | -1.224772 |
| 45  | 1 | 0 | 3.466594  | 3.230681  | 0.414638 |
| 46  | 1 | 0 | 2.185467  | 3.434109  | 1.625230 |
| 47  | 1 | 0 | 2.781376  | 1.815197  | 1.231084 |
| 48  | 1 | 0 | -0.068217 | 4.970077  | -2.448190 |
| 49  | 1 | 0 | 0.560725  | 3.380103  | -2.884268 |
| 50  | 1 | 0 | -0.782088 | 3.517718  | -1.738627 |
| 1e (conformer 8) |     |    |        |        |        |
| 1   | 6 | 0 | 4.654008 | -1.726000 | -1.017279 |
| 2   | 6 | 0 | 4.212699 | -2.253229 | 0.170491 |
| 3   | 6 | 0 | 2.964272 | -1.868788 | 0.725413 |
| 4   | 6 | 0 | 2.148124 | -0.914715 | 0.032426 |
| 5   | 6 | 0 | 2.645128 | -0.386568 | -1.189557 |
| 6   | 6 | 0 | 3.858337 | -0.781645 | -1.701443 |
| 7   | 6 | 0 | 2.512230 | -2.413268 | 1.954877 |
| 8   | 6 | 0 | 1.303388 | -2.036978 | 2.477444 |

S207
| 9  | 6  | 0   | 0.491673 | -1.106388 | 1.792129 |
| 10 | 6  | 0   | 0.881540 | -0.544434 | 0.596556 |
| 11 | 6  | 0   | -0.006524 | 0.485386 | -0.104250 |
| 12 | 6  | 0   | -1.480543 | 0.393237 | 0.288824 |
| 13 | 6  | 0   | -2.346765 | -0.567290 | -0.327261 |
| 14 | 6  | 0   | -1.987724 | 1.240947 | 1.249075 |
| 15 | 6  | 0   | -3.347525 | 1.200277 | 1.629345 |
| 16 | 6  | 0   | -2.006524 | 0.305347 | 1.039744 |
| 17 | 6  | 0   | -3.729017 | -0.598282 | 0.053431 |
| 18 | 6  | 0   | -1.902300 | -1.508926 | -1.296291 |
| 19 | 6  | 0   | -2.770224 | -2.409072 | -1.867013 |
| 20 | 6  | 0   | -4.133768 | -2.424329 | -1.499839 |
| 21 | 6  | 0   | -4.597488 | -1.539102 | -0.558930 |
| 22 | 8  | 0   | 0.554798  | 1.769962 | 0.185882 |
| 23 | 6  | 0   | 0.134745  | 2.867680 | -0.648828 |
| 24 | 6  | 0   | 0.415220  | 4.147551 | 0.148877 |
| 25 | 6  | 0   | 0.825132  | 2.846754 | -2.015266 |
| 26 | 6  | 0   | 1.877795  | 4.346151 | 0.560274 |
| 27 | 1  | 0   | 5.609731  | -2.028468 | -1.430166 |
| 28 | 1  | 0   | 4.815890  | -2.977681 | 0.707958 |
| 29 | 1  | 0   | 2.066671  | 0.351429 | -1.725684 |
| 30 | 1  | 0   | 4.210473  | -0.360282 | -2.636580 |
| 31 | 1  | 0   | 3.140010  | -3.132510 | 2.470583 |
| 32 | 1  | 0   | 0.957589  | -2.453453 | 3.416813 |
| 33 | 1  | 0   | -0.465441 | -0.835788 | 2.218816 |
| 34 | 1  | 0   | 0.053762  | 0.311071 | -1.184086 |
| 35 | 1  | 0   | -1.319613 | 1.954245 | 1.715409 |
| 36 | 1  | 0   | -3.709276 | 1.885563 | 2.387851 |
| 37 | 1  | 0   | -5.249873 | 0.271936 | 1.320151 |
| 38 | 1  | 0   | -0.858538 | -1.536345 | -1.581571 |
| 39 | 1  | 0   | -2.404305 | -3.117989 | -2.601286 |
| 40 | 1  | 0   | -4.807893 | -3.139141 | -1.958097 |
| 41 | 1  | 0   | -5.641655 | -1.548281 | -0.263619 |
| 42 | 1  | 0   | -0.949120 | 2.798847 | -0.804739 |
| 43 | 1  | 0   | 0.071625  | 5.000138 | -0.448149 |
| 44 | 1  | 0   | -0.211171 | 4.125109 | 1.046297 |
| 45 | 1  | 0   | 0.522226  | 3.720364 | -2.599785 |
| 46 | 1  | 0   | 1.911633  | 2.862063 | -1.908970 |
| 47 | 1  | 0   | 0.547523  | 1.962410 | -2.594318 |
| 48 | 1  | 0   | 1.981311  | 5.238294 | 1.183572 |
| 49 | 1  | 0   | 2.236228  | 3.487483 | 1.130176 |
| 50 | 1  | 0   | 2.533052  | 4.474850 | -0.305318 |

| 1e (conformer 9) |
|------------------|
| 1  | 6  | 0   | -3.833816 | -2.268564 | 2.105218 |
| 2  | 6  | 0   | -4.356538 | -1.781202 | 0.933537 |
| 3  | 6  | 0   | -3.566633 | -1.006299 | 0.044508 |
|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 4 | 6 | 0 | -2.202964 | -0.719643 | 0.384208 |
| 5 | 6 | 0 | -1.694303 | -1.255423 | 1.599958 |
| 6 | 6 | 0 | -2.486481 | -2.004879 | 2.436443 |
| 7 | 6 | 0 | -4.100050 | -0.517574 | -1.175852|
| 8 | 6 | 0 | -3.320888 | 0.221430  | -2.028315|
| 9 | 6 | 0 | -1.981627 | 0.516328  | -1.691082|
|10 | 6 | 0 | -1.418729 | 0.074755  | -0.513455|
|11 | 6 | 0 | 0.029365  | 0.435407  | -0.185367|
|12 | 6 | 0 | 1.038044  | -0.644264 | -0.585101|
|13 | 6 | 0 | 2.351198  | -0.656292 | -0.005358|
|14 | 6 | 0 | 1.694303  | -1.608157 | 1.599958 |
|15 | 6 | 0 | 2.436443  | -2.028315 | -1.691082|
|16 | 6 | 0 | 2.879595  | -2.648689 | -1.356074|
|17 | 6 | 0 | 3.274022  | -1.681752 | -0.395986|
|18 | 6 | 0 | 2.792928  | 0.301660  | 0.946246 |
|19 | 6 | 0 | 4.053941  | 0.242934  | 1.490577 |
|20 | 6 | 0 | 4.954648  | -0.775157 | 1.109155 |
|21 | 6 | 0 | 4.569103  | -1.712533 | 0.183876 |
|22 | 6 | 0 | 0.448631  | 1.644976  | -0.828405|
|23 | 6 | 0 | -0.147723 | 2.874417  | -0.365386|
|24 | 6 | 0 | 0.484291  | 3.351465  | 0.951528 |
|25 | 6 | 0 | 0.040137  | 3.864742  | -1.507283|
|26 | 6 | 0 | -0.207404 | 4.575087  | 1.563917 |
|27 | 1 | 0 | -4.448072 | -2.860415 | 2.774390 |
|28 | 1 | 0 | -5.387797 | -1.985976 | 0.664973 |
|29 | 1 | 0 | -0.659417 | -1.089567 | 1.870156 |
|30 | 1 | 0 | -2.072434 | -2.402647 | 3.356208 |
|31 | 1 | 0 | -5.132342 | -0.742527 | -1.422746|
|32 | 1 | 0 | -3.728017 | 0.588320  | -2.963977|
|33 | 1 | 0 | -1.374117 | 1.106904  | -2.365572|
|34 | 1 | 0 | 0.095385  | 0.572567  | 0.899807 |
|35 | 1 | 0 | -0.280447 | -1.608612 | -1.950872|
|36 | 1 | 0 | 1.323552  | -3.346723 | -2.639538|
|37 | 1 | 0 | 3.588089  | -3.418052 | -1.644967|
|38 | 1 | 0 | 2.132226  | 1.105165  | 1.235642 |
|39 | 1 | 0 | 4.362891  | 0.989153  | 2.214273 |
|40 | 1 | 0 | 5.947112  | -0.810234 | 1.544170 |
|41 | 1 | 0 | 5.253758  | -2.497132 | -0.121502|
|42 | 1 | 0 | -1.220864 | 2.711211  | -0.200190|
|43 | 1 | 0 | 0.442832  | 2.535120  | 1.679767 |
|44 | 1 | 0 | 1.544076  | 3.563373  | 0.772713 |
|45 | 1 | 0 | -0.386675 | 4.841328  | -1.262285|
|46 | 1 | 0 | 1.105247  | 3.993527  | -1.719132|
|47 | 1 | 0 | -0.444574 | 3.499979  | -2.414084|
|48 | 1 | 0 | 0.230357  | 4.821190  | 2.534616|
|   |   |   | 1e (conformer 10) |   |   |   |
|---|---|---|-----------------|---|---|---|
|   |   |   |      |   |   |   |
| 49 | 1  | 0  | -0.112742 | 5.459444 | 0.929455 |
| 50 | 1  | 0  | -1.274535 | 4.389292 | 1.720985 |
|  1 | 6  | 0  | 4.908587  | -1.239696 | -0.965297 |
|  2 | 6  | 0  | 4.505241  | -1.814662 | 0.213856  |
|  3 | 6  | 0  | 3.213231  | -1.566864 | 0.746608  |
|  4 | 6  | 0  | 2.313854  | -0.703063 | 0.039678  |
|  5 | 6  | 0  | 2.772622  | -0.120160 | -1.171966 |
|  6 | 6  | 0  | 4.029600  | -0.382727 | -1.662650 |
|  7 | 6  | 0  | 2.797525  | -2.160432 | 1.966297  |
|  8 | 6  | 0  | 1.545696  | -1.916091 | 2.465241  |
|  9 | 6  | 0  | 0.652085  | -1.074806 | 1.765240  |
| 10 | 6  | 0  | 1.003558  | -0.471205 | 0.578464  |
| 11 | 6  | 0  | 0.024976  | 0.443085  | -0.161736 |
| 12 | 6  | 0  | -1.430285 | 0.264183  | 0.264217  |
| 13 | 6  | 0  | -2.247312 | -0.757448 | -0.321045 |
| 14 | 6  | 0  | -1.969391 | 1.089110  | 1.227207  |
| 15 | 6  | 0  | -3.315253 | 0.968228  | 1.637828  |
| 16 | 6  | 0  | -4.124897 | 0.015141  | 1.076134  |
| 17 | 6  | 0  | -3.616878 | -0.869503 | 0.090292  |
| 18 | 6  | 0  | -1.765641 | -1.685704 | -1.285598 |
| 19 | 6  | 0  | -2.587430 | -2.646638 | -1.824438 |
| 20 | 6  | 0  | -3.939800 | -2.740306 | -1.428615 |
| 21 | 6  | 0  | -4.437862 | -1.871182 | -0.490491 |
| 22 | 8  | 0  | 0.502517  | 1.781130  | 0.027257  |
| 23 | 6  | 0  | -0.051649 | 2.820901  | -0.799643 |
| 24 | 6  | 0  | 0.508938  | 4.134807  | -0.252731 |
| 25 | 6  | 0  | 0.279980  | 2.651041  | -2.834525 |
| 26 | 6  | 0  | 0.148791  | 4.420942  | 1.206422  |
| 27 | 1  | 0  | 5.898253  | -1.437809 | -1.361218 |
| 28 | 1  | 0  | 5.172804  | -2.472418 | 0.760968  |
| 29 | 1  | 0  | 2.127264  | 0.557602  | -1.710886 |
| 30 | 1  | 0  | 4.352065  | 0.076985  | -2.590405 |
| 31 | 1  | 0  | 3.487755  | -2.811007 | 2.493292  |
| 32 | 1  | 0  | 1.227837  | -2.370117 | 3.397044  |
| 33 | 1  | 0  | -0.336416 | -0.910270 | 2.173988  |
| 34 | 1  | 0  | 0.085967  | 0.199186  | -1.227107 |
| 35 | 1  | 0  | -1.340802 | 1.849726  | 1.672303  |
| 36 | 1  | 0  | -3.702855 | 1.638351  | 2.397102  |
| 37 | 1  | 0  | -5.162203 | -0.080067 | 1.379658  |
| 38 | 1  | 0  | -0.728144 | -1.654321 | -1.592251 |
| 39 | 1  | 0  | -2.192987 | -3.342155 | -2.555752 |
| 40 | 1  | 0  | -4.577509 | -3.502258 | -1.862336 |
| 41 | 1  | 0  | -5.472965 | -1.940445 | -0.172190 |
| 42 | 1  | 0  | -1.147193 | 2.820680  | -0.683089 |
| 43 | 1  | 0  | 1.598492  | 4.105547  | -0.365233 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|44 | 1 | 0 | 0.146594 | 4.947827 | -0.891569 |
|45 | 1 | 0 | -0.163761 | 3.470692 | -2.855179 |
|46 | 1 | 0 | 1.361707 | 2.673970 | -2.441746 |
|47 | 1 | 0 | -0.116658 | 1.721413 | -0.112224 |
|48 | 1 | 0 | -0.935637 | 4.480780 | 1.343535 |
|49 | 1 | 0 | -0.116658 | 1.721413 | -2.697635 |
|50 | 1 | 0 | 0.533499 | 3.635584 | 1.858996 |

**1e (conformer 11)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
|1  | 6 | 0 | 4.984908 | -0.886142 | -1.028066 |
|2  | 6 | 0 | 4.629645 | -1.591033 | 0.094592 |
|3  | 6 | 0 | 3.332651 | -1.468827 | 0.657982 |
|4  | 6 | 0 | 2.375519 | -0.596823 | 0.041974 |
|5  | 6 | 0 | 2.786263 | 0.122920 | -1.028066 |
|6  | 6 | 0 | 4.050000 | -0.019284 | -1.112224 |
|7  | 6 | 0 | 2.969353 | -2.195133 | 1.820974 |
|8  | 6 | 0 | 1.712804 | -2.070895 | 2.351644 |
|9  | 6 | 0 | 0.762984 | -1.223364 | 1.739552 |
|10 | 6 | 0 | 1.061754 | -0.493532 | 0.610346 |
|11 | 6 | 0 | 0.019250 | 0.433227 | -0.018485 |
|12 | 6 | 0 | -1.420498 | 0.079892 | 0.352987 |
|13 | 6 | 0 | -2.131333 | -0.942769 | -0.355289 |
|14 | 6 | 0 | -2.048076 | 0.748120 | 1.381472 |
|15 | 6 | 0 | -3.834440 | 0.463482 | 1.743676 |
|16 | 6 | 0 | -4.092974 | -0.494645 | 1.066785 |
|17 | 6 | 0 | -3.490760 | -1.220348 | 0.006924 |
|18 | 6 | 0 | -1.550973 | -1.713611 | -1.400254 |
|19 | 6 | 0 | -2.272526 | -2.679547 | -2.060145 |
|20 | 6 | 0 | -3.616722 | -2.935990 | -1.711215 |
|21 | 6 | 0 | -4.207165 | -2.222583 | -0.698211 |
|22 | 8 | 0 | 0.372637 | 1.765435 | 0.369436 |
|23 | 6 | 0 | -0.239308 | 2.844747 | -0.365532 |
|24 | 6 | 0 | -0.086407 | 4.075952 | 0.531919 |
|25 | 6 | 0 | 0.399897 | 3.026304 | -1.742937 |
|26 | 6 | 0 | -0.793059 | 5.332932 | 0.015680 |
|27 | 1 | 0 | 5.978980 | -0.988992 | -1.448399 |
|28 | 1 | 0 | 5.340167 | -2.257402 | 0.572816 |
|29 | 1 | 0 | 2.098605 | 0.808846 | -1.584412 |
|30 | 1 | 0 | 4.333974 | 0.543652 | -2.516733 |
|31 | 1 | 0 | 3.703360 | -2.849501 | 2.279668 |
|32 | 1 | 0 | 1.434793 | -2.625628 | 3.240718 |
|33 | 1 | 0 | -0.227644 | -1.154981 | 2.170091 |
|34 | 1 | 0 | 0.104758 | 0.349589 | -1.107454 |
|35 | 1 | 0 | -1.497164 | 1.511098 | 1.917406 |
|36 | 1 | 0 | -3.842947 | 1.012883 | 2.557831 |
|37 | 1 | 0 | -5.121593 | -0.714361 | 1.332933 |
|38 | 1 | 0 | -0.515968 | -1.555410 | -1.673987 |
|   |   |   |   |   |
|---|---|---|---|---|
| 39 | 1 | 0 | -1.804590 | -3.254270 | -2.851545 |
| 40 | 1 | 0 | -4.175266 | -3.699797 | -2.240404 |
| 41 | 1 | 0 | -5.236641 | -2.418333 | 0.670155 |
| 42 | 1 | 0 | -1.308661 | 2.629712 | -0.492482 |
| 43 | 1 | 0 | -0.480650 | 3.813642 | 1.518026 |
| 44 | 1 | 0 | 0.983136 | 4.268479 | 0.743701 |
| 45 | 1 | 0 | -0.084367 | 3.840793 | -2.287061 |
| 46 | 1 | 0 | 1.463189 | 3.260897 | -1.642551 |
| 47 | 1 | 0 | 0.295797 | 2.130034 | -2.359133 |
| 48 | 1 | 0 | -0.711856 | 5.693899 | -0.921799 |
| 49 | 1 | 0 | -1.308661 | 2.629712 | -0.492482 |
| 50 | 1 | 0 | -0.480650 | 3.813642 | 1.518026 |

**1e (conformer 12)**

|   |   |   |   |   |
|---|---|---|---|---|
| 1  | 6 | 0 | 4.681780 | -1.222044 | -1.051599 |
| 2  | 6 | 0 | 4.701349 | -0.517412 | 0.125659 |
| 3  | 6 | 0 | 3.559141 | 0.194017 | 0.576576 |
| 4  | 6 | 0 | 2.354851 | 0.165865 | -0.204516 |
| 5  | 6 | 0 | 2.379254 | -0.571698 | -1.420021 |
| 6  | 6 | 0 | 3.506322 | -1.242559 | -1.832081 |
| 7  | 6 | 0 | 3.600036 | 0.943711 | 1.779482 |
| 8  | 6 | 0 | 2.502570 | 1.653782 | 2.187558 |
| 9  | 6 | 0 | 1.315879 | 1.633200 | 1.422704 |
| 10 | 6 | 0 | 1.211443 | 0.898015 | 0.261249 |
| 11 | 6 | 0 | -0.091687 | 0.948790 | -0.547681 |
| 12 | 6 | 0 | -0.809943 | -0.380317 | -0.811763 |
| 13 | 6 | 0 | -1.258704 | -1.257469 | 0.230630 |
| 14 | 6 | 0 | -1.092291 | -0.706000 | -2.123105 |
| 15 | 6 | 0 | -1.776834 | -1.889647 | -2.476352 |
| 16 | 6 | 0 | -2.186921 | -2.755957 | -1.498048 |
| 17 | 6 | 0 | -1.944932 | -2.464887 | -0.130497 |
| 18 | 6 | 0 | -1.074160 | -0.989584 | 1.613921 |
| 19 | 6 | 0 | -1.518360 | -1.865212 | 2.575793 |
| 20 | 6 | 0 | -2.176298 | -3.060916 | 2.214209 |
| 21 | 6 | 0 | -2.385095 | -3.348896 | 0.889028 |
| 22 | 8 | 0 | -0.986712 | 1.863272 | 0.092201 |
| 23 | 6 | 0 | -1.877742 | 2.587217 | -0.773672 |
| 24 | 6 | 0 | -3.075982 | 3.014179 | 0.075036 |
| 25 | 6 | 0 | -1.161167 | 3.785068 | -1.399477 |
| 26 | 6 | 0 | -3.912337 | 1.849390 | 0.607892 |
| 27 | 1 | 0 | 5.562853 | -1.758913 | -1.384651 |
| 28 | 1 | 0 | 5.599945 | -0.487720 | 0.733287 |
| 29 | 1 | 0 | 1.492362 | -0.620579 | -2.033892 |
| 30 | 1 | 0 | 3.490253 | -1.795870 | -2.764563 |
| 31 | 1 | 0 | 4.516583 | 0.952397 | 2.860223 |
| 32 | 1 | 0 | 2.535296 | 2.239635 | 3.099521 |
| 33 | 1 | 0 | 0.461445 | 2.209770 | 1.747812 |
|  |  |  |  |  |  |
|---|---|---|---|---|---|
| 34 | 1 | 0 | 0.177852 | 1.347605 | -1.534759 |
| 35 | 1 | 0 | -0.766975 | -0.037824 | -2.914939 |
| 36 | 1 | 0 | -1.970470 | -2.105222 | -3.521070 |
| 37 | 1 | 0 | -2.708390 | -3.672648 | -1.752733 |
| 38 | 1 | 0 | -0.580321 | -0.078725 | 1.913891 |
| 39 | 1 | 0 | -1.362933 | 3.672648 | -1.752733 |
| 40 | 1 | 0 | -2.518597 | -3.743919 | 2.983566 |
| 41 | 1 | 0 | -2.897556 | -3.099775 | 0.597848 |
| 42 | 1 | 0 | -2.229726 | 1.911957 | -1.565823 |
| 43 | 1 | 0 | -2.700133 | 3.619724 | 0.907786 |
| 44 | 1 | 0 | -3.701635 | 3.675984 | -0.534307 |
| 45 | 1 | 0 | -1.823253 | 4.308837 | -2.094990 |
| 46 | 1 | 0 | -0.848762 | 4.487179 | -0.622024 |
| 47 | 1 | 0 | -0.271528 | 1.913891 | -1.565823 |
| 48 | 1 | 0 | -4.745523 | 2.213809 | 1.214873 |
| 49 | 1 | 0 | -4.331427 | 1.256589 | -0.210913 |
| 50 | 1 | 0 | -3.066868 | 1.183710 | 1.224432 |
| 1e (conformer 15) |  |  |  |  |  |
| 1 | 6 | 0 | 2.673534 | -3.032679 | 2.091590 |
| 2 | 6 | 0 | 2.825354 | -3.272215 | 0.749178 |
| 3 | 6 | 0 | 2.264771 | -2.397995 | -0.218470 |
| 4 | 6 | 0 | 1.514064 | -1.254194 | 0.214616 |
| 5 | 6 | 0 | 1.393859 | -1.032656 | 1.613312 |
| 6 | 6 | 0 | 1.955105 | -1.896491 | 2.523142 |
| 7 | 6 | 0 | 2.450525 | -2.635338 | -1.604924 |
| 8 | 6 | 0 | 1.928881 | -1.773998 | -2.533246 |
| 9 | 6 | 0 | 1.181536 | -0.653743 | -2.108555 |
| 10 | 6 | 0 | 0.942096 | -0.387543 | -0.775769 |
| 11 | 6 | 0 | 0.124974 | 0.866728 | -0.430856 |
| 12 | 6 | 0 | -1.167489 | 0.641547 | 0.365297 |
| 13 | 6 | 0 | -2.268400 | -0.095683 | -0.187054 |
| 14 | 6 | 0 | -1.304656 | 1.210248 | 1.613389 |
| 15 | 6 | 0 | -2.479354 | 1.051896 | 2.380941 |
| 16 | 6 | 0 | -3.532455 | 0.327372 | 1.890060 |
| 17 | 6 | 0 | -3.459332 | -0.253805 | 0.589812 |
| 18 | 6 | 0 | -2.624184 | -0.640555 | -1.490374 |
| 19 | 6 | 0 | -3.349818 | -1.350003 | -1.980793 |
| 20 | 6 | 0 | -4.510213 | -1.516317 | -1.195212 |
| 21 | 6 | 0 | -4.557949 | -0.977020 | 0.065611 |
| 22 | 6 | 0 | 0.923099 | 1.808629 | 0.287942 |
| 23 | 6 | 0 | 1.945328 | 2.488357 | -0.463153 |
| 24 | 6 | 0 | 1.362430 | 3.672561 | -1.254714 |
| 25 | 6 | 0 | 3.017252 | 2.887220 | 0.544701 |
| 26 | 6 | 0 | 0.668800 | 4.741022 | -0.404412 |
| 27 | 1 | 0 | 3.107706 | -3.707344 | 2.820919 |
| 28 | 1 | 0 | 3.384135 | -4.135895 | 0.403810 |
|   | Conformer | 50% | 50%_DFT | Rmsd  | Dihedral | 1e (conformer 16) | 1e (conformer 16) |
|---|-----------|-----|---------|-------|----------|------------------|------------------|
| 29| 1         | 1   | 0       | 0.862760 | -0.162516 | 1.964154 | 1.708873 |
| 30| 1         | 0   | 1       | 1.846959 | -1.701964 | 3.584428 | 3.802568 |
| 31| 1         | 0   | 0       | 3.021327 | -3.504571 | 3.584428 | -3.593797 |
| 32| 1         | 0   | 0       | -0.171974 | 1.309508 | 2.472200 | 0.198446 |
| 33| 1         | 0   | 0       | 0.776100 | 0.014980 | 2.861935 | 0.203956 |
| 34| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 35| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 36| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 37| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 38| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 39| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 40| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 41| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 42| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 43| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 44| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 45| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 46| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 47| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 48| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 49| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
| 50| 1         | 0   | 0       | 2.083126 | -1.944806 | 3.561634 | 1.337907 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 24 | 6 | 0 | 2.001930 | -3.555552 | 0.364769 |
| 25 | 6 | 0 | 3.462049 | -2.053576 | -1.106273 |
| 26 | 6 | 0 | 3.095293 | -4.239264 | 1.192740 |
| 27 | 1 | 0 | 1.924300 | 4.654519 | -2.429021 |
| 28 | 1 | 0 | 2.326184 | 4.779159 | 0.004930 |
| 29 | 1 | 0 | 0.554699 | 0.616954 | -2.025540 |
| 30 | 1 | 0 | 0.942883 | -0.269580 | -1.631134 |
| 31 | 1 | 0 | 2.317339 | 3.754221 | 2.208878 |
| 32 | 1 | 0 | 1.880855 | 1.800841 | 3.665867 |
| 33 | 1 | 0 | 3.095293 | -4.239264 | 1.192740 |
| 34 | 1 | 0 | 0.554699 | 0.616954 | -2.025540 |
| 35 | 1 | 0 | 0.942883 | -0.269580 | -1.631134 |
| 36 | 1 | 0 | 2.317339 | 3.754221 | 2.208878 |
| 37 | 1 | 0 | 1.880855 | 1.800841 | 3.665867 |
| 38 | 1 | 0 | 0.554699 | 0.616954 | -2.025540 |
| 39 | 1 | 0 | 0.942883 | -0.269580 | -1.631134 |
| 40 | 1 | 0 | 2.639151 | -1.537021 | 0.808012 |
| 41 | 1 | 0 | 1.076626 | -3.527253 | 0.949955 |
| 42 | 1 | 0 | 3.174263 | -2.599378 | -2.009419 |
| 43 | 1 | 0 | 3.655434 | -1.014959 | -1.379974 |
| 44 | 1 | 0 | 2.768769 | -5.227779 | 1.525449 |
| 45 | 1 | 0 | 4.016663 | -4.375276 | 0.620937 |
| 46 | 1 | 0 | 3.341939 | -3.655775 | 2.085682 |
| 47 | 1 | 0 | 1.363140 | 0.662692 | 3.259128 |
| 48 | 1 | 0 | 5.582431 | -0.680254 | 2.030143 |
| 49 | 1 | 0 | 5.650605 | -0.019995 | -0.338093 |
| 50 | 1 | 0 | 3.174263 | -2.599378 | -2.009419 |

**1e (conformer 17)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | -4.850952 | 0.515671 | -1.204618 |
| 2  | 6 | 0 | -4.797575 | -0.096863 | 0.022048 |
| 3  | 6 | 0 | -3.577489 | -0.605566 | 0.538407 |
| 4  | 6 | 0 | -2.371140 | -0.463491 | -0.227128 |
| 5  | 6 | 0 | -2.472881 | 0.169905 | -1.496221 |
| 6  | 6 | 0 | -3.673186 | 0.642567 | -1.971392 |
| 7  | 6 | 0 | -3.541309 | -1.266759 | 1.792159 |
| 8  | 6 | 0 | -2.365506 | -1.785530 | 2.264515 |
| 9  | 6 | 0 | -1.175511 | -1.649168 | 1.517176 |
| 10 | 6 | 0 | -1.146399 | -0.987042 | 0.308206 |
| 11 | 6 | 0 | 0.174113 | -0.893117 | -0.468358 |
| 12 | 6 | 0 | 0.700618 | 0.518751 | -0.763227 |
| 13 | 6 | 0 | 1.043298 | 1.461343 | 0.262705 |
| 14 | 6 | 0 | 0.907795 | 0.867438 | -2.082279 |
| 15 | 6 | 0 | 1.401598 | 2.135479 | -2.459497 |
| 16 | 6 | 0 | 1.698421 | 3.063703 | -1.497112 |
| 17 | 6 | 0 | 1.534634 | 2.753350 | -0.122316 |
| 18 | 6 | 0 | 0.939523 | 1.178637 | 1.651648 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 19 | 6 | 0 | 1.273546 | 2.118514 | 2.597175 |
| 20 | 6 | 0 | 1.734580 | 3.396479 | 2.212725 |
| 21 | 6 | 0 | 1.864306 | 3.701463 | 0.881259 |
| 22 | 8 | 0 | 1.155203 | -1.655069 | 0.237394 |
| 23 | 6 | 0 | 2.283529 | -2.109651 | -0.530072 |
| 24 | 6 | 0 | 3.425614 | -2.290210 | 0.472287 |
| 25 | 6 | 0 | 1.926275 | -3.389567 | -1.286923 |
| 26 | 6 | 0 | 4.769242 | -2.662000 | -0.162092 |
| 27 | 1 | 0 | -5.790789 | 0.897421 | -1.587245 |
| 28 | 1 | 0 | -5.696274 | -0.208957 | 0.619827 |
| 29 | 1 | 0 | -1.589875 | 0.294605 | -2.104451 |
| 30 | 1 | 0 | -3.714316 | 1.120164 | -2.944098 |
| 31 | 1 | 0 | -4.817953 | 0.863287 | -0.856634 |
| 32 | 1 | 0 | -4.710676 | 0.082808 | 0.266763 |
| 33 | 1 | 0 | -3.481224 | -0.530615 | 0.622254 |
| 34 | 1 | 0 | -2.321897 | -0.318617 | -0.197803 |
| 35 | 1 | 0 | -2.479255 | 0.490131 | -1.356673 |
| 36 | 1 | 0 | -3.687662 | 1.061511 | -1.677783 |
| 37 | 1 | 0 | -3.391349 | -1.362530 | 1.766789 |
| 38 | 1 | 0 | -2.209193 | -1.977865 | 2.080674 |
| 39 | 1 | 0 | -1.065243 | -1.773545 | 1.278856 |
| 40 | 1 | 0 | -1.087032 | -0.949840 | 0.173674 |
| 41 | 1 | 0 | 0.182638 | -0.791559 | -0.674082 |
| 42 | 1 | 0 | 0.742813 | 0.630141 | -0.819655 |
| 43 | 1 | 0 | 1.179299 | 1.422812 | 0.293606 |

**1e (conformer 18)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.817953 | 0.863287 | -0.856634 |
| 2 | 6 | 0 | -4.710676 | 0.082808 | 0.266763 |
| 3 | 6 | 0 | -3.481224 | -0.530615 | 0.622254 |
| 4 | 6 | 0 | -2.321897 | -0.318617 | -0.197803 |
| 5 | 6 | 0 | -2.479255 | 0.490131 | -1.356673 |
| 6 | 6 | 0 | -3.687662 | 1.061511 | -1.677783 |
| 7 | 6 | 0 | -3.391349 | -1.362530 | 1.766789 |
| 8 | 6 | 0 | -2.209193 | -1.977865 | 2.080674 |
| 9 | 6 | 0 | -1.065243 | -1.773545 | 1.278856 |
| 10 | 6 | 0 | -1.087032 | -0.949840 | 0.173674 |
| 11 | 6 | 0 | 0.182638 | -0.791559 | -0.674082 |
| 12 | 6 | 0 | 0.742813 | 0.630141 | -0.819655 |
| 13 | 6 | 0 | 1.179299 | 1.422812 | 0.293606 |
|   | 6   | 0  | 0.884617 | 1.139391 | -2.094471 |
|---|-----|----|----------|----------|-----------|
|15 | 6   | 0  | 1.401407 | 2.430574 | -2.338834 |
|16 | 6   | 0  | 1.786869 | 3.219059 | -1.287393 |
|17 | 6   | 0  | 1.693093 | 2.739334 |  0.044714 |
|18 | 6   | 0  | 1.146410 | 0.968619 |  1.639852 |
|19 | 6   | 0  | 1.567890 | 1.770522 |  2.673413 |
|20 | 6   | 0  | 2.051094 | 3.073629 |  2.425060 |
|21 | 6   | 0  | 2.113588 | 3.542288 |  1.137046 |
|22 | 8   | 0  | 1.181397 | -1.666939| -0.146614 |
|23 | 6   | 0  | 2.212681 | -2.074417| -1.063189 |
|24 | 6   | 0  | 3.465766 | -2.370338| -0.230341 |
|25 | 6   | 0  | 1.738650 | -3.255630| -1.912850 |
|26 | 6   | 0  | 3.307209 | -3.469663|  0.824984 |
|27 | 1   | 0  | 5.764481 | 1.323503 | -1.116902 |
|28 | 1   | 0  | 5.573124 | 0.084727 |  0.903751 |
|29 | 1   | 0  | 1.632030 | 0.672532 |  1.999891 |
|30 | 1   | 0  | 3.771936 | 1.673115 | -2.569273 |
|31 | 1   | 0  | 4.275910 | -1.510262|  2.377409 |
|32 | 1   | 0  | 2.140641 | -2.627779|  2.946022 |
|33 | 1   | 0  | 0.143777 | -2.277992|  1.530819 |
|34 | 1   | 0  | 0.079113 | -1.121069| -1.689010 |
|35 | 1   | 0  | 0.578748 | 0.533474 | -2.942166 |
|36 | 1   | 0  | 1.486592 | 2.789583 | -3.358257 |
|37 | 1   | 0  | 2.178132 | 4.216692 | -1.457213 |
|38 | 1   | 0  | 0.793784 | -0.028406|  1.851045 |
|39 | 1   | 0  | 1.530536 | 1.397591 |  3.690945 |
|40 | 1   | 0  | 2.376251 | 3.696490 |  3.250841 |
|41 | 1   | 0  | 2.492114 | 4.538221 |  0.931383 |
|42 | 1   | 0  | 2.450069 | -1.231242| -1.723557 |
|43 | 1   | 0  | 4.274706 | -2.631896| -0.922260 |
|44 | 1   | 0  | 3.761314 | -1.438117|  0.260103 |
|45 | 1   | 0  | 2.524608 | -3.567741| -2.606990 |
|46 | 1   | 0  | 1.470082 | -4.107341| -1.285012 |
|47 | 1   | 0  | 0.860791 | -2.989336| -2.507165 |
|48 | 1   | 0  | 4.228023 | -3.576419|  1.404430 |
|49 | 1   | 0  | 2.500088 | -3.227853|  1.518928 |
|50 | 1   | 0  | 3.088316 | -4.442427|  0.377073 |

|   | 6   | 0  | -5.337696| 0.047094 | -0.029813 |
|1   | 6   | 0  | -4.852640| -1.177520| -0.414853 |
|2   | 6   | 0  | -3.466264| -1.472791| -0.343112 |
|3   | 6   | 0  | -2.554496| -0.471396|  0.127885 |
|4   | 6   | 0  | -3.096306|  0.785308|  0.512790 |
|5   | 6   | 0  | -4.446154|  1.035134|  0.441155 |
|6   | 6   | 0  | -2.972940| -2.748989| -0.718092 |
|7   | 6   | 0  | -1.637397| -3.031591| -0.616286 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|  9 |  6 |  0 | -0.735913 | -2.051151 | -0.144337 |
| 10 |  6 |  0 | -1.155040 | -0.788207 |  0.212353 |
| 11 |  6 |  0 | -0.175344 |  0.248042 |  0.770796 |
| 12 |  6 |  0 |  1.244069 | -0.259535 |  1.023731 |
| 13 |  6 |  0 |  2.202106 | -0.490312 | -0.019352 |
| 14 |  6 |  0 |  1.609362 | -0.501913 |  2.331657 |
| 15 |  6 |  0 |  2.893228 | -0.975864 |  2.677517 |
| 16 |  6 |  0 |  3.826513 | -1.196068 |  1.698441 |
| 17 |  6 |  0 |  3.510224 | -0.961358 |  0.335564 |
| 18 |  6 |  0 |  1.918039 | -0.287212 | -1.398601 |
| 19 |  6 |  0 |  2.867934 | -0.528939 | -2.362262 |
| 20 |  6 |  0 |  4.157024 | -0.984604 | -2.007280 |
| 21 |  6 |  0 |  4.466836 | -1.195145 | -0.687241 |
| 22 |  6 |  0 |  0.229060 |  1.397722 | -0.089046 |
| 23 |  6 |  0 |  0.281192 |  3.610330 | -0.787434 |
| 24 |  6 |  0 |  0.136764 |  3.097118 |  1.680225 |
| 25 |  6 |  0 |  0.679369 |  3.177345 | -2.199538 |
| 26 |  1 |  0 | -6.399565 |  0.258730 | -0.086528 |
| 27 |  1 |  0 | -5.26547 | -1.946767 | -0.777849 |
| 28 |  1 |  0 | -2.427570 |  1.566314 |  0.841148 |
| 29 |  1 |  0 | -4.830118 |  2.003383 |  0.743222 |
| 30 |  1 |  0 | -3.673229 | -3.496376 | -1.076391 |
| 31 |  1 |  0 | -1.259211 | -4.009242 | -0.893040 |
| 32 |  1 |  0 |  0.309901 | -2.312873 | -0.060320 |
| 33 |  1 |  0 | -0.567314 |  0.536806 |  1.755014 |
| 34 |  1 |  0 |  0.886112 | -0.326732 |  3.121915 |
| 35 |  1 |  0 |  3.134838 | -1.155839 |  3.718918 |
| 36 |  1 |  0 |  4.819624 | -1.553103 |  1.950426 |
| 37 |  1 |  0 |  0.938849 |  0.69072 | -1.681920 |
| 38 |  1 |  0 |  2.624995 | -0.367668 | -3.406634 |
| 39 |  1 |  0 |  4.896310 | -1.168753 | -2.778756 |
| 40 |  1 |  0 |  5.452510 | -1.548978 | -0.403054 |
| 41 |  1 |  0 |  1.592389 |  2.297527 |  0.311200 |
| 42 |  1 |  0 | -0.781134 |  3.879539 | -0.769322 |
| 43 |  1 |  0 |  0.838379 |  4.511114 | -0.506654 |
| 44 |  1 |  0 |  0.700234 |  4.010689 |  1.888086 |
| 45 |  1 |  0 | -0.928727 |  3.342078 |  1.720063 |
| 46 |  1 |  0 |  0.363112 |  2.390303 |  2.480508 |
| 47 |  1 |  0 |  0.516960 |  3.991220 | -2.911490 |
| 48 |  1 |  0 |  1.735347 |  2.895862 | -2.246890 |
| 49 |  1 |  0 |  0.086805 |  2.320976 | -2.524360 |

**1e (conformer 32)**

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|  1 |  6 |  0 | -5.270561 | -0.256680 |  0.034824 |
|  2 |  6 |  0 | -4.730736 | -1.453364 | -0.365129 |
|  3 |  6 |  0 | -3.330063 | -1.677910 | -0.319500 |
|   |   |   | 4.000000  | 6.000000  | 0.000000 |
|---|---|---|----------|----------|---------|
|4  | 6 | 0 | -2.462565 | -0.633922 | 0.142164 |
|5  | 6 | 0 | -3.060483 | 0.591470  | 0.543641 |
|6  | 6 | 0 | -4.422380 | 0.773159  | 0.496198 |
|7  | 6 | 0 | -2.778191 | -2.924384 | -0.712428|
|8  | 6 | 0 | -1.427862 | -3.137125 | -0.638041|
|9  | 6 | 0 | -0.569736 | -2.114293 | -0.175224|
|10 | 6 | 0 | -1.047576 | -0.877732 | 0.199699 |
|11 | 6 | 0 | -0.112808 | 0.207049  | 0.742147 |
|12 | 6 | 0 | 1.329358  | -0.236860 | 0.985324 |
|13 | 6 | 0 | 2.293127  | -0.406294 | -0.064921|
|14 | 6 | 0 | 1.709022  | -0.483672 | 2.288053 |
|15 | 6 | 0 | 3.012848  | -0.909044 | 2.622268 |
|16 | 6 | 0 | 3.950705  | -1.074323 | 1.636823 |
|17 | 6 | 0 | 3.620754  | -0.828657 | 0.278983 |
|18 | 6 | 0 | 1.998994  | -0.185888 | -1.440298|
|19 | 6 | 0 | 2.957316  | -0.368228 | -2.408900|
|20 | 6 | 0 | 4.264257  | -0.778478 | -2.064474|
|21 | 6 | 0 | 4.584314  | -1.002749 | -0.749171|
|22 | 6 | 0 | -0.215839 | 1.342216  | 0.199699 |
|23 | 6 | 0 | 2.215839  | 1.342216  | -0.064921|
|24 | 6 | 0 | 0.464278  | 2.545221  | 0.278444 |
|25 | 6 | 0 | 0.515899  | 3.447555  | -0.960598|
|26 | 6 | 0 | -0.198512 | 3.209992  | 1.488409 |
|27 | 6 | 0 | -0.847661 | 3.853329  | -1.530110|
|28 | 6 | 0 | -6.342598 | -0.098938 | -0.002659|
|29 | 6 | 0 | -5.371051 | -2.254099 | -0.720708|
|30 | 6 | 0 | -2.427707 | 1.402815  | 0.869638 |
|31 | 6 | 0 | -4.849574 | 1.719229  | 0.810216 |
|32 | 6 | 0 | -3.445176 | -3.705081 | -1.063151|
|33 | 6 | 0 | -1.004559 | -4.091725 | -0.929562|
|34 | 6 | 0 | 0.489721  | -2.321717 | -0.112991|
|35 | 6 | 0 | -0.508537 | 0.488986  | 1.727527 |
|36 | 6 | 0 | 0.982082  | -0.350406 | 3.083007 |
|37 | 6 | 0 | 3.265802  | -1.095356 | 3.659866 |
|38 | 6 | 0 | 4.958611  | -1.394207 | 1.879853 |
|39 | 6 | 0 | 1.006076  | 0.137893  | -1.715673|
|40 | 6 | 0 | 2.706618  | -0.195870 | -3.449735|
|41 | 6 | 0 | 5.009314  | -0.916664 | -2.840000|
|42 | 6 | 0 | 5.584132  | -1.321387 | -0.472810|
|43 | 6 | 0 | 1.496248  | 2.289362  | 0.548779 |
|44 | 6 | 0 | 1.096073  | 4.340626  | -0.701340|
|45 | 6 | 0 | 1.087408  | 2.918210  | -1.728652|
|46 | 6 | 0 | 0.333436  | 4.132038  | 1.739789 |
|47 | 6 | 0 | -1.241472 | 3.463930  | 1.286798 |
|48 | 6 | 0 | -0.165890 | 2.568331  | 2.371845 |
|49 | 6 | 0 | -0.719979 | 4.431257  | -2.449271|
| Conformer | Z | R | E(x) | E(y) | E(z) | E(RMS) | E(RMSd) |
|-----------|---|---|------|------|------|--------|---------|
| 1e (conformer 36) | 1 | 6 | 0 | -5.365048 | 0.276039 | -0.144003 |
| 2 | 6 | 0 | -4.949018 | -0.997202 | -0.442166 |
| 3 | 6 | 0 | -3.583639 | -1.368035 | -0.329376 |
| 4 | 6 | 0 | -2.619509 | -0.393357 | 0.090847 |
| 5 | 6 | 0 | -3.090580 | 0.914524 | 0.387365 |
| 6 | 6 | 0 | -4.422198 | 1.237989 | 0.278405 |
| 7 | 6 | 0 | -3.162967 | -2.692578 | -0.613924 |
| 8 | 6 | 0 | -1.847625 | -3.045298 | -0.474486 |
| 9 | 6 | 0 | -0.894788 | -2.090113 | -0.054688 |
| 10 | 6 | 0 | -1.241988 | -0.784166 | 0.214153 |
| 11 | 6 | 0 | -0.204130 | 0.226045 | 0.712718 |
| 12 | 6 | 0 | 1.182912 | -0.350086 | 0.995427 |
| 13 | 6 | 0 | 2.122300 | -0.685825 | -0.036613 |
| 14 | 6 | 0 | 1.537374 | -0.546868 | 2.313550 |
| 15 | 6 | 0 | 2.792363 | -1.078293 | 2.681615 |
| 16 | 6 | 0 | 3.706726 | -1.402960 | 1.713779 |
| 17 | 6 | 0 | 3.400711 | -1.216696 | 0.340881 |
| 18 | 6 | 0 | 1.847292 | -0.532187 | -1.424854 |
| 19 | 6 | 0 | 2.778700 | -0.87784 | -2.374991 |
| 20 | 6 | 0 | 4.038803 | -1.392780 | -1.997918 |
| 21 | 6 | 0 | 4.338810 | -1.557181 | -0.669114 |
| 22 | 8 | 0 | -0.178057 | 1.318013 | -0.218798 |
| 23 | 6 | 0 | 0.609475 | 2.468782 | 0.145720 |
| 24 | 6 | 0 | 0.798942 | 3.253009 | -1.155013 |
| 25 | 6 | 0 | -0.058797 | 3.289014 | 1.251205 |
| 26 | 6 | 0 | 1.724801 | 4.467263 | -1.033412 |
| 27 | 1 | 0 | -6.41158 | 0.545574 | -0.231562 |
| 28 | 1 | 0 | -5.662959 | -1.747333 | -0.766571 |
| 29 | 1 | 0 | -2.382403 | 1.674444 | 0.679365 |
| 30 | 1 | 0 | -4.751469 | 2.244414 | 0.512710 |
| 31 | 1 | 0 | -3.902288 | -3.419570 | -0.933672 |
| 32 | 1 | 0 | -1.524708 | -4.059214 | -0.682157 |
| 33 | 1 | 0 | 0.133073 | -2.406183 | 0.059225 |
| 34 | 1 | 0 | -0.575646 | 0.598313 | 1.677351 |
| 35 | 1 | 0 | 0.828911 | -0.287209 | 3.093918 |
| 36 | 1 | 0 | 3.027517 | -1.219143 | 3.730501 |
| 37 | 1 | 0 | 4.677573 | -1.806078 | 1.982466 |
| 38 | 1 | 0 | 0.891017 | -0.130258 | -1.725723 |
| 39 | 1 | 0 | 2.543051 | -0.754208 | -3.426204 |
| 40 | 1 | 0 | 4.763609 | -1.658645 | -2.759236 |
| 41 | 1 | 0 | 5.302153 | -1.955538 | -0.367749 |
| 42 | 1 | 0 | 1.592223 | 2.129457 | 0.498351 |
| 43 | 1 | 0 | 1.201410 | 2.559207 | -1.897965 |
| index | conformer 39 | index | 1e (conformer 39) |
|-------|-------------|-------|------------------|
| 44    | 1           | 6     | 1                |
| 45    | 1           | 6     | 2                |
| 46    | 1           | 6     | 3                |
| 47    | 1           | 6     | 4                |
| 48    | 1           | 6     | 5                |
| 49    | 1           | 6     | 6                |
| 50    | 1           | 6     | 7                |
|       |             | 6     | 8                |
|       |             | 6     | 9                |
|       |             | 6     | 10               |
|       |             | 6     | 11               |
|       |             | 6     | 12               |
|       |             | 6     | 13               |
|       |             | 6     | 14               |
|       |             | 6     | 15               |
|       |             | 6     | 16               |
|       |             | 6     | 17               |
|       |             | 6     | 18               |
|       |             | 6     | 19               |
|       |             | 6     | 20               |
|       |             | 6     | 21               |
|       |             | 8     | 22               |
|       |             | 6     | 23               |
|       |             | 6     | 24               |
|       |             | 6     | 25               |
|       |             | 6     | 26               |
|       |             | 1     | 27               |
|       |             | 1     | 28               |
|       |             | 1     | 29               |
|       |             | 1     | 30               |
|       |             | 1     | 31               |
|       |             | 1     | 32               |
|       |             | 1     | 33               |
|       |             | 1     | 34               |
|       |             | 1     | 35               |
|       |             | 1     | 36               |
|       |             | 1     | 37               |
|       |             | 1     | 38               |

```
44 1 0 -0.187612  3.562155 -1.517912
45 1 0 0.581365  4.122243  1.550888
46 1 0 -1.012586  3.698736  0.906073
47 1 0 -1.012586  3.698736  0.906073
48 1 0 -1.012586  3.698736  0.906073
49 1 0 -1.012586  3.698736  0.906073
50 1 0 -1.012586  3.698736  0.906073
1 6 0 -4.086809 -1.696769 -1.866390
2 6 0 -4.426216 -1.528289 -1.347634
3 6 0 -3.497518 -0.995687  0.894956
4 6 0 -2.186566 -0.621963 -0.062773
5 6 0 -1.871524 -0.812655 -1.437929
6 6 0 -2.795362 -1.336315 -2.310876
7 6 0 -3.844904 -0.837780  1.751628
8 6 0 -2.939207 -0.330701  2.646422
9 6 0 -1.651919  0.047203  2.206705
10 6 0 -1.257603 -0.088294  0.892259
11 6 0  0.159425  0.351305  0.526206
12 6 0  1.162528 -0.786234  0.310214
13 6 0  2.557411 -0.487715  0.132932
14 6 0  0.765206 -2.104777  0.354843
15 6 0  1.683988 -3.167497  0.203719
16 6 0  3.015523 -2.907724  0.132932
17 6 0  3.486861 -1.570104 -0.011383
18 6 0  3.077894  0.834865  0.114470
19 6 0  4.423862  1.072934 -0.032207
20 6 0  5.332814  0.003186 -0.180585
21 6 0  4.868671 -1.288156 -0.172015
22 8 0  0.197428  1.194033 -0.635502
23 6 0  0.540898  2.431284 -0.566835
24 6 0  0.198245  3.487765  0.270005
25 6 0 -0.750582  2.858591 -2.014429
26 6 0 -0.637400  4.740009  0.560262
27 1 0 -4.804711 -2.106893 -2.567863
28 1 0 -4.514058 -1.804912 -0.193913
29 1 0 -0.891619 -0.528937 -1.793134
30 1 0 -2.529554 -1.474427 -3.353056
31 1 0 -4.839802 -1.126244  2.074452
32 1 0 -3.205320 -0.209779  3.690400
33 1 0 -0.951333  0.456351  2.927821
34 1 0  0.526899  0.924970  1.388674
35 1 0 -0.276783 -2.345650  0.514744
36 1 0  1.322217 -4.188979  0.237216
37 1 0  3.729054 -3.717194 -0.093443
38 1 0  2.396814  1.668194  0.191083
```
|     |     |     |        |        |        |        |        |
|-----|-----|-----|--------|--------|--------|--------|--------|
| 39  | 1   | 0   | 4.790822 | 2.093460 | -0.041228 |
| 40  | 1   | 0   | 6.391268 | 0.204633 | -0.301768 |
| 41  | 1   | 0   | 5.555951 | -2.120428 | -0.284419 |
| 42  | 1   | 0   | -1.516728 | 2.236787 | -0.103149 |
| 43  | 1   | 0   | 0.497300 | 3.042414 | 1.224225 |
| 44  | 1   | 0   | 1.120323 | 3.764162 | -0.103149 |
| 45  | 1   | 0   | -1.306961 | 3.796652 | -2.072386 |
| 46  | 1   | 0   | -1.516728 | 2.236787 | -0.103149 |
| 47  | 1   | 0   | -0.894678 | 5.281725 | -0.353178 |
| 48  | 1   | 0   | -0.089593 | 5.430527 | 1.206477 |
| 49  | 1   | 0   | -0.894678 | 5.281725 | -0.353178 |
| 50  | 1   | 0   | -1.571614 | 4.482051 | 1.068738 |

**1e (conformer 43)**

|     |     |     |        |        |        |        |        |
|-----|-----|-----|--------|--------|--------|--------|--------|
| 1   | 6   | 0   | -4.270008 | -0.689963 | -2.050065 |
| 2   | 6   | 0   | -4.559952 | -1.031078 | -0.753243 |
| 3   | 6   | 0   | -3.580293 | -0.922987 | 0.269040 |
| 4   | 6   | 0   | -2.269604 | -0.440571 | -0.060422 |
| 5   | 6   | 0   | -2.007320 | -0.097732 | -1.416991 |
| 6   | 6   | 0   | -2.978761 | -0.223192 | -2.381220 |
| 7   | 6   | 0   | -3.878304 | -1.292459 | 1.605970 |
| 8   | 6   | 0   | -2.923738 | -1.194147 | 2.584619 |
| 9   | 6   | 0   | -1.636539 | -0.710984 | 2.265537 |
| 10  | 6   | 0   | -1.291428 | -0.336186 | 0.983767 |
| 11  | 6   | 0   | 0.133508  | 0.170289  | 0.757664 |
| 12  | 6   | 0   | 1.093773  | -0.859580 | 0.155165 |
| 13  | 6   | 0   | 2.506131  | -0.596927 | 0.162941 |
| 14  | 6   | 0   | 0.641503  | -2.053202 | -0.362316 |
| 15  | 6   | 0   | 1.524201  | -3.010671 | -0.911063 |
| 16  | 6   | 0   | 2.872653  | -2.774674 | -0.930994 |
| 17  | 6   | 0   | 3.398298  | -1.572334 | -0.391559 |
| 18  | 6   | 0   | 3.078850  | 0.581699  | 0.713159 |
| 19  | 6   | 0   | 4.438621  | 0.785025  | 0.716225 |
| 20  | 6   | 0   | 5.310525  | -0.174761 | 0.158151 |
| 21  | 6   | 0   | 4.796146  | -1.326483 | -0.382302 |
| 22  | 8   | 0   | 0.207153  | 1.354994  | -0.047033 |
| 23  | 6   | 0   | -0.003367 | 2.616075  | 0.612634 |
| 24  | 6   | 0   | 0.761274  | 3.668383  | -0.202502 |
| 25  | 6   | 0   | -1.485754 | 2.952329  | 0.795402 |
| 26  | 6   | 0   | 0.294495  | 3.830342  | -1.652671 |
| 27  | 1   | 0   | -0.026802 | -0.779107 | -2.821455 |
| 28  | 1   | 0   | -5.547236 | -1.394615 | -0.487398 |
| 29  | 1   | 0   | -1.029106 | 0.275460  | -1.681078 |
| 30  | 1   | 0   | -2.752355 | 0.044013  | -3.407727 |
| 31  | 1   | 0   | -4.874305 | -1.654700 | 1.838332 |
| 32  | 1   | 0   | -3.151265 | -1.477441 | 3.606090 |
| 33  | 1   | 0   | -0.897435 | -0.629590 | 3.056400 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 34 | 1 | 0 | 0.521696 | 0.421452 | 1.755327 |
| 35 | 1 | 0 | -0.416870 | -2.275052 | -0.352436 |
| 36 | 1 | 0 | 1.121169 | -3.932487 | -1.315034 |
| 37 | 1 | 0 | 3.558080 | -3.503702 | -1.350537 |
| 38 | 1 | 0 | 2.435054 | 1.339600 | 1.134881 |
| 39 | 1 | 0 | 4.845606 | -3.932487 | -1.350537 |
| 40 | 1 | 0 | 6.380546 | -0.000292 | 0.160937 |
| 41 | 1 | 0 | 5.455165 | -2.075177 | -0.809770 |
| 42 | 1 | 0 | 0.463146 | 2.558796 | 1.609028 |
| 43 | 1 | 0 | 0.680648 | 4.625557 | 0.325624 |
| 44 | 1 | 0 | 1.819889 | 3.392135 | -0.196646 |
| 45 | 1 | 0 | -1.589101 | 3.955211 | 1.221223 |
| 46 | 1 | 0 | -2.014560 | 2.248159 | 1.469439 |
| 47 | 1 | 0 | -1.974331 | 2.248159 | 1.469439 |
| 48 | 1 | 0 | 0.918405 | 4.561113 | -2.174052 |
| 49 | 1 | 0 | 0.367104 | 2.882168 | -2.188288 |
| 50 | 1 | 0 | -0.739824 | 4.178004 | -1.714914 |

### 1e (conformer 45)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | -4.358909 | -0.833240 | -2.002874 |
| 2  | 6 | 0 | -4.637383 | -1.017159 | -0.672130 |
| 3  | 6 | 0 | -3.640867 | -0.815831 | 0.319255 |
| 4  | 6 | 0 | -2.323740 | -0.408733 | -0.079358 |
| 5  | 6 | 0 | -2.073962 | -0.227267 | -1.469368 |
| 6  | 6 | 0 | -3.062914 | -0.435980 | -2.400715 |
| 7  | 6 | 0 | -3.928839 | -1.019005 | 1.693462 |
| 8  | 6 | 0 | -2.959040 | -0.830080 | 2.643402 |
| 9  | 6 | 0 | -1.664317 | -0.423945 | 2.255380 |
| 10 | 6 | 0 | -1.327621 | -0.213116 | 0.934516 |
| 11 | 6 | 0 | 0.112796 | 0.202625 | 0.634280 |
| 12 | 6 | 0 | 1.022451 | -0.940309 | 0.172190 |
| 13 | 6 | 0 | 2.445395 | -0.744198 | 0.147028 |
| 14 | 6 | 0 | 0.513718 | -2.169264 | -0.185574 |
| 15 | 6 | 0 | 1.349272 | -3.230137 | -0.601886 |
| 16 | 6 | 0 | 2.707164 | -3.061994 | -0.648349 |
| 17 | 6 | 0 | 3.289662 | -1.824670 | -0.270558 |
| 18 | 6 | 0 | 3.074226 | 0.469626 | 0.535861 |
| 19 | 6 | 0 | 4.441987 | 0.608592 | 0.514890 |
| 20 | 6 | 0 | 5.266653 | -0.456634 | 0.093285 |
| 21 | 6 | 0 | 4.697427 | -1.645111 | -0.289876 |
| 22 | 6 | 0 | 0.227856 | 1.261675 | -0.325757 |
| 23 | 6 | 0 | 0.108474 | 2.612093 | 0.155018 |
| 24 | 6 | 0 | 0.859852 | 3.474328 | -0.865161 |
| 25 | 6 | 0 | -1.346989 | 3.039365 | 0.347180 |
| 26 | 6 | 0 | 1.049187 | 4.935010 | -0.444476 |
| 27 | 6 | 0 | -5.128764 | -0.991818 | -2.749831 |
| 28 | 6 | 0 | -5.628747 | -1.323603 | -0.354510 |
29  1  0  -1.092494  0.093956  -1.785053  
30  1  0  -2.846261  -0.292312  -3.453518  
31  1  0  -4.929933  -1.326072  1.977686  
32  1  0  -3.179606  -0.984433  3.693619  
33  1  0  -0.911028  -0.273393  3.022490  
34  1  0  0.521861  0.569247  1.586431  
35  1  0  -0.553499  -2.339770  -0.148232  
36  1  0  0.902568  -4.177295  -0.882482  
37  1  0  3.56698  -3.870960  -0.966144  
38  1  0  2.468395  1.306192  0.852064  
39  1  0  4.891971  1.546368  0.821691  
40  1  0  6.343622  -0.333243  0.075937  
41  1  0  5.319550  -2.473860  -0.611959  
42  1  0  0.902568  -4.177295  -0.882482  
43  1  0  3.356698  -3.870960  -0.966144  
44  1  0  2.468395  1.306192  0.852064  
45  1  0  4.891971  1.546368  0.821691  
46  1  0  6.343622  -0.333243  0.075937  
47  1  0  5.319550  -2.473860  -0.611959  
48  1  0  0.902568  -4.177295  -0.882482  
49  1  0  3.356698  -3.870960  -0.966144  
50  1  0  2.468395  1.306192  0.852064  

1e (conformer 46)

1  6  0  2.681141  -2.962691  2.098154  
2  6  0  2.885148  -3.162078  0.755963  
3  6  0  2.330464  -2.279832  -0.207633  
4  6  0  1.528621  -1.172760  0.228859  
5  6  0  1.356767  -0.990494  1.627512  
6  6  0  1.914813  -1.860032  2.533932  
7  6  0  2.572649  -2.471416  -1.592704  
8  6  0  2.055329  -1.601161  -2.515207  
9  6  0  1.255527  -0.518775  -2.087638  
10  6  0  0.963198  -0.297368  -0.757434  
11  6  0  0.909098  0.918716  -0.411258  
12  6  0  -1.204026  0.631007  0.360103  
13  6  0  -2.258747  -0.154462  -0.215297  
14  6  0  -1.391890  1.190611  1.606262  
15  6  0  -2.573249  0.976965  2.349285  
16  6  0  -3.581987  0.205952  1.836505  
17  6  0  -3.456724  -0.368413  0.546257  
18  6  0  -2.202446  -0.718427  -1.519403  
19  6  0  -3.245634  -1.452164  -2.032304  
20  6  0  -4.412702  -1.673142  -1.270472  
21  6  0  -4.510342  -1.139528  -0.010102  
22  8  0  0.827447  1.898981  0.319483  
23  6  0  1.818448  2.651223  -0.408810
|   |   |   |    |          |          |          |          |          |          |          |          |          |          |
|---|---|---|----|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 24 | 6 | 0 | 1.529638 | 4.140288 | -0.196348 |          |          |          |          |          |          |          |          |
| 25 | 6 | 0 | 3.214798 | 2.255404 | 0.064811  |          |          |          |          |          |          |          |          |
| 26 | 6 | 0 | 0.177536 | 4.594958 | -0.749109 |          |          |          |          |          |          |          |          |
| 27 | 1 | 0 | 3.111481 | -3.643097 | 2.824417  |          |          |          |          |          |          |          |          |
| 28 | 1 | 0 | 3.482094 | -3.998879 | 0.408272  |          |          |          |          |          |          |          |          |
| 29 | 1 | 0 | 0.788190 | -0.145531 | 1.981745  |          |          |          |          |          |          |          |          |
| 30 | 1 | 0 | 1.767195 | -1.695886 | 3.595572  |          |          |          |          |          |          |          |          |
| 31 | 1 | 0 | 3.181594 | -3.313263 | -1.905239 |          |          |          |          |          |          |          |          |
| 32 | 1 | 0 | 2.250818 | -1.737777 | -3.572804 |          |          |          |          |          |          |          |          |
| 33 | 1 | 0 | 2.177148 | 0.154311 | -2.836978 |          |          |          |          |          |          |          |          |
| 34 | 1 | 0 | 3.482094 | -3.998879 | 0.408272  |          |          |          |          |          |          |          |          |
| 35 | 1 | 0 | 0.788190 | -0.145531 | 1.981745  |          |          |          |          |          |          |          |          |
| 36 | 1 | 0 | 1.720685 | 2.420381 | -1.477867 |          |          |          |          |          |          |          |          |
| 37 | 1 | 0 | 1.582158 | 4.345211 | 0.878990  |          |          |          |          |          |          |          |          |
| 38 | 1 | 0 | 2.337149 | 4.715146 | -0.664135 |          |          |          |          |          |          |          |          |
| 39 | 1 | 0 | 3.978534 | 2.835672 | -0.461378 |          |          |          |          |          |          |          |          |
| 40 | 1 | 0 | 3.16016  | 2.444477 | 1.136835  |          |          |          |          |          |          |          |          |
| 41 | 1 | 0 | 3.402530 | 1.196035 | -0.113860 |          |          |          |          |          |          |          |          |
| 42 | 1 | 0 | 0.09532  | 5.657042 | -0.552460 |          |          |          |          |          |          |          |          |
| 43 | 1 | 0 | 0.121412 | 4.447828 | -1.832685 |          |          |          |          |          |          |          |          |
| **1e (conformer 79)** |   |   |    |          |          |          |          |          |          |          |          |          |          |
| 1  | 6 | 0 | -4.873131 | -0.826177 | 1.250030  |          |          |          |          |          |          |          |          |
| 2  | 6 | 0 | -4.557899 | -1.608266 | 0.167213  |          |          |          |          |          |          |          |          |
| 3  | 6 | 0 | -3.294548 | -1.505936 | -0.471011 |          |          |          |          |          |          |          |          |
| 4  | 6 | 0 | -2.326154 | -0.570058 | 0.024370  |          |          |          |          |          |          |          |          |
| 5  | 6 | 0 | -2.694574 | 0.222324  | 1.145723  |          |          |          |          |          |          |          |          |
| 6  | 6 | 0 | -3.927354 | 0.098630  | 1.741966  |          |          |          |          |          |          |          |          |
| 7  | 6 | 0 | -2.977611 | -2.312633 | -1.593862 |          |          |          |          |          |          |          |          |
| 8  | 6 | 0 | -1.754521 | -2.206396 | -2.201227 |          |          |          |          |          |          |          |          |
| 9  | 6 | 0 | -0.794933 | -1.294333 | -1.710342 |          |          |          |          |          |          |          |          |
| 10 | 6 | 0 | -1.049540 | -0.483902 | -0.626143 |          |          |          |          |          |          |          |          |
| 11 | 6 | 0 | -0.003221 | 0.535924  | -0.166470 |          |          |          |          |          |          |          |          |
| 12 | 6 | 0 | 1.430281 | 0.111332  | -0.479167 |          |          |          |          |          |          |          |          |
| 13 | 6 | 0 | 2.088804 | -0.879558 | 0.319012  |          |          |          |          |          |          |          |          |
| 14 | 6 | 0 | 2.10037  | 0.681075  | -1.538507 |          |          |          |          |          |          |          |          |
| 15 | 6 | 0 | 3.429770 | 0.319818  | -1.851423 |          |          |          |          |          |          |          |          |
| 16 | 6 | 0 | 4.089689 | -0.612418 | -1.093522 |          |          |          |          |          |          |          |          |
| 17 | 6 | 0 | 3.442439 | -1.233293 | 0.006278  |          |          |          |          |          |          |          |          |
| 18 | 6 | 0 | 1.464080 | -1.537620 | 1.413988  |          |          |          |          |          |          |          |          |
|   |   |   |          |          |          |          |
|---|---|---|----------|----------|----------|----------|
| 19| 6 | 0 | 2.137455 | -2.474327| 2.161602 |
| 20| 6 | 0 | 3.474444 | -2.810792| 1.856171 |
| 21| 6 | 0 | 4.107807 | -2.202954| 0.800737 |
| 22| 6 | 0 | -0.337270| 1.786311 | -0.780836|
| 23| 6 | 0 | -0.330042| 2.957410 | 0.053374 |
| 24| 6 | 0 | 1.091145 | 3.427866 | 0.396483 |
| 25| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 26| 6 | 0 | -0.337270| 1.786311 | -0.780836|
| 27| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 28| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 29| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 30| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 31| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 32| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 33| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 34| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 35| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 36| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 37| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 38| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 39| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 40| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 41| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 42| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 43| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 44| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 45| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 46| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 47| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 48| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 49| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| 50| 6 | 0 | -1.150425| 3.994789 | -0.703484|
| **1e** (conformer 81) | | | | | | |
| 1 | 6 | 0 | 4.178383 | -2.026185| -1.853945|
| 2 | 6 | 0 | 4.635507 | -1.285170| -0.792754|
| 3 | 6 | 0 | 3.751585 | -0.486584| -0.021091|
| 4 | 6 | 0 | 2.359722 | -0.448846| -0.364070|
| 5 | 6 | 0 | 1.922969 | -1.240030| -1.462397|
| 6 | 6 | 0 | 2.806236 | -2.003919| -2.187388|
| 7 | 6 | 0 | 4.218297 | 0.269964 | 1.084808|
| 8 | 6 | 0 | 3.349176 | 1.034045 | 1.820123|
| 9 | 6 | 0 | 1.980158 | 1.085973 | 1.475989|
| 10| 6 | 0 | 1.478936 | 0.374531 | 0.408944|
| 11| 6 | 0 | -0.007038 | 0.466037 | 0.067773|
| 12| 6 | 0 | -0.824913 | -0.717330| 0.594596|
| 13| 6 | 0 | -2.096248 | -1.037196| 0.009426|
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 14 | 6 | 0 | -0.373116 | -1.463831 | 1.660026 |
| 15 | 6 | 0 | -1.125297 | -2.534091 | 2.193148 |
| 16 | 6 | 0 | -2.337438 | -2.863350 | 1.647518 |
| 17 | 6 | 0 | -2.852272 | -2.131006 | 0.546921 |
| 18 | 6 | 0 | -2.657249 | -0.325299 | -1.085142 |
| 19 | 6 | 0 | -3.875446 | -0.671853 | -1.620361 |
| 20 | 6 | 0 | -4.611840 | -1.752152 | -1.088502 |
| 21 | 6 | 0 | -4.106682 | -2.462231 | -0.028150 |
| 22 | 8 | 0 | -0.607992 | 1.657245 | 0.589575 |
| 23 | 6 | 0 | -0.736988 | 2.775258 | 0.305431 |
| 24 | 6 | 0 | -1.779582 | 3.689905 | 0.342930 |
| 25 | 6 | 0 | 0.595293 | 3.470742 | -0.586711 |
| 26 | 6 | 0 | -2.235146 | 4.855651 | -0.538124 |
| 27 | 1 | 0 | 4.864742 | -2.632611 | -2.434099 |
| 28 | 1 | 0 | 5.686823 | -1.300972 | -0.524218 |
| 29 | 1 | 0 | 0.873816 | -1.259255 | -1.728218 |
| 30 | 1 | 0 | 2.446405 | -2.599138 | -3.019183 |
| 31 | 1 | 0 | 5.272734 | 0.230947 | 1.337530 |
| 32 | 1 | 0 | 3.707295 | 1.608547 | 2.667243 |
| 33 | 1 | 0 | 1.301334 | 1.705213 | 2.047941 |
| 34 | 1 | 0 | -0.094351 | 0.489584 | -1.024850 |
| 35 | 1 | 0 | 0.586211 | -1.229373 | 2.103106 |
| 36 | 1 | 0 | -0.731569 | -3.092898 | 3.034633 |
| 37 | 1 | 0 | -2.921127 | -3.686253 | 2.046752 |
| 38 | 1 | 0 | -2.121516 | 0.512716 | -1.508671 |
| 39 | 1 | 0 | -4.275871 | -0.109011 | -2.456274 |
| 40 | 1 | 0 | -5.571827 | -2.015806 | -1.517702 |
| 41 | 1 | 0 | -4.663443 | -3.294069 | 0.390976 |
| 42 | 1 | 0 | -1.144058 | 2.407153 | -1.260807 |
| 43 | 1 | 0 | -2.637669 | 3.064795 | 0.605063 |
| 44 | 1 | 0 | -1.369008 | 4.066271 | 1.286465 |
| 45 | 1 | 0 | 1.022689 | 3.873037 | 0.335562 |
| 46 | 1 | 0 | 1.321797 | 2.784447 | -1.025250 |
| 47 | 1 | 0 | 0.451931 | 4.295294 | -1.290084 |
| 48 | 1 | 0 | -3.030606 | 5.420577 | -0.044782 |
| 49 | 1 | 0 | -1.423047 | 5.556514 | -0.750439 |
| 50 | 1 | 0 | -2.629780 | 4.502734 | -1.496109 |

| 3b (conformer 2) |
|---|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.630835 | -1.166069 | 0.211799 |
| 2 | 6 | 0 | 1.276784 | -0.697867 | -0.315553 |
| 3 | 6 | 0 | 0.789178 | 0.594112 | 0.357054 |
| 4 | 8 | 0 | 0.339763 | -1.759013 | -0.115458 |
| 5 | 6 | 0 | 2.715412 | -2.304853 | 0.982925 |
| 6 | 6 | 0 | 3.953620 | -2.763868 | 1.487574 |
| 7 | 6 | 0 | 5.110623 | -2.083390 | 1.210329 |
| 8 | 6 | 0 | 5.078703 | -0.911204 | 0.410990 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 9 | 6 | 0 | 3.825330 | -0.436452 | -0.098972 |
| 10 | 6 | 0 | 0.822689 | 0.658636 | 1.734990 |
| 11 | 6 | 0 | 0.361343 | 1.788542 | 2.440124 |
| 12 | 6 | 0 | -0.132244 | 2.871419 | 1.756126 |
| 13 | 6 | 0 | -0.194668 | 2.860018 | 0.340699 |
| 14 | 6 | 0 | 0.263753 | 0.658636 | -0.098972 |
| 15 | 6 | 0 | 6.269104 | 0.740342 | 0.340699 |
| 16 | 6 | 0 | 6.241334 | 1.193478 | 1.798770 |
| 17 | 6 | 0 | 5.010094 | 1.741367 | 2.463300 |
| 18 | 6 | 0 | 3.837988 | 1.704997 | 1.756126 |
| 19 | 6 | 0 | 3.837988 | 1.704997 | -0.381819 |
| 20 | 6 | 0 | 6.241334 | 1.193478 | 1.798770 |
| 21 | 6 | 0 | 0.167568 | 0.658636 | -0.098972 |
| 22 | 6 | 0 | 1.382830 | -0.537112 | -1.394022 |
| 23 | 6 | 0 | 1.812186 | -0.537112 | -1.394022 |
| 24 | 6 | 0 | 3.978782 | -0.537112 | -1.394022 |
| 25 | 6 | 0 | 6.064810 | -2.860893 | 1.193478 |
| 26 | 6 | 0 | 3.978782 | -0.537112 | -1.394022 |
| 27 | 6 | 0 | 6.064810 | -2.860893 | 1.193478 |
| 28 | 6 | 0 | 5.010094 | 1.741367 | 2.463300 |
| 29 | 6 | 0 | 3.837988 | 1.704997 | 1.756126 |
| 30 | 6 | 0 | 3.837988 | 1.704997 | -0.381819 |
| 31 | 6 | 0 | 6.241334 | 1.193478 | 1.798770 |
| 32 | 6 | 0 | 0.167568 | 0.658636 | -0.098972 |
| 33 | 1 | 0 | 1.382830 | -0.537112 | -1.394022 |
| 34 | 1 | 0 | 1.812186 | -0.537112 | -1.394022 |
| 35 | 1 | 0 | 3.978782 | -0.537112 | -1.394022 |
| 36 | 1 | 0 | 6.064810 | -2.860893 | 1.193478 |
| 37 | 1 | 0 | 3.978782 | -0.537112 | -1.394022 |
| 38 | 1 | 0 | 6.064810 | -2.860893 | 1.193478 |
| 39 | 1 | 0 | 0.167568 | 0.658636 | -0.098972 |
| 40 | 1 | 0 | 1.382830 | -0.537112 | -1.394022 |
| 41 | 1 | 0 | 1.812186 | -0.537112 | -1.394022 |
| 42 | 1 | 0 | 3.978782 | -0.537112 | -1.394022 |
| 43 | 1 | 0 | 6.064810 | -2.860893 | 1.193478 |
| 44 | 1 | 0 | 3.978782 | -0.537112 | -1.394022 |
| 45 | 1 | 0 | 6.064810 | -2.860893 | 1.193478 |
| 46 | 1 | 0 | 0.167568 | 0.658636 | -0.098972 |
| 47 | 1 | 0 | 1.382830 | -0.537112 | -1.394022 |
| 48 | 1 | 0 | 1.812186 | -0.537112 | -1.394022 |
| 49 | 1 | 0 | 3.978782 | -0.537112 | -1.394022 |
| 50 | 1 | 0 | 6.064810 | -2.860893 | 1.193478 |
| 51 | 1 | 0 | 0.167568 | 0.658636 | -0.098972 |
| 52 | 1 | 0 | 1.382830 | -0.537112 | -1.394022 |
| 53 | 1 | 0 | 1.812186 | -0.537112 | -1.394022 |
|   |   |   | 54 | 1 | 0 | -3.077563 | -5.144955 | -1.314791 |
|---|---|---|---|---|---|-----------|-----------|-----------|
|   |   |   | 55 | 1 | 0 | -3.996522 | -4.410445 | -0.002402 |
|   |   |   | 56 | 1 | 0 | -3.516387 | -0.852152 | -1.535201 |
|   |   |   | 57 | 1 | 0 | -4.862310 | -1.927961 | -1.816049 |
|   |   |   | 58 | 1 | 0 | -4.958374 | -2.418059 | 0.661999 |
|   |   |   | 59 | 1 | 0 | -3.657140 | -1.276784 | 0.926745 |
|   |   |   | 60 | 1 | 0 | -6.423244 | -0.602420 | -0.270636 |
|   |   |   | 61 | 1 | 0 | -3.905337 | 2.185542 | 1.413914 |
|   |   |   | 62 | 1 | 0 | -4.643475 | 1.440967 | 2.823988 |
|   |   |   | 63 | 1 | 0 | -3.489129 | 0.526268 | 1.847630 |
|   |   |   | 64 | 1 | 0 | -7.009408 | 1.987861 | 1.852381 |
|   |   |   | 65 | 1 | 0 | -6.265062 | 2.716614 | 0.436443 |
|   |   |   | 66 | 1 | 0 | -7.419060 | 1.386250 | 0.236540 |
|   | 3b (conformer 3) |   | 1 | 6 | 0 | -0.838823 | 1.055517 | 0.500864 |
|   |   |   | 2 | 6 | 0 | -1.177239 | -0.277902 | -0.161172 |
|   |   |   | 3 | 6 | 0 | -2.504347 | -0.882630 | 0.295785 |
|   |   |   | 4 | 8 | 0 | -0.076267 | -1.160655 | 0.079203 |
|   |   |   | 5 | 6 | 0 | -1.380723 | 1.394545 | 0.720750 |
|   |   |   | 6 | 6 | 0 | -1.062154 | 2.612191 | 2.362860 |
|   |   |   | 7 | 6 | 0 | -0.202748 | 3.500286 | 1.769893 |
|   |   |   | 8 | 6 | 0 | 0.381455 | 3.204171 | 0.510959 |
|   |   |   | 9 | 6 | 0 | 0.072468 | 1.962439 | -0.136225 |
|   |   |   | 10 | 6 | 0 | -2.510762 | -1.893936 | 1.231054 |
|   |   |   | 11 | 6 | 0 | -3.716404 | -2.484750 | 1.672909 |
|   |   |   | 12 | 6 | 0 | -4.919285 | -2.059025 | 1.169955 |
|   |   |   | 13 | 6 | 0 | -4.967888 | -1.017885 | 0.206480 |
|   |   |   | 14 | 6 | 0 | -3.747415 | -0.410582 | -0.238243 |
|   |   |   | 15 | 6 | 0 | 1.268997 | 4.117252 | -0.117211 |
|   |   |   | 16 | 6 | 0 | 1.837157 | 3.831774 | -1.334378 |
|   |   |   | 17 | 6 | 0 | 1.542557 | 2.607332 | -1.974184 |
|   |   |   | 18 | 6 | 0 | 0.689750 | 1.699943 | -1.389736 |
|   |   |   | 19 | 6 | 0 | -6.204259 | -0.562496 | -0.322452 |
|   |   |   | 20 | 6 | 0 | -6.249509 | 0.452449 | -1.246645 |
|   |   |   | 21 | 6 | 0 | -5.051088 | 1.062155 | -1.679930 |
|   |   |   | 22 | 6 | 0 | -3.836379 | 0.644321 | -1.188443 |
|   |   |   | 23 | 6 | 0 | 0.060875 | -2.202083 | -0.890103 |
|   |   |   | 24 | 6 | 0 | 1.123123 | -3.187882 | -0.420420 |
|   |   |   | 25 | 6 | 0 | 2.538462 | -2.621356 | -0.185533 |
|   |   |   | 26 | 6 | 0 | 3.402807 | -3.685243 | 0.507284 |
|   |   |   | 27 | 6 | 0 | 3.178771 | -2.125995 | -1.495964 |
|   |   |   | 28 | 6 | 0 | 4.554859 | -1.440108 | -1.351944 |
|   |   |   | 29 | 6 | 0 | 4.514308 | -0.201493 | -0.497393 |
|   |   |   | 30 | 6 | 0 | 5.323736 | 0.150304 | 0.510357 |
|   |   |   | 31 | 6 | 0 | 6.491694 | -0.664984 | 1.006781 |
|   |   |   | 32 | 6 | 0 | 5.114897 | 1.450519 | 1.248863 |
|   |   |   |  |   |   |   |
|---|---|---|---|---|---|---|
| 33| 1 | 0 | -1.248572| -0.115153| -1.243874 |
| 34| 1 | 0 | -2.073729| 0.715781 | 2.201760 |
| 35| 1 | 0 | -1.508650| 2.839504 | 3.324344 |
| 36| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 37| 1 | 0 | -1.564465| 2.839504 | 3.324344 |
| 38| 1 | 0 | -2.073729| 0.715781 | 2.201760 |
| 39| 1 | 0 | -1.508650| 2.839504 | 3.324344 |
| 40| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 41| 1 | 0 | 2.512159 | 4.538399 | -1.803839 |
| 42| 1 | 0 | 1.997646 | 2.379319 | -2.931720 |
| 43| 1 | 0 | -2.073729| 0.715781 | 2.201760 |
| 44| 1 | 0 | 2.512159 | 4.538399 | -1.803839 |
| 45| 1 | 0 | 1.997646 | 2.379319 | -2.931720 |
| 46| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 47| 1 | 0 | -2.936845| 1.143991 | -1.524656 |
| 48| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 49| 1 | 0 | -2.936845| 1.143991 | -1.524656 |
| 50| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 51| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 52| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 53| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 54| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 55| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 56| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 57| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 58| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 59| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 60| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 61| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 62| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 63| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 64| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 65| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| 66| 1 | 0 | 0.041427 | 4.441412 | 2.251633 |
| **3b (conformer 4)** | | | | | | |
| 1 | 6 | 0 | 0.872417 | 0.717097 | -0.090186 |
| 2 | 6 | 0 | 1.371403 | -0.457785 | 0.763604 |
| 3 | 6 | 0 | 2.400593 | -1.324677 | 0.042707 |
| 4 | 8 | 0 | 0.282098 | -1.300094 | 1.147660 |
| 5 | 6 | 0 | 0.460075 | 0.451582 | -1.379869 |
| 6 | 6 | 0 | -0.056114 | 1.458771 | -2.220024 |
| 7 | 6 | 0 | -0.152851 | 2.750248 | -1.765282 |
| 8 | 6 | 0 | 0.253849 | 3.081572 | -0.449077 |
| 9 | 6 | 0 | 0.770584 | 2.055356 | 0.414740 |
| 10| 6 | 0 | 2.070945 | -2.602380 | -0.353887 |
| 11| 6 | 0 | 3.001566 | -3.431706 | -1.020642 |

5230
|    |   |   |         |         |         |         |         |
|----|---|---|--------|--------|--------|--------|--------|
| 12 | 6 | 0  | 4.269342 | -2.981000 | -1.281431 |       |        |
| 13 | 6 | 0  | 4.662218 | -1.676611 | -0.883435 |       |        |
| 14 | 6 | 0  | 3.720960 | -0.827689 | 0.212821  |       |        |
| 15 | 6 | 0  | 0.152926 | 4.415112  | 0.030002  |       |        |
| 16 | 6 | 0  | 0.539062 | 4.744576  | 1.304943  |       |        |
| 17 | 6 | 0  | 1.045128 | 3.742137  | 2.162273  |       |        |
| 18 | 6 | 0  | 1.156484 | -1.676611 | 0.883435  |       |        |
| 19 | 6 | 0  | 5.975164 | -1.198886 | 1.134694  |       |        |
| 20 | 6 | 0  | 6.359338 | 0.061194  | 0.746234  |       |        |
| 21 | 6 | 0  | 5.436871 | 0.902053  | 0.085758  |       |        |
| 22 | 6 | 0  | 4.156221 | 0.470492  | 0.171366  |       |        |
| 23 | 6 | 0  | 0.152926 | 4.415112  | 0.030002  |       |        |
| 24 | 6 | 0  | 0.539062 | 4.744576  | 1.304943  |       |        |
| 25 | 6 | 0  | 1.045128 | 3.742137  | 2.162273  |       |        |
| 26 | 6 | 0  | 1.156484 | -1.676611 | 0.883435  |       |        |
| 27 | 6 | 0  | 5.975164 | -1.198886 | 1.134694  |       |        |
| 28 | 6 | 0  | 6.359338 | 0.061194  | 0.746234  |       |        |
| 29 | 6 | 0  | 5.436871 | 0.902053  | 0.085758  |       |        |
| 30 | 6 | 0  | 4.156221 | 0.470492  | 0.171366  |       |        |
| 31 | 6 | 0  | 0.152926 | 4.415112  | 0.030002  |       |        |
| 32 | 6 | 0  | 0.539062 | 4.744576  | 1.304943  |       |        |
| 33 | 1 | 0  | 1.845667 | -0.077688 | 1.674998  |       |        |
| 34 | 1 | 0  | 0.542826 | -0.560144 | 1.759626  |       |        |
| 35 | 1 | 0  | 0.366590 | 1.207269  | 0.322792  |       |        |
| 36 | 1 | 0  | 0.540544 | 3.535391  | 2.406036  |       |        |
| 37 | 1 | 0  | 1.080575 | -2.977483 | -0.135691 |       |        |
| 38 | 1 | 0  | 2.703170 | -4.430666 | -1.319100 |       |        |
| 39 | 1 | 0  | 4.990110 | -3.613362 | -1.789293 |       |        |
| 40 | 1 | 0  | 0.239251 | 5.174959  | 0.638200  |       |        |
| 41 | 1 | 0  | 0.456791 | 5.766645  | 1.565743  |       |        |
| 42 | 1 | 0  | 1.347904 | 4.000713  | 3.170894  |       |        |
| 43 | 1 | 0  | 1.545371 | 1.703181  | 2.419513  |       |        |
| 44 | 1 | 0  | 6.675258 | -1.854011 | -1.643024 |       |        |
| 45 | 1 | 0  | 7.365403 | 0.412995  | -0.945197 |       |        |
| 46 | 1 | 0  | 5.739399 | 1.898052  | 0.218037  |       |        |
| 47 | 1 | 0  | 3.471075 | 1.145265  | 0.666215  |       |        |
| 48 | 1 | 0  | -0.041993| -0.503224 | 3.031217  |       |        |
| 49 | 1 | 0  | -1.039111| 0.190317  | 1.743310  |       |        |
| 50 | 1 | 0  | -1.188480| -2.665553 | 2.831330  |       |        |
| 51 | 1 | 0  | -2.298619| -1.369288 | 3.251765  |       |        |
| 52 | 1 | 0  | -1.941455| -2.456938 | 0.423289  |       |        |
| 53 | 1 | 0  | -2.770082| -4.236445 | 1.965051  |       |        |
| 54 | 1 | 0  | -4.092028| -3.184476 | 2.486389  |       |        |
| 55 | 1 | 0  | -4.031245| -3.777404 | 0.822458  |       |        |
| 56 | 1 | 0  | -4.205289| -0.768137 | 1.590991  |       |        |
|      |      |      | Pe          | C              | H              | Ge          | C              |
|------|------|------|-------------|----------------|----------------|-------------|----------------|
|      |      |      | 57          | 1              | 0              | -2.873409   | -0.117999    | 0.655188      |
|      |      |      | 58          | 1              | 0              | -4.955748   | -2.097521    | -0.389282     |
|      |      |      | 59          | 1              | 0              | -3.534056   | -1.588978    | -1.278519     |
|      |      |      | 60          | 1              | 0              | -4.305050   | 0.802845     | -1.224142     |
|      |      |      | 61          | 1              | 0              | -6.960630   | -1.818806    | -0.575049     |
|      |      |      | 62          | 1              | 0              | -8.091272   | -0.499930    | -0.247948     |
|      |      |      | 63          | 1              | 0              | -7.891645   | -1.091881    | -1.889528     |
|      |      |      | 64          | 1              | 0              | -5.989814   | 2.200364     | -1.864947     |
|      |      |      | 65          | 1              | 0              | -7.340285   | 1.361506     | -2.648653     |
|      |      |      | 66          | 1              | 0              | -7.506382   | 1.921963     | -0.990940     |
| 3b (conformer 5) | | | 1   | 6   | 0  | -1.530135 | 1.413873   | 0.402775     |
|      |      |      | 2   | 6   | 0  | -1.113800 | -0.051774  | 0.306535     |
|      |      |      | 3   | 6   | 0  | -2.259808 | -1.044076  | 0.497522     |
|      |      |      | 4   | 8   | 0  | -0.063914 | -0.253202  | 1.258663     |
|      |      |      | 5   | 6   | 0  | -2.697198 | 1.779157   | 1.036399     |
|      |      |      | 6   | 6   | 0  | -3.086434 | 3.132640   | 1.153320     |
|      |      |      | 7   | 6   | 0  | -2.303805 | 4.123834   | 0.620775     |
|      |      |      | 8   | 6   | 0  | -1.093236 | 3.803972   | -0.047432    |
|      |      |      | 9   | 6   | 0  | -0.688508 | 2.433029   | -0.155988    |
|      |      |      |10  | 6   | 0  | -2.444836 | -1.648914  | 1.721507     |
|      |      |      |11  | 6   | 0  | -3.481950 | -2.584950  | 1.934564     |
|      |      |      |12  | 6   | 0  | -4.333808 | -2.916520  | 0.911906     |
|      |      |      |13  | 6   | 0  | -4.190712 | -2.316872  | -0.366433    |
|      |      |      |14  | 6   | 0  | -3.145516 | -1.359194  | -0.583625    |
|      |      |      |15  | 6   | 0  | -0.274740 | 4.819778   | -0.607572    |
|      |      |      |16  | 6   | 0  | 0.899043  | 4.511028   | -1.250164    |
|      |      |      |17  | 6   | 0  | 1.306648  | 3.162740   | -1.355130    |
|      |      |      |18  | 6   | 0  | 0.536936  | 2.155926   | -0.820670    |
|      |      |      |19  | 6   | 0  | -5.067711 | -2.643119  | -1.434304    |
|      |      |      |20  | 6   | 0  | -4.935754 | -2.051187  | -2.666520    |
|      |      |      |21  | 6   | 0  | -3.916173 | -1.097382  | -2.882453    |
|      |      |      |22  | 6   | 0  | -3.048716 | -0.759559  | -1.870140    |
|      |      |      |23  | 6   | 0  | 0.783240  | -1.369514  | 0.978385     |
|      |      |      |24  | 6   | 0  | 1.806470  | -1.502404  | 2.098191     |
|      |      |      |25  | 6   | 0  | 2.778140  | -0.317044  | 2.265196     |
|      |      |      |26  | 6   | 0  | 3.576978  | -0.469241  | 3.568922     |
|      |      |      |27  | 6   | 0  | 3.696786  | -0.083155  | 1.044366     |
|      |      |      |28  | 6   | 0  | 4.642812  | -1.239927  | 0.660514     |
|      |      |      |29  | 6   | 0  | 5.572754  | -0.856254  | -0.458743    |
|      |      |      |30  | 6   | 0  | 5.670326  | -1.379779  | -1.688127    |
|      |      |      |31  | 6   | 0  | 4.835730  | -2.522676  | -2.210010    |
|      |      |      |32  | 6   | 0  | 6.672413  | -0.840615  | -2.680719    |
|      |      |      |33  | 1   | 0  | -0.695949 | -0.224167  | -0.693820    |
|      |      |      |34  | 1   | 0  | -3.339130 | 1.013293   | 1.453119     |
|      |      |      |35  | 1   | 0  | -4.011281 | 3.378028   | 1.663161     |

5232
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 36| 1 | 0 | -2.598122 | 5.165209 | 0.700782 |
| 37| 1 | 0 | -1.771010 | -1.398960 | 2.532010 |
| 38| 1 | 0 | -3.595935 | -3.041048 | -2.911741 |
| 39| 1 | 0 | -5.129063 | -3.638492 | 1.065570 |
| 40| 1 | 0 | -0.596269 | 5.852306 | -0.517123 |
| 41| 1 | 0 | 1.514842  | 5.296449  | -1.673667 |
| 42| 1 | 0 | 2.237524  | 2.920453  | -1.855690 |
| 43| 1 | 0 | 0.883827  | 1.134435  | -0.898986 |
| 44| 1 | 0 | -5.852132 | -3.371719 | 1.256703 |
| 45| 1 | 0 | -5.613599 | -2.308664 | 3.472540 |
| 46| 1 | 0 | -3.821124 | -0.623670 | 3.853148 |
| 47| 1 | 0 | 0.883827  | 1.134435  | -0.898986 |
| 48| 1 | 0 | -5.852132 | -3.371719 | -1.256703 |
| 49| 1 | 0 | -5.613599 | -2.308664 | 3.472540 |
| 50| 1 | 0 | -3.821124 | -0.623670 | 3.853148 |
| 51| 1 | 0 | 2.237524  | 2.920453  | -1.855690 |
| 52| 1 | 0 | 0.187675  | -2.288609 | 0.910658 |
| 53| 1 | 0 | 1.270843  | -1.222652 | 0.003052 |
| 54| 1 | 0 | 1.257725  | -1.639811 | 3.036681 |
| 55| 1 | 0 | 2.366488  | -2.431031 | 1.935677 |
| 56| 1 | 0 | 2.163449  | 0.584474  | 2.361406 |
| 57| 1 | 0 | 4.158942  | -1.396147 | 3.587424 |
| 58| 1 | 0 | 4.273030  | 0.363935  | 3.706021 |
| 59| 1 | 0 | 3.086746  | 0.169346  | 0.170902 |
| 60| 1 | 0 | 4.300130  | 0.810507  | 1.244913 |
| 61| 1 | 0 | 4.064039  | -2.128099 | 0.397575 |
| 62| 1 | 0 | 5.246451  | -1.516518 | 1.533974 |
| 63| 1 | 0 | 6.240771  | -0.028215 | -0.220789 |
| 64| 1 | 0 | 5.475448  | -3.366132 | -2.495994 |
| 65| 1 | 0 | 4.103789  | -2.888589 | -1.490330 |
| 66| 1 | 0 | 4.296951  | -2.221704 | -3.116281 |

|   | 3b (conformer 7) |
|---|----------------|
| 1 | 6 | 0 | -0.583634 | 1.549110 | -0.125938 |
| 2 | 6 | 0 | -0.654221 | 0.079518 | -0.530098 |
| 3 | 6 | 0 | -1.501228 | -0.763362 | 0.435265 |
| 4 | 8 | 0 | 0.683235  | -0.420335 | -0.603368 |
| 5 | 6 | 0 | 0.587521  | 2.072151  | 0.377618 |
| 6 | 6 | 0 | 0.682782  | 3.428836  | 0.763452 |
| 7 | 6 | 0 | -0.395522 | 4.264978  | 0.633227 |
| 8 | 6 | 0 | -1.620859 | 3.777713  | 0.108982 |
| 9 | 6 | 0 | -1.727735 | 2.400360  | -0.275246 |
| 10| 6 | 0 | -1.252285 | -0.645950 | 1.787377 |
| 11| 6 | 0 | -1.949034 | -1.412006 | 2.743517 |
| 12| 6 | 0 | -2.914514 | -2.300608 | 2.340891 |
| 13| 6 | 0 | -3.212038 | -2.464418 | 0.965282 |
| 14| 6 | 0 | -2.495690 | -1.693651 | -0.013946 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 15 | 6 | 0 | -2.743819 | 4.632720 | -0.043956 |
| 16 | 6 | 0 | -3.929951 | 4.163613 | -0.553105 |
| 17 | 6 | 0 | -4.042250 | 2.807572 | -0.930931 |
| 18 | 6 | 0 | -2.973637 | 1.952159 | -0.794209 |
| 19 | 6 | 0 | -4.206648 | -3.385380 | 0.540513 |
| 20 | 6 | 0 | -4.497594 | -3.555472 | -0.789783 |
| 21 | 6 | 0 | -3.796037 | -2.805073 | -1.759748 |
| 22 | 6 | 0 | -2.827223 | -1.905120 | -1.383198 |
| 23 | 6 | 0 | -4.042250 | 2.807572 | -0.930931 |
| 24 | 6 | 0 | 2.973637 | -1.952159 | -0.794209 |
| 25 | 6 | 0 | 4.206648 | -3.385380 | 0.540513 |
| 26 | 6 | 0 | 4.497594 | -3.555472 | -0.789783 |
| 27 | 6 | 0 | 3.796037 | -2.805073 | -1.759748 |
| 28 | 6 | 0 | 2.827223 | -1.905120 | -1.383198 |
| 29 | 6 | 0 | 4.042250 | 2.807572 | -0.930931 |
| 30 | 6 | 0 | 2.973637 | -1.952159 | -0.794209 |
| 31 | 6 | 0 | 4.206648 | -3.385380 | 0.540513 |
| 32 | 6 | 0 | 4.497594 | -3.555472 | -0.789783 |
| 33 | 1 | 0 | -1.086603 | 0.036443 | -1.535538 |
| 34 | 1 | 0 | 1.451929 | 1.428168 | 0.466026 |
| 35 | 1 | 0 | 1.619826 | 3.803324 | 1.160787 |
| 36 | 1 | 0 | -0.327806 | 5.308070 | 0.924235 |
| 37 | 1 | 0 | -0.503443 | 0.061360 | 2.124092 |
| 38 | 1 | 0 | -1.722907 | -1.287104 | 3.796497 |
| 39 | 1 | 0 | -3.463452 | -2.889416 | 3.068365 |
| 40 | 1 | 0 | -2.646192 | 5.672463 | 0.251273 |
| 41 | 1 | 0 | -4.779485 | 4.828049 | -0.664105 |
| 42 | 1 | 0 | -4.980215 | 2.436327 | -1.328726 |
| 43 | 1 | 0 | -3.098724 | 0.916720 | -1.080550 |
| 44 | 1 | 0 | -4.736595 | -3.957070 | 1.295482 |
| 45 | 1 | 0 | -5.259895 | -4.261440 | -1.099116 |
| 46 | 1 | 0 | -4.022878 | -2.941232 | -2.811349 |
| 47 | 1 | 0 | -2.308027 | -1.354306 | -2.156226 |
| 48 | 1 | 0 | 0.421411 | -1.579938 | -2.298024 |
| 49 | 1 | 0 | 0.247569 | -2.446141 | -0.763580 |
| 50 | 1 | 0 | 2.389680 | -2.952605 | -1.934552 |
| 51 | 1 | 0 | 2.811229 | -1.245897 | -1.914536 |
| 52 | 1 | 0 | 2.887764 | -1.308778 | 0.589387 |
| 53 | 1 | 0 | 2.458319 | -4.329667 | 0.266997 |
| 54 | 1 | 0 | 2.901553 | -3.511945 | 1.769471 |
| 55 | 1 | 0 | 1.330039 | -3.205224 | 1.036465 |
| 56 | 1 | 0 | 4.941097 | -2.800696 | 0.778938 |
| 57 | 1 | 0 | 4.653579 | -3.328972 | -0.866335 |
| 58 | 1 | 0 | 6.366745 | -1.651818 | -0.883143 |
| 59 | 1 | 0 | 4.971725 | -0.948565 | -1.663284 |
|    |   |   |          |          |          |
|----|---|---|----------|----------|----------|
| 60 | 1 | 0 | 5.725474 | -0.448333 | 1.292041 |
| 61 | 1 | 0 | 4.661823 | 1.037909  | -2.025971|
| 62 | 1 | 0 | 3.804832 | 2.286769  | -1.116308|
| 63 | 1 | 0 | 5.493609 | 2.519294  | -1.543676|
| 64 | 1 | 0 | 5.635889 | 1.661880  | 2.148909 |
| 65 | 1 | 0 | 6.083408 | 2.909581  | 0.972842 |
| 66 | 1 | 0 | 4.394248 | 2.680950  | 1.399802 |

3b (conformer 8)

|    |   |   |          |          |          |
|----|---|---|----------|----------|----------|
| 1  | 6 | 0 | -0.727953| 1.331852  | 0.269504 |
| 2  | 6 | 0 | -0.886424| 0.040600  | -0.530181|
| 3  | 6 | 0 | -1.810060| -0.900553 | 0.114348 |
| 4  | 8 | 0 | 0.429077 | -0.475796 | -0.756071|
| 5  | 6 | 0 | -1.055841| 1.387977  | 1.605906 |
| 6  | 6 | 0 | -0.900156| 2.574005  | -1.116308|
| 7  | 6 | 0 | -0.421796| 3.711996  | 1.763168 |
| 8  | 6 | 0 | -0.071050| 3.711178  | 0.387796 |
| 9  | 6 | 0 | -0.215503| 2.506884  | -0.375813|
| 10 | 6 | 0 | -1.272298| -2.028705 | 0.842987 |
| 11 | 6 | 0 | -2.090834| -3.011967 | 1.443320 |
| 12 | 6 | 0 | -3.454498| -2.952872 | 1.307060 |
| 13 | 6 | 0 | -4.059072| -1.900295 | 0.571650 |
| 14 | 6 | 0 | -3.232321| -0.894965 | -0.030284|
| 15 | 6 | 0 | 0.422721 | 4.883098  | -0.243704|
| 16 | 6 | 0 | 0.765865 | 4.880842  | -1.573378|
| 17 | 6 | 0 | 0.631934 | 3.695360  | -2.329750|
| 18 | 6 | 0 | 0.158560 | 2.542999  | -1.746791|
| 19 | 6 | 0 | -5.469074| -1.820959 | 0.424821 |
| 20 | 6 | 0 | -6.052523| -0.793769 | -0.275616|
| 21 | 6 | 0 | -5.243937| 0.207355  | -0.858446|
| 22 | 6 | 0 | -3.874806| 0.159186  | -0.737420|
| 23 | 6 | 0 | 0.542404 | -1.323267 | -1.901333|
| 24 | 6 | 0 | 2.004980 | -1.707004 | -2.087042|
| 25 | 6 | 0 | 2.599511 | -2.620343 | -0.995736|
| 26 | 6 | 0 | 2.025213 | -4.042461 | -1.080133|
| 27 | 6 | 0 | 4.138971 | -2.660101 | -1.085115|
| 28 | 6 | 0 | 4.863708 | -1.394516 | -0.577456|
| 29 | 6 | 0 | 4.752021 | -1.214280 | 0.912841 |
| 30 | 6 | 0 | 4.265067 | -0.173484 | 1.601631 |
| 31 | 6 | 0 | 3.708016 | 1.085483  | 0.987961 |
| 32 | 6 | 0 | 4.238618 | -0.192162 | 3.111228 |
| 33 | 1 | 0 | -1.314870| 0.298349  | -1.507758|
| 34 | 1 | 0 | -1.448860| 0.505894  | 2.095644 |
| 35 | 1 | 0 | -1.168874| 2.575989  | 3.409420 |
| 36 | 1 | 0 | -0.305907| 4.628504  | 2.332430|
| 37 | 1 | 0 | -0.196028| -2.087979 | 0.948071 |
| 38 | 1 | 0 | -1.631554| -3.815136 | 2.008855 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 39 | 1 | 0 | -4.089356 | -3.707392 | 1.759845 |
| 40 | 1 | 0 | 0.524391 | 5.786974 | 0.348233 |
| 41 | 1 | 0 | 1.141462 | 5.782536 | -2.043835 |
| 42 | 1 | 0 | 0.910166 | 3.693808 | -3.378999 |
| 43 | 1 | 0 | 0.086258 | 1.644246 | -2.344259 |
| 44 | 1 | 0 | -6.081848 | -2.591092 | 0.882099 |
| 45 | 1 | 0 | -7.130675 | -0.744726 | -0.378619 |
| 46 | 1 | 0 | -5.707719 | 1.023204 | -1.401584 |
| 47 | 1 | 0 | -3.283424 | 0.951382 | -1.178581 |
| 48 | 1 | 0 | -0.095991 | -2.207749 | -1.784419 |
| 49 | 1 | 0 | 0.186107 | -0.780698 | -2.790384 |
| 50 | 1 | 0 | 2.101196 | -2.206128 | -3.060552 |
| 51 | 1 | 0 | 2.580714 | -0.778884 | -2.154593 |
| 52 | 1 | 0 | 2.334578 | -2.196564 | -0.020893 |
| 53 | 1 | 0 | 2.402688 | -4.664545 | -0.263295 |
| 54 | 1 | 0 | 0.933547 | -4.052568 | -1.021437 |
| 55 | 1 | 0 | 2.311261 | -4.523815 | -2.022530 |
| 56 | 1 | 0 | 4.504134 | -3.517197 | -0.506217 |
| 57 | 1 | 0 | 4.432734 | -2.851788 | -2.125556 |
| 58 | 1 | 0 | 5.925675 | -1.491183 | -0.840255 |
| 59 | 1 | 0 | 4.503085 | -0.512053 | -1.110687 |
| 60 | 1 | 0 | 5.121638 | -2.061735 | 1.491712 |
| 61 | 1 | 0 | 3.759677 | 1.096263 | -0.099714 |
| 62 | 1 | 0 | 2.658153 | 1.218769 | 1.270552 |
| 63 | 1 | 0 | 4.249352 | 1.963209 | 1.360718 |
| 64 | 1 | 0 | 4.638908 | -1.124926 | 3.514243 |
| 65 | 1 | 0 | 4.824611 | 0.637797 | 3.524277 |
| 66 | 1 | 0 | 3.215487 | -0.067071 | 3.485289 |

**3b (conformer 9)**

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1  | 6 | 0 | 1.476604 | -0.788302 | 0.612607 |
| 2  | 6 | 0 | 0.667683 | -0.029546 | -0.449772 |
| 3  | 6 | 0 | 0.663425 | 1.480614 | -0.230487 |
| 4  | 8 | 0 | -0.691012 | -0.474358 | -0.463079 |
| 5  | 6 | 0 | 1.242602 | -0.492116 | 1.939788 |
| 6  | 6 | 0 | 1.902891 | -1.171631 | 2.983308 |
| 7  | 6 | 0 | 2.815845 | -2.154813 | 2.693963 |
| 8  | 6 | 0 | 3.096462 | -2.501976 | 1.349204 |
| 9  | 6 | 0 | 2.416992 | -1.819145 | 0.282267 |
| 10 | 6 | 0 | -0.487995 | 2.114569 | 0.183072 |
| 11 | 6 | 0 | -0.526071 | 3.512522 | 0.390315 |
| 12 | 6 | 0 | 0.590528 | 4.276911 | 0.171822 |
| 13 | 6 | 0 | 1.797978 | 3.673272 | -0.266075 |
| 14 | 6 | 0 | 1.846304 | 2.254640 | -0.469615 |
| 15 | 6 | 0 | 4.036814 | -3.521296 | 1.041703 |
| 16 | 6 | 0 | 4.310293 | -3.868900 | -0.257413 |
| 17 | 6 | 0 | 3.644675 | -3.205915 | -1.312675 |
|    |   |   |    |  |  |  |
|----|---|---|----|---|---|---|
| 18 | 6 | 0 | 2.728430 | -2.215002 | -1.050376 |
| 19 | 6 | 0 | 2.959342 | 4.451924  | -0.511560 |
| 20 | 6 | 0 | 4.127387 | 3.870295  | -0.940209 |
| 21 | 6 | 0 | 4.182999 | 2.473198  | -1.138843 |
| 22 | 6 | 0 | 3.075379 | 1.689565  | -0.908402 |
| 23 | 6 | 0 | -0.895465| -1.777718 | -1.001609 |
| 24 | 6 | 0 | -2.385810| -2.094966 | -0.975194 |
| 25 | 6 | 0 | -3.294394| -1.139020 | -1.772548 |
| 26 | 6 | 0 | -2.929999| -1.110230 | -3.264201 |
| 27 | 6 | 0 | -4.781149| -1.511510 | -1.602985 |
| 28 | 6 | 0 | -5.375174| -3.870295 | -0.940209 |
| 29 | 6 | 0 | -3.075379| 1.689565  | -0.908402 |
| 30 | 6 | 0 | -0.895465| -1.777718 | -1.001609 |
| 31 | 6 | 0 | -2.385810| -2.094966 | -0.975194 |
| 32 | 6 | 0 | -3.294394| -1.139020 | -1.772548 |
| 33 | 6 | 0 | -2.929999| -1.110230 | -3.264201 |
| 34 | 6 | 0 | -4.781149| -1.511510 | -1.602985 |
| 35 | 6 | 0 | -5.375174| -3.870295 | -0.940209 |
| 36 | 6 | 0 | -3.075379| 1.689565  | -0.908402 |
| 37 | 6 | 0 | -0.895465| -1.777718 | -1.001609 |
| 38 | 6 | 0 | -2.385810| -2.094966 | -0.975194 |
| 39 | 6 | 0 | -3.294394| -1.139020 | -1.772548 |
| 40 | 6 | 0 | -2.929999| -1.110230 | -3.264201 |
| 41 | 6 | 0 | -4.781149| -1.511510 | -1.602985 |
| 42 | 6 | 0 | -5.375174| -3.870295 | -0.940209 |
| 43 | 6 | 0 | -3.075379| 1.689565  | -0.908402 |
| 44 | 6 | 0 | -0.895465| -1.777718 | -1.001609 |
| 45 | 6 | 0 | -2.385810| -2.094966 | -0.975194 |
| 46 | 6 | 0 | -3.294394| -1.139020 | -1.772548 |
| 47 | 6 | 0 | -2.929999| -1.110230 | -3.264201 |
| 48 | 6 | 0 | -4.781149| -1.511510 | -1.602985 |
| 49 | 6 | 0 | -5.375174| -3.870295 | -0.940209 |
| 50 | 6 | 0 | -3.075379| 1.689565  | -0.908402 |
| 51 | 6 | 0 | -0.895465| -1.777718 | -1.001609 |
| 52 | 6 | 0 | -2.385810| -2.094966 | -0.975194 |
| 53 | 6 | 0 | -3.294394| -1.139020 | -1.772548 |
| 54 | 6 | 0 | -2.929999| -1.110230 | -3.264201 |
| 55 | 6 | 0 | -4.781149| -1.511510 | -1.602985 |
| 56 | 6 | 0 | -5.375174| -3.870295 | -0.940209 |
| 57 | 6 | 0 | -3.075379| 1.689565  | -0.908402 |
| 58 | 6 | 0 | -0.895465| -1.777718 | -1.001609 |
| 59 | 6 | 0 | -2.385810| -2.094966 | -0.975194 |
| 60 | 6 | 0 | -3.294394| -1.139020 | -1.772548 |
| 61 | 6 | 0 | -2.929999| -1.110230 | -3.264201 |
| 62 | 6 | 0 | -4.781149| -1.511510 | -1.602985 |
|   |   |   |    |    |    |    |
|---|---|---|----|----|----|----|
| 63| 1 | 0 | -3.369174 | 0.221821 | 2.795654 |
| 64| 1 | 0 | -5.532867 | 2.644243 | 0.842183 |
| 65| 1 | 0 | -5.719608 | 2.304174 | 2.571494 |
| 66| 1 | 0 | -4.114228 | 2.553032 | 1.901595 |
| 3b (conformer 10) |   |   |    |    |    |    |
| 1 | 6 | 0 | -2.247404 | -0.960072 | -0.288436 |
| 2 | 6 | 0 | -1.140015 | -0.197207 | 0.436590 |
| 3 | 6 | 0 | -0.736473 | 1.113381 | -0.234823 |
| 4 | 8 | 0 | 0.049578 | -0.982955 | 0.576793 |
| 5 | 6 | 0 | -1.926483 | -2.021810 | -1.105419 |
| 6 | 6 | 0 | -2.922582 | -2.761578 | -1.782284 |
| 7 | 6 | 0 | -4.246260 | -2.434383 | -1.634223 |
| 8 | 6 | 0 | -4.629901 | -1.345529 | -0.808677 |
| 9 | 6 | 0 | -3.621521 | -0.586817 | -0.127527 |
| 10| 6 | 0 | -0.997075 | 1.336530 | -1.568660 |
| 11| 6 | 0 | -0.610730 | 2.535168 | -2.210071 |
| 12| 6 | 0 | 0.031507 | 3.519261 | -1.504384 |
| 13| 6 | 0 | 0.323309 | 3.343261 | -0.126680 |
| 14| 6 | 0 | -0.054672 | 2.122911 | 0.523801 |
| 15| 6 | 0 | -5.995006 | -0.990118 | -0.647636 |
| 16| 6 | 0 | -6.363032 | 0.071461 | 0.142154 |
| 17| 6 | 0 | -5.373021 | 0.830846 | 0.804734 |
| 18| 6 | 0 | -4.041662 | 0.512440 | 0.671696 |
| 19| 6 | 0 | 0.986690 | 4.354264 | 0.617208 |
| 20| 6 | 0 | 1.275955 | 4.181246 | 1.948449 |
| 21| 6 | 0 | 0.913806 | 2.977968 | 2.593219 |
| 22| 6 | 0 | 0.270757 | 1.978991 | 1.900066 |
| 23| 6 | 0 | -0.001300 | -1.934410 | 1.642548 |
| 24| 6 | 0 | 1.246228 | -2.809914 | 1.642986 |
| 25| 6 | 0 | 2.571190 | -2.144736 | 2.073161 |
| 26| 6 | 0 | 3.620167 | -3.225440 | 2.385708 |
| 27| 6 | 0 | 3.116024 | -1.082117 | 1.091936 |
| 28| 6 | 0 | 3.476744 | -1.584515 | -0.321061 |
| 29| 6 | 0 | 3.944814 | -0.462952 | -1.207868 |
| 30| 6 | 0 | 5.138558 | -0.298383 | -1.793184 |
| 31| 6 | 0 | 6.296991 | -1.258006 | -1.679050 |
| 32| 6 | 0 | 5.420155 | 0.912970 | 2.649496 |
| 33| 1 | 0 | -1.508679 | 0.034708 | 1.443922 |
| 34| 1 | 0 | -0.884230 | -2.292148 | -1.221653 |
| 35| 1 | 0 | -2.631349 | -3.591717 | -2.416252 |
| 36| 1 | 0 | -5.017520 | -3.001026 | -2.145472 |
| 37| 1 | 0 | -1.516301 | 0.580007 | 2.143678 |
| 38| 1 | 0 | -0.832942 | 2.670567 | 3.262568 |
| 39| 1 | 0 | 0.324721 | 4.445774 | 1.987157 |
| 40| 1 | 0 | -6.747574 | -1.575548 | -1.165884 |
| 41| 1 | 0 | -7.409188 | 0.332688 | 0.255075 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 42| 1 | 0 | -5.665652 | 1.675207 | 1.418827 |
| 43| 1 | 0 | -3.304759 | 1.125325 | 1.174854 |
| 44| 1 | 0 | 1.264052  | 5.272702 | 0.110043 |
| 45| 1 | 0 | 1.783871  | 4.960957 | 2.504727 |
| 46| 1 | 0 | 1.150811  | 2.838919 | 3.642210 |
| 47| 1 | 0 | 0.023137  | 1.060683 | 2.415328 |
| 48| 1 | 0 | -0.094789 | -1.402119 | 2.602836 |
| 49| 1 | 0 | -0.890364 | -2.568227 | 1.530327 |
| 50| 1 | 0 | 1.040297  | -3.631990 | 2.339796 |
| 51| 1 | 0 | 1.352816  | -3.274079 | 0.656413 |
| 52| 1 | 0 | 2.367346  | -1.614307 | 3.014276 |
| 53| 1 | 0 | 3.284380  | -3.878747 | 3.196960 |
| 54| 1 | 0 | 3.818058  | -3.859895 | 1.516231 |
| 55| 1 | 0 | 4.569617  | -2.775222 | 2.690710 |
| 56| 1 | 0 | 2.383428  | -0.278115 | 0.995404 |
| 57| 1 | 0 | 4.012721  | -0.636652 | 1.539675 |
| 58| 1 | 0 | 4.227416  | -2.375842 | -0.262808 |
| 59| 1 | 0 | 2.584910  | -2.031513 | -0.776474 |
| 60| 1 | 0 | 3.199217  | 0.314204  | -1.372981 |
| 61| 1 | 0 | 6.578039  | -1.642320 | -2.667158 |
| 62| 1 | 0 | 7.181876  | -0.745548 | -1.282935 |
| 63| 1 | 0 | 6.088861  | -2.112215 | -1.035172 |
| 64| 1 | 0 | 6.269012  | 1.484711  | -2.254861 |
| 65| 1 | 0 | 5.690492  | 0.618726  | -3.671144 |
| 66| 1 | 0 | 4.557092  | 1.579436  | -2.704419 |

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| **3b (conformer 14)** |   |   |   |   |   |   |
| 1 | 6 | 0 | -0.235142 | -2.020455 | -0.029152 |
| 2 | 6 | 0 | 0.610184  | -1.203934 | -1.005673 |
| 3 | 6 | 0 | 2.115301  | -1.197015 | -0.739265 |
| 4 | 8 | 0 | 0.041890  | 0.110248  | -1.081026 |
| 5 | 6 | 0 | 0.291284  | -2.527716 | 1.138345 |
| 6 | 6 | 0 | -0.485226 | -3.303137 | 2.029492 |
| 7 | 6 | 0 | -1.794924 | -3.583459 | 1.740225 |
| 8 | 6 | 0 | -2.383295 | -3.106034 | 0.540139 |
| 9 | 6 | 0 | -1.602059 | -2.312105 | -0.362088 |
| 10| 6 | 0 | 2.902965  | -2.005586 | -1.532702 |
| 11| 6 | 0 | 4.302913  | -2.084510 | -1.367989 |
| 12| 6 | 0 | 4.920521  | -1.330327 | -0.403562 |
| 13| 6 | 0 | 4.162820  | -0.473643 | 0.436401 |
| 14| 6 | 0 | 2.738065  | -0.397852 | 0.277081 |
| 15| 6 | 0 | -3.730715 | -3.413352 | 0.213982 |
| 16| 6 | 0 | -4.295176 | -2.971338 | -0.957102 |
| 17| 6 | 0 | -3.528640 | -2.194279 | -1.853646 |
| 18| 6 | 0 | -2.224251 | -1.870148 | -1.561915 |
| 19| 6 | 0 | 4.794244  | 0.306114  | 1.441626 |
| 20| 6 | 0 | 4.063271  | 1.127067  | 2.264025 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 21| 6 | 0 | 2.660292 | 1.202879 | 2.113588 |
| 22| 6 | 0 | 2.015214 | 0.464860 | 1.149134 |
| 23| 6 | 0 | 0.440507 | 0.856581 | -2.231709 |
| 24| 6 | 0 | -0.341831 | 2.163502 | -2.269083 |
| 25| 6 | 0 | -0.010388 | 3.176363 | -1.153995 |
| 26| 6 | 0 | 1.394058 | 3.770488 | -1.334841 |
| 27| 6 | 0 | -1.063676 | 4.301742 | -1.096239 |
| 28| 6 | 0 | -2.431283 | 3.905235 | -0.500191 |
| 29| 6 | 0 | -2.367903 | 3.609575 | 0.974896 |
| 30| 6 | 0 | -2.802860 | 2.529618 | 1.637749 |
| 31| 6 | 0 | -3.471881 | 1.337118 | 1.003630 |
| 32| 6 | 0 | -2.651908 | 2.431397 | 3.137020 |
| 33| 1 | 0 | 0.489486 | -1.673123 | -1.993907 |
| 34| 1 | 0 | 1.326093 | -2.336179 | 1.388657 |
| 35| 1 | 0 | -0.032322 | -3.675541 | 2.941468 |
| 36| 1 | 0 | -2.396805 | -4.180605 | 2.417481 |
| 37| 1 | 0 | 2.433210 | -2.602450 | -2.308278 |
| 38| 1 | 0 | 4.882189 | -2.736590 | -2.011928 |
| 39| 1 | 0 | 5.996312 | -1.376413 | -0.269672 |
| 40| 1 | 0 | -4.307914 | -4.013157 | 0.910267 |
| 41| 1 | 0 | -5.324033 | -3.215867 | -1.196245 |
| 42| 1 | 0 | -3.975480 | -1.845974 | -2.778413 |
| 43| 1 | 0 | -1.668214 | -1.252869 | -2.253162 |
| 44| 1 | 0 | 5.872001 | 0.238432 | 1.548818 |
| 45| 1 | 0 | 4.557706 | 1.716573 | 3.028079 |
| 46| 1 | 0 | 2.085751 | 1.852395 | 2.764669 |
| 47| 1 | 0 | 0.943567 | 0.543406 | 1.038379 |
| 48| 1 | 0 | 1.522766 | 1.033708 | -2.213630 |
| 49| 1 | 0 | 0.223279 | 0.267981 | -3.136989 |
| 50| 1 | 0 | -0.158877 | 2.636228 | -3.243447 |
| 51| 1 | 0 | -1.406134 | 1.910090 | -2.241311 |
| 52| 1 | 0 | -0.036769 | 2.645087 | -0.196716 |
| 53| 1 | 0 | 2.168559 | 2.999950 | -1.354517 |
| 54| 1 | 0 | 1.461544 | 4.338799 | -2.270009 |
| 55| 1 | 0 | 1.636479 | 4.452073 | -0.514513 |
| 56| 1 | 0 | -0.660295 | 5.129551 | -0.500365 |
| 57| 1 | 0 | -1.214590 | 4.704301 | -2.106595 |
| 58| 1 | 0 | -3.118370 | 4.747720 | -0.658585 |
| 59| 1 | 0 | -2.858031 | 3.065440 | -1.053391 |
| 60| 1 | 0 | -1.906547 | 4.400947 | 1.567310 |
| 61| 1 | 0 | -2.921017 | 0.418468 | 1.232266 |
| 62| 1 | 0 | -4.482162 | 1.206279 | 1.409879 |
| 63| 1 | 0 | -3.553963 | 1.412306 | -0.079631 |
| 64| 1 | 0 | -3.628518 | 2.319411 | 3.623994 |
| 65| 1 | 0 | -2.063978 | 1.548149 | 3.413876 |
|   |   |   | 66          | 1           | 0          | -2.162956 | 3.313596 | 3.555887 |
|---|---|---|-------------|-------------|------------|-----------|----------|----------|
| **3b (conformer 15)** |   |   | 1           | 6           | 0          | 2.536740  | -0.948541 | 0.143706 |
|   | 2 | 6 | 0           | 1.193097    | -0.268799  | -0.116283 |
|   | 3 | 6 | 0           | 0.988016    | 1.029482   | 0.660112  |
|   | 4 | 8 | 0           | 0.088469    | -1.124291  | 0.198197  |
|   | 5 | 6 | 0           | 2.607751    | -2.033822  | 0.988982  |
|   | 6 | 6 | 0           | 3.830718    | -2.697552  | 1.238307  |
|   | 7 | 6 | 0           | 4.984877    | -2.270455  | 0.632988  |
|   | 8 | 6 | 0           | 4.966806    | -1.153268  | -0.242396 |
|   | 9 | 6 | 0           | 3.730164    | -0.471499  | -0.490189 |
|   | 10| 6 | 0           | 1.650318    | 1.251564   | 1.847108  |
|   | 11| 6 | 0           | 1.453385    | 2.432489   | 2.597308  |
|   | 12| 6 | 0           | 0.595775    | 3.401653   | 2.145105  |
|   | 13| 6 | 0           | -0.110270   | 3.226490   | 0.926646  |
|   | 14| 6 | 0           | 0.072952    | 2.021112   | 0.172010  |
|   | 15| 6 | 0           | 6.152443    | -0.694118  | -0.874155 |
|   | 16| 6 | 0           | 6.134000    | 0.394641   | -1.711208 |
|   | 17| 6 | 0           | 4.920748    | 1.078161   | -1.948621 |
|   | 18| 6 | 0           | 3.753739    | 0.658412   | -1.353942 |
|   | 19| 6 | 0           | -0.997461   | 4.224327   | 0.443966  |
|   | 20| 6 | 0           | -1.685680   | 4.053391   | -0.732053 |
|   | 21| 6 | 0           | -1.518089   | 2.863722   | -1.474809 |
|   | 22| 6 | 0           | -0.667906   | 1.876763   | -1.033021 |
|   | 23| 6 | 0           | -0.214008   | -2.088090  | -0.814129 |
|   | 24| 6 | 0           | -1.255088   | -3.087363  | -0.321232 |
|   | 25| 6 | 0           | -2.702695   | -2.581274  | -0.141365 |
|   | 26| 6 | 0           | -3.660655   | -3.783266  | -0.104644 |
|   | 27| 6 | 0           | -2.856827   | -1.689243  | 1.106993  |
|   | 28| 6 | 0           | -4.235777   | -1.018021  | 1.281552  |
|   | 29| 6 | 0           | -4.572738   | -0.049429  | 0.179925  |
|   | 30| 6 | 0           | -5.693828   | 0.041207   | -0.548168 |
|   | 31| 6 | 0           | -6.894386   | -0.860656  | -0.403666 |
|   | 32| 6 | 0           | -5.846472   | 1.109705   | -1.604323 |
|   | 33| 1 | 0           | 1.148972    | -0.039769  | -1.187969 |
|   | 34| 1 | 0           | 1.699724    | -2.382451  | 1.465317  |
|   | 35| 1 | 0           | 3.847261    | -3.549335  | 1.909200  |
|   | 36| 1 | 0           | 5.926404    | -2.778210  | 0.814745  |
|   | 37| 1 | 0           | 2.344799    | 0.506716   | 2.215679  |
|   | 38| 1 | 0           | 1.992098    | 2.567605   | 3.528432  |
|   | 39| 1 | 0           | 0.445422    | 4.315674   | 2.710233  |
|   | 40| 1 | 0           | 7.080826    | -1.221543  | -0.680134 |
|   | 41| 1 | 0           | 7.047252    | 0.735157   | -2.186058 |
|   | 42| 1 | 0           | 4.911163    | 1.944130   | -2.601072 |
|   | 43| 1 | 0           | 2.843566    | 1.214587   | -1.538489 |
|   | 44| 1 | 0           | -1.122605   | 5.131400   | 1.026423  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|45 | 1 | 0 | -2.358917 | 4.824145 | -1.089953 |
|46 | 1 | 0 | -2.067922 | 2.726048 | -2.399272 |
|47 | 1 | 0 | -0.575098 | 0.968829 | -1.614172 |
|48 | 1 | 0 | 0.699750  | -2.628883 | -1.092212 |
|49 | 1 | 0 | -0.578978 | -1.569243 | -1.714508 |
|50 | 1 | 0 | -1.264300 | -3.898548 | -1.059827 |
|51 | 1 | 0 | -0.899121 | -3.533871 | 0.615678  |
|52 | 1 | 0 | -2.957130 | -1.977930 | -1.023276 |
|53 | 1 | 0 | -0.578978 | -1.569243 | -1.714508 |
|54 | 1 | 0 | -1.264300 | -3.898548 | -1.059827 |
|55 | 1 | 0 | -0.899121 | -3.533871 | 0.615678  |
|56 | 1 | 0 | -2.957130 | -1.977930 | -1.023276 |
|57 | 1 | 0 | -0.578978 | -1.569243 | -1.714508 |
|58 | 1 | 0 | -1.264300 | -3.898548 | -1.059827 |
|59 | 1 | 0 | -0.899121 | -3.533871 | 0.615678  |
|60 | 1 | 0 | -2.957130 | -1.977930 | -1.023276 |
|61 | 1 | 0 | -0.578978 | -1.569243 | -1.714508 |
|62 | 1 | 0 | -1.264300 | -3.898548 | -1.059827 |
|63 | 1 | 0 | -0.899121 | -3.533871 | 0.615678  |
|64 | 1 | 0 | -2.957130 | -1.977930 | -1.023276 |
|65 | 1 | 0 | -0.578978 | -1.569243 | -1.714508 |
|66 | 1 | 0 | -1.264300 | -3.898548 | -1.059827 |

3b (conformer 17)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.304767 | 1.660097 | 0.027546 |
| 2 | 6 | 0 | -1.029438 | 0.226349  | -0.416821 |
| 3 | 6 | 0 | -1.788671 | -0.816260 | 0.417088 |
| 4 | 6 | 0 | 0.381159  | 0.004878  | -0.339029 |
| 5 | 6 | 0 | -0.322515 | 2.387146  | 0.663823 |
| 6 | 6 | 0 | -0.545749 | 3.717774  | 1.085532 |
| 7 | 6 | 0 | -1.754096 | 4.323655  | 0.858339 |
| 8 | 6 | 0 | -2.794783 | 3.621556  | 0.196515 |
| 9 | 6 | 0 | -2.578108 | 2.268479  | -0.225594 |
|10| 6 | 0 | -1.723512 | -0.718010 | 1.791841 |
|11| 6 | 0 | -2.349436 | -1.656077 | 2.637241 |
|12| 6 | 0 | -3.058062 | -2.700893 | 2.098661 |
|13| 6 | 0 | -3.158656 | -2.852757 | 0.693533 |
|14| 6 | 0 | -2.511343 | -1.905482 | -0.172408 |
|15| 6 | 0 | -4.047534 | 4.238523  | -0.059144 |
|16| 6 | 0 | -5.054377 | 3.562413  | -0.703687 |
|17| 6 | 0 | -4.847798 | 2.228834  | -1.115983 |
|18| 6 | 0 | -3.646446 | 1.600914  | -0.885208 |
|19| 6 | 0 | -3.887333 | -3.933392 | 0.128644 |
|20| 6 | 0 | -3.984942 | -4.092648 | -1.230869 |
|21| 6 | 0 | -3.348120 | -3.169268 | -2.089928 |
|22| 6 | 0 | -2.635006 | -2.117166 | -1.576664 |
|23| 6 | 0 | 0.852784  | -1.136145 | -1.051856 |
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
|24 | 6 | 0 | 2.370969 | -1.191824 | -0.935136 |
|25 | 6 | 0 | 2.923678 | -1.401955 | 0.488985 |
|26 | 6 | 0 | 2.532910 | -2.776140 | 1.053043 |
|27 | 6 | 0 | 4.455177 | -1.227595 | 0.531854 |
|28 | 6 | 0 | 4.961698 | 0.210002 | 0.300780 |
|29 | 6 | 0 | 6.445217 | 0.335588 | 0.516858 |
|30 | 6 | 0 | 7.393652 | 0.696603 | 0.055120 |
|31 | 6 | 0 | 7.143054 | 1.074651 | -1.796323 |
|32 | 6 | 0 | 8.844590 | 0.757690 | 0.531854 |
|33 | 1 | 0 | -1.326423 | 0.147111 | -1.468145 |
|34 | 1 | 0 | 0.642541 | 1.928284 | 0.828961 |
|35 | 1 | 0 | 0.251450 | 5.346354 | 1.174912 |
|36 | 1 | 0 | -3.551467 | -3.424216 | 2.739454 |
|37 | 1 | 0 | -4.195351 | 5.263299 | 0.266068 |
|38 | 1 | 0 | -6.005863 | 4.046601 | -0.892761 |
|39 | 1 | 0 | -5.644304 | 1.693549 | -1.624453 |
|40 | 1 | 0 | -3.526978 | 0.574344 | -1.203897 |
|41 | 1 | 0 | -4.369496 | -4.637110 | 0.799434 |
|42 | 1 | 0 | -4.544952 | -4.922088 | -1.647528 |
|43 | 1 | 0 | -3.421058 | -3.296830 | -3.164286 |
|44 | 1 | 0 | -2.156566 | -1.430208 | -2.267544 |
|45 | 1 | 0 | 0.387277 | -2.049083 | -0.662322 |
|46 | 1 | 0 | 0.569082 | -1.047759 | -2.111246 |
|47 | 1 | 0 | 2.726204 | -2.006398 | -1.580379 |
|48 | 1 | 0 | 2.766599 | -0.262904 | -1.356639 |
|49 | 1 | 0 | 2.481715 | -0.633073 | 1.133980 |
|50 | 1 | 0 | 1.449599 | -2.911738 | 1.093404 |
|51 | 1 | 0 | 2.950003 | -3.584422 | 0.441337 |
|52 | 1 | 0 | 2.914578 | -2.901281 | 2.070565 |
|53 | 1 | 0 | 4.813369 | -1.562442 | 1.512978 |
|54 | 1 | 0 | 4.921957 | -1.897314 | -0.202352 |
|55 | 1 | 0 | 4.683741 | 0.555335 | -0.696484 |
|56 | 1 | 0 | 4.444704 | 0.873185 | 1.008252 |
|57 | 1 | 0 | 6.774120 | 0.085439 | 1.525743 |
|58 | 1 | 0 | 6.094370 | 1.008636 | -2.084591 |
|59 | 1 | 0 | 7.481113 | 2.099974 | -1.988193 |
|60 | 1 | 0 | 7.718940 | 0.427466 | -2.468371 |
|61 | 1 | 0 | 9.457551 | 0.089929 | -0.562177 |
|62 | 1 | 0 | 9.249338 | 1.767803 | -0.081237 |
|63 | 1 | 0 | 8.981652 | 0.475262 | 1.100962 |
|3b (conformer 19) | 1 | 6 | 0 | 2.505153 | -1.261360 | 0.242119 |
|   | 2 | 6 | 0 | 1.498823 | -0.186657 | -0.165495 |
|   |   |   | 1.615008 | 1.114292 | 0.624765 |
|---|---|---|----------|----------|----------|
| 4 | 8 | 0 | 0.146450 | -0.636991 | -0.034517 |
| 5 | 6 | 0 | 2.118254 | -2.278756 | 0.133377 |
| 6 | 6 | 0 | 3.013 | -3.298303 | 1.477287 |
| 7 | 6 | 0 | 4.300942 | -3.304202 | 1.004772 |
| 8 | 6 | 0 | 2.118254 | -2.278756 | 0.133377 |
| 9 | 6 | 0 | 3.013 | -3.298303 | 1.477287 |
| 10 | 6 | 0 | 2.277192 | 1.142297 | 1.858126 |
| 11 | 6 | 0 | 2.327411 | 2.334581 | 2.610180 |
| 12 | 6 | 0 | 1.819848 | 3.536750 | 0.847615 |
| 13 | 6 | 0 | 1.181777 | 3.536750 | 0.847615 |
| 14 | 6 | 0 | 1.181777 | 3.536750 | 0.847615 |
| 15 | 6 | 0 | 6.083046 | -2.265657 | -0.360262 |
| 16 | 6 | 0 | 6.521160 | -1.264483 | -1.190203 |
| 17 | 6 | 0 | 5.641041 | -0.223535 | -1.563242 |
| 18 | 6 | 0 | 4.34451 | -0.207239 | -1.104992 |
| 19 | 6 | 0 | 0.653846 | 4.744771 | 0.320235 |
| 20 | 6 | 0 | 0.030287 | 4.772418 | -0.903012 |
| 21 | 6 | 0 | -0.096821 | 3.581186 | -1.651328 |
| 22 | 6 | 0 | 0.402017 | 2.394313 | -1.167235 |
| 23 | 6 | 0 | -0.292445 | 1.506716 | -1.080051 |
| 24 | 6 | 0 | -1.725948 | 1.932477 | -0.791388 |
| 25 | 6 | 0 | -2.768689 | -0.796486 | -0.762916 |
| 26 | 6 | 0 | -2.989154 | -0.198043 | -2.160333 |
| 27 | 6 | 0 | -4.082784 | -1.312311 | -0.144942 |
| 28 | 6 | 0 | -5.152401 | -0.232750 | 0.111512 |
| 29 | 6 | 0 | -6.332171 | -0.766206 | 0.877606 |
| 30 | 6 | 0 | -7.614638 | -0.842430 | 0.497698 |
| 31 | 6 | 0 | -8.150666 | -0.375874 | -0.832750 |
| 32 | 6 | 0 | -8.661386 | -1.422698 | 1.418109 |
| 33 | 1 | 0 | 1.674301 | 0.040161 | -1.225030 |
| 34 | 1 | 0 | 1.100458 | -2.282533 | 1.461761 |
| 35 | 1 | 0 | 2.672058 | -4.080348 | 2.146493 |
| 36 | 1 | 0 | 4.992618 | -4.089735 | 1.290772 |
| 37 | 1 | 0 | 2.649014 | 0.231496 | 2.264118 |
| 38 | 1 | 0 | 2.814415 | 2.313386 | 3.578609 |
| 39 | 1 | 0 | 1.899242 | 4.428858 | 2.682291 |
| 40 | 1 | 0 | 6.753779 | -3.065585 | -0.063751 |
| 41 | 1 | 0 | 7.540829 | -1.266223 | -1.560421 |
| 42 | 1 | 0 | 5.993177 | 0.571921 | -2.210490 |
| 43 | 1 | 0 | 3.699276 | 0.614096 | -1.389459 |
| 44 | 1 | 0 | 0.753031 | 5.652477 | 0.906622 |
| 45 | 1 | 0 | -0.367895 | 5.701789 | -1.294325 |
| 46 | 1 | 0 | -0.597358 | 3.602454 | -2.613063 |
| 47 | 1 | 0 | 0.272482 | 1.494337 | -1.753293 |
|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 48 | 1 | 0 | -0.212658 | -0.986424 | -2.045982 |
| 49 | 1 | 0 | 0.353642  | -2.392027 | -1.133241 |
| 50 | 1 | 0 | -2.015213 | -2.677282 | -1.544425 |
| 51 | 1 | 0 | -1.729892 | -2.449295 | 0.174660  |
| 52 | 1 | 0 | -2.376405 | -0.009468 | -0.108359 |
| 53 | 1 | 0 | -3.424477 | -0.942032 | -2.837824 |
| 54 | 1 | 0 | -3.663041 | -2.392027 | -1.133241 |
| 55 | 1 | 0 | -2.053023 | 0.148330  | -2.605564 |
| 56 | 1 | 0 | -2.053023 | 0.148330  | -2.605564 |
| 57 | 1 | 0 | -3.850058 | -1.799845 | 0.809557  |
| 58 | 1 | 0 | -4.690449 | 0.577236  | 0.693122  |
| 59 | 1 | 0 | -5.471224 | 0.212562  | -0.832402 |
| 60 | 1 | 0 | -6.087945 | -1.146066 | 1.869858  |
| 61 | 1 | 0 | -8.652497 | -1.199719 | -1.353857 |
| 62 | 1 | 0 | -8.905709 | 0.406406  | -0.689747 |
| 63 | 1 | 0 | -7.380917 | 0.019725  | 1.494806  |
| 64 | 1 | 0 | -9.447687 | -0.688333 | 1.630963  |
| 65 | 1 | 0 | -9.157015 | -2.285049 | 0.956036  |
| 66 | 1 | 0 | -8.232115 | -1.745999 | 2.368563  |

**3b (conformer 20)**

|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 1  | 6 | 0 | -0.470996 | -1.293961 | 1.051641 |
| 2  | 6 | 0 | -1.398200 | -0.129729 | 0.704479 |
| 3  | 6 | 0 | -2.767576 | -0.518149 | 0.147573 |
| 4  | 8 | 0 | -0.804664 | 0.809622  | -0.201553|
| 5  | 6 | 0 | -0.344250 | -1.632365 | 2.383000 |
| 6  | 6 | 0 | 0.475776  | -2.698914 | 2.811504 |
| 7  | 6 | 0 | 1.186522  | -3.426160 | 1.891537 |
| 8  | 6 | 0 | 1.101945  | -3.118713 | 0.508781 |
| 9  | 6 | 0 | 0.264871  | -2.038399 | 0.069576 |
| 10 | 6 | 0 | -3.068215 | -1.819960 | -0.188106|
| 11 | 6 | 0 | -4.344668 | -2.188863 | -0.670375|
| 12 | 6 | 0 | -5.330860 | -1.247119 | -0.803594|
| 13 | 6 | 0 | -5.083819 | 0.105811  | -0.453477|
| 14 | 6 | 0 | -3.788168 | 0.486100  | 0.027604 |
| 15 | 6 | 0 | 1.827248  | -3.873204 | -0.451501|
| 16 | 6 | 0 | 1.738081  | -3.586717 | -1.791125|
| 17 | 6 | 0 | 0.915373  | -2.524437 | -2.228875|
| 18 | 6 | 0 | 0.200637  | -1.770461 | -1.327667|
| 19 | 6 | 0 | -6.104736 | 1.086623  | -0.561985|
| 20 | 6 | 0 | -5.874700 | 2.392185  | -0.204305|
| 21 | 6 | 0 | -4.602289 | 2.771975  | 0.276924 |
| 22 | 6 | 0 | -3.589144 | 1.847973  | 0.384485 |
| 23 | 6 | 0 | 0.268833  | 1.567240  | 0.359228 |
| 24 | 6 | 0 | 0.726219  | 2.572304  | -0.691708|
| 25 | 6 | 0 | 1.803261  | 3.579732  | -0.230142|
| 26 | 6 | 0 | 1.276278  | 4.537111  | 0.851248 |
|   |     | 0 | 2.797337 | -0.490717 | 0.179266 |
|---|-----|---|---------|-----------|---------|
| 1 | 6   | 0 | 2.797337 | -0.490717 | 0.179266 |
| 2 | 6   | 0 | 1.414638 | -0.172853 | 0.747496 |
| 3 | 6   | 0 | 0.815498 | 0.827297 | -0.087154 |
| 4 | 8   | 0 | 0.815498 | 0.827297 | -0.087154 |
| 5 | 6   | 0 | 3.128056 | -1.757171 | -0.250081 |

**3b (conformer 21)**

|   |     | 0 | 2.797337 | -0.490717 | 0.179266 |
|---|-----|---|---------|-----------|---------|
| 1 | 6   | 0 | 2.797337 | -0.490717 | 0.179266 |
| 2 | 6   | 0 | 1.414638 | -0.172853 | 0.747496 |
| 3 | 6   | 0 | 0.503580 | -1.376578 | 0.984802 |
| 4 | 8   | 0 | 0.815498 | 0.827297 | -0.087154 |
| 5 | 6   | 0 | 3.128056 | -1.757171 | -0.250081 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 6 | 6 | 0 | 4.416329 | -2.063375 | -0.744712 |
| 7 | 6 | 0 | 5.384027 | -1.094839 | -0.796472 |
| 8 | 6 | 0 | 5.105862 | 0.222606  | 0.348242  |
| 9 | 6 | 0 | 3.798451 | 0.539678  | 0.146667  |
|10 | 6 | 0 | 0.363754 | -1.825168 | 2.281817  |
|11 | 6 | 0 | -0.444240| -1.094839 | -0.796472 |
|12 | 6 | 0 | -1.130291| -3.595554 | 1.621014  |
|13 | 6 | 0 | -1.032141| -3.173390 | 0.269770  |
|14 | 6 | 0 | -0.205944| -2.048686 | -0.066413 |
|15 | 6 | 0 | 6.107336 | 1.228872  | -0.372325 |
|16 | 6 | 0 | 5.847467 | 2.498946  | 0.080030  |
|17 | 6 | 0 | 4.563517 | 2.815893  | 0.575785  |
|18 | 6 | 0 | 3.798451 | 0.539678  | 0.146667  |
|19 | 6 | 0 | 0.363754 | -1.825168 | 2.281817  |
|20 | 6 | 0 | -1.631172| -3.457813 | -2.069735 |
|21 | 6 | 0 | -0.817917| -2.352284 | -2.406392 |
|22 | 6 | 0 | -0.126035| -1.666027 | -1.435880 |
|23 | 6 | 0 | -0.284761| 1.511332  | 0.512276  |
|24 | 6 | 0 | -0.749731| 2.595565  | -0.450343 |
|25 | 6 | 0 | -1.813796| 3.547454  | 0.129725  |
|26 | 6 | 0 | -2.065526| 4.714189  | -0.838188 |
|27 | 6 | 0 | -3.128044| 2.849967  | 0.552530  |
|28 | 6 | 0 | -3.893117| 2.103993  | -0.560386 |
|29 | 6 | 0 | -5.235629| 1.614397  | -0.088109 |
|30 | 6 | 0 | -5.686160| 0.356193  | 0.004418  |
|31 | 6 | 0 | -4.899018| -0.833959 | -0.372055 |
|32 | 6 | 0 | -7.079747| 0.070751  | 0.510617  |
|33 | 1 | 0 | 1.577087 | 0.278116  | 1.738363  |
|34 | 1 | 0 | 2.399812 | -2.547570 | -0.208291 |
|35 | 1 | 0 | 4.629983 | -3.072165 | -1.075591 |
|36 | 1 | 0 | 6.376429 | -1.321691 | -1.172107 |
|37 | 1 | 0 | 0.892527 | -1.310593 | 3.078143  |
|38 | 1 | 0 | -0.529180| -3.256913 | 3.641095  |
|39 | 1 | 0 | -1.757801| -4.448451 | 1.858175  |
|40 | 1 | 0 | 7.090306 | 0.971748  | -0.753547 |
|41 | 1 | 0 | 6.621705 | 3.257640  | 0.058345  |
|42 | 1 | 0 | 4.359138 | 3.819507  | 0.932285  |
|43 | 1 | 0 | 2.587535 | 2.141514  | 0.962870  |
|44 | 1 | 0 | -2.353269| -4.704531 | -0.489709 |
|45 | 1 | 0 | -2.170509| -3.988677 | -2.846323 |
|46 | 1 | 0 | -0.737897| -2.041776 | -3.442358 |
|47 | 1 | 0 | 0.483546 | -0.816595 | -1.707804 |
|48 | 1 | 0 | 0.038936 | 1.959336  | 1.466314  |
|49 | 1 | 0 | -1.089778| 0.802891  | 0.741284  |
|50 | 1 | 0 | 0.128042 | 3.182581  | -0.740890 |

5247
|   |   |   | 1 | 0 | -1.118904 | 2.124801 | -1.367599 |
|---|---|---|---|---|-----------|----------|-----------|
| 52 | 1 | 0 | -1.393141 | 3.980356 | 1.048189 |
| 53 | 1 | 0 | -2.813228 | 5.405587 | -0.437684 |
| 54 | 1 | 0 | -1.146310 | 5.281059 | -1.012388 |
| 55 | 1 | 0 | -2.421310 | 4.364892 | -1.811835 |
| 56 | 1 | 0 | -2.926989 | 2.145305 | 1.366790 |
| 57 | 1 | 0 | -3.789754 | 3.613157 | 0.980408 |
| 58 | 1 | 0 | -4.052136 | 2.785279 | -1.405693 |
| 59 | 1 | 0 | -3.287888 | 1.279290 | -0.942373 |
| 60 | 1 | 0 | -5.915519 | 2.407505 | -0.224160 |
| 61 | 1 | 0 | -5.410195 | -1.426874 | 1.168795 |
| 62 | 1 | 0 | -3.887607 | -0.656576 | 0.713089 |
| 63 | 1 | 0 | -4.825110 | -1.556639 | 0.481863 |
| 64 | 1 | 0 | -7.051433 | -0.572581 | 1.398268 |
| 65 | 1 | 0 | -7.613672 | 0.987043 | 0.770941 |
| 66 | 1 | 0 | -7.668929 | -0.464802 | -0.243658 |

**3b (conformer 23)**

|   |   |   | 1 | 0 | -1.023670 | 0.790494 | -1.023362 |
|---|---|---|---|---|-----------|----------|-----------|
| 1 | 6 | 0 | -1.495213 | -0.671192 | -1.017784 |
| 2 | 6 | 0 | -2.569703 | -1.045547 | 0.011049 |
| 3 | 6 | 0 | -0.395883 | -1.567019 | -0.850854 |
| 4 | 8 | 0 | -1.129846 | 1.494203 | -2.205646 |
| 5 | 6 | 0 | -0.715824 | 2.839220 | -2.323526 |
| 6 | 6 | 0 | -0.179665 | 3.484256 | -1.239455 |
| 7 | 6 | 0 | -0.019189 | 2.804310 | -0.004299 |
| 8 | 6 | 0 | -0.432127 | 1.434611 | 0.114002 |
| 9 | 6 | 0 | -2.304600 | -2.022655 | 0.947248 |
| 10 | 6 | 0 | -3.264460 | -2.418229 | 1.904771 |
| 11 | 6 | 0 | -4.506268 | -1.839244 | 1.918697 |
| 12 | 6 | 0 | -4.844660 | -0.852606 | 0.957930 |
| 13 | 6 | 0 | -3.874388 | -0.447545 | -0.019744 |
| 14 | 6 | 0 | 0.557878 | 3.459159 | 1.115732 |
| 15 | 6 | 0 | 0.739324 | 2.799318 | 2.305850 |
| 16 | 6 | 0 | 0.352526 | 1.445887 | 2.422057 |
| 17 | 6 | 0 | -0.213732 | 0.783131 | 1.358531 |
| 18 | 6 | 0 | -6.139863 | -0.271293 | 0.940123 |
| 19 | 6 | 0 | -6.489063 | 0.660349 | -0.005906 |
| 20 | 6 | 0 | -5.546612 | 1.049662 | -0.982267 |
| 21 | 6 | 0 | -4.279760 | 0.513856 | -0.986315 |
| 22 | 6 | 0 | 0.504701 | -1.625061 | -1.955562 |
| 23 | 6 | 0 | 1.538077 | -2.711730 | -1.689404 |
| 24 | 6 | 0 | 2.448532 | -2.496870 | -0.462372 |
| 25 | 6 | 0 | 3.234477 | -3.785543 | -0.176421 |
| 26 | 6 | 0 | 3.378193 | -1.281599 | -0.642914 |
| 27 | 6 | 0 | 4.186665 | -0.894594 | 0.612173 |
| 28 | 6 | 0 | 4.930205 | 0.401453 | 0.436718 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 30| 6 | 0 | 6.252828 | 0.614342 | 0.426654 |
| 31| 6 | 0 | 7.301469 | -0.454688 | 0.607943 |
| 32| 6 | 0 | 6.810666 | 2.003104 | 0.226641 |
| 33| 1 | 0 | -1.930159 | -0.852860 | -2.012587 |
| 34| 1 | 0 | -1.552808 | 1.002336 | -3.076631 |
| 35| 1 | 0 | -0.825955 | 3.352987 | -3.271893 |
| 36| 1 | 0 | 0.137368 | 4.519404 | -1.312148 |
| 37| 1 | 0 | -1.333942 | -0.252961 | 1.468181 |
| 38| 1 | 0 | -3.007891 | 1.002336 | -3.076631 |
| 39| 1 | 0 | -5.249668 | -0.585491 | 1.691868 |
| 40| 1 | 0 | -1.552808 | 1.002336 | -3.076631 |
| 41| 1 | 0 | -0.825955 | 3.352987 | -3.271893 |
| 42| 1 | 0 | 0.137368 | 4.519404 | -1.312148 |
| 43| 1 | 0 | -1.333942 | -0.252961 | 1.468181 |
| 44| 1 | 0 | -6.856704 | -0.585491 | 1.691868 |
| 45| 1 | 0 | -7.482945 | 1.093543 | -0.008653 |
| 46| 1 | 0 | -5.822840 | 1.779997 | -1.734770 |
| 47| 1 | 0 | -3.579858 | 0.842010 | -1.739708 |
| 48| 1 | 0 | -0.977561 | -0.648718 | -2.111766 |
| 49| 1 | 0 | -0.504907 | 0.923592 | 3.360105 |
| 50| 1 | 0 | -1.004754 | -3.661993 | -2.869937 |
| 51| 1 | 0 | 2.159076 | -2.809505 | -2.589742 |
| 52| 1 | 0 | 1.798352 | -2.297146 | 0.397782 |
| 53| 1 | 0 | 3.835830 | -3.705735 | 0.732061 |
| 54| 1 | 0 | 2.558664 | -4.636223 | -0.047710 |
| 55| 1 | 0 | 3.912079 | -4.022178 | -1.004972 |
| 56| 1 | 0 | 4.072703 | -1.475725 | -1.471124 |
| 57| 1 | 0 | 2.784461 | -0.411052 | -0.940183 |
| 58| 1 | 0 | 3.485170 | -0.785360 | 1.450563 |
| 59| 1 | 0 | 4.868784 | -1.701768 | 0.884811 |
| 60| 1 | 0 | 4.287842 | 1.269302 | 0.288609 |
| 61| 1 | 0 | 7.978528 | -0.476836 | -0.254212 |
| 62| 1 | 0 | 7.923361 | -0.238944 | 1.485035 |
| 63| 1 | 0 | 6.883385 | -1.453428 | 0.731026 |
| 64| 1 | 0 | 6.018301 | 2.743428 | 0.099148 |
| 65| 1 | 0 | 7.426819 | 2.306249 | 1.081919 |
| 66| 1 | 0 | 7.460910 | 2.042790 | -0.655667 |

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 3b (conformer 24) | 1 | 6 | 0 | -1.181857 | 0.663386 | 0.553682 |
| 2 | 6 | 0 | -1.496203 | -0.636166 | -0.202010 |
| 3 | 6 | 0 | -2.807361 | -1.280065 | 0.241240 |
| 4 | 8 | 0 | -0.453774 | -1.596274 | -0.014160 |
| 5 | 6 | 0 | -1.257625 | 0.645428 | 1.931181 |
| 6 | 6 | 0 | -0.939721 | 1.776158 | 2.710176 |
| 7 | 6 | 0 | -0.549962 | 2.942905 | 2.101297 |
| 8 | 6 | 0 | -0.453420 | 3.019641 | 0.689783 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 9 | 6 | 0 | -0.764536 | 1.865045 | -0.107961 |
| 10 | 6 | 0 | -2.790146 | -2.449924 | 0.969107 |
| 11 | 6 | 0 | -3.986251 | -3.072180 | 1.393988 |
| 12 | 6 | 0 | -5.202676 | -2.524476 | 1.079150 |
| 13 | 6 | 0 | -5.274738 | -1.326507 | 0.321747 |
| 14 | 6 | 0 | -4.065120 | -0.685822 | -0.105655 |
| 15 | 6 | 0 | -0.047792 | 4.222506 | 0.052233 |
| 16 | 6 | 0 | 0.054458 | 4.304699 | -0.762186 |
| 17 | 6 | 0 | -3.986251 | -3.072180 | 1.079150 |
| 18 | 6 | 0 | -5.202676 | -2.524476 | 1.079150 |
| 19 | 6 | 0 | -5.274738 | -1.326507 | 0.321747 |
| 20 | 6 | 0 | -4.065120 | -0.685822 | -0.105655 |
| 21 | 6 | 0 | -0.047792 | 4.222506 | 0.052233 |
| 22 | 6 | 0 | 0.054458 | 4.304699 | -0.762186 |
| 23 | 6 | 0 | -3.986251 | -3.072180 | 1.079150 |
| 24 | 6 | 0 | -5.202676 | -2.524476 | 1.079150 |
| 25 | 6 | 0 | -5.274738 | -1.326507 | 0.321747 |
| 26 | 6 | 0 | -4.065120 | -0.685822 | -0.105655 |
| 27 | 6 | 0 | -0.047792 | 4.222506 | 0.052233 |
| 28 | 6 | 0 | 0.054458 | 4.304699 | -0.762186 |
| 29 | 6 | 0 | -3.986251 | -3.072180 | 1.079150 |
| 30 | 6 | 0 | -5.202676 | -2.524476 | 1.079150 |
| 31 | 6 | 0 | -5.274738 | -1.326507 | 0.321747 |
| 32 | 6 | 0 | -4.065120 | -0.685822 | -0.105655 |
| 33 | 1 | 0 | -1.578281 | -0.429836 | -1.274546 |
| 34 | 1 | 0 | -1.575988 | -0.263909 | 2.427526 |
| 35 | 1 | 0 | -1.013443 | 1.719141 | 3.790391 |
| 36 | 1 | 0 | -0.311214 | 3.822218 | 2.690447 |
| 37 | 1 | 0 | -1.837268 | -2.903004 | 1.205998 |
| 38 | 1 | 0 | -3.931227 | -3.990704 | 1.967884 |
| 39 | 1 | 0 | -6.124828 | -2.998810 | 1.398480 |
| 40 | 1 | 0 | 0.181302 | 5.083073 | 0.672411 |
| 41 | 1 | 0 | 0.363657 | 5.229966 | -1.786568 |
| 42 | 1 | 0 | -0.160379 | 3.236448 | -3.185230 |
| 43 | 1 | 0 | -0.852826 | 1.147803 | -2.161954 |
| 44 | 1 | 0 | -7.432373 | -1.250290 | 0.305958 |
| 45 | 1 | 0 | -7.561268 | 0.829924 | -1.019745 |
| 46 | 1 | 0 | -5.467577 | 1.954979 | -1.763657 |
| 47 | 1 | 0 | -3.291466 | 1.031530 | -1.190754 |
| 48 | 1 | 0 | 1.183574 | -0.347110 | -0.281717 |
| 49 | 1 | 0 | 0.598290 | -1.166705 | -1.742360 |
| 50 | 1 | 0 | 1.847022 | -2.549218 | 0.685612 |
| 51 | 1 | 0 | 1.255232 | -3.369037 | -0.750817 |
| 52 | 1 | 0 | 3.672278 | -3.234367 | -0.744474 |
| 53 | 1 | 0 | 4.056601 | -2.424318 | -3.026987 |
|   |   |   |   |
|---|---|---|---|
| 54| 1 | 0 | 2.459710 -3.163679 -2.945392 |
| 55| 1 | 0 | 2.622105 -1.403289 -2.967192 |
| 56| 1 | 0 | 3.500392 -0.189847 -0.868148 |
| 57| 1 | 0 | 3.859192 -2.093208 -0.434888 |
| 58| 1 | 0 | 5.570382 -1.170724 -1.895883 |
| 59| 1 | 0 | 5.840398 0.990783 -0.661813 |
| 60| 1 | 0 | 8.782744 -1.219062 1.172852 |
| 61| 1 | 0 | 7.592554 -1.055967 2.454044 |
| 62| 1 | 0 | 7.243557 -2.079673 1.056279 |
| 63| 1 | 0 | 7.289804 2.227293 0.593121 |
| 64| 1 | 0 | 7.600346 1.532861 2.193744 |
| 65| 1 | 0 | 8.816292 1.393192 0.932015 |
| 66| 1 | 0 | 5.3b (conformer 25) |
| 1 | 6 | 0 | 1.932245 -1.483199 0.170281 |
| 2 | 6 | 0 | 1.358798 -0.112250 -0.183796 |
| 3 | 6 | 0 | 1.894986 1.032628 0.672043 |
| 4 | 8 | 0 | -0.068265 -0.083316 -0.074006 |
| 5 | 6 | 0 | 1.209399 -2.339596 0.971719 |
| 6 | 6 | 0 | 1.697387 -3.620793 1.314059 |
| 7 | 6 | 0 | 2.915239 -4.043815 0.845796 |
| 8 | 6 | 0 | 3.701737 -3.198101 0.020884 |
| 9 | 6 | 0 | 3.213945 -1.893700 -0.321393 |
| 10 | 6 | 0 | 2.466590 0.791322 1.901580 |
| 11 | 6 | 0 | 2.945991 1.841711 2.716452 |
| 12 | 6 | 0 | 2.861056 3.140867 2.288026 |
| 13 | 6 | 0 | 2.285362 3.446601 1.027322 |
| 14 | 6 | 0 | 1.785005 2.384705 0.204447 |
| 15 | 6 | 0 | 4.966760 -3.617849 -0.468296 |
| 16 | 6 | 0 | 5.731907 -2.793146 -1.256039 |
| 17 | 6 | 0 | 5.262185 -1.502324 -1.585915 |
| 18 | 6 | 0 | 4.040536 -1.064876 -1.130065 |
| 19 | 6 | 0 | 2.194169 4.787163 0.568999 |
| 20 | 6 | 0 | 1.632924 5.084034 -0.648677 |
| 21 | 6 | 0 | 1.131713 4.043087 -1.461217 |
| 22 | 6 | 0 | 1.202730 2.734266 -1.044351 |
| 23 | 6 | 0 | -0.758075 -0.692968 -1.166619 |
| 24 | 6 | 0 | -2.253961 -0.671773 -0.878139 |
| 25 | 6 | 0 | -2.877125 0.731138 -0.731483 |
| 26 | 6 | 0 | -2.931563 1.485325 -2.069155 |
| 27 | 6 | 0 | -4.256171 0.670894 -0.038165 |
| 28 | 6 | 0 | -5.357174 -0.122699 -0.772365 |
| 29 | 6 | 0 | -6.678018 -0.049601 -0.055428 |
| 30 | 6 | 0 | -7.394222 -1.042179 0.489158 |
| 31 | 6 | 0 | -7.001200 -2.498397 0.476183 |
| 32 | 6 | 0 | -8.705006 -0.760227 1.183270 |
|     |     |     |        |        |        |
|-----|-----|-----|--------|--------|--------|
| 33  | 1   | 0   | 1.618122 | 0.091373 | -1.230694 |
| 34  | 1   | 0   | 0.243556 | -2.016130 | 1.340197  |
| 35  | 1   | 0   | 1.099692 | -4.267265 | 3.679912  |
| 36  | 1   | 0   | 3.294971 | -5.028041 | 1.099665  |
| 37  | 1   | 0   | 2.556961 | -0.227641 | 2.256101  |
| 38  | 1   | 0   | 3.85504  | 1.609240  | 3.679912  |
| 39  | 1   | 0   | 3.232410 | 3.952914  | 2.904572  |
| 40  | 1   | 0   | 6.967774 | -3.126157 | -0.204337 |
| 41  | 1   | 0   | 5.872921 | -0.849314 | -2.199335 |
| 42  | 1   | 0   | 6.696774 | -3.126157 | -1.621513 |
| 43  | 1   | 0   | 5.872921 | -0.849314 | -2.199335 |
| 44  | 1   | 0   | 3.385504 | 1.609240  | 3.679912  |
| 45  | 1   | 0   | 3.232410 | 3.952914  | 2.904572  |
| 46  | 1   | 0   | 5.321847 | -4.608781 | -0.204337 |
| 47  | 1   | 0   | 1.569532 | 6.112137  | -0.986899 |
| 48  | 1   | 0   | 3.716596 | -0.063407 | -1.383173 |
| 49  | 1   | 0   | 2.978442 | 5.578728  | 1.203895  |
| 50  | 1   | 0   | 6.939128 | -2.887827 | 1.499295  |
| 51  | 1   | 0   | 4.126873 | 0.949835  | -2.815578 |
| 52  | 1   | 0   | 4.609965 | 1.697122  | 0.120064  |
| 53  | 1   | 0   | 7.083693 | -0.958409 | -1.780524 |
| 54  | 1   | 0   | 7.762487 | -3.097364 | -0.37839  |
| 55  | 1   | 0   | 6.044496 | -2.683802 | -0.011350 |
| 56  | 1   | 0   | 8.674636 | -1.089699 | 2.228845  |
| 57  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 58  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 59  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 60  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 61  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 62  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 63  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 64  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 65  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 66  | 1   | 0   | 3.551787 | -3.250426 | 0.207671  |

| 3b (conformer 27) |
|-------------------|
| 1     | 6   | 0   | 1.986815 | -1.348908 | 0.381024  |
| 2     | 6   | 0   | 1.494859 | 0.028077  | -0.059689 |
| 3     | 6   | 0   | 2.230261 | 1.198912  | 0.587495  |
| 4     | 8   | 0   | 0.099918 | 0.211600  | 0.204473  |
| 5     | 6   | 0   | 1.307503 | -2.034114 | 1.364625  |
| 6     | 6   | 0   | 1.718556 | -3.317538 | 1.789893  |
| 7     | 6   | 0   | 2.813791 | -3.916095 | 1.220657  |
| 8     | 6   | 0   | 3.551787 | -3.250426 | 0.207671  |
| 9     | 6   | 0   | 3.144100 | -1.943292 | -0.218792 |
| 10    | 6   | 0   | 2.975836 | 1.027965  | 1.732552  |
| 11    | 6   | 0   | 3.651600 | 2.107291  | 2.345956  |
|   |   |   | 3.586178 | 3.362493 | 1.799431 |
|---|---|---|----------|----------|----------|
| 12| 6 | 0 | 2.834005 | 3.594956 | 0.618480 |
| 13| 6 | 0 | 2.135684 | 2.505737 | 0.001920 |
| 14| 6 | 0 | 4.690494 | -3.853110| -0.389184|
| 15| 6 | 0 | 5.410411 | -3.201703| -1.360499|
| 16| 6 | 0 | 5.021866 | -1.907999| -1.774451|
| 17| 6 | 0 | 3.923185 | -1.296012| -1.217913|
| 18| 6 | 0 | 2.759071 | 4.889052 | 0.039275 |
| 19| 6 | 0 | 2.026670 | 5.114716 | -1.100284|
| 20| 6 | 0 | 1.330024 | 4.046881 | -1.708230|
| 21| 6 | 0 | 1.380450 | 2.782127 | -1.170007|
| 22| 6 | 0 | 0.766788 | -0.439324| -0.724931|
| 23| 6 | 0 | 3.253069 | -0.658109| -1.809184|
| 24| 6 | 0 | 3.332974 | -2.193975| -1.813100|
| 25| 6 | 0 | 3.636831 | -0.003914| 0.043859 |
| 26| 6 | 0 | 5.021866 | -1.907999| -1.774451|
| 27| 6 | 0 | 3.923185 | -1.296012| -1.217913|
| 28| 6 | 0 | 2.759071 | 4.889052 | 0.039275 |
| 29| 6 | 0 | 2.026670 | 5.114716 | -1.100284|
| 30| 6 | 0 | 1.330024 | 4.046881 | -1.708230|
| 31| 6 | 0 | 1.380450 | 2.782127 | -1.170007|
| 32| 6 | 0 | 0.766788 | -0.439324| -0.724931|
| 33| 6 | 0 | 3.253069 | -0.658109| -1.809184|
| 34| 6 | 0 | 3.332974 | -2.193975| -1.813100|
| 35| 6 | 0 | 3.636831 | -0.003914| 0.043859 |
| 36| 6 | 0 | 5.021866 | -1.907999| -1.774451|
| 37| 6 | 0 | 3.923185 | -1.296012| -1.217913|
| 38| 6 | 0 | 2.759071 | 4.889052 | 0.039275 |
| 39| 6 | 0 | 2.026670 | 5.114716 | -1.100284|
| 40| 6 | 0 | 1.330024 | 4.046881 | -1.708230|
| 41| 6 | 0 | 1.380450 | 2.782127 | -1.170007|
| 42| 6 | 0 | 0.766788 | -0.439324| -0.724931|
| 43| 6 | 0 | 3.253069 | -0.658109| -1.809184|
| 44| 6 | 0 | 3.332974 | -2.193975| -1.813100|
| 45| 6 | 0 | 3.636831 | -0.003914| 0.043859 |
| 46| 6 | 0 | 5.021866 | -1.907999| -1.774451|
| 47| 6 | 0 | 3.923185 | -1.296012| -1.217913|
| 48| 6 | 0 | 2.759071 | 4.889052 | 0.039275 |
| 49| 6 | 0 | 2.026670 | 5.114716 | -1.100284|
| 50| 6 | 0 | 1.330024 | 4.046881 | -1.708230|
| 51| 6 | 0 | 1.380450 | 2.782127 | -1.170007|
| 52| 6 | 0 | 0.766788 | -0.439324| -0.724931|
| 53| 6 | 0 | 3.253069 | -0.658109| -1.809184|
| 54| 6 | 0 | 3.332974 | -2.193975| -1.813100|
| 55| 6 | 0 | 3.636831 | -0.003914| 0.043859 |
| 56| 6 | 0 | 5.021866 | -1.907999| -1.774451|
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 57 | 1 | 0 | -5.309785 | -0.344978 | -1.917004 |
| 58 | 1 | 0 | -5.467859 | -1.339479 | 0.377566  |
| 59 | 1 | 0 | -4.647023 | 0.057953  | 1.043041  |
| 60 | 1 | 0 | -6.515551 | 1.564775  | 0.338071  |
| 61 | 1 | 0 | -8.920246 | -1.732584 | -0.227363 |
| 62 | 1 | 0 | -7.338326 | -2.131212 | 0.452589  |
| 63 | 1 | 0 | -8.690247 | -1.719846 | 1.513809  |
| 64 | 1 | 0 | -9.765136 | 0.724974  | -0.192467 |
| 65 | 1 | 0 | -9.584190 | 0.749028  | 1.555694  |
| 66 | 1 | 0 | -8.750798 | 1.962676  | 0.569550  |

### 3b (conformer 28)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
|  1 | 6 | 0 | 0.992162 | 1.753790 | 1.039315 |
|  2 | 6 | 0 | 1.732600 | 0.422174 | 0.924790 |
|  3 | 6 | 0 | 2.827449 | 0.355459 | -0.139168|
|  4 | 8 | 0 | 0.855813 | -0.695055 | 0.723209 |
|  5 | 6 | 0 | 1.320823 | 2.575339  | 2.097804  |
|  6 | 6 | 0 | 0.699707 | 3.827601  | 2.296787  |
|  7 | 6 | 0 | -0.273388 | 4.252972  | 1.429334  |
|  8 | 6 | 0 | -0.657862 | 3.447041  | 0.326444  |
|  9 | 6 | 0 | -0.022568 | 2.177001  | 0.117514  |
| 10 | 6 | 0 | 3.001336 | 1.361027  | -1.064483 |
| 11 | 6 | 0 | 4.031201 | 1.312663  | -2.031682 |
| 12 | 6 | 0 | 4.901288 | 0.254681  | -2.061625 |
| 13 | 6 | 0 | 4.784579 | -0.798101 | -1.117237 |
| 14 | 6 | 0 | 3.736919 | -0.757098 | -0.139682 |
| 15 | 6 | 0 | -1.657809 | 3.884090  | -0.582565 |
| 16 | 6 | 0 | -2.020723 | 3.114030  | -1.659613 |
| 17 | 6 | 0 | -1.395840 | 1.864303  | -1.871691 |
| 18 | 6 | 0 | -0.428154 | 1.406062  | -1.008697 |
| 19 | 6 | 0 | 5.698052 | -1.885227 | -1.118082 |
| 20 | 6 | 0 | 5.601612 | -2.892929 | -0.190397 |
| 21 | 6 | 0 | 4.576591 | -2.854305 | 0.780607  |
| 22 | 6 | 0 | 3.669247 | -1.820878 | 0.801397  |
| 23 | 6 | 0 | -0.000721 | -0.978022 | 1.830803  |
| 24 | 6 | 0 | -0.633687 | -2.349342 | 1.630021  |
| 25 | 6 | 0 | -1.555753 | -2.503409 | 0.403224  |
| 26 | 6 | 0 | -1.848236 | -3.993268 | 0.167253  |
| 27 | 6 | 0 | -2.847275 | -1.677091 | 0.554426  |
| 28 | 6 | 0 | -3.751656 | -1.650505 | -0.694033 |
| 29 | 6 | 0 | -4.890122 | -0.676833 | -0.553516 |
| 30 | 6 | 0 | -6.205830 | -0.926321 | -0.514866 |
| 31 | 6 | 0 | -6.828557 | -2.295869 | -0.622608 |
| 32 | 6 | 0 | -7.202457 | 0.196803  | -0.356048 |
| 33 | 1 | 0 | 2.228443 | 0.277301  | 1.896787  |
| 34 | 1 | 0 | 2.081298 | 2.251217  | 2.801373  |
| 35 | 1 | 0 | 0.992049 | 4.442472  | 3.140533  |
|   |   |   |   |   |
|---|---|---|---|---|
| 36 | 1 | 0 | -0.762862 | 5.210594 | 1.573296 |
| 37 | 1 | 0 | 2.340153 | 2.217137 | -1.057955 |
| 38 | 1 | 0 | 4.125859 | 2.122388 | -2.746417 |
| 39 | 1 | 0 | 5.695709 | 0.211009 | -2.799460 |
| 40 | 1 | 0 | -2.129200 | 4.846306 | -0.410650 |
| 41 | 1 | 0 | -2.783279 | 3.460661 | -2.348127 |
| 42 | 1 | 0 | -1.683464 | 1.260246 | -2.725106 |
| 43 | 1 | 0 | 4.501503 | -2.746417 | 1.512626 |
| 44 | 1 | 0 | 6.482367 | -1.901460 | -1.867952 |
| 45 | 1 | 0 | 6.307144 | -3.716126 | 0.061215 |
| 46 | 1 | 0 | 4.501503 | -3.650938 | 1.512626 |
| 47 | 1 | 0 | 2.870044 | -1.828524 | 1.537230 |
| 48 | 1 | 0 | 0.592458 | -0.981223 | 2.758178 |
| 49 | 1 | 0 | 6.482367 | -1.901460 | -1.867952 |
| 50 | 1 | 0 | 6.307144 | -3.716126 | 0.061215 |
| 51 | 1 | 0 | 4.501503 | -3.650938 | 1.512626 |
| 52 | 1 | 0 | 2.870044 | -1.828524 | 1.537230 |
| 53 | 1 | 0 | 0.592458 | -0.981223 | 2.758178 |
| 54 | 1 | 0 | 6.482367 | -1.901460 | -1.867952 |
| 55 | 1 | 0 | 6.307144 | -3.716126 | 0.061215 |
| 56 | 1 | 0 | 4.501503 | -3.650938 | 1.512626 |
| 57 | 1 | 0 | 2.870044 | -1.828524 | 1.537230 |
| 58 | 1 | 0 | 0.592458 | -0.981223 | 2.758178 |
| 59 | 1 | 0 | 6.482367 | -1.901460 | -1.867952 |
| 60 | 1 | 0 | 6.307144 | -3.716126 | 0.061215 |
| 61 | 1 | 0 | 4.501503 | -3.650938 | 1.512626 |
| 62 | 1 | 0 | 2.870044 | -1.828524 | 1.537230 |
| 63 | 1 | 0 | 0.592458 | -0.981223 | 2.758178 |
| 64 | 1 | 0 | 6.482367 | -1.901460 | -1.867952 |
| 65 | 1 | 0 | 6.307144 | -3.716126 | 0.061215 |
| 66 | 1 | 0 | 4.501503 | -3.650938 | 1.512626 |

**3b (conformer 29)**

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6 | 0 | -2.791096 | 0.302658 | 0.068450 |
| 2 | 6 | 0 | -1.455296 | 0.200914 | 0.804107 |
| 3 | 6 | 0 | -0.761800 | 1.528487 | 1.107645 |
| 4 | 6 | 0 | -0.618593 | -0.708037 | 0.076668 |
| 5 | 6 | 0 | -3.251570 | 1.501320 | -0.430410 |
| 6 | 6 | 0 | -4.502741 | 1.606051 | -1.080024 |
| 7 | 6 | 0 | -5.303342 | 0.502824 | -1.218152 |
| 8 | 6 | 0 | -4.889297 | -0.753806 | -0.704840 |
| 9 | 6 | 0 | -3.617788 | -0.866370 | -0.052417 |
| 10 | 6 | 0 | -0.839927 | 2.010751 | 2.397646 |
| 11 | 6 | 0 | -0.234667 | 3.227409 | 2.781466 |
| 12 | 6 | 0 | 0.470317 | 3.959868 | 1.861153 |
| 13 | 6 | 0 | 0.590674 | 3.509539 | 0.520790 |
| 14 | 6 | 0 | -0.033145 | 2.278919 | 0.124815 |
|    |    |    |         |         |         |         |         |         |         |         |         |         |         |         |
|----|----|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 15 | 6  | 0  | -5.720993 | -1.899056 | -0.817580 |
| 16 | 6  | 0  | -5.332160 | -3.111113 | -0.302703 |
| 17 | 6  | 0  | -4.083689 | -3.226996 | 0.347625  |
| 18 | 6  | 0  | -3.250331 | -2.139103 | 0.464293  |
| 19 | 6  | 0  | 1.312814  | 4.266237  | -0.440298 |
| 20 | 6  | 0  | 1.417313  | 3.841971  | -1.741795 |
| 21 | 6  | 0  | 0.799342  | 2.634628  | -2.138360 |
| 22 | 6  | 0  | 0.096606  | 1.873353  | -1.234084 |
| 23 | 6  | 0  | 0.488135  | -1.212171 | 0.824566  |
| 24 | 6  | 0  | 1.262441  | -2.177887 | -0.062742 |
| 25 | 6  | 0  | 2.488304  | -2.816222 | 0.621285  |
| 26 | 6  | 0  | 2.075042  | -3.835788 | 1.694413  |
| 27 | 6  | 0  | 3.419811  | -3.484135 | -0.411304 |
| 28 | 6  | 0  | 4.234910  | -2.518333 | 1.782936  |
| 29 | 6  | 0  | 5.268299  | -1.742385 | -0.524805 |
| 30 | 6  | 0  | 5.487116  | -0.420904 | -0.500402 |
| 31 | 6  | 0  | 4.699151  | 0.599840  | -1.281701 |
| 32 | 6  | 0  | 6.596718  | 0.162484  | 0.341148  |
| 33 | 1  | 0  | -1.669121 | -0.255242 | 1.782936  |
| 34 | 1  | 0  | -2.649188 | 2.393558  | -0.324427 |
| 35 | 1  | 0  | -4.821882 | 2.568219  | -1.464541 |
| 36 | 1  | 0  | -6.266226 | 0.574972  | -1.713191 |
| 37 | 1  | 0  | -1.383798 | 1.438627  | 3.142868  |
| 38 | 1  | 0  | -0.325039 | 3.570971  | 3.805788  |
| 39 | 1  | 0  | 0.945707  | 4.893380  | 2.143908  |
| 40 | 1  | 0  | -6.678463 | -1.796133 | -1.317951 |
| 41 | 1  | 0  | -5.977651 | -3.977525 | -0.393314 |
| 42 | 1  | 0  | -3.777320 | -4.184988 | 0.753187  |
| 43 | 1  | 0  | -2.288582 | -2.260677 | 0.941476  |
| 44 | 1  | 0  | 1.779181  | 5.194016  | -0.124882 |
| 45 | 1  | 0  | 1.969255  | 4.430358  | -2.466333 |
| 46 | 1  | 0  | 0.879969  | 2.304888  | -3.168340 |
| 47 | 1  | 0  | -0.360309 | 0.947051  | -1.550370 |
| 48 | 1  | 0  | 1.137948  | -0.387918 | 1.147094  |
| 49 | 1  | 0  | 0.112820  | -1.709867 | 1.731113  |
| 50 | 1  | 0  | 0.584175  | -2.967327 | -0.408103 |
| 51 | 1  | 0  | 1.573418  | -1.623991 | -0.953179 |
| 52 | 1  | 0  | 3.060718  | -2.018952 | 1.113567  |
| 53 | 1  | 0  | 1.440531  | -3.392266 | 2.466047  |
| 54 | 1  | 0  | 1.520838  | -4.668650 | 1.246881  |
| 55 | 1  | 0  | 2.953598  | -4.253163 | 2.194887  |
| 56 | 1  | 0  | 4.123572  | -4.135031 | 0.121796  |
| 57 | 1  | 0  | 2.824248  | -4.145111 | -1.053720 |
| 58 | 1  | 0  | 4.746530  | -3.121240 | -2.059326 |
| 59 | 1  | 0  | 3.565494  | -1.851980 | -1.845070 |
|   |   |   |   |   |
|---|---|---|---|---|
|   |   |   |   |   |
| 60 | 1 | 0 | 5.924631 | -2.362620 | 0.086978 |
| 61 | 1 | 0 | 3.889510 | 0.166900 | -1.867901 |
| 62 | 1 | 0 | 4.264644 | 1.349964 | -0.611207 |
| 63 | 1 | 0 | 5.357342 | 1.143405 | -1.970131 |
| 64 | 1 | 0 | 7.315001 | 0.709778 | -0.281195 |
| 65 | 1 | 0 | 6.201462 | 0.882862 | 1.067390 |
| 66 | 1 | 0 | 7.140820 | -0.609878 | 0.888666 |

3b (conformer 31)

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6 | 0 | 0.825868 | -0.700303 | -0.999806 |
| 2 | 6 | 0 | 1.384458 | 0.729626 | -0.964703 |
| 3 | 6 | 0 | 2.539086 | 0.994598 | 0.009082 |
| 4 | 8 | 0 | 0.353802 | 1.680919 | -0.698246 |
| 5 | 6 | 0 | 0.806232 | -1.350563 | -2.216757 |
| 6 | 6 | 0 | 0.312525 | -2.665637 | -2.362472 |
| 7 | 6 | 0 | -0.173049 | -3.335672 | -1.269841 |
| 8 | 6 | 0 | -0.205147 | -2.708896 | 0.002852 |
| 9 | 6 | 0 | 0.283720 | -1.367073 | 0.149092 |
|10 | 6 | 0 | 2.393156 | 1.947418 | 0.995144 |
|11 | 6 | 0 | 3.432649 | 2.244994 | 1.903680 |
|12 | 6 | 0 | 4.634360 | 1.592298 | 1.817380 |
|13 | 6 | 0 | 4.851029 | 0.626402 | 0.801840 |
|14 | 6 | 0 | 3.799080 | 0.320258 | -0.126051 |
|15 | 6 | 0 | -0.726917 | -3.389424 | 1.134596 |
|16 | 6 | 0 | -0.786305 | -2.779213 | 2.362908 |
|17 | 6 | 0 | -0.330284 | -1.450225 | 2.507034 |
|18 | 6 | 0 | 0.186718 | -0.764346 | 1.432921 |
|19 | 6 | 0 | 6.104358 | -0.029526 | 0.680479 |
|20 | 6 | 0 | 6.336754 | -0.941330 | -0.319243 |
|21 | 6 | 0 | 5.313656 | -1.234016 | -1.246764 |
|22 | 6 | 0 | 4.084344 | -0.624263 | -1.150774 |
|23 | 6 | 0 | -0.574606 | 1.875046 | -1.764809 |
|24 | 6 | 0 | -1.495013 | 3.032465 | -1.400417 |
|25 | 6 | 0 | -2.452445 | 2.775789 | -0.217259 |
|26 | 6 | 0 | -2.977795 | 4.113769 | 0.324514 |
|27 | 6 | 0 | -3.601404 | 1.830529 | -0.622190 |
|28 | 6 | 0 | -4.427829 | 1.271968 | 0.553197 |
|29 | 6 | 0 | -5.588875 | 0.433811 | 0.091258 |
|30 | 6 | 0 | -5.808769 | -0.873460 | 0.284948 |
|31 | 6 | 0 | -4.893351 | -1.798434 | 1.046545 |
|32 | 6 | 0 | -7.046228 | -1.539135 | -0.267519 |
|33 | 1 | 0 | 1.772261 | 0.928008 | -1.975507 |
|34 | 1 | 0 | 1.192520 | -0.840558 | -3.094299 |
|35 | 1 | 0 | 0.324449 | -3.137811 | -3.338366 |
|36 | 1 | 0 | -0.546211 | -4.350241 | -1.363278 |
|37 | 1 | 0 | 1.456059 | 2.481742 | 1.068517 |
|38 | 1 | 0 | 3.269526 | 2.995961 | 2.668839 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 39 | 1 | 0 | 5.438156 | 1.812325 | 2.512189 |
| 40 | 1 | 0 | -1.083808 | -4.406347 | 1.007830 |
| 41 | 1 | 0 | -1.186699 | -1.083808 | 1.007830 |
| 42 | 1 | 0 | 0.520049  | 0.253031  | 1.565460 |
| 43 | 1 | 0 | 6.883819  | 0.211549  | 1.396018 |
| 44 | 1 | 0 | 7.299908  | -1.432299 | -0.401304|
| 45 | 1 | 0 | 5.497283  | -1.948464 | -2.041652|
| 46 | 1 | 0 | 3.321978  | -0.881392 | 3.475327 |
| 47 | 1 | 0 | -0.388279 | -0.965331 | 3.475327 |
| 48 | 1 | 0 | -1.139155 | 0.953346  | -1.950583|
| 49 | 1 | 0 | -0.021850 | 2.114912  | -2.685350|
| 50 | 1 | 0 | 2.081412  | 3.294736  | -2.290749|
| 51 | 1 | 0 | -0.863672 | 3.899587  | -1.178131|
| 52 | 1 | 0 | -1.872889 | 2.289857  | 0.576814 |
| 53 | 1 | 0 | -3.641503 | 3.979405  | 1.182001 |
| 54 | 1 | 0 | -3.537567 | 4.653577  | -0.448043|
| 55 | 1 | 0 | -2.153271 | 4.756698  | 0.646400 |
| 56 | 1 | 0 | -4.267642 | 2.362533  | -1.315260|
| 57 | 1 | 0 | -3.200893 | 0.979097  | -1.182254|
| 58 | 1 | 0 | -3.768105 | 0.706618  | 1.216441 |
| 59 | 1 | 0 | -4.819898 | 2.105729  | 1.148142 |
| 60 | 1 | 0 | -6.335743 | 0.980825  | -0.484688|
| 61 | 1 | 0 | -5.409316 | -2.215623 | 1.919938 |
| 62 | 1 | 0 | -3.979632 | -1.317579 | 1.393368 |
| 63 | 1 | 0 | -4.604095 | -2.650482 | 0.420570 |
| 64 | 1 | 0 | -6.781445 | -2.349916 | -0.956937|
| 65 | 1 | 0 | -7.639585 | -1.993596 | 0.535154 |
| 66 | 1 | 0 | -7.683611 | -0.831978 | -0.802399|

**3b (conformer 36)**

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1  | 6 | 0 | 2.350319 | -0.475265 | 0.258776 |
| 2  | 6 | 0 | 1.726768 | 0.325962  | -0.883911|
| 3  | 6 | 0 | 1.710577 | 1.842828  | -0.701168|
| 4  | 8 | 0 | 0.428708 | -0.221942 | -1.149726|
| 5  | 6 | 0 | 2.713387 | 0.121597  | 1.446182 |
| 6  | 6 | 0 | 3.318950 | -0.610039 | 2.493130 |
| 7  | 6 | 0 | 3.573256 | -1.947948 | 2.343275 |
| 8  | 6 | 0 | 3.240965 | -2.610595 | 1.133174|
| 9  | 6 | 0 | 2.621693 | -1.873843 | 0.070730 |
| 10 | 6 | 0 | 2.637012 | 2.580730  | -1.408466|
| 11 | 6 | 0 | 2.710854 | 3.987224  | -1.307633|
| 12 | 6 | 0 | 1.834293 | 4.660944  | -0.496419|
| 13 | 6 | 0 | 0.854306 | 3.955343  | 0.248941 |
| 14 | 6 | 0 | 0.781132 | 2.525052  | 0.153281 |
| 15 | 6 | 0 | 3.524399 | -3.990414 | 0.954819 |
| 16 | 6 | 0 | 3.225997 | -4.629001 | -0.223515|
| 17 | 6 | 0 | 2.625225 | -3.906457 | -1.277994|

5258
|   |   |   | 2.328177 | -2.571342 | -1.133126 |
|---|---|---|---|---|---|
|18 | 6 | 0 | -0.052392 | 4.644329 | 1.097724 |
|19 | 6 | 0 | -0.993087 | 3.963157 | 1.829754 |
|20 | 6 | 0 | -1.068362 | 2.554966 | 1.739883 |
|21 | 6 | 0 | -0.209886 | 1.854822 | 0.925194 |
|22 | 6 | 0 | -0.123136 | 0.159569 | -2.410802 |
|23 | 6 | 0 | -1.352457 | -0.694369 | -2.693745 |
|24 | 6 | 0 | -2.544356 | -0.508365 | -1.733474 |
|25 | 6 | 0 | -1.068362 | 2.554966 | 1.739883 |
|26 | 6 | 0 | -0.209886 | 1.854822 | 0.925194 |
|27 | 6 | 0 | -0.123136 | 0.159569 | -2.410802 |
|28 | 6 | 0 | -1.352457 | -0.694369 | -2.693745 |
|29 | 6 | 0 | -2.544356 | -0.508365 | -1.733474 |
|30 | 6 | 0 | -1.068362 | 2.554966 | 1.739883 |
|31 | 6 | 0 | -0.209886 | 1.854822 | 0.925194 |
|32 | 6 | 0 | -0.123136 | 0.159569 | -2.410802 |
|33 | 1 | 0 | 2.348559 | 0.141880 | -1.773592 |
|34 | 1 | 0 | 2.537982 | 1.179048 | 3.413598 |
|35 | 1 | 0 | 3.581080 | -0.100596 | 3.413598 |
|36 | 1 | 0 | 4.039192 | -2.516795 | 3.141276 |
|37 | 1 | 0 | 3.333182 | 2.066070 | -2.063418 |
|38 | 1 | 0 | 3.457553 | 4.526738 | -1.879301 |
|39 | 1 | 0 | 1.876448 | 5.742008 | -0.413424 |
|40 | 1 | 0 | 3.989329 | -4.532945 | 1.771669 |
|41 | 1 | 0 | 3.449977 | -5.682518 | -0.347956 |
|42 | 1 | 0 | 2.390764 | -4.411503 | -2.208632 |
|43 | 1 | 0 | 1.844396 | -2.047541 | -1.944931 |
|44 | 1 | 0 | 0.015231 | 5.725679 | 1.159074 |
|45 | 1 | 0 | -1.677715 | 4.501122 | 2.476027 |
|46 | 1 | 0 | -1.812754 | 2.019943 | 2.319030 |
|47 | 1 | 0 | -0.287723 | 0.779295 | 0.859045 |
|48 | 1 | 0 | 0.627317 | -0.004727 | -3.199711 |
|49 | 1 | 0 | -0.362307 | 1.229907 | -2.411565 |
|50 | 1 | 0 | -1.677917 | -0.479559 | -3.720604 |
|51 | 1 | 0 | -1.039852 | -1.744326 | -2.678356 |
|52 | 1 | 0 | -2.167641 | -0.620420 | -0.710955 |
|53 | 1 | 0 | -3.984635 | 1.033850 | -1.157723 |
|54 | 1 | 0 | -2.438457 | 1.678281 | -1.677355 |
|55 | 1 | 0 | -3.571846 | 1.038435 | -2.876903 |
|56 | 1 | 0 | -3.997271 | -1.508663 | -2.987876 |
|57 | 1 | 0 | -3.055677 | -2.589675 | -1.976756 |
|58 | 1 | 0 | -5.330018 | -0.784949 | -0.998163 |
|59 | 1 | 0 | -5.414022 | -2.502187 | -1.304041 |
|60 | 1 | 0 | -3.601785 | -2.862064 | 0.502414 |
|61 | 1 | 0 | -5.054784 | 0.609989 | 2.194428 |
|62 | 1 | 0 | -5.922883 | 0.121403 | 0.732897 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 63 | 1  | 0 | -6.418800 | -0.489794 | 2.313395 |
| 64 | 1  | 0 | -3.498471 | -1.088679 | 3.403111 |
| 65 | 1  | 0 | -4.860758 | -2.184616 | 3.582319 |
| 66 | 1  | 0 | -3.386584 | -2.739438 | 2.769995 |

### 3b (conformer 37)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6  | 0 | 1.273867 | 1.684953 | 0.157195 |
| 2 | 6  | 0 | 1.174339 | 0.256052 | 0.689845 |
| 3 | 6  | 0 | 2.493562 | -0.369573 | 1.144912 |
| 4 | 8  | 0 | 0.485326 | -0.528930 | -0.293233 |
| 5 | 6  | 0 | 2.490569 | 2.274756 | -0.106948 |
| 6 | 6  | 0 | 2.587510 | 3.602848 | -0.580676 |
| 7 | 6  | 0 | 1.455906 | 4.349816 | -0.777678 |
| 8 | 6  | 0 | 0.176964 | 3.801712 | -0.499421 |
| 9 | 6  | 0 | 0.073633 | 2.452298 | -0.026840 |
| 10 | 6  | 0 | 2.739413 | -0.413958 | 2.501700 |
| 11 | 6  | 0 | 3.928130 | -0.960724 | 3.031860 |
| 12 | 6  | 0 | 4.873977 | -1.485171 | 2.188812 |
| 13 | 6  | 0 | 4.671807 | -1.476160 | 0.784407 |
| 14 | 6  | 0 | 3.469632 | -0.909640 | 0.241506 |
| 15 | 6  | 0 | -1.001760 | 4.574790 | -0.669751 |
| 16 | 6  | 0 | -2.238463 | 4.055646 | -0.376193 |
| 17 | 6  | 0 | -2.346113 | 2.729433 | 0.097538 |
| 18 | 6  | 0 | -1.224876 | 1.949426 | 0.259581 |
| 19 | 6  | 0 | 5.648285 | -2.014410 | -0.095527 |
| 20 | 6  | 0 | 5.462232 | -1.997242 | -1.455505 |
| 21 | 6  | 0 | 4.283224 | -1.436145 | -1.995496 |
| 22 | 6  | 0 | 3.314490 | -0.908774 | -1.74107 |
| 23 | 6  | 0 | 0.051335 | -1.808115 | 0.173845 |
| 24 | 6  | 0 | -0.613384 | -2.550523 | -0.978111 |
| 25 | 6  | 0 | -1.950598 | -1.970169 | -1.484345 |
| 26 | 6  | 0 | -2.277727 | -2.556927 | -2.866015 |
| 27 | 6  | 0 | -3.082795 | -2.219971 | -0.468580 |
| 28 | 6  | 0 | -4.429791 | -1.549649 | -0.802491 |
| 29 | 6  | 0 | -5.474863 | -1.825125 | 0.244715 |
| 30 | 6  | 0 | -6.220850 | -0.956671 | 0.940234 |
| 31 | 6  | 0 | -6.164417 | 0.542888 | 0.789830 |
| 32 | 6  | 0 | -7.220953 | -1.440287 | 1.962721 |
| 33 | 1  | 0 | 0.540197 | 0.293974 | 1.588691 |
| 34 | 1  | 0 | 3.403365 | 1.716890 | 0.052394 |
| 35 | 1  | 0 | 3.565956 | 4.023594 | -0.783309 |
| 36 | 1  | 0 | 1.520946 | 5.371052 | -1.138584 |
| 37 | 1  | 0 | 1.996175 | -0.016229 | 3.185693 |
| 38 | 1  | 0 | 4.081265 | -0.970369 | 4.105102 |
| 39 | 1  | 0 | 5.788745 | -1.915707 | 2.582747 |
| 40 | 1  | 0 | -0.905205 | 5.593017 | -1.032505 |
| 41 | 1  | 0 | -3.130537 | 4.658177 | -0.505561 |
|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
| 42| 1 | 0 | -3.322908 | 2.322272 | 0.333041 |
| 43| 1 | 0 | -1.336402 | 0.928765 | 0.597125 |
| 44| 1 | 0 | 6.550882  | -2.440107| 0.330792 |
| 45| 1 | 0 | 6.216245  | -2.410561| -2.116070|
| 46| 1 | 0 | 4.140708  | -1.421116| -3.070433|
| 47| 1 | 0 | 2.414201  | -0.492124| -1.601704|
| 48| 1 | 0 | -0.633466 | -1.674117| 1.024956 |
| 49| 1 | 0 | 0.909768  | -2.386595| 0.535784 |
| 50| 1 | 0 | 0.105277  | -2.579428| -1.803935|
| 51| 1 | 0 | -0.766994 | -3.591901| -0.666378|
| 52| 1 | 0 | -1.820422 | -0.887272| -1.598963|
| 53| 1 | 0 | -3.189051 | -2.129061| -3.289950|
| 54| 1 | 0 | -1.465870 | -2.362284| -3.572724|
| 55| 1 | 0 | -2.414949 | -3.643162| -2.808108|
| 56| 1 | 0 | -3.236431 | -3.303705| -0.371602|
| 57| 1 | 0 | -2.770135 | -1.871539| 0.521901 |
| 58| 1 | 0 | -4.274626 | -0.476019| -0.939093 |
| 59| 1 | 0 | -4.793205 | -1.931013| -1.764846|
| 60| 1 | 0 | -5.629360 | -2.884156| 0.452943 |
| 61| 1 | 0 | -5.911394 | 1.017244 | 1.745570 |
| 62| 1 | 0 | -5.441521 | 0.873031 | 0.044318 |
| 63| 1 | 0 | -7.146036 | 0.935748 | 0.499288 |
| 64| 1 | 0 | -7.230245 | -2.529549| 2.037781 |
| 65| 1 | 0 | -6.996598 | -1.031632| 2.955412 |
| 66| 1 | 0 | -8.234704 | -1.106966| 1.709986 |

3b (conformer 38)

|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
| 1 | 6 | 0 | -1.592496 | 1.589876| -0.397888|
| 2 | 6 | 0 | -1.042392 | 0.185588| -0.645921|
| 3 | 6 | 0 | -2.077807 | -0.864765| -1.049826|
| 4 | 8 | 0 | -0.274405 | -0.193307| 0.504398 |
| 5 | 6 | 0 | -2.946675 | 1.833436 | -0.328784|
| 6 | 6 | 0 | -3.459723 | 3.134465 | -0.123623|
| 7 | 6 | 0 | -2.608597 | 4.201113 | -0.000421|
| 8 | 6 | 0 | -1.204689 | 4.012533 | -0.085377|
| 9 | 6 | 0 | -0.679894 | 2.693635 | -0.285648|
|10| 6 | 0 | -2.154203 | -1.200100| -2.385830|
|11| 6 | 0 | -3.082273 | -2.147493| -2.870090|
|12| 6 | 0 | -3.933441 | -2.776864| -1.998458|
|13| 6 | 0 | -3.894096 | -2.479757| -0.611540|
|14| 6 | 0 | -2.958083 | -1.509720| -0.117404|
|15| 6 | 0 | -0.312040 | 5.112209 | 0.014051 |
|16| 6 | 0 | 1.045713  | 4.934894 | -0.088671|
|17| 6 | 0 | 1.568807  | 3.638817 | -0.292802|
|18| 6 | 0 | 0.731153  | 2.551658 | -0.383127|
|19| 6 | 0 | -4.775622 | -3.124082| 0.296842 |
|20| 6 | 0 | -4.749052 | -2.830638| 1.637632|
|   |   |   |   |   |
|---|---|---|---|---|
| 21| 6 | 0 | -3.832434 | -1.873901 | 2.128770 |
| 22| 6 | 0 | -2.961372 | -1.232717 | 1.279550 |
| 23| 6 | 0 | 0.571270 | -1.326394 | 3.555251 |
| 24| 6 | 0 | 1.295241 | -1.642529 | 1.602976 |
| 25| 6 | 0 | 2.239446 | -0.546030 | 2.134507 |
| 26| 6 | 0 | 2.709169 | -0.895472 | 3.555251 |
| 27| 6 | 0 | 3.423790 | -0.228329 | 1.193816 |
| 28| 6 | 0 | 4.410454 | -1.381719 | 0.915755 |
| 29| 6 | 0 | 5.579836 | -0.933996 | 0.081136 |
| 30| 6 | 0 | 5.946711 | -1.344621 | 1.140229 |
| 31| 6 | 0 | 5.228051 | -2.376934 | 0.007314 |
| 32| 6 | 0 | 7.162941 | -1.381719 | 0.915755 |
| 33| 1 | 0 | -0.349504 | 0.260606 | 1.497689 |
| 34| 1 | 0 | -3.645626 | 1.015059 | 0.436770 |
| 35| 1 | 0 | -4.532866 | 3.278549 | -0.068023 |
| 36| 1 | 0 | -2.994326 | 5.203363 | 0.155028 |
| 37| 1 | 0 | -1.481428 | -0.719787 | -3.089493 |
| 38| 1 | 0 | -3.110419 | 2.376934 | -3.929321 |
| 39| 1 | 0 | -4.647483 | -3.511505 | -2.355868 |
| 40| 1 | 0 | -0.726775 | 6.102965 | 0.169287 |
| 41| 1 | 0 | 1.716478 | 5.783421 | -0.013562 |
| 42| 1 | 0 | 2.641199 | 3.498795 | -0.372410 |
| 43| 1 | 0 | 1.157882 | 1.567577 | -0.513345 |
| 44| 1 | 0 | -5.476364 | -3.855503 | -0.092542 |
| 45| 1 | 0 | -5.428503 | -3.328842 | 2.320168 |
| 46| 1 | 0 | -3.815829 | -1.642664 | 3.188157 |
| 47| 1 | 0 | -2.259414 | -0.511421 | 1.671847 |
| 48| 1 | 0 | -0.027033 | -2.192760 | -0.007314 |
| 49| 1 | 0 | 1.278865 | -1.111620 | -0.514926 |
| 50| 1 | 0 | 0.535246 | -1.850396 | 2.364077 |
| 51| 1 | 0 | 1.846331 | -2.580053 | 1.461750 |
| 52| 1 | 0 | 1.649083 | 0.374172 | 2.204000 |
| 53| 1 | 0 | 1.856771 | -0.975586 | 4.236278 |
| 54| 1 | 0 | 3.242900 | -1.850644 | 3.587335 |
| 55| 1 | 0 | 3.379135 | -0.125948 | 3.950896 |
| 56| 1 | 0 | 3.043442 | 0.137207 | 0.233953 |
| 57| 1 | 0 | 3.980924 | 0.611531 | 1.626415 |
| 58| 1 | 0 | 4.792928 | -1.765080 | 1.869856 |
| 59| 1 | 0 | 3.889268 | -2.215276 | 0.440026 |
| 60| 1 | 0 | 6.192868 | -0.162594 | 0.547674 |
| 61| 1 | 0 | 5.896892 | -3.235582 | -2.169202 |
| 62| 1 | 0 | 4.342775 | -2.792282 | -1.454653 |
| 63| 1 | 0 | 4.917530 | -1.985398 | -2.918860 |
| 64| 1 | 0 | 7.898008 | -1.543853 | -2.046555 |
| 65| 1 | 0 | 6.895351 | -0.298424 | -2.776378 |
|      |   |   |           |           |           |
|------|---|---|-----------|-----------|-----------|
| 66   | 1 | 0 | 7.650779  | -0.007339 | -1.199446 |
| **3b** (conformer 40) |   |   |           |           |           |
|  1   | 6 | 0 | -2.757739 | 0.078153  | 0.709925  |
|  2   | 6 | 0 | -1.352397 | 0.645245  | 0.910751  |
|  3   | 6 | 0 | -0.953937 | 1.779768  | -0.032579 |
|  4   | 8 | 0 | -0.327369 | -0.356127 | 0.847245  |
|  5   | 6 | 0 | -3.735388 | 0.473818  | 1.599144  |
|  6   | 6 | 0 | -5.067702 | 0.016925  | 1.502001  |
|  7   | 6 | 0 | -5.417782 | -0.861002 | 0.508490  |
|  8   | 6 | 0 | -4.452128 | -1.311422 | -0.428686 |
|  9   | 6 | 0 | -3.098973 | -0.840345 | -0.338940 |
| 10   | 6 | 0 | -1.722972 | 2.118225  | -1.124315 |
| 11   | 6 | 0 | -1.367891 | 3.183126  | -1.983582 |
| 12   | 6 | 0 | -0.240003 | 3.921624  | -1.738812 |
| 13   | 6 | 0 | 0.578652  | 3.631376  | -0.616623 |
| 14   | 6 | 0 | 0.226056  | 2.547985  | 0.253336  |
| 15   | 6 | 0 | -4.807039 | -2.219084 | -1.461939 |
| 16   | 6 | 0 | -3.878149 | -2.648728 | -2.376914 |
| 17   | 6 | 0 | -2.545954 | -2.184754 | -2.295808 |
| 18   | 6 | 0 | -2.165233 | -1.308377 | -1.306798 |
| 19   | 6 | 0 | 1.736099  | 4.404702  | -0.363332 |
| 20   | 6 | 0 | 2.518147  | 4.138507  | 0.760518  |
| 21   | 6 | 0 | 2.172202  | 3.077053  | 1.625645  |
| 22   | 6 | 0 | 1.062868  | 2.303210  | 1.376335  |
| 23   | 6 | 0 | -0.376422 | -1.317334 | 1.903652  |
| 24   | 6 | 0 | 0.781561  | -2.292372 | 1.730991  |
| 25   | 6 | 0 | 2.190352  | -1.684579 | 1.880212  |
| 26   | 6 | 0 | 2.486349  | -1.298781 | 3.337520  |
| 27   | 6 | 0 | 3.282074  | -2.645909 | 1.366511  |
| 28   | 6 | 0 | 3.291975  | -2.931276 | -0.153052 |
| 29   | 6 | 0 | 3.504821  | -1.709358 | -1.006676 |
| 30   | 6 | 0 | 4.584551  | -1.381369 | -1.729868 |
| 31   | 6 | 0 | 5.840992  | -2.209657 | -1.832435 |
| 32   | 6 | 0 | 4.618073  | -0.101863 | -2.530504 |
| 33   | 1 | 0 | -1.345015 | 1.061960  | 1.929414  |
| 34   | 1 | 0 | -3.474040 | 1.159088  | 2.399425  |
| 35   | 1 | 0 | -5.804717 | 0.357656  | 2.220411  |
| 36   | 1 | 0 | -6.436478 | -1.225367 | 0.425701  |
| 37   | 1 | 0 | -2.627027 | 1.563752  | -1.337717 |
| 38   | 1 | 0 | -1.998676 | 3.409583  | -2.835813 |
| 39   | 1 | 0 | 0.038318  | 4.741809  | -2.392471 |
| 40   | 1 | 0 | -5.833672 | -2.566625 | -1.515732 |
| 41   | 1 | 0 | -4.162741 | -3.341022 | -3.161414 |
| 42   | 1 | 0 | -1.815163 | -2.523917 | -3.021686 |
| 43   | 1 | 0 | -1.140636 | -0.971026 | -1.250764 |
| 44   | 1 | 0 | 1.989711  | 5.218730  | -1.007766 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 45 | 1 | 0 | 3.398144 | 4.738113 | 0.964553 |
| 46 | 1 | 0 | 2.790657 | 2.867160 | 2.491311 |
| 47 | 1 | 0 | 0.834301 | 1.481685 | 2.039701 |
| 48 | 1 | 0 | -0.329394 | -0.797240 | 2.872520 |
| 49 | 1 | 0 | -1.327824 | -1.862478 | 1.873071 |
| 50 | 1 | 0 | 0.655453 | -3.100067 | 2.464226 |
| 51 | 1 | 0 | 0.671826 | -2.751760 | 1.873071 |
| 52 | 1 | 0 | 0.671826 | -2.751760 | 1.873071 |
| 53 | 1 | 0 | 2.225715 | -0.772786 | 1.275933 |
| 54 | 1 | 0 | 3.460570 | -0.808422 | 3.420711 |
| 55 | 1 | 0 | 1.739215 | -0.611986 | 3.744843 |
| 56 | 1 | 0 | 1.332207 | 0.273293 | 0.740588 |
| 57 | 1 | 0 | 2.630094 | -0.444738 | 1.111686 |
| 58 | 1 | 0 | 5.802990 | -3.129611 | -1.249348 |
| 59 | 1 | 0 | 6.039520 | -2.479610 | -2.876611 |
| 60 | 1 | 0 | 6.708768 | -1.632402 | -1.491736 |
| 61 | 1 | 0 | 3.694050 | 0.468792 | -2.421323 |
| 62 | 1 | 0 | 5.452709 | 0.536498 | -2.216318 |
| 63 | 1 | 0 | 4.769041 | -0.310283 | -3.596789 |
|   |   |   |   |   |   |
| 3b (conformer 41) |   |   |   |   |   |
| 1 | 6 | 0 | 1.494684 | 1.668054 | 0.138926 |
| 2 | 6 | 0 | 1.332207 | 0.273293 | 0.740588 |
| 3 | 6 | 0 | 2.630094 | -0.444738 | 1.111686 |
| 4 | 8 | 0 | 0.501184 | -0.489237 | -0.145279 |
| 5 | 6 | 0 | 2.721733 | 2.143920 | -0.268171 |
| 6 | 6 | 0 | 2.874899 | 3.441588 | -0.807353 |
| 7 | 6 | 0 | 1.792124 | 4.272914 | -0.925323 |
| 8 | 6 | 0 | 0.507810 | 3.843653 | -0.501032 |
| 9 | 6 | 0 | 0.346333 | 2.525256 | 0.037748 |
| 10 | 6 | 0 | 2.987347 | -0.461439 | 2.444185 |
| 11 | 6 | 0 | 4.165465 | -1.093405 | 2.897603 |
| 12 | 6 | 0 | 4.986195 | -1.730837 | 2.002904 |
| 13 | 6 | 0 | 4.665240 | -1.754553 | 0.620961 |
| 14 | 6 | 0 | 3.474054 | -1.102596 | 0.155080 |
| 15 | 6 | 0 | -0.617740 | 4.704571 | -0.591007 |
| 16 | 6 | 0 | -1.857124 | 4.298698 | -0.161413 |
| 17 | 6 | 0 | -2.021776 | 3.002850 | 0.375990 |
| 18 | 6 | 0 | -0.953522 | 2.141231 | 0.466934 |
| 19 | 6 | 0 | 5.512196 | -2.409352 | -0.312477 |
| 20 | 6 | 0 | 5.212090 | -2.423894 | -1.651953 |
| 21 | 6 | 0 | 4.043876 | -1.778860 | -2.116668 |
| 22 | 6 | 0 | 3.197952 | -1.138647 | -1.241611 |
| 23 | 6 | 0 | -0.028326 | 1.684855 | 0.429792 |

5264
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 24 | 6 | 0 | -0.826475 | -2.429377 | -0.632278 |   |
| 25 | 6 | 0 | -2.071691 | -1.703116 | -1.182444 |   |
| 26 | 6 | 0 | -2.546293 | -2.397544 | -2.467895 |   |
| 27 | 6 | 0 | -3.190412 | -1.683050 | -0.429828 |   |
| 28 | 6 | 0 | -4.396097 | -0.745463 | -0.521730 |   |
| 29 | 6 | 0 | -5.376175 | -0.577525 | 0.607005 |   |
| 30 | 6 | 0 | -6.655077 | -0.971260 | 0.673550 |   |
| 31 | 6 | 0 | -7.397344 | -1.683050 | -0.429828 |   |
| 32 | 6 | 0 | -7.479761 | -0.717149 | 1.912325 |   |
| 33 | 1 | 0 | 0.783762 | 0.397596 | 1.686426 |   |
| 34 | 1 | 0 | 3.598972 | 1.517922 | -0.174734 |   |
| 35 | 1 | 0 | 3.858085 | 3.772057 | -1.122946 |   |
| 36 | 1 | 0 | 1.901800 | 5.271674 | -1.335052 |   |
| 37 | 1 | 0 | 2.342818 | 0.025463 | 0.521730 |   |
| 38 | 1 | 0 | 4.408878 | -1.078416 | 3.953981 |   |
| 39 | 1 | 0 | 5.890904 | -2.227187 | 2.338335 |   |
| 40 | 1 | 0 | -0.477517 | 5.698391 | -1.003751 |   |
| 41 | 1 | 0 | -2.707981 | 4.966874 | 0.232591 |   |
| 42 | 1 | 0 | -3.001290 | 2.683651 | 0.714631 |   |
| 43 | 1 | 0 | -1.111101 | 1.146416 | 0.858785 |   |
| 44 | 1 | 0 | 6.408111 | -2.898597 | 0.055789 |   |
| 45 | 1 | 0 | 5.868047 | -2.926261 | 2.354130 |   |
| 46 | 1 | 0 | 3.811741 | -1.789114 | -3.175946 |   |
| 47 | 1 | 0 | 2.302574 | -0.659705 | -1.610109 |   |
| 48 | 1 | 0 | 0.787443 | -2.323923 | 0.789584 |   |
| 49 | 1 | 0 | -0.648316 | -1.426393 | 1.301794 |   |
| 50 | 1 | 0 | -0.144348 | -2.650164 | -1.460286 |   |
| 51 | 1 | 0 | -1.125180 | -3.398740 | -0.211842 |   |
| 52 | 1 | 0 | -1.768977 | -0.681351 | -1.440183 |   |
| 53 | 1 | 0 | -3.386437 | -1.875053 | -2.931396 |   |
| 54 | 1 | 0 | -1.741082 | -2.440541 | -3.207008 |   |
| 55 | 1 | 0 | -2.864807 | -3.426321 | -2.262880 |   |
| 56 | 1 | 0 | -3.545162 | -2.635477 | 0.103228 |   |
| 57 | 1 | 0 | -2.778691 | -1.229186 | 0.810479 |   |
| 58 | 1 | 0 | -4.019942 | 0.243784 | -0.816719 |   |
| 59 | 1 | 0 | -4.886121 | -1.160381 | -1.403973 |   |
| 60 | 1 | 0 | -4.968348 | -0.779991 | 1.486319 |   |
| 61 | 1 | 0 | -7.790796 | -2.640974 | -0.069821 |   |
| 62 | 1 | 0 | -8.263784 | -1.093506 | -0.752633 |   |
| 63 | 1 | 0 | -6.782234 | -1.881816 | -1.306993 |   |
| 64 | 1 | 0 | -7.849688 | -1.657756 | 2.337830 |   |
| 65 | 1 | 0 | -6.905928 | -0.197906 | 2.682679 |   |
| 66 | 1 | 0 | -8.363802 | -0.111467 | 1.679063 |   |

**3b (conformer 42)**

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.798916 | 1.028889 | -0.646543 |   |
| 2 | 6 | 0 | 0.586212 | -0.131153 | 0.333311 |   |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 3 | 6 | 0 | 1.844907 | -0.699622 | 1.006428 |
| 4 | 8 | 0 | -0.150094 | -1.148471 | -0.345352 |
| 5 | 6 | 0 | 0.445043 | 0.878152 | -1.970722 |
| 6 | 6 | 0 | 0.601531 | 1.922726 | -2.908170 |
| 7 | 6 | 0 | 1.103393 | 3.135411 | -2.514384 |
| 8 | 6 | 0 | 1.453130 | 3.357040 | -1.158089 |
| 9 | 6 | 0 | 1.297621 | 2.298770 | -0.200430 |
| 10 | 6 | 0 | 1.892424 | -0.692581 | 2.385395 |
| 11 | 6 | 0 | 2.998917 | -1.193393 | 3.105806 |
| 12 | 6 | 0 | 4.070376 | -1.717086 | 2.430411 |
| 13 | 6 | 0 | 4.065200 | -1.779877 | 1.012883 |
| 14 | 6 | 0 | 2.938204 | -1.279081 | 0.280037 |
| 15 | 6 | 0 | 1.939252 | 4.620854 | -0.731220 |
| 16 | 6 | 0 | 2.250632 | 4.856165 | 0.585033 |
| 17 | 6 | 0 | 2.085502 | 3.825413 | 1.535492 |
| 18 | 6 | 0 | 1.626161 | 2.586541 | 1.153235 |
| 19 | 6 | 0 | 5.161507 | -2.346093 | 0.308337 |
| 20 | 6 | 0 | 5.153158 | -2.436999 | -1.061435 |
| 21 | 6 | 0 | 4.033964 | -1.966921 | -1.780687 |
| 22 | 6 | 0 | 2.959619 | -1.407046 | -1.135518 |
| 23 | 6 | 0 | -0.728083 | -2.139599 | 0.502423 |
| 24 | 6 | 0 | -1.634905 | -3.032122 | -0.335486 |
| 25 | 6 | 0 | -2.830763 | -2.335014 | -1.016499 |
| 26 | 6 | 0 | -3.473570 | -3.291250 | -2.032505 |
| 27 | 6 | 0 | -3.854222 | -1.815449 | 0.012256 |
| 28 | 6 | 0 | -4.944853 | -0.893726 | -0.569462 |
| 29 | 6 | 0 | -5.903973 | -0.405060 | 0.481865 |
| 30 | 6 | 0 | -6.117883 | 0.848799 | 0.902736 |
| 31 | 6 | 0 | -5.410835 | 2.070227 | 0.370506 |
| 32 | 6 | 0 | -7.131939 | 1.139956 | 1.982838 |
| 33 | 1 | 0 | -0.044949 | 0.252459 | 1.149222 |
| 34 | 1 | 0 | 0.032512 | -0.066976 | -2.295722 |
| 35 | 1 | 0 | 0.318005 | 1.755303 | -3.941398 |
| 36 | 1 | 0 | 1.228916 | 3.943727 | -3.227207 |
| 37 | 1 | 0 | 1.053949 | -0.283027 | 2.940791 |
| 38 | 1 | 0 | 2.993259 | -1.159059 | 4.189434 |
| 39 | 1 | 0 | 4.931142 | -2.099866 | 2.968800 |
| 40 | 1 | 0 | 2.054720 | 5.405952 | -1.471488 |
| 41 | 1 | 0 | 2.618275 | 5.827304 | 0.896792 |
| 42 | 1 | 0 | 2.325926 | 4.010904 | 2.576540 |
| 43 | 1 | 0 | 1.523534 | 1.817881 | 1.904225 |
| 44 | 1 | 0 | 6.009275 | -2.713192 | 0.877629 |
| 45 | 1 | 0 | 5.993297 | -2.872904 | -1.587501 |
| 46 | 1 | 0 | 4.022103 | -2.050451 | -2.867214 |
| 47 | 1 | 0 | 2.112042 | -1.066533 | -1.708699 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 48 | 1 | 0 | 0.058376 | -2.744348 | 0.970212 |
| 49 | 1 | 0 | -1.286085 | -1.646487 | 1.311090 |
| 50 | 1 | 0 | -1.016544 | -3.510865 | -1.102772 |
| 51 | 1 | 0 | -2.001645 | -3.838715 | 0.313218 |
| 52 | 1 | 0 | -2.434593 | -1.471304 | -1.563366 |
| 53 | 1 | 0 | -2.737190 | -3.638672 | -2.763335 |
| 54 | 1 | 0 | -3.885266 | -4.174545 | 1.530678 |
| 55 | 1 | 0 | -3.885266 | -4.174545 | -2.587532 |
| 56 | 1 | 0 | -4.328862 | -2.672318 | 0.510059 |
| 57 | 1 | 0 | -3.336345 | -1.257438 | 0.798789 |
| 58 | 1 | 0 | -4.466014 | -0.058520 | -1.087758 |
| 59 | 1 | 0 | -5.514928 | -1.440030 | -1.330465 |
| 60 | 1 | 0 | -6.486273 | -1.193040 | 0.959974 |
| 61 | 1 | 0 | -6.130602 | 2.767075 | -0.075434 |
| 62 | 1 | 0 | -4.918363 | 2.613249 | 1.185626 |
| 63 | 1 | 0 | -7.906780 | 1.825519 | 1.618956 |
| 64 | 1 | 0 | -7.621923 | 0.230304 | 2.336106 |
| 65 | 1 | 0 | -6.660642 | 1.630622 | 2.842958 |
| 66 | 1 | 0 |   |   |   |

**3b (conformer 50)**

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1  | 6  | 0  | 2.336535 | 1.412352 | 0.014596 |
| 2  | 6  | 0  | 1.713539 | 0.349093 | 0.918461 |
| 3  | 6  | 0  | 2.456048 | 0.984655 | 0.989918 |
| 4  | 8  | 0  | 0.337320 | 0.197755 | 0.542394 |
| 5  | 6  | 0  | 3.410615 | 1.127708 | -0.799833 |
| 6  | 6  | 0  | 4.011664 | 2.115498 | -1.612788 |
| 7  | 6  | 0  | 3.539376 | 3.401473 | -1.599224 |
| 8  | 6  | 0  | 2.450376 | 3.757598 | -0.761826 |
| 9  | 6  | 0  | 1.833835 | 2.757776 | 0.060131 |
| 10 | 6  | 0  | 3.194809 | 1.246642 | 2.124984 |
| 11 | 6  | 0  | 3.912751 | -2.451334 | 2.290984 |
| 12 | 6  | 0  | 3.876027 | -3.409219 | 1.310473 |
| 13 | 6  | 0  | 3.127749 | -3.197576 | 0.123346 |
| 14 | 6  | 0  | 2.403956 | -1.970615 | -0.051774 |
| 15 | 6  | 0  | 1.970524 | 5.093152 | -0.717372 |
| 16 | 6  | 0  | 0.933434 | 5.446889 | 0.109955 |
| 17 | 6  | 0  | 0.328464 | 4.469002 | 0.930001 |
| 18 | 6  | 0  | 0.761854 | 3.163943 | 0.901597 |
| 19 | 6  | 0  | 3.092254 | -4.180028 | -0.901834 |
| 20 | 6  | 0  | 2.382518 | -3.970885 | -2.058239 |
| 21 | 6  | 0  | 1.671979 | -2.762644 | -2.237503 |
| 22 | 6  | 0  | 1.678524 | -1.791899 | -1.263662 |
| 23 | 6  | 0  | -0.473224 | -0.433592 | 1.534261 |
| 24 | 6  | 0  | -1.929761 | -0.393758 | 1.088500 |
| 25 | 6  | 0  | -2.253092 | -1.198371 | -0.186290 |
| 26 | 6  | 0  | -2.099271 | -2.712615 | 0.024833 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 27 | 6 | 0 | -3.638246 | -0.822886 | -0.758021 |
| 28 | 6 | 0 | -4.856081 | -1.140791 | 0.134210 |
| 29 | 6 | 0 | -6.155656 | -0.807752 | -0.547240 |
| 30 | 6 | 0 | -7.098467 | 0.068941 | -0.176831 |
| 31 | 6 | 0 | -7.042756 | -0.758021 | 1.064384 |
| 32 | 6 | 0 | -8.340645 | 0.269092 | -0.176831 |
| 33 | 1 | 0 | 1.732536 | 0.755814 | 1.941243 |
| 34 | 1 | 0 | 3.815060 | -0.823908 | 0.134210 |
| 35 | 1 | 0 | 4.850052 | 1.844547 | -2.244594 |
| 36 | 1 | 0 | 3.995396 | 4.166365 | -2.244594 |
| 37 | 1 | 0 | 3.226104 | -0.504947 | 2.917040 |
| 38 | 1 | 0 | 4.483348 | -2.614198 | 3.198334 |
| 39 | 1 | 0 | 4.418353 | -4.341708 | 1.427540 |
| 40 | 1 | 0 | 2.446312 | 5.835149 | -1.350407 |
| 41 | 1 | 0 | 0.578271 | 6.470921 | 0.136825 |
| 42 | 1 | 0 | -0.490097 | 4.749453 | 1.583799 |
| 43 | 1 | 0 | 0.263737 | 2.430305 | 1.519004 |
| 44 | 1 | 0 | 3.644160 | -5.102684 | -0.754358 |
| 45 | 1 | 0 | 2.366101 | -4.727917 | -2.834339 |
| 46 | 1 | 0 | 1.113878 | -2.601116 | -3.152974 |
| 47 | 1 | 0 | 1.121127 | -0.878279 | -1.410312 |
| 48 | 1 | 0 | -0.362875 | 0.105144 | 2.488477 |
| 49 | 1 | 0 | -0.133880 | -0.895794 | 0.944710 |
| 50 | 1 | 0 | -2.536448 | -0.759584 | 1.926035 |
| 51 | 1 | 0 | -2.206793 | 0.655127 | 0.932876 |
| 52 | 1 | 0 | -1.522811 | -0.895794 | -0.944710 |
| 53 | 1 | 0 | -2.369358 | -3.260681 | -0.882935 |
| 54 | 1 | 0 | -1.068824 | -2.981852 | 0.267998 |
| 55 | 1 | 0 | -2.737410 | -3.076928 | 0.836296 |
| 56 | 1 | 0 | -3.645552 | 0.249291 | -0.986551 |
| 57 | 1 | 0 | -3.766531 | -1.336787 | -1.718821 |
| 58 | 1 | 0 | -4.854391 | -2.211478 | 0.374404 |
| 59 | 1 | 0 | -4.769169 | -0.613338 | 1.086526 |
| 60 | 1 | 0 | -6.328900 | -1.357247 | -1.472802 |
| 61 | 1 | 0 | -6.133404 | 0.780771 | 1.647117 |
| 62 | 1 | 0 | -7.111358 | 1.986463 | 0.801599 |
| 63 | 1 | 0 | -7.897801 | 0.710026 | 1.716691 |
| 64 | 1 | 0 | -8.426865 | 1.310692 | -1.343790 |
| 65 | 1 | 0 | -8.343763 | -0.371057 | -1.896000 |
| 66 | 1 | 0 | -9.244546 | 0.051528 | -0.429595 |

**3b (conformer 56)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.291062 | 1.467833 | 0.257985 |
| 2 | 6 | 0 | 1.364253 | 0.299382 | 0.591218 |
| 3 | 6 | 0 | 2.056597 | -0.992344 | 1.024716 |
| 4 | 8 | 0 | 0.475773 | 0.114086 | -0.518629 |
| 5 | 6 | 0 | 3.656766 | 1.306697 | 0.176971 |

5268
|   |   |   | 4.519125 | 2.391691 | -0.100809 |
|---|---|---|----------|----------|-----------|
| 7 | 6 | 0 | 4.008508 | 3.649408 | -0.286724 |
| 8 | 6 | 0 | 2.610943 | 3.878084 | -0.193891 |
| 9 | 6 | 0 | 1.731889 | 2.779516 | 0.080573 |
|10 | 6 | 0 | 2.069942 | -1.286789 | 2.372384 |
|11 | 6 | 0 | 2.690532 | -2.448834 | 2.880343 |
|12 | 6 | 0 | 3.291729 | -3.332969 | 0.193891 |
|13 | 6 | 0 | 3.009194 | -3.087305 | 0.624067 |
|14 | 6 | 0 | 2.069942 | -1.286789 | 2.372384 |
|15 | 6 | 0 | 2.071171 | 5.180982 | -0.358349 |
|16 | 6 | 0 | 0.721590 | 5.408580 | -0.247768 |
|17 | 6 | 0 | -0.148997 | 4.331900 | 0.031055 |
|18 | 6 | 0 | 0.341029 | 3.056076 | 0.185296 |
|19 | 6 | 0 | 3.926026 | -3.995473 | -0.271450 |
|20 | 6 | 0 | 3.947319 | -3.755176 | -1.622888 |
|21 | 6 | 0 | 3.339345 | -2.588379 | -2.138315 |
|22 | 6 | 0 | 2.721679 | -1.688289 | -1.301926 |
|23 | 6 | 0 | -0.674672 | -0.678981 | -0.222593 |
|24 | 6 | 0 | -1.547494 | -0.710233 | -1.471568 |
|25 | 6 | 0 | -2.870176 | -1.498424 | -1.343461 |
|26 | 6 | 0 | -2.630734 | -2.998510 | -1.104185 |
|27 | 6 | 0 | -3.816495 | -0.878136 | -0.294453 |
|28 | 6 | 0 | -5.284668 | -1.335074 | -0.411733 |
|29 | 6 | 0 | -6.159506 | -0.745467 | 0.660760 |
|30 | 6 | 0 | -7.177493 | 0.115945 | 0.532764 |
|31 | 6 | 0 | -7.672151 | 0.678704 | -0.776228 |
|32 | 6 | 0 | -7.937373 | 0.601268 | 1.743672 |
|33 | 6 | 0 | 0.755969 | 0.614657 | 1.452920 |
|34 | 6 | 0 | 4.092092 | 0.328612 | 0.332144 |
|35 | 6 | 0 | 5.587517 | 2.217840 | -0.162464 |
|36 | 6 | 0 | 4.663650 | 4.488193 | -0.498178 |
|37 | 6 | 0 | 1.590096 | 0.603703 | 3.066424 |
|38 | 6 | 0 | 2.681152 | -2.638248 | 3.947807 |
|39 | 6 | 0 | 3.767471 | -4.232838 | 2.397536 |
|40 | 6 | 0 | 2.751155 | 5.999902 | -0.569821 |
|41 | 6 | 0 | 0.322480 | 6.408904 | -0.372733 |
|42 | 6 | 0 | -1.214739 | 4.512740 | 0.118233 |
|43 | 6 | 0 | -0.348635 | 2.245347 | 0.371665 |
|44 | 6 | 0 | 4.391508 | -4.887057 | 0.136085 |
|45 | 6 | 0 | 4.429202 | -4.455977 | -2.295513 |
|46 | 6 | 0 | 3.359917 | -2.400669 | -3.206208 |
|47 | 6 | 0 | 2.252020 | -0.806141 | -1.712066 |
|48 | 6 | 0 | -0.367995 | -1.688786 | 0.074296 |
|49 | 6 | 0 | -1.212029 | -0.232448 | 0.627307 |
|50 | 6 | 0 | -1.771010 | 0.323794 | -1.755437 |
|     |     |     |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|-----|-----|-----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 51  | 1   | 0   | -0.953950 | -1.135534 | -2.287958 |
| 52  | 1   | 0   | -3.365119 | -1.400068 | -2.319076 |
| 53  | 1   | 0   | -1.941379 | -3.408507 | -1.848213 |
| 54  | 1   | 0   | -2.201750 | -3.186330 | -0.114962 |
| 55  | 1   | 0   | -3.560423 | -3.568724 | -1.170837 |
| 56  | 1   | 0   | -3.453375 | -1.105921 | 0.715449  |
| 57  | 1   | 0   | -3.791048 | 0.213930  | -0.388772 |
| 58  | 1   | 0   | -5.656261 | -1.085611 | -1.409413 |
| 59  | 1   | 0   | -3.329382 | -2.428297 | -0.332989 |
| 60  | 1   | 0   | -5.907884 | -1.066446 | 1.671711  |
| 61  | 1   | 0   | -8.721994 | 0.407261  | -0.388772 |
| 62  | 1   | 0   | -7.634171 | 1.774265  | -0.760405 |
| 63  | 1   | 0   | -7.100012 | 0.336244  | 1.668695  |
| 64  | 1   | 0   | -7.453375 | 0.169035  | 2.667629  |
| 65  | 1   | 0   | -3.207063 | -1.765387 | 2.204756  |
| 66  | 1   | 0   | -4.405151 | -1.987143 | 1.270205  |
| 67  | 1   | 0   | -4.396454 | -1.004628 | 0.093301  |
| 68  | 1   | 0   | -3.090405 | -1.070061 | 0.725158  |
| 69  | 1   | 0   | -1.889704 | -0.837475 | 0.210860  |
| 70  | 1   | 0   | -1.904727 | -1.820712 | 1.390409  |
| 71  | 1   | 0   | -3.081505 | -0.150267 | 1.975014  |
| 72  | 1   | 0   | -4.039214 | -0.665684 | 3.060660  |
| 73  | 1   | 0   | -3.266691 | 1.329617  | 1.669585  |
| 74  | 1   | 0   | -0.690342 | -1.013239 | 0.560936  |
| 75  | 1   | 0   | 0.499873  | -0.403007 | 0.050264  |
| 76  | 1   | 0   | 1.695948  | -1.253891 | 0.472818  |
| 77  | 1   | 0   | 1.534240  | -2.260219 | 1.399250  |
| 78  | 1   | 0   | 2.617802  | -3.073196 | 1.802401  |
| 79  | 1   | 0   | 3.863496  | -2.884233 | 1.265000  |
| 80  | 1   | 0   | 4.080841  | -1.868705 | 0.298066  |
| 81  | 1   | 0   | 2.988749  | -1.032291 | 0.106243  |
| 82  | 1   | 0   | 3.248437  | -0.027128 | 1.077561  |
| 83  | 1   | 0   | 4.501180  | 0.138240  | 1.619389  |
| 84  | 1   | 0   | 5.571835  | -0.690024 | 1.219199  |
| 85  | 1   | 0   | 5.361211  | -1.669101 | 0.280340  |
| 86  | 1   | 0   | 0.589172  | 1.048341  | 0.539793  |
| 87  | 1   | 0   | 0.896503  | 1.269383  | 1.866327  |
| 88  | 1   | 0   | 0.941295  | 2.566115  | 2.415110  |
| 89  | 1   | 0   | 0.680617  | 3.656756  | 1.624851  |
| 90  | 1   | 0   | 0.362149  | 3.491526  | 0.254483  |
| 91  | 1   | 0   | 0.307729  | 2.169850  | 0.307746  |
| 92  | 1   | 0   | -0.016405 | 2.061379  | 1.691086  |
| 93  | 1   | 0   | -0.268356 | 3.170747  | 2.462114  |

4b (conformer 1)
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|  30 | 6 | 0 | -0.214302 | 4.465056 | 1.899639 |
|  31 | 6 | 0 | 0.093814 | 4.615010 | 0.571589 |
|  32 | 6 | 0 | -3.188176 | -2.764037 | 3.366138 |
|  33 | 1 | 0 | -3.299366 | -0.754763 | 2.628509 |
|  34 | 1 | 0 | -4.374527 | -3.017271 | 0.890312 |
|  35 | 1 | 0 | -5.340824 | -1.889696 | 1.831862 |
|  36 | 1 | 0 | -5.250975 | -1.204616 | -0.559320 |
|  37 | 1 | 0 | -4.535993 | 0.011196 | 0.481528 |
|  38 | 1 | 0 | -2.983412 | -2.099451 | -1.096433 |
|  39 | 1 | 0 | -1.929082 | 0.191983 | 0.590602 |
|  40 | 1 | 0 | -1.767913 | -2.831149 | 0.986046 |
|  41 | 1 | 0 | -1.048997 | -1.630541 | 2.047567 |
|  42 | 1 | 0 | -2.068137 | -0.214357 | -2.380590 |
|  43 | 1 | 0 | -3.933810 | -0.077381 | -3.979696 |
|  44 | 1 | 0 | -3.832746 | -1.710746 | -3.311378 |
|  45 | 1 | 0 | -5.086579 | -0.596325 | -2.750411 |
|  46 | 1 | 0 | -3.233504 | 1.930320 | -2.574670 |
|  47 | 1 | 0 | -4.384501 | 1.486378 | -1.316143 |
|  48 | 1 | 0 | -2.677406 | 1.732324 | -0.918093 |
|  49 | 1 | 0 | 0.468491 | -0.421161 | 1.041920 |
|  50 | 1 | 0 | 0.549661 | -2.434019 | -1.810313 |
|  51 | 1 | 0 | 2.450651 | -3.853111 | -2.537114 |
|  52 | 1 | 0 | 4.698743 | -3.508338 | -1.565233 |
|  53 | 1 | 0 | 2.454267 | 0.634996 | 1.394514 |
|  54 | 1 | 0 | 4.669115 | 0.914770 | 2.357318 |
|  55 | 1 | 0 | 6.555629 | -0.549048 | 1.652535 |
|  56 | 1 | 0 | 6.176864 | -2.311235 | -0.035996 |
|  57 | 1 | 0 | 1.118033 | 0.419897 | -2.501668 |
|  58 | 1 | 0 | 1.189104 | 2.694455 | -3.462763 |
|  59 | 1 | 0 | 0.717950 | 4.660337 | -2.035354 |
|  60 | 1 | 0 | -0.070825 | 1.086846 | 2.158361 |
|  61 | 1 | 0 | -0.512346 | 3.051136 | 3.511803 |
|  62 | 1 | 0 | -0.416019 | 5.332320 | 2.517895 |
|  63 | 1 | 0 | 0.138512 | 5.603736 | 0.126753 |
|  64 | 1 | 0 | -4.108240 | -2.703477 | 3.955008 |
|  65 | 1 | 0 | -3.095649 | -3.790819 | 2.996837 |
|  66 | 1 | 0 | -2.346740 | -2.576273 | 4.039784 |

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|  4b (conformer 2) | 1 | 6 | 0 | 2.959427 | -2.598769 | -1.504820 |
|   | 2 | 6 | 0 | 4.310991 | -2.435864 | -0.797000 |
|   | 3 | 6 | 0 | 4.524844 | -1.003661 | -0.295818 |
|   | 4 | 6 | 0 | 3.868000 | -0.498035 | 0.618919 |
|   | 5 | 6 | 0 | 2.047005 | -0.652156 | -0.123827 |
|   | 6 | 6 | 0 | 1.833883 | -2.102709 | -0.583267 |
|   | 7 | 6 | 0 | 3.712011 | 0.922196 | 1.169838 |
|   | 8 | 6 | 0 | 3.444665 | 2.054191 | 0.167081 |
|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
| 9 | 6 | 0 | 3.040903 | 1.219771 | 2.519820 |
| 10| 8 | 0 | 0.995746 | -0.197520 | 0.744809 |
| 11| 6 | 0 | -0.312619 | -0.072001 | 0.169280 |
| 12| 6 | 0 | -1.236937 | -1.198069 | 0.631494 |
| 13| 6 | 0 | -0.898156 | -1.964588 | 1.723900 |
| 14| 6 | 0 | -1.730051 | -3.013823 | 2.176252 |
| 15| 6 | 0 | -2.900033 | -3.299845 | 1.522573 |
| 16| 6 | 0 | -3.293564 | -2.541805 | 0.389236 |
| 17| 6 | 0 | -2.460172 | -1.467366 | -0.064832 |
| 18| 6 | 0 | -2.894207 | -0.720636 | -1.194495 |
| 19| 6 | 0 | -4.068578 | -1.023039 | -1.842249 |
| 20| 6 | 0 | -4.881312 | -2.087463 | -1.395519 |
| 21| 6 | 0 | -3.246608 | -1.825847 | -0.696111 |
| 22| 6 | 0 | -0.846243 | 1.317422  | 0.527936  |
| 23| 6 | 0 | -1.424728 | 1.516249  | 1.763011  |
| 24| 6 | 0 | -1.877307 | 2.786070  | 2.178221  |
| 25| 6 | 0 | -1.761327 | 3.865114  | 1.341224  |
| 26| 6 | 0 | -1.181402 | 3.718877  | 0.055907  |
| 27| 6 | 0 | -0.706115 | 2.430939  | -0.365945 |
| 28| 6 | 0 | -0.125227 | 2.340692  | -1.662178 |
| 29| 6 | 0 | -0.023533 | 3.437457  | -2.484840 |
| 30| 6 | 0 | -0.495148 | 4.698894  | -2.062162 |
| 31| 6 | 0 | -1.060271 | 4.830103  | -0.817999 |
| 32| 6 | 0 | 2.717451  | -4.040360 | -1.963151 |
| 33| 1 | 0 | 2.971245  | -1.957665 | -2.398587 |
| 34| 1 | 0 | 4.351270  | -3.129839 | 0.053538  |
| 35| 1 | 0 | 5.125773  | -2.722747 | -1.471028 |
| 36| 1 | 0 | 5.470107  | -0.940599 | 0.252485  |
| 37| 1 | 0 | 4.625367  | -0.331201 | -1.157201 |
| 38| 1 | 0 | 3.339878  | -1.173327 | 1.484519  |
| 39| 1 | 0 | 2.060887  | -0.004010 | -1.013824 |
| 40| 1 | 0 | 1.775890  | -2.746243 | 0.302705  |
| 41| 1 | 0 | 0.871195  | -2.194986 | -1.095631 |
| 42| 1 | 0 | 4.794338  | 0.910007  | 1.357666  |
| 43| 1 | 0 | 2.374536  | 2.188716  | -0.003891 |
| 44| 1 | 0 | 3.835608  | 3.000439  | 0.552094  |
| 45| 1 | 0 | 3.925435  | 1.873295  | -0.798863 |
| 46| 1 | 0 | 3.407858  | 2.168109  | 2.925760  |
| 47| 1 | 0 | 1.957844  | 1.283257  | 2.418371  |
| 48| 1 | 0 | 3.267343  | 0.437208  | 3.251166  |
| 49| 1 | 0 | -0.223655 | -0.148949 | -0.917057 |
| 50| 1 | 0 | 0.033380  | -1.756546 | 2.233642  |
| 51| 1 | 0 | -1.430898 | -3.593509 | 3.042539  |
| 52| 1 | 0 | -3.541063 | -4.107512 | 1.860101  |
| 53| 1 | 0 | -2.303646 | 0.113686  | -1.550061 |
|   |   |   |   |
|---|---|---|---|
| 54 | 1 | 0 | -4.376469 -0.435679 -2.700075 |
| 55 | 1 | 0 | -5.805823 -2.315239 -1.914037 |
| 56 | 1 | 0 | -5.119540 -3.642811 0.051419 |
| 57 | 1 | 0 | -5.805823 -2.315239 -1.914037 |
| 58 | 1 | 0 | -5.119540 -3.642811 0.051419 |
| 59 | 1 | 0 | -2.112032 4.845064 1.647531 |
| 60 | 1 | 0 | 0.425509 3.333086 -3.466255 |
| 61 | 1 | 0 | -0.408718 5.556709 -2.719302 |
| 62 | 1 | 0 | -1.425892 5.794320 -0.481065 |
| 63 | 1 | 0 | 3.511419 -4.380599 -2.634671 |
| 64 | 1 | 0 | 2.689315 -4.722834 -1.107200 |
|   |   |   |   |
| **4b (conformer 3)** |   |   |   |
| 1 | 6 | 0 | 4.249709 0.284688 -0.617174 |
| 2 | 6 | 0 | 4.887036 -1.070758 -0.279556 |
| 3 | 6 | 0 | 4.030654 -1.869233 0.710424 |
| 4 | 6 | 0 | 2.592856 -2.090601 0.200589 |
| 5 | 6 | 0 | 1.946731 -0.731728 -0.139353 |
| 6 | 6 | 0 | 2.811260 0.075287 -1.115626 |
| 7 | 6 | 0 | 1.717871 -2.964996 1.137847 |
| 8 | 6 | 0 | 2.131538 -4.443537 1.080527 |
| 9 | 6 | 0 | 1.676109 -2.478772 2.595928 |
| 10 | 8 | 0 | 0.659117 -0.970270 -0.736570 |
| 11 | 6 | 0 | 0.465997 -0.282160 -0.185912 |
| 12 | 6 | 0 | 0.471665 1.193219 -0.613602 |
| 13 | 6 | 0 | 0.759731 1.484307 -1.930942 |
| 14 | 6 | 0 | 0.726985 2.801845 -2.428342 |
| 15 | 6 | 0 | 0.406194 3.843307 -1.594923 |
| 16 | 6 | 0 | 0.105438 3.605712 -0.231151 |
| 17 | 6 | 0 | 0.131284 2.262052 0.279273 |
| 18 | 6 | 0 | 0.178112 2.082120 1.658244 |
| 19 | 6 | 0 | 0.492694 3.143789 2.471904 |
| 20 | 6 | 0 | 0.518039 4.459636 1.960025 |
| 21 | 6 | 0 | 0.224308 4.678645 0.638572 |
| 22 | 6 | 0 | 0.726961 -1.026182 -0.623254 |
| 23 | 6 | 0 | 0.165667 -1.973285 -1.630425 |
| 24 | 6 | 0 | 2.804672 -2.686188 -2.055244 |
| 25 | 6 | 0 | 0.402918 -2.455516 -1.457468 |
| 26 | 6 | 0 | 0.414996 -1.498068 -0.409892 |
| 27 | 6 | 0 | 2.989278 -0.763727 0.016141 |
| 28 | 6 | 0 | 0.153092 0.187931 1.068516 |
| 29 | 6 | 0 | 0.4383003 0.397479 1.668826 |
| 30 | 6 | 0 | 5.521441 -0.330617 1.247857 |
| 31 | 6 | 0 | 5.402087 -1.257783 0.227230 |
| 32 | 6 | 0 | 5.083393 1.078187 -1.628082 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 33| 1 | 0 | 4.201725 | 0.869783 | 0.312829 |
| 34| 1 | 0 | 5.011046 | -1.647392 | -1.206260 |
| 35| 1 | 0 | 5.891866 | -0.920655 | 0.130792 |
| 36| 1 | 0 | 4.503497 | -2.834675 | -1.206260 |
| 37| 1 | 0 | 4.004349 | -1.333064 | 1.666932 |
| 38| 1 | 0 | 2.659455 | -2.630711 | -0.754564 |
| 39| 1 | 0 | 1.815041 | -0.152862 | 0.782964 |
| 40| 1 | 0 | 2.829142 | -0.464243 | -2.071256 |
| 41| 1 | 0 | 2.331599 | 1.038469 | -1.308493 |
| 42| 1 | 0 | 0.701412 | -2.904853 | 0.737082 |
| 43| 1 | 0 | 1.464800 | -5.056122 | 1.694655 |
| 44| 1 | 0 | 2.086257 | -4.827283 | 0.057111 |
| 45| 1 | 0 | 3.149383 | -0.920655 | 1.452375 |
| 46| 1 | 0 | 9.05595 | -3.018984 | 3.153352 |
| 47| 1 | 0 | 2.628020 | -2.648541 | 3.108066 |
| 48| 1 | 0 | 1.446049 | -1.412107 | 2.673950 |
| 49| 1 | 0 | -0.412121 | -0.350164 | 0.904661 |
| 50| 1 | 0 | -1.022323 | 0.674039 | -2.600833 |
| 51| 1 | 0 | -0.961529 | 2.985399 | -3.470818 |
| 52| 1 | 0 | -0.381965 | 4.862826 | -1.965178 |
| 53| 1 | 0 | 0.165724 | 1.089967 | 2.089286 |
| 54| 1 | 0 | 0.722869 | 2.969423 | 3.517025 |
| 55| 1 | 0 | 0.767449 | 5.288977 | 2.611999 |
| 56| 1 | 0 | 0.238677 | 5.684864 | 0.232632 |
| 57| 1 | 0 | -0.698113 | -2.175460 | -2.088378 |
| 58| 1 | 0 | -2.710253 | -3.418435 | -2.850365 |
| 59| 1 | 0 | -4.913612 | -3.000541 | -1.772340 |
| 60| 1 | 0 | -2.306616 | 0.772282 | 1.403749 |
| 61| 1 | 0 | -4.475940 | 1.128174 | 2.465269 |
| 62| 1 | 0 | -4.80718 | -0.158099 | 1.724085 |
| 63| 1 | 0 | -6.267718 | -1.821744 | -0.106585 |
| 64| 1 | 0 | 6.100393 | 1.243992 | -1.260014 |
| 65| 1 | 0 | 5.156639 | 0.541865 | -2.580287 |
| 66| 1 | 0 | 4.636552 | 2.055885 | -1.830514 |

**4b (conformer S)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 1 | 6 | 0 | -3.618772 | -2.673267 | 1.015949 |
| 2 | 6 | 0 | -4.767997 | -2.075441 | 0.191989 |
| 3 | 6 | 0 | -4.599949 | -0.563800 | -0.002769 |
| 4 | 6 | 0 | -3.254253 | -0.193186 | -0.658897 |
| 5 | 6 | 0 | -2.101328 | -0.789217 | 0.168409 |
| 6 | 6 | 0 | -2.276537 | -2.302223 | 0.366086 |
| 7 | 6 | 0 | -3.087552 | 1.324607 | -0.940775 |
| 8 | 6 | 0 | -4.004264 | 1.788936 | -2.083231 |
| 9 | 6 | 0 | -3.273360 | 2.218994 | 0.295151 |
| 10| 8 | 0 | -0.871265 | -0.525455 | -0.527813 |
| 11| 6 | 0 | 0.318598 | -0.541197 | 0.268004 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 12| 6 | 0 | 1.465011 | -1.114123 | -0.575905 |
| 13| 6 | 0 | 1.234464 | -1.450268 | -1.892834 |
| 14| 6 | 0 | 2.241619 | -2.015661 | -2.704915 |
| 15| 6 | 0 | 3.486920 | -2.260779 | -2.190933 |
| 16| 6 | 0 | 3.771737 | -1.961925 | -0.834251 |
| 17| 6 | 0 | 2.753490 | -1.383634 | -0.003602 |
| 18| 6 | 0 | 3.080298 | -1.136052 | 1.358076 |
| 19| 6 | 0 | 4.324991 | -1.427954 | 1.863622 |
| 20| 6 | 0 | 5.325139 | -1.983192 | 1.037320 |
| 21| 6 | 0 | 5.048329 | -2.242411 | -0.281476 |
| 22| 6 | 0 | 0.532238 | 0.837896  | 0.903861 |
| 23| 6 | 0 | 0.351355 | 0.948425  | 2.267866 |
| 24| 6 | 0 | 0.486435 | 2.177677  | 2.950028 |
| 25| 6 | 0 | 0.804077 | 3.312231  | 2.251592 |
| 26| 6 | 0 | 0.982907 | 3.265500  | 0.844711 |
| 27| 6 | 0 | 0.835887 | 2.019288  | 0.148654 |
| 28| 6 | 0 | 0.986545 | 2.029066  | -1.264382 |
| 29| 6 | 0 | 1.285141 | 3.186794  | -1.942564 |
| 30| 6 | 0 | 1.447221 | 4.406535  | -1.250488 |
| 31| 6 | 0 | 1.295313 | 4.440845  | 0.112813 |
| 32| 6 | 0 | -3.760224 | -4.188553 | 1.190703 |
| 33| 1 | 0 | -3.651361 | -2.213418 | 2.014593 |
| 34| 1 | 0 | -4.799438 | -2.571852 | -0.787358 |
| 35| 1 | 0 | -5.726785 | -2.285622 | 0.678821 |
| 36| 1 | 0 | -5.423503 | -0.176413 | -0.609068 |
| 37| 1 | 0 | -4.679648 | -0.072630 | 0.974186 |
| 38| 1 | 0 | -3.212365 | -0.697216 | -1.635190 |
| 39| 1 | 0 | -2.071267 | -0.292673 | 1.148046 |
| 40| 1 | 0 | -2.203120 | -2.780828 | -0.618287 |
| 41| 1 | 0 | -1.450959 | -2.698359 | 0.967271 |
| 42| 1 | 0 | -2.057022 | 1.451784  | -1.282671 |
| 43| 1 | 0 | -3.794313 | 2.830270  | -2.344278 |
| 44| 1 | 0 | -3.855915 | 1.184950  | -2.983716 |
| 45| 1 | 0 | -5.062951 | 1.730052  | -1.811252 |
| 46| 1 | 0 | -4.305842 | 2.204693  | 0.657850 |
| 47| 1 | 0 | -2.619469 | 1.925115  | 1.119961 |
| 48| 1 | 0 | -3.030004 | 3.255710  | 0.046509 |
| 49| 1 | 0 | 0.176993 | -1.239467 | 1.102721 |
| 50| 1 | 0 | 0.251167 | -1.274974 | -2.306037 |
| 51| 1 | 0 | 2.016883 | -2.255958 | -3.738216 |
| 52| 1 | 0 | 4.267781 | -2.695060 | -2.806423 |
| 53| 1 | 0 | 2.342663 | -0.698291 | 2.013938 |
| 54| 1 | 0 | 4.541191 | -1.225986 | 2.906885 |
| 55| 1 | 0 | 6.304543 | -2.204619 | 1.446194 |
| 56| 1 | 0 | 5.805789 | -2.674736 | -0.927187 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 57 | 1 | 0 | 0.108392 | 0.059498 | 2.842165 |
| 58 | 1 | 0 | 0.340242 | 2.213524 | 4.023688 |
| 59 | 1 | 0 | 0.917756 | 3.163208 | -3.020983 |
| 60 | 1 | 0 | 0.860943 | 1.110183 | 0.340242 |
| 61 | 1 | 0 | 1.395662 | -3.020983 | 1.395662 |
| 62 | 1 | 0 | 1.685587 | -1.797857 | 1.685587 |
| 63 | 1 | 0 | 1.408796 | -0.655833 | 1.408796 |
| 64 | 1 | 0 | -4.708442 | -4.444509 | -4.708442 |
| 65 | 1 | 0 | -3.730831 | 0.221622 | -3.730831 |
| 66 | 1 | 0 | -2.951918 | 1.804921 | -2.951918 |

4b (conformer 11)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | 4.263999 | 0.966925 | 0.227676 |
| 2  | 6 | 0 | 5.086126 | -0.282078 | -0.121108 |
| 3  | 6 | 0 | 4.386366 | -1.567439 | 0.337316 |
| 4  | 6 | 0 | 2.966441 | -1.707135 | -0.246878 |
| 5  | 6 | 0 | 2.138341 | -0.454189 | 0.105886 |
| 6  | 6 | 0 | 2.843276 | 0.831690 | -0.340933 |
| 7  | 6 | 0 | 2.256782 | -3.035916 | 0.127309 |
| 8  | 6 | 0 | 2.869794 | -4.233076 | 0.615651 |
| 9  | 6 | 0 | 2.200195 | -3.318161 | 1.637619 |
| 10 | 8 | 0 | 0.857539 | -0.541304 | -0.546498 |
| 11 | 6 | 0 | -0.300980 | -0.373009 | 0.271848 |
| 12 | 6 | 0 | -0.460002 | 1.084350 | 0.729652 |
| 13 | 6 | 0 | -0.298407 | 1.354301 | 2.073282 |
| 14 | 6 | 0 | -0.410326 | 2.659382 | 2.600751 |
| 15 | 6 | 0 | -0.685863 | 3.709334 | 1.765546 |
| 16 | 6 | 0 | -0.837254 | 3.498717 | 0.370358 |
| 17 | 6 | 0 | -0.710544 | 2.174848 | -0.168650 |
| 18 | 6 | 0 | -0.817805 | 2.020185 | -1.577100 |
| 19 | 6 | 0 | -1.063430 | 3.096371 | -2.395942 |
| 20 | 6 | 0 | -1.213198 | 4.392919 | -1.857788 |
| 21 | 6 | 0 | -1.097961 | 4.585833 | -0.504137 |
| 22 | 6 | 0 | -1.495198 | -0.990856 | -0.467713 |
| 23 | 6 | 0 | -1.332816 | -1.452143 | -1.756856 |
| 24 | 6 | 0 | -2.390881 | -2.053855 | -2.472515 |
| 25 | 6 | 0 | -3.620275 | -2.206853 | -1.889234 |
| 26 | 6 | 0 | -3.836312 | -1.778039 | -0.555243 |
| 27 | 6 | 0 | -2.765314 | -1.164826 | 0.178293 |
| 28 | 6 | 0 | -3.025388 | -0.788901 | 1.524727 |
| 29 | 6 | 0 | -4.255505 | -0.990940 | 2.104178 |
| 30 | 6 | 0 | -5.307991 | -1.579655 | 1.371401 |
| 31 | 6 | 0 | -5.096403 | -1.963166 | 0.071116 |
| 32 | 6 | 0 | 4.940384 | 2.254845 | -0.252722 |
| 33 | 1 | 0 | 4.184707 | 1.016532 | 1.323618 |
| 34 | 1 | 0 | 5.241000 | -0.314950 | -1.208044 |
| 35 | 1 | 0 | 6.080970 | -0.215489 | 0.333311 |
|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
|36| 1| 0| 4.989035 | -2.436724 | 0.058074 |
|37| 1| 0| 4.334839 | -1.568208 | 1.432782 |
|38| 1| 0| 3.057388 | -1.702014 | -1.342324 |
|39| 1| 0| 1.983387 | -0.417229 | 1.191925 |
|40| 1| 0| 2.886636 | 0.828597 | -1.437388 |
|41| 1| 0| 2.347457 | 1.692738 | -0.053739 |
|42| 1| 0| 1.227312 | -2.934208 | 0.229679 |
|43| 1| 0| 2.298359 | -5.144638 | -0.417425 |
|44| 1| 0| 1.983387 | -0.417229 | 1.191925 |
|45| 1| 0| 3.901994 | -4.422399 | -0.304667 |
|46| 1| 0| 1.564670 | -4.185858 | 1.836308 |
|47| 1| 0| 3.190361 | -3.539680 | 2.046664 |
|48| 1| 0| 1.788381 | -2.477739 | 2.203630 |
|49| 1| 0| 1.629666 | -0.963303 | 1.188734 |
|50| 1| 0| 0.535553 | 2.754903 |
|51| 1| 0| 2.819976 | 3.665159 |
|52| 1| 0| 4.717126 | 2.155352 |
|53| 1| 0| 1.040478 | 2.009990 |
|54| 1| 0| 2.948589 | -3.467418 |
|55| 1| 0| 5.231912 | -2.515453 |
|56| 1| 0| 5.579112 | -0.079023 |
|57| 1| 0| -1.351755 | -2.224992 |
|58| 1| 0| -2.393844 | -3.487601 |
|59| 1| 0| -2.66405 | -2.430727 |
|60| 1| 0| -0.324021 | 2.110142 |
|61| 1| 0| -0.691941 | 3.133612 |
|62| 1| 0| -6.275356 | 1.837438 |
|63| 1| 0| -5.894318 | -2.515453 |
|64| 1| 0| 2.362270 | 0.178553 |
|65| 1| 0| 2.256953 | -1.342900 |
|66| 1| 0| 4.357588 | 0.026351 |

**4b (conformer 12)**

|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
|1 | 6| 0| 2.551379 | -2.679530 | -1.766524 |
|2 | 6| 0| 2.741402 | -3.722279 | -0.658096 |
|3 | 6| 0| 2.698474 | -3.074841 | 0.729343 |
|4 | 6| 0| 1.395694 | -2.288111 | 0.973516 |
|5 | 6| 0| 1.206777 | -1.231370 | -0.135727 |
|6 | 6| 0| 1.255202 | -1.886429 | -1.525729 |
|7 | 6| 0| 1.278935 | -1.717227 | 2.413369 |
|8 | 6| 0| 0.983343 | -2.828930 | 3.432926 |
|9 | 6| 0| 2.495760 | -0.890909 | 2.857677 |
|10| 8| 0| -0.053221 | -0.583380 | 0.134061 |
|11| 6| 0| -0.557285 | 0.365423 | -0.819567 |
|12| 6| 0| -1.964054 | 0.765100 | -0.362367 |
|13| 6| 0| -2.292252 | 2.081233 | -0.120881 |
|14| 6| 0| -3.596600 | 2.468480 | 0.260280 |
|   |   | x | y | z |   |   |   |
|---|---|---|---|---|---|---|---|
| 15| 6 | 0 | -4.585362 | 1.530432 | 0.387341 |   |   |
| 16| 6 | 0 | -4.313486 | 0.162833 | 0.126146 |   |   |
| 17| 6 | 0 | -2.990055 | -0.236454 | 0.387341 |   |   |
| 18| 6 | 0 | -2.771997 | -1.613698 | -0.532866 |   |   |
| 19| 6 | 0 | -3.789892 | -2.531233 | -0.441370 |   |   |
| 20| 6 | 0 | -5.087990 | -2.134744 | -0.055568 |   |   |
| 21| 6 | 0 | -5.338196 | -0.814571 | 0.222905 |   |   |
| 22| 6 | 0 | -2.990055 | -0.236454 | 0.387341 |   |   |
| 23| 6 | 0 | -2.771997 | -1.613698 | -0.532866 |   |   |
| 24| 6 | 0 | -3.789892 | -2.531233 | -0.441370 |   |   |
| 25| 6 | 0 | -5.087990 | -2.134744 | -0.055568 |   |   |
| 26| 6 | 0 | -5.338196 | -0.814571 | 0.222905 |   |   |
| 27| 6 | 0 | -2.990055 | -0.236454 | 0.387341 |   |   |
| 28| 6 | 0 | -2.771997 | -1.613698 | -0.532866 |   |   |
| 29| 6 | 0 | -3.789892 | -2.531233 | -0.441370 |   |   |
| 30| 6 | 0 | -5.087990 | -2.134744 | -0.055568 |   |   |
| 31| 6 | 0 | -5.338196 | -0.814571 | 0.222905 |   |   |
| 32| 1 | 0 |  0.399753 |  1.524677 | -1.095518 |   |   |
| 33| 1 | 0 |  0.676594 |  1.820938 | -2.414135 |   |   |
| 34| 1 | 0 |  1.543801 |  2.871982 | -2.782558 |   |   |
| 35| 1 | 0 |  1.901885 |  3.372986 | -0.440418 |   |   |
| 36| 1 | 0 |  2.148669 |  3.629342 | -1.813796 |   |   |
| 37| 1 | 0 |  2.771997 |  3.069342 | -1.813796 |   |   |
| 38| 1 | 0 |  3.389022 |  3.723149 | -1.813796 |   |   |
| 39| 1 | 0 |  4.059022 |  4.372149 | -1.813796 |   |   |
| 40| 1 | 0 |  4.729022 |  5.021149 | -1.813796 |   |   |
| 41| 1 | 0 |  5.399022 |  5.672149 | -1.813796 |   |   |
| 42| 1 | 0 |  6.069022 |  6.321149 | -1.813796 |   |   |
| 43| 1 | 0 |  6.739022 |  6.972149 | -1.813796 |   |   |
| 44| 1 | 0 |  7.409022 |  7.621149 | -1.813796 |   |   |
| 45| 1 | 0 |  8.079022 |  8.272149 | -1.813796 |   |   |
| 46| 1 | 0 |  8.749022 |  8.921149 | -1.813796 |   |   |
| 47| 1 | 0 |  9.419022 |  9.572149 | -1.813796 |   |   |
| 48| 1 | 0 | 10.089022| 10.221149| -1.813796|   |   |
| 49| 1 | 0 | 10.759022| 10.872149| -1.813796|   |   |
| 50| 1 | 0 | 11.429022|11.521149| -1.813796|   |   |
| 51| 1 | 0 | 12.099022|12.172149| -1.813796|   |   |
| 52| 1 | 0 | 12.769022|12.821149| -1.813796|   |   |
| 53| 1 | 0 | 13.439022|13.472149| -1.813796|   |   |
| 54| 1 | 0 | 14.109022|14.121149| -1.813796|   |   |
| 55| 1 | 0 | 14.779022|14.772149| -1.813796|   |   |
| 56| 1 | 0 | 15.449022|15.421149| -1.813796|   |   |
| 57| 1 | 0 | 16.119022|16.072149| -1.813796|   |   |
| 58| 1 | 0 | 16.789022|16.721149| -1.813796|   |   |
| 59| 1 | 0 | 17.459022|17.372149| -1.813796|   |   |
|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 60 | 1 | 0 | 0.114731 | 1.300870 | 1.623180 |
| 61 | 1 | 0 | 1.171281 | 2.715406 | 3.323999 |
| 62 | 1 | 0 | 2.716825 | 4.548997 | 2.660439 |
| 63 | 1 | 0 | 3.177110 | 4.964322 | -0.269907 |
| 64 | 1 | 0 | 3.502381 | -3.851627 | -3.339289 |
| 65 | 1 | 0 | 1.743922 | -4.020603 | -3.282040 |
| 66 | 1 | 0 | 2.469881 | -2.550920 | -3.944788 |

### 4b (conformer 13)

|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 1  | 6 | 0 | 3.865084 | -2.229968 | -0.760718 |
| 2  | 6 | 0 | 5.013872 | -1.482718 | -0.071088 |
| 3  | 6 | 0 | 4.804237 | 0.034971 | -0.100614 |
| 4  | 6 | 0 | 3.453649 | -0.485541 | 0.501680 |
| 5  | 6 | 0 | 2.316663 | -0.265778 | -0.212813 |
| 6  | 6 | 0 | 2.529123 | -1.786285 | -0.145777 |
| 7  | 6 | 0 | 3.352670 | 2.040080 | 0.515415 |
| 8  | 6 | 0 | 2.954597 | 2.652712 | -0.835965 |
| 9  | 6 | 0 | 2.460078 | 2.577755 | 1.643946 |
| 10 | 8 | 0 | 1.062446 | 0.103673 | 0.386792 |
| 11 | 6 | 0 | -0.111743 | -0.251258 | -0.355930 |
| 12 | 6 | 0 | -0.975685 | -1.221924 | 0.455598 |
| 13 | 6 | 0 | -0.616332 | -1.502504 | 1.737334 |
| 14 | 6 | 0 | -1.343153 | -2.405901 | 2.534414 |
| 15 | 6 | 0 | -2.440709 | -3.046076 | 2.028929 |
| 16 | 6 | 0 | -2.846167 | -2.815257 | 0.697355 |
| 17 | 6 | 0 | -2.109873 | -1.892983 | -0.115839 |
| 18 | 6 | 0 | -2.541219 | -1.720161 | -1.458861 |
| 19 | 6 | 0 | -3.622844 | -2.400926 | -1.956872 |
| 20 | 6 | 0 | -4.346246 | -3.295400 | -1.143599 |
| 21 | 6 | 0 | -3.962185 | -3.493521 | 0.151367 |
| 22 | 6 | 0 | -0.786549 | 1.029414 | -0.856696 |
| 23 | 6 | 0 | -0.723472 | 1.308086 | -2.208888 |
| 24 | 6 | 0 | -1.288929 | 2.476182 | -2.765796 |
| 25 | 6 | 0 | -1.923276 | 3.374200 | -1.955233 |
| 26 | 6 | 0 | -2.002393 | 3.148722 | -0.556215 |
| 27 | 6 | 0 | -1.418233 | 1.968416 | 0.010157 |
| 28 | 6 | 0 | -1.484577 | 1.801595 | 1.416776 |
| 29 | 6 | 0 | -2.108277 | 2.727318 | 2.216727 |
| 30 | 6 | 0 | -2.701453 | 3.880861 | 1.656062 |
| 31 | 6 | 0 | -2.643724 | 4.084531 | 0.296678 |
| 32 | 6 | 0 | 4.041275 | -3.750251 | -0.692739 |
| 33 | 1 | 0 | 3.864259 | -1.936776 | -1.820861 |
| 34 | 1 | 0 | 5.082432 | -1.822686 | 0.971112 |
| 35 | 1 | 0 | 5.968264 | -1.737887 | -0.544924 |
| 36 | 1 | 0 | 5.613134 | 0.530857 | 0.445103 |
| 37 | 1 | 0 | 4.874572 | 0.386649 | -1.137802 |
| 38 | 1 | 0 | 3.435562 | 0.153733 | 1.548933 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 39 | 1 | 0 | 2.299678 | 0.043929 | -1.268447 |
| 40 | 1 | 0 | 2.492095 | -2.092974 | 0.906653  |
| 41 | 1 | 0 | 1.702784 | -2.299958 | -0.647583 |
| 42 | 1 | 0 | 4.371541 | 2.387452  | 0.733933  |
| 43 | 1 | 0 | 3.053534 | 3.741443  | -0.798724 |
| 44 | 1 | 0 | 3.588709 | 2.297252  | -1.653853 |
| 45 | 1 | 0 | 1.915131 | 2.427893  | -1.085796 |
| 46 | 1 | 0 | 2.521606 | 3.669719  | 1.691980  |
| 47 | 1 | 0 | 1.417345 | 2.300600  | 1.493537  |
| 48 | 1 | 0 | 4.371541 | 2.387452  | 0.733933  |
| 49 | 1 | 0 | 3.053534 | 3.741443  | -0.798724 |
| 50 | 1 | 0 | 3.588709 | 2.297252  | -1.653853 |
| 51 | 1 | 0 | 1.915131 | 2.427893  | -1.085796 |
| 52 | 1 | 0 | 2.521606 | 3.669719  | 1.691980  |
| 53 | 1 | 0 | 1.417345 | 2.300600  | 1.493537  |
| 54 | 1 | 0 | 4.371541 | 2.387452  | 0.733933  |
| 55 | 1 | 0 | 3.053534 | 3.741443  | -0.798724 |
| 56 | 1 | 0 | 3.588709 | 2.297252  | -1.653853 |
| 57 | 1 | 0 | 1.915131 | 2.427893  | -1.085796 |
| 58 | 1 | 0 | 2.521606 | 3.669719  | 1.691980  |
| 59 | 1 | 0 | 1.417345 | 2.300600  | 1.493537  |
| 60 | 1 | 0 | 4.371541 | 2.387452  | 0.733933  |
| 61 | 1 | 0 | 3.053534 | 3.741443  | -0.798724 |
| 62 | 1 | 0 | 3.588709 | 2.297252  | -1.653853 |
| 63 | 1 | 0 | 1.915131 | 2.427893  | -1.085796 |
| 64 | 1 | 0 | 2.521606 | 3.669719  | 1.691980  |
| 65 | 1 | 0 | 1.417345 | 2.300600  | 1.493537  |
| 66 | 1 | 0 | 4.371541 | 2.387452  | 0.733933  |

### 5b (conformer 1)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | -0.029116 | 0.626500 | -0.035354 |
| 2  | 6 | 0 | 1.458160 | 0.841290 | 0.231961  |
| 3  | 6 | 0 | 1.875194 | 1.913780 | 0.989258  |
| 4  | 6 | 0 | 2.433484 | -0.057364 | -0.312407 |
| 5  | 6 | 0 | 3.244319 | 2.142644 | 1.253709  |
| 6  | 6 | 0 | 3.821517 | 0.186032 | -0.047074 |
| 7  | 6 | 0 | 4.197685 | 1.298974 | 0.748436  |
| 8  | 6 | 0 | -0.607052 | -0.580590 | 0.717201  |
| 9  | 6 | 0 | -1.427262 | -1.570773 | 0.083000  |
| 10 | 6 | 0 | -0.369494 | -0.671598 | 2.072807  |
| 11 | 6 | 0 | -1.962341 | -2.638324 | 0.882567  |
| 12 | 6 | 0 | -0.901536 | -1.716189 | 2.854046  |
| 13 | 6 | 0 | -1.680225 | -2.683046 | 2.269988  |
| 14 | 8 | 0 | -0.714300 | 1.825333 | 0.344297  |
| 15 | 1 | 0 | -0.146787 | 0.479963 | -1.113078 |
| 16 | 1 | 0 | 1.133716 | 2.598460 | 1.376256  |
| 17 | 6 | 0 | 2.100163 | -1.182367 | -1.114964 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 18 | 1 | 0 | 3.532131 | 2.996817 | 1.856523 |
| 19 | 6 | 0 | 4.797408 | -0.690145 | -0.588998 |
| 20 | 1 | 0 | 5.251107 | 1.470182 | 0.943779 |
| 21 | 6 | 0 | -1.751413 | -1.566585 | -1.304421 |
| 22 | 1 | 0 | 0.252168 | 0.078650 | 2.547047 |
| 23 | 6 | 0 | -2.773784 | -3.630683 | 0.271390 |
| 24 | 1 | 0 | -0.686047 | -1.752579 | 3.915911 |
| 25 | 6 | 0 | -1.751413 | -1.566585 | -1.304421 |
| 26 | 1 | 0 | 0.252168 | 0.078650 | 2.547047 |
| 27 | 6 | 0 | -2.773784 | -3.630683 | 0.271390 |
| 28 | 6 | 0 | -2.251822 | 4.295588 | -0.268224 |
| 29 | 8 | 0 | -3.060053 | 1.879225 | -2.040818 |
| 30 | 1 | 0 | -1.295049 | 2.087599 | -2.119436 |
| 31 | 6 | 0 | -2.888942 | 5.178551 | -0.191262 |
| 32 | 1 | 0 | -2.613937 | 1.010153 | 0.140904 |
| 33 | 6 | 0 | -2.540657 | -2.543145 | -1.862893 |
| 34 | 6 | 0 | -3.059155 | -3.590191 | -1.069517 |
| 35 | 6 | 0 | -1.375511 | -0.780097 | -1.945658 |
| 36 | 1 | 0 | -3.167936 | -4.91647 | -0.378933 |
| 37 | 6 | 0 | -2.768279 | -2.508876 | -2.922425 |
| 38 | 6 | 0 | -3.679798 | -4.354974 | -1.522173 |
| 39 | 6 | 0 | -5.192937 | -2.425512 | -1.770323 |
| 40 | 1 | 0 | -5.843388 | -0.491647 | -0.378933 |
| 41 | 6 | 0 | -5.843388 | -0.491647 | -0.378933 |
| 42 | 6 | 0 | -2.768279 | -2.508876 | -2.922425 |
| 43 | 6 | 0 | -3.679798 | -4.354974 | -1.522173 |
| 44 | 1 | 0 | -3.679798 | -4.354974 | -1.522173 |
| 45 | 6 | 0 | -2.768279 | -2.508876 | -2.922425 |
| 46 | 6 | 0 | -3.679798 | -4.354974 | -1.522173 |
| 47 | 6 | 0 | -3.679798 | -4.354974 | -1.522173 |
| 48 | 6 | 0 | -3.679798 | -4.354974 | -1.522173 |
| 49 | 6 | 0 | -3.679798 | -4.354974 | -1.522173 |

**5b (conformer 2)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.048960 | 0.612993 | -0.044457 |
| 2 | 6 | 0 | 0.575931 | -0.621247 | 0.701077 |
| 3 | 6 | 0 | 0.343178 | -0.704089 | 2.058153 |
| 4 | 6 | 0 | 1.347188 | -1.645615 | 0.060013 |
| 5 | 6 | 0 | 0.833023 | -1.772845 | 2.834124 |
| 6 | 6 | 0 | 1.383690 | -2.737919 | 0.854369 |
| 7 | 6 | 0 | 1.563760 | -2.772565 | 2.243438 |
| 8 | 6 | 0 | -1.424816 | 0.898151 | 0.233155 |
| 9 | 6 | 0 | -2.445220 | 0.042070 | -0.297151 |
| 10 | 6 | 0 | -1.785832 | 1.995576 | 0.983649 |
| 11 | 6 | 0 | -3.818404 | 0.351886 | -0.023739 |
| 12 | 6 | 0 | -3.140903 | 2.290221 | 1.255808 |
| 13 | 6 | 0 | -4.136305 | 1.487549 | 0.765114 |
|   |   |   |   |   |
|---|---|---|---|---|
| 14 | 8  | 0  | 0.795158 | 1.774718 | 0.337407 |
| 15 | 1  | 0  | 0.153086 | 0.465555 | -1.123473 |
| 16 | 1  | 0  | -0.240616 | 0.072492 | 2.538041 |
| 17 | 6  | 0  | 1.662323 | -1.653447 | -1.329454 |
| 18 | 1  | 0  | 0.623142 | -1.801391 | 3.897339 |
| 19 | 6  | 0  | 2.600364 | -3.764804 | 0.236259 |
| 20 | 1  | 0  | 1.941158 | -3.603646 | 2.829868 |
| 21 | 6  | 0  | -2.170723 | -1.102696 | -1.094086 |
| 22 | 1  | 0  | -1.010618 | 2.648527 | 1.359348 |
| 23 | 6  | 0  | -4.838089 | -0.481869 | -0.551616 |
| 24 | 1  | 0  | -3.383783 | 3.161834 | 1.853389 |
| 25 | 1  | 0  | -5.179092 | 1.709205 | 0.966749 |
| 26 | 6  | 0  | 2.132136 | 1.854487 | -0.165558 |
| 27 | 6  | 0  | 2.865847 | 2.942719 | 0.646597 |
| 28 | 6  | 0  | 2.175329 | 2.414082 | -1.599936 |
| 29 | 8  | 0  | 3.082094 | 4.060490 | -0.219200 |
| 30 | 6  | 0  | 2.213989 | 3.920068 | -1.342635 |
| 31 | 1  | 0  | 3.840642 | 2.605906 | 1.007296 |
| 32 | 1  | 0  | 2.443595 | 3.222705 | 1.504173 |
| 33 | 1  | 0  | 1.322657 | 2.094094 | -2.202060 |
| 34 | 1  | 0  | 3.095578 | 2.094925 | -2.097811 |
| 35 | 1  | 0  | 1.208886 | 4.299711 | -1.111573 |
| 36 | 1  | 0  | 2.633385 | 4.504490 | -2.162745 |
| 37 | 1  | 0  | 2.621676 | 0.881527 | -0.076157 |
| 38 | 6  | 0  | -3.183330 | -1.888190 | -1.591968 |
| 39 | 6  | 0  | -4.533143 | -1.577807 | -1.319792 |
| 40 | 6  | 0  | 2.878156 | -3.734952 | -1.106497 |
| 41 | 6  | 0  | 2.402540 | -2.663823 | -1.894693 |
| 42 | 1  | 0  | 1.320435 | -0.847742 | -1.965731 |
| 43 | 1  | 0  | 2.962242 | -4.580586 | 0.853473 |
| 44 | 1  | 0  | -1.147369 | -1.377940 | -1.309163 |
| 45 | 1  | 0  | -5.872040 | -0.233493 | -0.335169 |
| 46 | 1  | 0  | -2.942532 | -2.756060 | -2.195711 |
| 47 | 1  | 0  | -5.322917 | -2.205507 | -1.716849 |
| 48 | 1  | 0  | 3.460590 | -4.526211 | -1.564405 |
| 49 | 1  | 0  | 2.625220 | -2.637655 | -2.955528 |

**5b (conformer 4)**

|   |   |   |   |   |
|---|---|---|---|---|
| 1  | 6  | 0  | 0.047772 | 0.227080 | -0.075417 |
| 2  | 6  | 0  | -1.393064 | -0.106468 | -0.447550 |
| 3  | 6  | 0  | -1.947640 | 0.444415 | -1.581961 |
| 4  | 6  | 0  | -2.176231 | -0.994428 | 0.358980 |
| 5  | 6  | 0  | -3.282180 | 0.174972 | -1.958026 |
| 6  | 6  | 0  | -3.535225 | -1.253714 | -0.018571 |
| 7  | 6  | 0  | -4.062510 | -0.649002 | -1.188854 |
| 8  | 6  | 0  | 1.072829 | -0.799826 | -0.555764 |
| 9  | 6  | 0  | 2.390161 | -0.810350 | 0.014461 |
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 10 | 6 | 0 | 0.760951 | -1.710626 | -1.540064 |   |   |   |   |
| 11 | 6 | 0 | 3.340600 | -1.776183 | -0.452552 |   |   |   |   |
| 12 | 6 | 0 | 1.704309 | -2.654030 | -2.005572 |   |   |   |   |
| 13 | 6 | 0 | 2.965374 | -2.688583 | -1.472560 |   |   |   |   |
| 14 | 8 | 0 | 0.456809 | 1.503905 | -0.591054 |   |   |   |   |
| 15 | 1 | 0 | 0.104874 | 0.280640 | 1.018451 |   |   |   |   |
| 16 | 1 | 0 | -1.340090 | 1.103381 | 2.189024 |   |   |   |   |
| 17 | 6 | 0 | -1.671942 | -1.645473 | 1.518639 |   |   |   |   |
| 18 | 1 | 0 | -3.684720 | 0.091642 | 1.029225 |   |   |   |   |
| 19 | 6 | 0 | -4.325842 | -2.118516 | 0.782208 |   |   |   |   |
| 20 | 1 | 0 | -5.091374 | -0.854439 | 1.465161 |   |   |   |   |
| 21 | 6 | 0 | 2.809499 | 0.091642 | 1.029225 |   |   |   |   |
| 22 | 1 | 0 | -0.232707 | -1.711347 | 1.812370 |   |   |   |   |
| 23 | 1 | 0 | -1.199204 | 3.267255 | 0.128732 |   |   |   |   |
| 24 | 1 | 0 | 3.694759 | -3.412800 | -1.820080 |   |   |   |   |
| 25 | 6 | 0 | 0.195646 | 2.626851 | 0.239541 |   |   |   |   |
| 26 | 1 | 0 | -5.353995 | 2.301149 | 0.487277 |   |   |   |   |
| 27 | 1 | 0 | 0.702996 | 5.652136 | 0.964433 |   |   |   |   |
| 28 | 6 | 0 | 0.872181 | 0.834614 | 0.655852 |   |   |   |   |
| 29 | 6 | 0 | 0.469008 | -1.575195 | 1.744762 |   |   |   |   |
| 30 | 6 | 0 | 2.144882 | -1.118118 | 0.053877 |   |   |   |   |
| 31 | 6 | 0 | 1.274236 | -2.601590 | 2.285229 |   |   |   |   |
| **5b (conformer S)** |   |   |   |   |   |   |   |   |   |
| 1 | 6 | 0 | -0.003009 | 0.298053 | 0.124142 |   |   |   |   |
| 2 | 6 | 0 | 0.872181 | -0.834614 | 0.655852 |   |   |   |   |
| 3 | 6 | 0 | 0.469008 | -1.575195 | 1.744762 |   |   |   |   |
| 4 | 6 | 0 | 2.144882 | -1.118118 | 0.053877 |   |   |   |   |
| 5 | 6 | 0 | 1.274236 | -2.601590 | 2.285229 |   |   |   |   |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 6 | 6 | 0 | 2.954594 | -2.162411 | 0.598938 |
| 7 | 6 | 0 | 2.489532 | -2.891405 | 1.723291 |
| 8 | 6 | 0 | -1.492046 | 0.126119 | 0.419237 |
| 9 | 6 | 0 | -2.303306 | -0.733619 | -0.390180 |
|10 | 6 | 0 | -2.066795 | 0.805810 | 1.470427 |
|11 | 6 | 0 | -3.702455 | -0.842898 | -0.096921 |
|12 | 6 | 0 | -3.443713 | 0.685427 | 1.763805 |
|13 | 6 | 0 | -4.245961 | -0.116170 | 0.994093 |
|14 | 8 | 0 | 0.515513 | 1.513913 | 0.685469 |
|15 | 1 | 0 | 0.109908 | 0.343410 | -0.964521 |
|16 | 1 | 0 | -0.492708 | -1.371474 | 2.198150 |
|17 | 6 | 0 | 2.655182 | -0.400214 | -1.065498 |
|18 | 6 | 0 | 4.210933 | -2.454173 | 0.006516 |
|19 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|20 | 1 | 0 | -0.492708 | -1.371474 | 2.198150 |
|21 | 6 | 0 | 2.655182 | -0.400214 | -1.065498 |
|22 | 6 | 0 | 4.210933 | -2.454173 | 0.006516 |
|23 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|24 | 6 | 0 | 4.210933 | -2.454173 | 0.006516 |
|25 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|26 | 6 | 0 | 4.210933 | -2.454173 | 0.006516 |
|27 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|28 | 6 | 0 | 4.210933 | -2.454173 | 0.006516 |
|29 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|30 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|31 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|32 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|33 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|34 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|35 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|36 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|37 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|38 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|39 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|40 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|41 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|42 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|43 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|44 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|45 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|46 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|47 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|48 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |
|49 | 6 | 0 | 3.113279 | -3.681554 | 2.128040 |

**5b (conformer 6)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.006669 | -0.694060 | -0.068680 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 2 | 6 | 0 | -0.434871 | 0.540108 | 0.730300 |
| 3 | 6 | 0 | -0.203860 | 0.543576 | 2.090280 |
| 4 | 6 | 0 | -1.125561 | 1.646120 | 0.135439 |
| 5 | 6 | 0 | -0.618047 | 1.609211 | 2.913303 |
| 6 | 6 | 0 | -1.538833 | 2.734977 | 0.977515 |
| 7 | 6 | 0 | -1.269442 | 2.686107 | 2.367268 |
| 8 | 6 | 0 | 1.465575 | -1.071580 | 0.175647 |
| 9 | 6 | 0 | 2.526317 | -0.267282 | -0.356300 |
|10 | 6 | 0 | 1.772729 | -2.201789 | 0.901022 |
|11 | 6 | 0 | 3.882902 | -0.660546 | -0.108566 |
|12 | 6 | 0 | 3.112016 | -2.579347 | 2.990388 |
|13 | 6 | 0 | 4.145409 | -1.826620 | 0.655728 |
|14 | 8 | 0 | -0.79398 | -1.830479 | 0.283246 |
|15 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|16 | 1 | 0 | 0.108100 | -0.506110 | -1.140029 |
|17 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|18 | 1 | 0 | 0.108100 | -0.506110 | -1.140029 |
|19 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|20 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|21 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|22 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|23 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|24 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|25 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|26 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|27 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|28 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|29 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|30 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|31 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|32 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|33 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|34 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|35 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|36 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|37 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|38 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|39 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|40 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|41 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|42 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|43 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|44 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|45 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|46 | 1 | 0 | 0.318705 | -0.294881 | 2.535292 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 47 | 1 | 0 | 5.509623 | 1.834680 | -1.781387 |
| 48 | 1 | 0 | -3.012172 | 4.745548 | -1.360337 |
| 49 | 1 | 0 | -2.311279 | 2.865229 | -2.834179 |
| 5b (conformer 7) | | | | | |
| 1 | 6 | 0 | -0.039709 | 0.223255 | -0.080131 |
| 2 | 6 | 0 | -1.046772 | -0.824911 | -0.552845 |
| 3 | 6 | 0 | -0.718454 | -1.737097 | -1.530596 |
| 4 | 6 | 0 | -2.363851 | -0.855151 | 0.017446 |
| 5 | 6 | 0 | -1.644274 | -2.701092 | -1.988995 |
| 6 | 6 | 0 | -3.296606 | -1.841253 | -0.442933 |
| 7 | 6 | 0 | -2.904588 | -2.754435 | -1.455877 |
| 8 | 6 | 0 | 1.406297  | -0.086887 | -0.453101 |
| 9 | 6 | 0 | 2.208022  | -0.951848 | 0.359701  |
| 10| 6 | 0 | 1.947995  | 0.464611  | -1.593315 |
| 11| 6 | 0 | 3.571637  | -1.187114 | -0.017451 |
| 12| 6 | 0 | 3.286575  | 0.217586  | -1.969732 |
| 13| 6 | 0 | 4.084807  | -0.583384 | -1.194321 |
| 14| 8 | 0 | -0.470874 | 1.489912  | -0.602785 |
| 15| 1 | 0 | -0.096798 | 0.282074  | 1.013502  |
| 16| 1 | 0 | 0.274746  | -1.722668 | -1.960410 |
| 17| 6 | 0 | -2.800442 | 0.046390  | 1.025293  |
| 18| 1 | 0 | -1.345222 | -3.399015 | -2.762758 |
| 19| 6 | 0 | -4.598002 | -1.887967 | 0.121035  |
| 20| 1 | 0 | -3.620771 | -3.494115 | -1.798222 |
| 21| 6 | 0 | 1.718695  | -1.602374 | 1.526225  |
| 22| 1 | 0 | 1.327381  | 1.108327  | -2.203581 |
| 23| 6 | 0 | 4.380821  | -2.027940 | 0.790471  |
| 24| 1 | 0 | 3.678123  | 0.671319  | -2.873331 |
| 25| 1 | 0 | 5.116929  | -0.771375 | -1.470951 |
| 26| 6 | 0 | -0.238994 | 2.622315  | 0.221653  |
| 27| 6 | 0 | -1.191130 | 3.747288  | -0.203420 |
| 28| 6 | 0 | 1.129998  | 3.313008  | 0.109730  |
| 29| 8 | 0 | -0.558530 | 4.976767  | 0.154005  |
| 30| 6 | 0 | 0.788664  | 4.723014  | 0.586563  |
| 31| 1 | 0 | -2.165281 | 3.683937  | 0.288587  |
| 32| 1 | 0 | -1.342963 | 3.692771  | -1.288131 |
| 33| 1 | 0 | 1.439248  | 3.321880  | -0.938152 |
| 34| 1 | 0 | 1.912972  | 2.833999  | 0.699212  |
| 35| 1 | 0 | 1.438906  | 5.490927  | 0.161290  |
| 36| 1 | 0 | 0.841842  | 4.798528  | 1.681364  |
| 37| 1 | 0 | -0.419703 | 2.350739  | 1.272294  |
| 38| 6 | 0 | 2.529100  | -2.414082 | 2.283509  |
| 39| 6 | 0 | 3.876358  | -2.627322 | 1.917469  |
| 40| 6 | 0 | -4.979743 | -1.003829 | 1.098930  |
| 41| 6 | 0 | -4.067572 | -0.027222 | 1.553772  |
| 42| 1 | 0 | -2.129081 | 0.814261  | 1.383848  |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 43| 1 | 0 | -5.290695 | -2.641741 | -0.238723 |
| 44| 1 | 0 | 0.684374 | -1.476538 | 1.819319 |
| 45| 1 | 0 | 5.411941 | -2.192858 | 0.495408 |
| 46| 1 | 0 | 2.129838 | -2.900010 | 3.166692 |
| 47| 1 | 0 | 4.505124 | -3.268935 | 2.524342 |
| 48| 1 | 0 | -5.977113 | -1.050295 | 1.521174 |
| 49| 1 | 0 | -4.371568 | 0.673996 | 2.322969 |
| 5b (conformer 8) | | | | | | |
| 1 | 6 | 0 | 0.070115 | 0.293069 | -0.131447 |
| 2 | 6 | 0 | -0.707848 | -0.960293 | -0.534532 |
| 3 | 6 | 0 | -0.141524 | -1.912680 | -1.352535 |
| 4 | 6 | 0 | -2.038957 | -1.167674 | -0.035059 |
| 5 | 6 | 0 | -0.832730 | -3.092001 | -1.710651 |
| 6 | 6 | 0 | -2.728576 | -2.374348 | -0.387722 |
| 7 | 6 | 0 | -2.095904 | -3.320952 | -1.234678 |
| 8 | 6 | 0 | 1.549162 | 0.267912 | -0.507770 |
| 9 | 6 | 0 | 2.528998 | -0.306746 | 0.364338 |
| 10 | 6 | 0 | 1.949351 | 0.811181 | -1.709576 |
| 11 | 6 | 0 | 3.909213 | -0.267912 | -0.024758 |
| 12 | 6 | 0 | 3.307228 | 0.834858 | -2.095669 |
| 13 | 6 | 0 | 4.268223 | 0.319800 | -1.267605 |
| 14 | 8 | 0 | -0.609254 | 1.413311 | -0.717088 |
| 15 | 1 | 0 | 0.000781 | 0.381720 | 0.958286 |
| 16 | 1 | 0 | 0.862625 | -1.764890 | -1.727907 |
| 17 | 6 | 0 | -2.716945 | -0.236328 | 0.790890 |
| 18 | 1 | 0 | -0.349582 | -3.814810 | -2.358349 |
| 19 | 6 | 0 | -4.035504 | -2.604457 | 0.115490 |
| 20 | 1 | 0 | -2.630983 | -4.228020 | -1.496149 |
| 21 | 6 | 0 | 2.204181 | -0.930140 | 1.601197 |
| 22 | 1 | 0 | 1.196014 | 1.233687 | -2.363444 |
| 23 | 6 | 0 | 4.890716 | -0.819879 | 0.839447 |
| 24 | 1 | 0 | 3.583249 | 1.272417 | -3.048558 |
| 25 | 1 | 0 | 5.315108 | 0.335494 | -1.551748 |
| 26 | 6 | 0 | -0.262560 | 2.716274 | -0.233202 |
| 27 | 6 | 0 | -0.674339 | 2.976599 | 1.217674 |
| 28 | 6 | 0 | -1.184268 | 3.697551 | -0.961893 |
| 29 | 8 | 0 | -2.082792 | 3.199243 | 1.193876 |
| 30 | 6 | 0 | -2.471970 | 3.638537 | -0.123258 |
| 31 | 1 | 0 | -0.142553 | 3.865279 | 1.588030 |
| 32 | 1 | 0 | -0.468574 | 2.154628 | 1.905718 |
| 33 | 1 | 0 | -1.336608 | 3.403244 | -2.000302 |
| 34 | 1 | 0 | -0.744099 | 4.697894 | -0.940067 |
| 35 | 1 | 0 | -3.184180 | 2.914600 | -0.528124 |
| 36 | 1 | 0 | -2.965535 | 4.611411 | -0.042391 |
| 37 | 1 | 0 | 0.800995 | 2.916772 | -0.397253 |
| 38 | 6 | 0 | 3.180005 | -1.458356 | 2.411985 |
|    |   |   |       |       |       |
|----|---|---|-------|-------|-------|
| 39 | 6 | 0 | 4.539251 | -1.399589 | 2.032705 |
| 40 | 6 | 0 | -4.651830 | -1.688554 | 0.931032 |
| 41 | 6 | 0 | -3.983404 | -0.492262 | 1.269438 |
| 42 | 1 | 0 | -2.258094 | 0.710842 | 1.040907 |
| 43 | 1 | 0 | -4.540997 | -3.524351 | -0.160131 |
| 44 | 1 | 0 | 1.169273 | -1.011196 | 1.907380 |
| 45 | 1 | 0 | 5.931231 | -0.778177 | 0.534367 |
| 46 | 1 | 0 | 2.904198 | -1.929658 | 3.348624 |
| 47 | 1 | 0 | 5.299190 | -1.818666 | 2.682438 |
| 48 | 1 | 0 | -5.650658 | -1.876245 | 1.308944 |
| 49 | 1 | 0 | -4.474943 | 0.240854 | 0.160131 |

**5b (conformer 9)**

|    |   |   |       |       |       |
|----|---|---|-------|-------|-------|
| 1  | 6 | 0 | 0.004128 | 0.461195 | 0.026328 |
| 2  | 6 | 0 | 1.508240 | 0.471762 | 0.306177 |
| 3  | 6 | 0 | 2.041449 | 1.386138 | 1.187450 |
| 4  | 6 | 0 | 2.377724 | -0.459502 | -0.350398 |
| 5  | 6 | 0 | 3.428626 | 1.435898 | 1.453802 |
| 6  | 6 | 0 | 3.785271 | -0.398557 | -0.085396 |
| 7  | 6 | 0 | 4.283377 | 0.567256 | 0.827543 |
| 8  | 6 | 0 | -0.738092 | -0.674063 | 0.728770 |
| 9  | 6 | 0 | -1.816058 | -1.374402 | 0.092839 |
| 10 | 6 | 0 | -0.405687 | -0.987883 | 2.028511 |
| 11 | 6 | 0 | -2.512351 | -2.388074 | 0.834039 |
| 12 | 6 | 0 | -1.099092 | -1.977526 | 2.756114 |
| 13 | 6 | 0 | -2.130247 | -2.664920 | 2.170766 |
| 14 | 8 | 0 | -0.625904 | 1.677801 | 0.448382 |
| 15 | 1 | 0 | -0.121248 | 0.358834 | -1.055386 |
| 16 | 1 | 0 | 1.376016 | 2.081947 | 1.682634 |
| 17 | 6 | 0 | 1.912730 | -1.454077 | -1.253739 |
| 18 | 1 | 0 | 3.809738 | 2.170738 | 2.154175 |
| 19 | 6 | 0 | 4.655128 | -1.309491 | -0.738915 |
| 20 | 1 | 0 | 5.350395 | 0.603288 | 1.020541 |
| 21 | 6 | 0 | -2.239705 | -1.134568 | -1.243837 |
| 22 | 1 | 0 | 0.413662 | -0.463684 | 2.504638 |
| 23 | 6 | 0 | -3.576559 | -3.097698 | 0.218555 |
| 24 | 1 | 0 | -0.806707 | -2.191278 | 3.777914 |
| 25 | 1 | 0 | -2.667457 | -3.431437 | 2.719336 |
| 26 | 6 | 0 | -0.470932 | 2.793546 | -0.439686 |
| 27 | 6 | 0 | -0.700208 | 4.080815 | 0.389155 |
| 28 | 6 | 0 | -1.592278 | 2.862978 | -1.495665 |
| 29 | 8 | 0 | -1.861762 | 4.727800 | -0.129265 |
| 30 | 6 | 0 | -2.636437 | 3.730366 | -0.792918 |
| 31 | 1 | 0 | 0.131446 | 4.785141 | 0.321794 |
| 32 | 1 | 0 | -0.846705 | 3.792357 | 1.436944 |
| 33 | 1 | 0 | -1.960968 | 1.875565 | -1.775131 |
| 34 | 1 | 0 | -1.230010 | 3.372697 | -2.393093 |
|   |   |   |   |   |
|---|---|---|---|---|
| 35 | 1 | 0 | -3.212322 | 3.135811 | -0.069700 |
| 36 | 1 | 0 | -3.327734 | 4.238565 | -1.466176 |
| 37 | 1 | 0 | 0.525054  | 2.767754 | -0.890479 |
| 38 | 6 | 0 | -3.274383 | -1.840204 | -1.810548 |
| 39 | 6 | 0 | -3.954237 | -2.834047 | -1.073864 |
| 40 | 6 | 0 | 4.169907  | -2.250468 | -1.612836 |
| 41 | 6 | 0 | 2.783257  | -2.322818 | -1.868217 |
| 42 | 6 | 0 | 0.853438  | -1.548636 | -1.453434 |
| 43 | 6 | 0 | -1.742525 | -0.381036 | -1.839443 |
| 44 | 6 | 0 | 4.089711  | -2.041373 | -2.103892 |
| 45 | 6 | 0 | 5.718415  | -1.249878 | -0.530690 |
| 46 | 6 | 0 | 3.486225  | -0.128207 | -1.970548 |
| 47 | 6 | 0 | 3.786933  | -1.238122 | -1.530764 |
| 48 | 6 | 0 | 2.783257  | -2.322818 | -1.868217 |
| 49 | 6 | 0 | 0.853438  | -1.548636 | -1.453434 |

### 5b (conformer 11)

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6 | 0 | 0.000999 | 0.291056 | -0.132251 |
| 2 | 6 | 0 | -1.481786 | 0.090222 | -0.439425 |
| 3 | 6 | 0 | -2.053855 | 0.731691 | -1.516109 |
| 4 | 6 | 0 | -2.290584 | -0.758200 | 0.384236 |
| 5 | 6 | 0 | -3.425962 | 0.586268 | -1.819859 |
| 6 | 6 | 0 | -3.685319 | -0.892804 | 0.080170 |
| 7 | 6 | 0 | -4.226492 | -0.202843 | -1.035499 |
| 8 | 6 | 0 | 0.899983  | -0.831439 | -0.646715 |
| 9 | 6 | 0 | 2.177302  | -1.073350 | -0.039372 |
| 10 | 6 | 0 | 0.512759  | -1.598974 | -1.722822 |
| 11 | 6 | 0 | 3.008874  | -2.116012 | -0.566230 |
| 12 | 6 | 0 | 1.339206  | -2.617796 | -2.245335 |
| 13 | 6 | 0 | 2.559762  | -2.873254 | -1.678265 |
| 14 | 8 | 0 | 0.508404  | 1.510094  | 0.696773 |
| 15 | 1 | 0 | 0.104659  | 0.347657  | 0.956655 |
| 16 | 1 | 0 | -1.431010 | 1.364309  | -2.136383 |
| 17 | 6 | 0 | -1.777077 | -1.487838 | 1.491707 |
| 18 | 1 | 0 | -3.840084 | 1.108523  | -2.675059 |
| 19 | 6 | 0 | -4.498051 | -1.719548 | 0.898734 |
| 20 | 1 | 0 | -5.282791 | -0.313828 | 1.256829 |
| 21 | 6 | 0 | 2.671685  | -0.332768 | 1.068230 |
| 22 | 1 | 0 | -4.524333 | -1.423719 | -2.180555 |
| 23 | 6 | 0 | 4.270289  | -2.372307 | 0.031787 |
| 24 | 1 | 0 | 0.996362  | -3.196896 | -3.095239 |
| 25 | 1 | 0 | 3.199751  | -3.657112 | -2.069670 |
| 26 | 6 | 0 | 0.113554  | 2.706521  | -0.034258 |
| 27 | 6 | 0 | 0.351694  | 3.891420  | -0.982477 |
| 28 | 6 | 0 | 0.958461  | 3.102545  | 1.188603 |
| 29 | 8 | 0 | 0.702581  | 5.015802  | -0.171872 |
| 30 | 6 | 0 | 0.764460  | 4.616799  | 1.203520 |
|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 31 | 1 | 0 | -0.533332 | 4.132721 | -1.578968 |
| 32 | 1 | 0 | 1.177768  | 3.644926 | -1.658448 |
| 33 | 1 | 0 | 2.003407  | 2.848468 | 0.991100  |
| 34 | 1 | 0 | 0.641132  | 2.626565 | 2.119018  |
| 35 | 1 | 0 | 1.586816  | 5.155218 | 1.679212  |
| 36 | 1 | 0 | -0.168357 | 4.891816 | 1.716159  |
| 37 | 1 | 0 | -0.944641 | 2.646938 | 0.246144  |
| 38 | 1 | 0 | -2.592366 | -2.282200| 2.262239  |
| 39 | 1 | 0 | -0.720240 | -1.436986| 1.727809  |
| 40 | 1 | 0 | 5.552666  | -1.808637| 0.659352  |
| 41 | 1 | 0 | 2.079770  | 0.472101 | 1.480264  |
| 42 | 1 | 0 | 4.247508  | -0.024451| 2.470925  |
| 43 | 1 | 0 | 5.675387  | -1.844067| 1.551755  |
| 44 | 1 | 0 | 0.099685  | -0.709127| -0.261142 |
| 45 | 1 | 0 | -0.430630 | 0.446317 | 0.598258  |
| 46 | 1 | 0 | -0.265647 | 0.364604 | 1.965373  |
| 47 | 1 | 0 | -1.141321 | 1.561956 | 0.044642  |
| 48 | 1 | 0 | -0.778266 | 1.344724 | 2.838117  |
| 49 | 1 | 0 | -1.656143 | 2.562881 | 0.938464  |
| 50 | 1 | 0 | -1.459786 | 2.423421 | 2.334674  |
| 51 | 1 | 0 | -1.546346 | -1.074402| 0.060908  |
| 52 | 1 | 0 | 2.619128  | -0.204086| -0.321675 |
| 53 | 1 | 0 | 1.832248  | -2.54811 | 0.710918  |
| 54 | 1 | 0 | 3.965368  | -0.589332| -0.012792 |
| 55 | 1 | 0 | 3.160721  | -2.623252| 1.021214  |
| 56 | 1 | 0 | 4.205347  | -1.810465| 0.668384  |
| 57 | 1 | 0 | -0.692548 | -1.889016| -0.084209 |
| 58 | 1 | 0 | 0.059337  | -0.434099| -1.319591 |
| 59 | 1 | 0 | 0.279546  | -0.475893| 2.378548  |
| 60 | 1 | 0 | -1.372543 | 1.749029 | -1.348381 |
| 61 | 1 | 0 | -0.626021 | 1.241344 | 3.906473  |
| 62 | 1 | 0 | 3.677270  | 2.360283 | 0.410693  |
| 63 | 1 | 0 | -1.855668 | 3.186607 | 2.996305  |
| 64 | 1 | 0 | 1.026810  | 2.422520 | 1.005222  |
| 65 | 1 | 0 | 1.017788  | 3.443848 | 1.536862  |
| 66 | 1 | 0 | 5.522836  | -2.088640| 0.899064  |
| 67 | 1 | 0 | -1.990666 | -1.885262| -0.662869 |

5b (conformer 12)
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 27 | 6 | 0 | -3.126112 | -1.469902 | 0.288147 |
| 28 | 6 | 0 | -2.400387 | -3.324432 | -1.028133 |
| 29 | 8 | 0 | -4.287140 | -2.057240 | -0.279899 |
| 30 | 6 | 0 | -3.920749 | -3.359722 | -0.758908 |
| 31 | 1 | 0 | -3.291394 | -0.395705 | 0.355259 |
| 32 | 1 | 0 | -2.912052 | -1.865832 | 1.292781 |
| 33 | 1 | 0 | -1.857924 | -4.007486 | -0.371274 |
| 34 | 1 | 0 | -2.144117 | -3.574810 | -1.028133 |
| 35 | 1 | 0 | -4.175156 | -4.119771 | -0.009015 |
| 36 | 1 | 0 | -4.513018 | -3.552801 | -1.655148 |
| 37 | 1 | 0 | -2.004118 | -1.245208 | -1.552623 |
| 38 | 6 | 0 | 3.483845 | 1.822747 | -1.366068 |
| 39 | 6 | 0 | 4.807099 | 1.437052 | -0.049890 |
| 40 | 6 | 0 | -2.560413 | 3.818338 | -0.938859 |
| 41 | 6 | 0 | -2.058946 | 2.840082 | -1.825001 |
| 42 | 1 | 0 | -1.006210 | 1.021274 | -2.060071 |
| 43 | 1 | 0 | -2.740781 | 4.421077 | 1.103016 |
| 44 | 1 | 0 | 1.420987 | 1.360310 | -1.239555 |
| 45 | 1 | 0 | 6.049756 | -0.048940 | -0.157491 |
| 46 | 1 | 0 | 3.303349 | 2.757049 | -1.885473 |
| 47 | 1 | 0 | 5.635789 | 2.073653 | -1.350225 |
| 48 | 1 | 0 | -3.100464 | 4.674088 | -1.327371 |
| 49 | 1 | 0 | -2.218003 | 2.950116 | -2.891824 |

**5b (conformer 13)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | -0.059539 | -0.638829 | -0.322261 |
| 2  | 6 | 0 | -1.492090 | -1.027798 | 0.034069 |
| 3  | 6 | 0 | -1.747468 | -2.230341 | 0.655459 |
| 4  | 6 | 0 | -2.583151 | -0.155753 | -0.287871 |
| 5  | 6 | 0 | -3.062641 | -2.620560 | 0.994581 |
| 6  | 6 | 0 | -3.915981 | -0.563108 | 0.049286 |
| 7  | 6 | 0 | -4.124420 | -1.807189 | 0.698793 |
| 8  | 6 | 0 | 0.483531 | 0.498498 | 0.554894 |
| 9  | 6 | 0 | 1.199218 | 1.617780 | 0.015511 |
| 10 | 6 | 0 | 0.330213 | 0.393910 | 1.921737 |
| 11 | 6 | 0 | 1.738079 | 2.593814 | 0.922515 |
| 12 | 6 | 0 | 0.864639 | 1.350569 | 2.807594 |
| 13 | 6 | 0 | 1.556452 | 2.429219 | 2.317966 |
| 14 | 8 | 0 | 0.749922 | -1.814265 | -0.210472 |
| 15 | 1 | 0 | -0.057327 | -0.329209 | -1.372243 |
| 16 | 1 | 0 | -0.919249 | -2.889589 | 0.874723 |
| 17 | 6 | 0 | -2.417468 | 1.097935 | -0.937538 |
| 18 | 1 | 0 | -3.222537 | -3.573746 | 1.486175 |
| 19 | 6 | 0 | -5.005774 | 0.285318 | -0.276916 |
| 20 | 1 | 0 | -5.137498 | -2.102235 | 0.951358 |
| 21 | 6 | 0 | 1.410475 | 1.833337 | -1.376517 |
| 22 | 1 | 0 | -0.219664 | -0.448351 | 2.324874 |
|    |    |    |        |        |        |
|----|----|----|--------|--------|--------|
| 23 | 6  | 0  | 2.448604 | 3.710459 | 0.408253 |
| 24 | 1  | 0  | 0.720980  | 1.229168  | 3.875294 |
| 25 | 1  | 0  | 1.969728 | 3.173998  | 2.989904 |
| 26 | 6  | 0  | 1.995531 | -1.816918 | -0.912590 |
| 27 | 6  | 0  | 2.295258 | -3.279370 | -1.331998 |
| 28 | 6  | 0  | 3.020942 | -1.461742 | -0.019231 |
| 29 | 8  | 0  | 3.519920 | -3.663685 | -0.711835 |
| 30 | 6  | 0  | 3.678127 | -2.838925 | 0.442065 |
| 31 | 1  | 0  | 2.416528 | -3.397782 | -2.410705 |
| 32 | 1  | 0  | 1.463610 | -3.909279 | -0.993801 |
| 33 | 1  | 0  | 2.927224 | -0.790141 | 0.792102 |
| 34 | 1  | 0  | 3.981482 | -0.986705 | -0.622568 |
| 35 | 8  | 0  | 3.519920 | -3.663685 | -0.711835 |
| 36 | 6  | 0  | 3.678127 | -2.838925 | 0.442065 |
| 37 | 1  | 0  | 4.726909 | -2.878150 | 0.738524 |
| 38 | 6  | 0  | 4.805955 | 1.487277  | -0.908990 |
| 39 | 6  | 0  | 3.495881 | 1.894812  | -1.241012 |
| 40 | 6  | 0  | -2.621221 | -0.188144 | -0.325522 |
| 41 | 6  | 0  | -3.189206 | -2.590959 | 1.035822 |
| 42 | 1  | 0  | 1.029926 | 1.127545  | -2.097981 |
| 43 | 1  | 0  | 2.847392 | 4.435184  | 1.110496 |
| 44 | 1  | 0  | 2.246949 | 3.060293  | -2.907049 |
| 45 | 1  | 0  | 3.173629 | 4.736807  | -1.319025 |
| 46 | 1  | 0  | 5.648400 | 2.124900  | -1.152275 |
| 47 | 1  | 0  | 3.336213 | 2.846652  | -1.735774 |
| 48 | 1  | 0  | -0.105967 | -0.705484 | -0.234764 |
| 49 | 1  | 0  | -1.557185 | -1.060040 | 0.077182 |
| 50 | 1  | 0  | -1.855581 | -2.232530 | 0.735738 |
| 51 | 1  | 0  | -2.621221 | -0.188144 | -0.325522 |
| 52 | 1  | 0  | -3.189206 | -2.590959 | 1.035822 |
| 53 | 1  | 0  | -3.972454 | -0.563066 | -0.026369 |
| 54 | 1  | 0  | -4.225760 | -1.776103 | 0.664483 |
| 55 | 1  | 0  | 0.420531  | 0.463518  | 0.608388 |
| 56 | 1  | 0  | 1.160436  | 1.554104  | 0.043521 |
| 57 | 1  | 0  | 0.225141  | 0.418032  | 1.972936 |
| 58 | 1  | 0  | 1.676059  | 2.566396  | 0.924005 |
| 59 | 1  | 0  | 0.736626  | 1.410171  | 2.832743 |
| 60 | 1  | 0  | 1.448865  | 2.463782  | 2.318796 |
| 61 | 1  | 0  | 0.681446  | -1.883041 | -0.025488 |
| 62 | 1  | 0  | -0.053584 | -0.450663 | -1.297819 |
| 63 | 1  | 0  | -1.047413 | -2.893737 | 1.015358 |
| 64 | 1  | 0  | -2.410908 | 1.034280  | -1.020101 |
| 65 | 1  | 0  | -3.383046 | -3.521060 | 1.558430 |

**5b (conformer 15)**

|    |    |    |        |        |        |
|----|----|----|--------|--------|--------|
| 1  | 6  | 0  | -0.105967 | -0.705484 | -0.234764 |
| 2  | 6  | 0  | -1.557185 | -1.060040 | 0.077182 |
| 3  | 6  | 0  | -1.855581 | -2.232530 | 0.735738 |
| 4  | 6  | 0  | -2.621221 | -0.188144 | -0.325522 |
| 5  | 6  | 0  | -3.189206 | -2.590959 | 1.035822 |
| 6  | 6  | 0  | -3.972454 | -0.563066 | -0.026369 |
| 7  | 6  | 0  | -4.225760 | -1.776103 | 0.664483 |
| 8  | 6  | 0  | 0.420531  | 0.463518  | 0.608388 |
| 9  | 6  | 0  | 1.160436  | 1.554104  | 0.043521 |
| 10 | 6  | 0  | 0.225141  | 0.418032  | 1.972936 |
| 11 | 6  | 0  | 1.676059  | 2.566396  | 0.924005 |
| 12 | 6  | 0  | 0.736626  | 1.410171  | 2.832743 |
| 13 | 6  | 0  | 1.448865  | 2.463782  | 2.318796 |
| 14 | 8  | 0  | 0.681446  | -1.883041 | -0.025488 |
| 15 | 1  | 0  | -0.053584 | -0.450663 | -1.297819 |
| 16 | 1  | 0  | -1.047413 | -2.893737 | 1.015358 |
| 17 | 6  | 0  | -2.410908 | 1.034280  | -1.020101 |
| 18 | 1  | 0  | -3.383046 | -3.521060 | 1.558430 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 19 | 6 | 0 | -5.035469 | 0.285395 | -0.431232 |
| 20 | 1 | 0 | -5.252530 | -2.046692 | 0.887353 |
| 21 | 6 | 0 | 1.419481 | 1.706014 | -1.348944 |
| 22 | 1 | 0 | -0.342709 | -0.403129 | 2.394337 |
| 23 | 6 | 0 | 2.410815 | 3.655230 | 0.384615 |
| 24 | 1 | 0 | 0.559266 | 1.335863 | 3.899667 |
| 25 | 1 | 0 | 1.844599 | 3.235596 | 2.970470 |
| 26 | 1 | 0 | 1.981326 | -1.900788 | -0.595094 |
| 27 | 6 | 0 | 2.360956 | -3.342212 | -0.944875 |
| 28 | 6 | 0 | 3.125346 | -1.513938 | 0.358372 |
| 29 | 8 | 0 | 3.779601 | 3.235596 | 2.970470 |
| 30 | 1 | 0 | 0.342709 | -0.403129 | 2.394337 |
| 31 | 6 | 0 | 1.419481 | 3.235596 | 2.970470 |
| 32 | 1 | 0 | 0.559266 | 1.335863 | 3.899667 |
| 33 | 1 | 0 | 1.844599 | 3.235596 | 2.970470 |
| 34 | 6 | 0 | 1.981326 | -1.900788 | -0.595094 |
| 35 | 6 | 0 | 2.134825 | -2.719685 | 0.572721 |
| 36 | 6 | 0 | 2.360956 | -3.342212 | -0.944875 |
| 37 | 6 | 0 | 3.125346 | -1.513938 | 0.358372 |
| 38 | 6 | 0 | 2.360956 | -3.342212 | -0.944875 |
| 39 | 6 | 0 | 1.419481 | 3.235596 | 2.970470 |
| 40 | 6 | 0 | 1.981326 | -1.900788 | -0.595094 |
| 41 | 6 | 0 | 1.419481 | 3.235596 | 2.970470 |
| 42 | 6 | 0 | 2.555556 | -1.900788 | 0.358372 |
| 43 | 6 | 0 | 1.419481 | 3.235596 | 2.970470 |
| 44 | 6 | 0 | 1.981326 | -1.900788 | -0.595094 |
| 45 | 6 | 0 | 2.134825 | -2.719685 | 0.572721 |
| 46 | 6 | 0 | 2.360956 | -3.342212 | -0.944875 |
| 47 | 6 | 0 | 3.125346 | -1.513938 | 0.358372 |
| 48 | 6 | 0 | 2.360956 | -3.342212 | -0.944875 |
| 49 | 6 | 0 | 3.125346 | -1.513938 | 0.358372 |

**5b (conformer 16)**

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.030234 | 0.126128 | 0.660451 |
| 2 | 6 | 0 | -0.871559 | -1.086530 | 0.260096 |
| 3 | 6 | 0 | -0.294000 | -2.324380 | 0.082164 |
| 4 | 6 | 0 | -2.298281 | -0.956054 | 0.139361 |
| 5 | 6 | 0 | -1.061885 | -3.466112 | -0.238545 |
| 6 | 6 | 0 | -3.072674 | -2.121358 | -0.176416 |
| 7 | 6 | 0 | -2.421124 | -3.367130 | -0.367702 |
| 8 | 6 | 0 | 1.445027 | -0.151153 | 0.942999 |
| 9 | 6 | 0 | 2.418193 | -0.362662 | -0.090540 |
| 10 | 6 | 0 | 1.848737 | -0.183954 | 2.261236 |
| 11 | 6 | 0 | 3.782266 | -0.600184 | 0.286119 |
| 12 | 6 | 0 | 3.189233 | -0.430293 | 2.628924 |
| 13 | 6 | 0 | 4.137269 | -0.629825 | 1.659542 |
| 14 | 8 | 0 | -0.218982 | 1.134157 | -0.345611 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 15 | 1 | 0 | -0.453842 | 0.495787 | 1.604037 |
| 16 | 1 | 0 | 0.775738 | -2.437904 | 0.194992 |
| 17 | 6 | 0 | -2.995925 | 0.268093 | 0.336063 |
| 18 | 1 | 0 | -0.563350 | -4.418820 | -0.376983 |
| 19 | 6 | 0 | -4.484056 | -2.015768 | -0.282461 |
| 20 | 1 | 0 | -3.020518 | -4.238755 | -0.609458 |
| 21 | 6 | 0 | 2.100314 | -0.357803 | -1.478222 |
| 22 | 1 | 0 | 1.113364 | -0.018338 | 3.042300 |
| 23 | 6 | 0 | 4.757021 | -0.810664 | 0.336063 |
| 24 | 1 | 0 | 3.461319 | -0.452068 | 3.678071 |
| 25 | 6 | 0 | -0.563350 | -4.418820 | -0.376983 |
| 26 | 1 | 0 | 3.020518 | -4.238755 | -0.609458 |
| 27 | 6 | 0 | -0.489281 | 3.180082 | 1.021353 |
| 28 | 6 | 0 | -0.010843 | 3.304687 | -1.278920 |
| 29 | 8 | 0 | -1.689734 | 3.621409 | 0.390552 |
| 30 | 6 | 0 | -1.466554 | 3.733641 | -1.029511 |
| 31 | 1 | 0 | 0.103043 | 4.033886 | 1.382257 |
| 32 | 1 | 0 | -0.762203 | 2.570277 | 1.884513 |
| 33 | 1 | 0 | 0.120238 | 2.748805 | -2.207087 |
| 34 | 1 | 0 | 0.659427 | 4.168066 | -1.291548 |
| 35 | 1 | 0 | -2.174915 | 3.074044 | -1.537914 |
| 36 | 1 | 0 | -1.659457 | 4.764394 | -1.341588 |
| 37 | 1 | 0 | 1.369452 | 2.361742 | 0.171697 |
| 38 | 6 | 0 | 3.070506 | -0.570232 | -2.428405 |
| 39 | 6 | 0 | 4.413178 | -0.796756 | -2.052755 |
| 40 | 6 | 0 | -5.122333 | -0.818144 | -0.078779 |
| 41 | 6 | 0 | -4.366053 | 0.331604 | 0.235000 |
| 42 | 1 | 0 | -2.449694 | 1.177368 | 0.538999 |
| 43 | 1 | 0 | -5.051991 | -2.908193 | -0.524816 |
| 44 | 1 | 0 | 1.079235 | -0.175417 | -1.779593 |
| 45 | 1 | 0 | 5.784516 | -0.987483 | -0.423845 |
| 46 | 1 | 0 | 2.802162 | -0.564205 | -3.479032 |
| 47 | 1 | 0 | 5.166963 | -0.960947 | -2.814627 |
| 48 | 1 | 0 | -6.201476 | -0.751413 | -0.159492 |
| 49 | 1 | 0 | -4.867431 | 1.280146 | 0.392139 |

**5b (conformer 17)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.328236 | -0.615090 | -0.464709 |
| 2 | 6 | 0 | -0.918677 | -1.009629 | 0.336532 |
| 3 | 6 | 0 | -0.775000 | -1.614348 | 1.566953 |
| 4 | 6 | 0 | -2.238327 | -0.823302 | -0.196764 |
| 5 | 6 | 0 | -1.888989 | -2.011885 | 2.337653 |
| 6 | 6 | 0 | -3.366608 | -1.228783 | 0.592886 |
| 7 | 6 | 0 | -3.159622 | -1.814582 | 1.867316 |
| 8 | 6 | 0 | 0.499065 | 0.879710 | -0.771656 |
| 9 | 6 | 0 | 0.636122 | 1.883082 | 0.244437 |
| 10 | 6 | 0 | 0.571343 | 1.260623 | -2.096075 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 11 | 6 | 0 | 0.780738 | 3.254119 | -0.154084 |
| 12 | 6 | 0 | 0.724252 | 2.608650 | -2.486977 |
| 13 | 6 | 0 | 0.814490 | 3.587159 | -1.438409 |
| 14 | 8 | 0 | 1.471584 | -1.130007 | 0.224690 |
| 15 | 1 | 0 | 0.248333 | -1.118502 | 1.945959 |
| 16 | 1 | 0 | 0.221265 | -2.486977 | 1.945959 |
| 17 | 6 | 0 | -2.501523 | -0.282786 | -1.485258 |
| 18 | 1 | 0 | -1.726388 | -2.475933 | 3.304046 |
| 19 | 6 | 0 | -4.678024 | -1.055214 | 0.078926 |
| 20 | 1 | 0 | -4.022909 | -2.113448 | 2.452514 |
| 21 | 6 | 0 | 0.656360 | 1.592467 | 0.839477 |
| 22 | 1 | 0 | 0.499371 | -1.438409 | 0.839477 |
| 23 | 6 | 0 | 2.679794 | -1.203227 | -1.485258 |
| 24 | 1 | 0 | 2.702163 | -2.426696 | -1.485258 |
| 25 | 1 | 0 | 3.812631 | -1.525407 | 0.436912 |
| 26 | 1 | 0 | 0.903151 | 4.260370 | -0.802353 |
| 27 | 6 | 0 | -3.726499 | -3.048646 | 0.525092 |
| 28 | 6 | 0 | -3.229087 | -2.204760 | -2.413258 |
| 29 | 6 | 0 | 3.677455 | -1.011342 | 1.388773 |
| 30 | 1 | 0 | 4.769432 | -1.224798 | 0.001191 |
| 31 | 1 | 0 | 2.941695 | -3.357230 | 1.227729 |
| 32 | 1 | 0 | 4.664560 | -3.527349 | 0.812532 |
| 33 | 1 | 0 | 2.838349 | -0.263141 | -1.075369 |
| 34 | 6 | 0 | 0.784052 | 2.591284 | 2.570715 |
| 35 | 6 | 0 | 0.902052 | 3.941011 | -0.539745 |
| 36 | 6 | 0 | 2.702163 | -2.426696 | -1.478675 |
| 37 | 6 | 0 | 3.812631 | -1.525407 | 0.436912 |
| 38 | 6 | 0 | 3.406317 | -3.474567 | -0.802353 |
| 39 | 6 | 0 | 3.726499 | -3.048646 | 0.525092 |
| 40 | 6 | 0 | 3.229087 | -2.204760 | -2.413258 |
| 41 | 6 | 0 | 3.677455 | -1.011342 | 1.388773 |
| 42 | 1 | 0 | 4.769432 | -1.224798 | 0.001191 |
| 43 | 1 | 0 | 2.941695 | -3.357230 | 1.227729 |
| 44 | 1 | 0 | 4.664560 | -3.527349 | 0.812532 |
| 45 | 1 | 0 | 2.838349 | -0.263141 | -1.075369 |
| 46 | 1 | 0 | 0.784052 | 2.591284 | 2.570715 |
| 47 | 1 | 0 | 0.902052 | 3.941011 | 2.173849 |
| 48 | 1 | 0 | 2.702163 | -2.426696 | -1.478675 |
| 49 | 1 | 0 | 3.812631 | -1.525407 | 0.436912 |

5b (conformer 18)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.326279 | -0.605758 | -0.491343 |
| 2 | 6 | 0 | -0.459588 | 0.895796 | -0.779803 |
| 3 | 6 | 0 | -0.530169 | 1.295049 | -2.098932 |
| 4 | 6 | 0 | -0.569833 | 1.888214 | 0.250239 |
| 5 | 6 | 0 | -0.656543 | 2.651200 | -2.471227 |
| 6 | 6 | 0 | -0.687759 | 3.267010 | -0.129639 |
|   | 6  | 0  | -0.721651 | 3.618619 | -1.503796 |
|---|---|---|-----------|---------|-----------|
| 8 | 6  | 0  | 0.905663  | -1.046253 | 0.309859  |
| 9 | 6  | 0  | 2.234244  | -0.868961 | -0.204188 |
| 10| 6  | 0  | 0.737199  | -1.686356 | 1.519238  |
| 11| 6  | 0  | 3.346100  | -1.322309 | 0.582844  |
| 12| 6  | 0  | 1.835315  | -2.130866 | 2.287266  |
| 13| 6  | 0  | 3.114352  | -1.944836 | 1.835487  |
| 14| 8  | 0  | -1.488121 | -1.092216 | 0.189006  |
| 15| 1  | 0  | -0.258046 | -1.100166 | 1.470370  |
| 16| 1  | 0  | -0.477130 | 0.544166  | 2.881670  |
| 17| 6  | 0  | -0.588111 | 1.579767  | 1.637257  |
| 18| 1  | 0  | -0.699218 | 1.989503  | 2.419164  |
| 19| 6  | 0  | -0.784195 | 4.624241  | 0.877553  |
| 20| 1  | 0  | -0.811520 | 4.665756  | -1.773083 |
| 21| 6  | 0  | 2.521623  | -0.290885 | -1.471119 |
| 22| 1  | 0  | -0.266401 | -1.853631 | 1.883731  |
| 23| 6  | 0  | 4.666037  | -1.157246 | 0.883121  |
| 24| 1  | 0  | 1.653568  | -2.621298 | 3.237082  |
| 25| 1  | 0  | 3.965455  | -2.279503 | 2.419164  |
| 26| 6  | 0  | -2.677364 | -1.184090 | -0.601767 |
| 27| 6  | 0  | -3.86952  | -1.340001 | 0.368064  |
| 28| 6  | 0  | -2.726932 | -2.491677 | -1.413310 |
| 29| 8  | 0  | -4.345585 | -2.683847 | 0.256240  |
| 30| 6  | 0  | -3.344785 | -3.457867 | -0.403114 |
| 31| 1  | 0  | -4.693334 | -0.668902 | 0.121746  |
| 32| 1  | 0  | -3.525734 | -1.126703 | 1.386733  |
| 33| 1  | 0  | -1.744245 | -2.799993 | -1.775001 |
| 34| 1  | 0  | -3.393831 | -2.371609 | -2.272202 |
| 35| 1  | 0  | -2.587020 | -3.810378 | 0.310526  |
| 36| 1  | 0  | -3.835010 | -4.322467 | -0.852974 |
| 37| 1  | 0  | -2.774026 | -0.292509 | -1.227022 |
| 38| 6  | 0  | 3.812197  | -0.155633 | -1.925001 |
| 39| 6  | 0  | 4.900728  | -0.586378 | -1.137124 |
| 40| 6  | 0  | -0.782844 | 3.925549  | 2.207632  |
| 41| 6  | 0  | -0.690423 | 2.568632  | 2.586222  |
| 42| 1  | 0  | -0.531478 | 0.548998  | 1.948857  |
| 43| 1  | 0  | -0.865590 | 5.300604  | 0.572772  |
| 44| 1  | 0  | 1.713482  | 0.061200  | -2.094026 |
| 45| 1  | 0  | 5.492672  | -1.500311 | 0.701862  |
| 46| 1  | 0  | 3.995330  | 0.289578  | -2.896671 |
| 47| 1  | 0  | 5.914534  | -0.468792 | -1.502807 |
| 48| 1  | 0  | -0.858882 | 4.695139  | 2.967515  |
| 49| 1  | 0  | -0.701880 | 2.303560  | 3.637589  |

**5b (conformer 19)**

|   | 6  | 0  | 0.261383  | -0.714332 | -0.314352 |
|---|---|---|----------|----------|----------|
| 2 | 6  | 0  | -1.044750 | -1.031941 | 0.423881  |
|   |   |   |                  |                  |                  |
|---|---|---|------------------|------------------|------------------|
| 3 | 6 | 0 | -0.998067       | -1.537287       | 1.705601         |
| 4 | 6 | 0 | -2.319871       | -0.877453       | -0.217072        |
| 5 | 6 | 0 | -2.170232       | -1.860529       | 2.422829         |
| 6 | 6 | 0 | -3.507605       | -1.207899       | 0.518428         |
| 7 | 6 | 0 | -3.400863       | -1.690590       | 1.847229         |
| 8 | 6 | 0 | 0.475942        | 0.747775        | -0.728184        |
| 9 | 6 | 0 | 0.554087        | 1.829599        | 0.210952         |
| 10| 6 | 0 | 0.653801        | 1.016961        | -2.069867        |
| 11| 6 | 0 | 0.753339        | 3.161125        | -0.286157        |
| 12| 6 | 0 | 0.860139        | 2.326144        | -2.556371        |
| 13| 6 | 0 | 0.967771        | 3.378717        | -1.680809        |
| 14| 8 | 0 | 1.346773        | -1.177340       | 0.500550         |
| 15|   | 0 | 0.247927        | -1.297761       | -1.245108        |
| 16|   | 0 | -0.034135       | -1.690405       | 2.168373         |
| 17| 6 | 0 | -2.482297       | -0.440344       | -1.560280        |
| 18| 1 | 0 | -2.084251       | -2.245693       | 3.432766         |
| 19| 6 | 0 | -4.776246       | -1.065338       | -0.101477        |
| 20| 1 | 0 | -4.307978       | -1.933748       | 2.390463         |
| 21| 6 | 0 | 0.464165        | 1.654839        | 1.618478         |
| 22| 1 | 0 | 0.626531        | 0.197389        | -2.781748        |
| 23| 6 | 0 | 0.818963        | 4.244672        | 0.628296         |
| 24| 1 | 0 | 0.986531        | 2.488536        | -3.620683        |
| 25| 1 | 0 | 1.046825        | 4.391843        | -2.038763        |
| 26| 6 | 0 | 2.589977        | -1.342411       | -0.164716        |
| 27| 6 | 0 | 2.723303        | -2.656132       | -0.952536        |
| 28| 6 | 0 | 3.713663        | -1.496137       | 0.867225         |
| 29| 8 | 0 | 4.123455        | -2.863721       | -1.059099        |
| 30| 6 | 0 | 4.752181        | -2.372350       | 0.140203         |
| 31| 1 | 0 | 2.317631        | -2.623708       | -1.965267        |
| 32| 1 | 0 | 2.224911        | -3.462625       | -0.392783        |
| 33| 1 | 0 | 3.301314        | -2.005621       | 1.741614         |
| 34| 1 | 0 | 4.115453        | -0.535618       | 1.191461         |
| 35| 1 | 0 | 5.078664        | -3.215520       | 0.759714         |
| 36| 1 | 0 | 5.637899        | -1.810377       | -0.165541        |
| 37| 1 | 0 | 2.787448        | -0.490775       | -0.824544        |
| 38| 6 | 0 | 0.538459        | 2.726339        | 2.475904         |
| 39| 6 | 0 | 0.710616        | 4.037070        | 1.980181         |
| 40| 6 | 0 | -4.889758       | -0.632659       | -1.398573        |
| 41| 6 | 0 | -3.725958       | -0.324059       | -2.134358        |
| 42| 1 | 0 | -1.614347       | -0.183679       | -2.148489        |
| 43| 1 | 0 | -5.661693       | -1.314650       | 0.471461         |
| 44| 1 | 0 | 0.348385        | 0.660587        | 2.019197         |
| 45| 1 | 0 | 0.962813        | 5.245595        | 0.234822         |
| 46| 1 | 0 | 0.466629        | 2.563078        | 3.545485         |
| 47| 1 | 0 | 0.763510        | 4.873051        | 2.668553         |
| 48 | 1 | 0 | -5.865518 | -0.531523 | -1.860089 |
| 49 | 1 | 0 | -3.813228 | 0.011074 | -3.161929 |

**5b (conformer 20)**

| 1  | 6 | 0 | 0.240509 | 0.091066 | 0.691282  |
| 2  | 6 | 0 | -1.125404 | -0.532422 | 0.965129  |
| 3  | 6 | 0 | -1.494539 | -0.710453 | 2.282142  |
| 4  | 6 | 0 | -2.030078 | -0.931934 | -0.074623 |
| 5  | 6 | 0 | -2.734572 | -1.280904 | 2.641640  |
| 6  | 6 | 0 | -3.291931 | -1.506069 | 0.294351  |
| 7  | 6 | 0 | -3.616261 | -1.667666 | 1.666047  |
| 8  | 6 | 0 | 1.330917  | -0.879240 | 0.234871  |
| 9  | 6 | 0 | 2.691868  | -0.425701 | 0.151232  |
| 10 | 6 | 0 | 1.048783  | 2.198688  | -0.042310 |
| 11 | 6 | 0 | 3.708826  | -1.353526 | -0.249009 |
| 12 | 6 | 0 | 2.054381  | -3.108627 | -0.438793 |
| 13 | 6 | 0 | 3.354950  | -2.694897 | -0.546789 |
| 14 | 8 | 0 | 0.187400  | 1.169057  | 0.258982  |
| 15 | 1 | 0 | 0.574510  | 0.516573  | 1.648801  |
| 16 | 1 | 0 | -0.811528 | -0.403310 | 3.067903  |
| 17 | 6 | 0 | -1.738264 | -0.797372 | -1.461490 |
| 18 | 1 | 0 | -2.984370 | -1.402947 | 3.689411  |
| 19 | 6 | 0 | -4.196609 | -1.911036 | -0.722505 |
| 20 | 1 | 0 | -4.575164 | -2.102314 | 1.928119  |
| 21 | 6 | 0 | 3.096923  | 0.899662  | 0.468104  |
| 22 | 1 | 0 | 0.032901  | -2.559135 | 0.044699  |
| 23 | 6 | 0 | 5.058225  | -0.920852 | -0.328079 |
| 24 | 1 | 0 | 1.783948  | -4.135746 | -0.655869 |
| 25 | 1 | 0 | 4.133903  | -3.386078 | -0.851388 |
| 26 | 6 | 0 | -0.342785 | 2.399066  | 0.223224  |
| 27 | 6 | 0 | -1.867680 | 2.572295  | 0.102875  |
| 28 | 6 | 0 | 0.176296  | 3.560821  | -0.644827 |
| 29 | 8 | 0 | -2.050924 | 3.980818  | 0.115233  |
| 30 | 6 | 0 | -1.012446 | 4.546281  | -0.696928 |
| 31 | 1 | 0 | -2.437231 | 2.151066  | 0.930267  |
| 32 | 1 | 0 | -2.214850 | 2.123090  | -0.838807 |
| 33 | 1 | 0 | 0.422119  | 3.164955  | -1.632066 |
| 34 | 1 | 0 | 1.079324  | 4.010510  | -0.229629 |
| 35 | 1 | 0 | -1.372315 | 4.680450  | -1.725340 |
| 36 | 1 | 0 | -0.778421 | 5.529071  | -0.284751 |
| 37 | 1 | 0 | -0.048168 | 2.537714  | 1.272313  |
| 38 | 6 | 0 | 4.414956  | 1.283241  | 0.393549  |
| 39 | 6 | 0 | 5.409303  | 0.368100  | -0.014434 |
| 40 | 6 | 0 | -3.879785 | -1.766607 | -2.049483 |
| 41 | 6 | 0 | -2.636666 | -1.205603 | -2.418079 |
| 42 | 1 | 0 | -0.798300 | -0.355909 | -1.758181 |
| 43 | 1 | 0 | -5.148064 | -2.341214 | -0.427488 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 44 | 1 | 0 | 2.354153 | 1.626293 | 0.762540 |
| 45 | 1 | 0 | 5.812859 | -1.636238 | -0.638308 |
| 46 | 1 | 0 | 4.693641 | 2.300556 | 0.645407 |
| 47 | 1 | 0 | 6.444190 | 0.685223 | -0.076156 |
| 48 | 1 | 0 | -4.578966 | -2.081095 | -2.816135 |
| 49 | 1 | 0 | -2.389483 | -1.094100 | -3.467944 |

5b (conformer 26)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | -0.183132 | 0.107295 | 0.626844 |
| 2  | 6 | 0 | -1.219471 | -0.949691 | 0.239697 |
| 3  | 6 | 0 | -0.862826 | -2.269994 | 0.072393 |
| 4  | 6 | 0 | -2.603302 | -0.583066 | 0.113987 |
| 5  | 6 | 0 | -1.813460 | -3.265827 | -0.244967 |
| 6  | 6 | 0 | -3.565142 | -1.598743 | -0.201118 |
| 7  | 6 | 0 | -3.135587 | -2.938306 | -0.382871 |
| 8  | 6 | 0 | 1.756192  | 0.120395  | 2.271716  |
| 9  | 6 | 0 | 3.429452  | -1.335585 | 0.347822  |
| 10 | 6 | 0 | 2.836839  | -1.002838 | 2.673514  |
| 11 | 6 | 0 | 3.745723  | 1.403152  | 1.729210  |
| 12 | 6 | 0 | 0.176940  | 1.110201  | -0.408822 |
| 13 | 6 | 0 | -0.543877 | 0.578491  | 1.552133  |
| 14 | 6 | 0 | 0.170741  | 2.565670  | 0.189478  |
| 15 | 6 | 0 | -3.825857 | 0.740736  | 0.307130  |
| 16 | 6 | 0 | -1.483685 | -4.290371 | -0.374631 |
| 17 | 6 | 0 | -4.936598 | -1.251531 | -0.315153 |
| 18 | 6 | 0 | -3.873376 | 3.696512  | -0.623771 |
| 19 | 6 | 0 | 1.862177  | -0.802188 | -1.458409 |
| 20 | 6 | 0 | 0.872005  | -0.189823 | 3.032778  |
| 21 | 6 | 0 | 4.364426  | -1.748132 | -0.636946 |
| 22 | 6 | 0 | 3.080461  | 1.052916  | 3.728597  |
| 23 | 6 | 0 | 4.720980  | 1.776658  | 2.032383  |
| 24 | 6 | 0 | 0.615701  | 2.262811  | -0.151859 |
| 25 | 6 | 0 | 0.035483  | 3.263202  | 0.862791  |
| 26 | 6 | 0 | 0.682739  | 3.124767  | -1.416874 |
| 27 | 8 | 0 | 0.673179  | 4.492935  | 0.550860  |
| 28 | 6 | 0 | 0.914314  | 4.544501  | -0.896096 |
| 29 | 8 | 0 | 0.258717  | 3.031274  | 1.905630  |
| 30 | 6 | 0 | 1.056107  | 3.333125  | 0.735886  |
| 31 | 6 | 0 | -0.277466 | 3.041693  | -1.931981 |
| 32 | 6 | 0 | 1.466431  | 2.798591  | -2.101389 |
| 33 | 6 | 0 | 0.242708  | 5.276585  | -1.331802 |
| 34 | 6 | 0 | 1.942332  | 4.886951  | -1.011600 |
| 35 | 6 | 0 | 1.621286  | 1.969624  | 0.168336  |
| 36 | 6 | 0 | 2.791794  | -1.215353 | -2.382878 |
| 37 | 6 | 0 | 4.056765  | -1.691657 | -1.972891 |
| 38 | 6 | 0 | -1.091000 | -3.467944 | -0.244967 |

S
|   |   |   | 40          6           0          | -5.360254          | 0.038716          | -0.118097          |
|---|---|---|--------------------------------------|---------------------|-------------------|-------------------|
| 41 | 6 | 0 |                                      | -4.419504          | 1.041996          | 0.199772          |
| 42 | 1 | 0 |                                      | -2.377849          | 1.530335          | 0.519035          |
| 43 | 1 | 0 |                                      | -5.648854          | 2.033199          | -0.558452         |
| 44 | 1 | 0 |                                      | 0.902444           | -0.430195         | -1.786017         |
| 45 | 1 | 0 |                                      | 5.332096           | -2.114521         | -0.310146         |
| 46 | 1 | 0 |                                      | 2.550937           | -1.175844         | 3.439406          |
| 47 | 1 | 0 |                                      | 4.779734           | -2.012221         | -2.714588         |
| 48 | 1 | 0 |                                      | -6.411223          | 0.290238          | -0.205467         |
| 49 | 1 | 0 |                                      | -4.754581          | 2.061735          | 0.354306          |
| 50 | 1 | 0 |                                      | -0.227763          | 0.085170          | 0.682926          |
| 51 | 6 | 0 |                                      | -1.308636          | -0.898410         | 0.232702          |
| 52 | 6 | 0 |                                      | -1.012152          | -2.214073         | -0.047139         |
| 53 | 6 | 0 |                                      | -2.674847          | -0.460201         | 0.154427          |
| 54 | 6 | 0 |                                      | -2.008698          | -3.135076         | -0.440872         |
| 55 | 6 | 0 |                                      | -3.682452          | -1.399025         | -0.243642         |
| 56 | 6 | 0 |                                      | -3.314246          | -2.735960         | -0.543924         |
| 57 | 6 | 0 |                                      | 1.143497           | -0.524787         | 0.961978          |
| 58 | 6 | 0 |                                      | 2.056876           | -0.915178         | -0.073367         |
| 59 | 6 | 0 |                                      | 1.507037           | -0.701428         | 2.280614          |
| 60 | 6 | 0 |                                      | 3.321672           | -1.478956         | 0.301595          |
| 61 | 6 | 0 |                                      | 2.749809           | -1.262327         | 2.646118          |
| 62 | 6 | 0 |                                      | 3.640002           | -1.640255         | 1.674835          |
| 63 | 8 | 0 |                                      | -0.185113          | 1.155540          | -0.276100         |
| 64 | 1 | 0 |                                      | -0.566113          | 0.514565          | 1.637119          |
| 65 | 1 | 0 |                                      | 0.008230           | -2.562767         | 0.035235          |
| 66 | 6 | 0 |                                      | -3.094149          | 0.860150          | 0.473666          |
| 67 | 6 | 0 |                                      | -1.727388          | -4.158785         | -0.660163         |
| 68 | 6 | 0 |                                      | -5.036831          | -0.981490         | -0.318695         |
| 69 | 6 | 0 |                                      | -4.086262          | -3.435597         | -0.846827         |
| 70 | 6 | 0 |                                      | 1.771597           | -0.780819         | -1.461509         |
| 71 | 6 | 0 |                                      | 0.816835           | -0.402052         | 3.063145          |
| 72 | 6 | 0 |                                      | 4.235495           | -1.874212         | -0.710902         |
| 73 | 6 | 0 |                                      | 2.994410           | -1.384968         | 3.695089          |
| 74 | 6 | 0 |                                      | 4.600741           | -2.068145         | 1.941388          |
| 75 | 6 | 0 |                                      | 0.318757           | 2.398788          | 0.193543          |
| 76 | 6 | 0 |                                      | -0.231911          | 3.521931          | -0.695987         |
| 77 | 6 | 0 |                                      | 1.834973           | 2.621654          | 0.073536          |
| 78 | 8 | 0 |                                      | 0.718458           | 4.585476          | -0.653482         |
| 79 | 6 | 0 |                                      | 1.913152           | 4.145719          | 0.014959          |
| 80 | 6 | 0 |                                      | -1.202927          | 3.893645          | -0.357229         |
| 81 | 6 | 0 |                                      | -0.341172          | 3.141934          | -1.718971         |
| 82 | 6 | 0 |                                      | 2.181632           | 2.175171          | -0.861530         |
| 83 | 6 | 0 |                                      | 2.406277           | 2.192750          | 0.897182          |
| 84 | 6 | 0 |                                      | 2.777563           | 4.510623          | -0.544638         |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 36 | 1 | 0 | 1.947863 | 4.583889 | 1.021694 |
| 37 | 1 | 0 | 0.003404 | 2.546766 | 1.236967 |
| 38 | 6 | 0 | 2.679170 | -1.178781 | -2.413891 |
| 39 | 6 | 0 | 3.925047 | -1.729637 | -2.039439 |
| 40 | 6 | 0 | -5.401507 | 0.303270 | -0.003431 |
| 41 | 6 | 0 | -4.416517 | 1.229201 | 0.402804 |
| 42 | 6 | 0 | -2.360008 | 0.065257 | 0.669336 |
| 43 | 6 | 0 | -1.407827 | -0.187031 | 3.019789 |
| 44 | 6 | 0 | -1.860639 | -0.159397 | 2.223738 |
| 45 | 6 | 0 | -2.329953 | -0.499423 | -0.132530 |
| 46 | 6 | 0 | -3.203879 | -0.441894 | 2.555368 |
| 47 | 6 | 0 | -3.695802 | -0.777388 | 0.206557 |
| 48 | 6 | 0 | -4.103011 | -0.742085 | 0.156547 |
| 49 | 6 | 0 | -0.947804 | -1.077935 | 0.333214 |
| 1 | 6 | 0 | 0.244696 | 1.118022 | -0.353776 |
| 2 | 6 | 0 | -1.163509 | 0.082487 | 3.019789 |
| 3 | 6 | 0 | -1.636509 | 0.082487 | 3.019789 |
| 4 | 6 | 0 | -1.956745 | -0.556860 | -1.504679 |
| 5 | 6 | 0 | -3.166858 | -2.087947 | -0.079323 |
| 6 | 6 | 0 | -3.516601 | -1.092115 | -0.825512 |
| 7 | 6 | 0 | -4.618513 | -0.956922 | 1.805697 |
| 8 | 6 | 0 | -5.139060 | -0.956922 | 1.805697 |
| 9 | 6 | 0 | -5.084644 | -2.484360 | 0.504151 |
| 10 | 6 | 0 | -4.567887 | -1.952972 | -0.261619 |
| 11 | 6 | 0 | -7.40969 | -4.72954 | 0.10961 |
| 12 | 6 | 0 | -3.180055 | -4.243058 | -0.247920 |
| 13 | 6 | 0 | -3.62187 | 2.393710 | -0.121094 |
| 14 | 6 | 0 | -3.247908 | 3.279908 | -1.326008 |
| 15 | 6 | 0 | -4.275556 | 3.181413 | 1.072906 |
| 16 | 6 | 0 | -4.040173 | -0.940693 | 0.073413 |
| 17 | 6 | 0 | -0.876382 | 4.421673 | 0.407189 |
| 18 | 6 | 0 | -0.858050 | 3.948121 | -1.558059 |

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 36 | 1 | 0 | 1.947863 | 4.583889 | 1.021694 |
| 37 | 1 | 0 | 0.003404 | 2.546766 | 1.236967 |
| 38 | 6 | 0 | 2.679170 | -1.178781 | -2.413891 |
| 39 | 6 | 0 | 3.925047 | -1.729637 | -2.039439 |
| 40 | 6 | 0 | -5.401507 | 0.303270 | -0.003431 |
| 41 | 6 | 0 | -4.416517 | 1.229201 | 0.402804 |
| 42 | 6 | 0 | -2.360008 | 0.065257 | 0.669336 |
| 43 | 6 | 0 | -1.407827 | -0.187031 | 3.019789 |
| 44 | 6 | 0 | -1.860639 | -0.159397 | 2.223738 |
| 45 | 6 | 0 | -2.329953 | -0.499423 | -0.132530 |
| 46 | 6 | 0 | -3.203879 | -0.441894 | 2.555368 |
| 47 | 6 | 0 | -3.695802 | -0.777388 | 0.206557 |
| 48 | 6 | 0 | -4.103011 | -0.742085 | 0.156547 |
| 49 | 6 | 0 | -0.947804 | -1.077935 | 0.333214 |
| 1 | 6 | 0 | 0.244696 | 1.118022 | -0.353776 |
| 2 | 6 | 0 | -1.163509 | 0.082487 | 3.019789 |
| 3 | 6 | 0 | -1.636509 | 0.082487 | 3.019789 |
| 4 | 6 | 0 | -1.956745 | -0.556860 | -1.504679 |
| 5 | 6 | 0 | -3.166858 | -2.087947 | -0.079323 |
| 6 | 6 | 0 | -3.516601 | -2.484360 | 0.504151 |
| 7 | 6 | 0 | -4.618513 | -1.092115 | -0.825512 |
| 8 | 6 | 0 | -5.139060 | -0.956922 | 1.805697 |
| 9 | 6 | 0 | -5.084644 | -2.484360 | 0.504151 |
| 10 | 6 | 0 | -4.567887 | -1.952972 | -0.261619 |
| 11 | 6 | 0 | -7.40969 | -4.72954 | 0.10961 |
| 12 | 6 | 0 | -3.180055 | -4.243058 | -0.247920 |
| 13 | 6 | 0 | -3.62187 | 2.393710 | -0.121094 |
| 14 | 6 | 0 | -3.247908 | 3.279908 | -1.326008 |
| 15 | 6 | 0 | -4.275556 | 3.181413 | 1.072906 |
| 16 | 6 | 0 | -4.040173 | -0.940693 | 0.073413 |
| 17 | 6 | 0 | -0.876382 | 4.421673 | 0.407189 |
| 18 | 6 | 0 | -0.858050 | 3.948121 | -1.558059 |

**5b (conformer 39)**
|   |   |   |    |    |    |
|---|---|---|----|----|----|
| 32| 1 | 0 | 0.237642 | 2.690892 | -2.206297 |
| 33| 1 | 0 | 1.016049 | 2.581944 | 1.563167 |
| 34| 1 | 0 | -0.501176 | 3.443611 | 1.822665 |
| 35| 1 | 0 | 1.824308 | 4.728216 | 0.850354 |
| 36| 1 | 0 | 0.182557 | 5.275928 | 0.438968 |
| 37| 1 | 0 | -1.443206 | 2.265541 | -0.012930 |
| 38| 6 | 0 | 4.385984 | 0.435699 | -0.045714 |
| 39| 6 | 0 | 5.170857 | -0.720671 | -0.240531 |
| 40| 6 | 0 | -4.222036 | -1.138166 | -2.138426 |
| 41| 6 | 0 | -2.877334 | -0.868678 | -2.476616 |
| 42| 1 | 0 | -0.933936 | -0.341829 | -1.777721 |
| 43| 1 | 0 | -5.648365 | -1.299898 | -0.554066 |
| 44| 1 | 0 | 2.440965 | 1.244830 | 0.214419 |
| 45| 1 | 0 | 5.156641 | -2.851227 | -0.416887 |
| 46| 1 | 0 | 4.858525 | 1.411683 | -0.045653 |
| 47| 1 | 0 | 6.242427 | -0.631572 | -0.379926 |
| 48| 1 | 0 | -4.936184 | -1.381698 | -2.917053 |
| 49| 1 | 0 | -2.567833 | -0.908498 | -3.515073 |

5b (conformer 41)

|   |   |   |    |    |    |
|---|---|---|----|----|----|
| 1 | 6 | 0 | 0.169056 | 0.110181 | 0.628398 |
| 2 | 6 | 0 | -1.237083 | -0.399254 | 0.936711 |
| 3 | 6 | 0 | -1.617613 | -0.462175 | 2.260328 |
| 4 | 6 | 0 | -2.167351 | -0.806961 | -0.077980 |
| 5 | 6 | 0 | -2.891190 | -0.928258 | 2.653014 |
| 6 | 6 | 0 | -3.464702 | -1.270040 | 0.323926 |
| 7 | 6 | 0 | -3.796880 | -1.321058 | 1.702676 |
| 8 | 6 | 0 | 1.188928 | -0.967339 | 0.253100 |
| 9 | 6 | 0 | 2.578819 | -0.625627 | 0.122027 |
| 10| 6 | 0 | 0.811198 | -2.284580 | 0.109994 |
| 11| 6 | 0 | 3.524690 | -1.663754 | -0.168607 |
| 12| 6 | 0 | 1.745876 | -3.302172 | -0.184855 |
| 13| 6 | 0 | 3.073702 | -2.999606 | -0.324043 |
| 14| 8 | 0 | 0.190045 | 1.113391 | -0.405780 |
| 15| 1 | 0 | 0.532262 | 0.578001 | 1.554450 |
| 16| 1 | 0 | -0.914843 | -0.147994 | 3.025617 |
| 17| 6 | 0 | -1.868672 | -0.782135 | -1.469427 |
| 18| 1 | 0 | -3.146750 | -0.965248 | 3.705840 |
| 19| 6 | 0 | -4.396123 | -1.676608 | -0.667312 |
| 20| 1 | 0 | -4.781525 | -1.674907 | 1.989568 |
| 21| 6 | 0 | 3.079365 | 0.694354 | 0.286202 |
| 22| 1 | 0 | -0.227365 | -2.560881 | 0.230025 |
| 23| 6 | 0 | 4.902069 | -1.341679 | -0.285144 |
| 24| 1 | 0 | 1.399493 | -4.323530 | -0.294768 |
| 25| 1 | 0 | 3.799616 | -3.774682 | -0.546436 |
| 26| 6 | 0 | -0.603751 | 2.270653 | -0.165321 |
| 27| 6 | 0 | -0.548317 | 3.161807 | -1.423141 |
|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 28 | 6 | 0 | -0.116943 | 3.217357 | 0.947711 |
| 29 | 8 | 0 | -0.429486 | 4.517803 | -0.979751 |
| 30 | 6 | 0 | -0.635050 | 4.558032 | 0.432554 |
| 31 | 1 | 0 | -1.444349 | 3.045716 | -2.042069 |
| 32 | 1 | 0 | 0.330715 | 2.903097 | -2.019425 |
| 33 | 1 | 0 | 0.976193 | 3.226576 | 0.975308 |
| 34 | 1 | 0 | -0.498426 | 2.960491 | 1.937868 |
| 35 | 1 | 0 | -0.095222 | 5.420432 | 0.827091 |
| 36 | 1 | 0 | -0.635050 | 4.558032 | 0.432554 |
| 37 | 1 | 0 | -1.635967 | 1.968905 | 0.043177 |
| 38 | 6 | 0 | 4.421352 | 0.970930 | 0.176280 |
| 39 | 6 | 0 | 5.346432 | -0.054670 | -0.114585 |
| 40 | 6 | 0 | -4.073022 | -1.636624 | -2.000318 |
| 41 | 6 | 0 | -2.795798 | -1.186073 | -2.400534 |
| 42 | 1 | 0 | -0.899153 | -0.430298 | -1.790349 |
| 43 | 1 | 0 | -5.373610 | -2.032348 | -0.348466 |
| 44 | 1 | 0 | 2.385211 | 1.499563 | 0.471313 |
| 45 | 1 | 0 | 5.601974 | -2.139835 | -0.509882 |
| 46 | 1 | 0 | 4.772212 | 1.987338 | 0.306375 |
| 47 | 1 | 0 | 6.401653 | 0.177322 | -0.204592 |
| 48 | 1 | 0 | -4.793789 | -1.950398 | -2.747006 |
| 49 | 1 | 0 | -2.543146 | -1.158454 | -3.454609 |

**5b (conformer 43)**

|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 1  | 6 | 0 | -0.378122 | -0.585262 | -0.469758 |
| 2  | 6 | 0 | -0.423106 | 0.919100 | -0.767365 |
| 3  | 6 | 0 | -0.520167 | 1.314536 | -2.085823 |
| 4  | 6 | 0 | -0.432498 | 1.921213 | 0.258804 |
| 5  | 6 | 0 | -0.578420 | 2.674190 | -2.462671 |
| 6  | 6 | 0 | -0.481638 | 3.302658 | -0.125932 |
| 7  | 6 | 0 | -0.547658 | 3.648636 | -1.500438 |
| 8  | 6 | 0 | 0.842068 | -1.107341 | 0.301012 |
| 9  | 6 | 0 | 2.172274 | -0.985509 | -0.224577 |
| 10 | 6 | 0 | 0.651967 | -1.774061 | 1.493029 |
| 11 | 6 | 0 | 3.267176 | -1.517867 | 0.536510 |
| 12 | 6 | 0 | 1.733843 | -2.295654 | 2.235224 |
| 13 | 6 | 0 | 3.016236 | -2.161861 | 1.774571 |
| 14 | 8 | 0 | -1.547803 | -0.984479 | 0.249647 |
| 15 | 1 | 0 | -0.372748 | -1.091365 | -1.446002 |
| 16 | 1 | 0 | -0.540313 | 0.557279 | -2.864022 |
| 17 | 6 | 0 | -0.412941 | 1.619745 | 1.647454 |
| 18 | 1 | 0 | -0.644675 | 2.937172 | -3.512319 |
| 19 | 6 | 0 | -0.477711 | 4.306486 | 0.877524 |
| 20 | 1 | 0 | -0.584044 | 4.697951 | -1.773925 |
| 21 | 6 | 0 | 2.476208 | -0.391639 | -1.480320 |
| 22 | 1 | 0 | -0.356282 | -1.903658 | 1.859928 |
| 23 | 6 | 0 | 4.588514 | -1.409891 | 0.030213 |

S303
|   |   |   | 1.536349 | -2.804334 | 3.172215 |
|---|---|---|----------|----------|----------|
| 24| 1 | 0 | 3.854772 | -2.556206 | 2.338911 |
| 25| 1 | 0 | -2.761021 | -1.017422 | -0.501749 |
| 26| 6 | 0 | -3.912726 | -1.206143 | 0.491268 |
| 27| 6 | 0 | -2.867034 | -2.283434 | -1.395818 |
| 28| 8 | 0 | -4.105585 | -2.609791 | 0.599277 |
| 29| 6 | 0 | -3.988075 | -3.110965 | 0.728043 |
| 30| 1 | 0 | -4.822764 | -0.719585 | 0.105995 |
| 31| 1 | 0 | -3.676080 | -0.804939 | 1.475579 |
| 32| 1 | 0 | -1.916586 | -2.818808 | -1.371887 |
| 33| 6 | 0 | -3.99915  | -2.044703 | -2.435549 |
| 34| 6 | 0 | -3.768511 | -4.177016 | -0.664568 |
| 35| 1 | 0 | -4.939095 | -2.980881 | -1.266837 |
| 36| 1 | 0 | -2.868275 | -0.313750 | -1.946798 |
| 37| 6 | 0 | 4.839863  | -0.821187 | -1.183477 |
| 38| 6 | 0 | -0.443260 | 3.975691  | 2.208736  |
| 39| 6 | 0 | -0.417039 | 2.617307  | 2.592825  |
| 40| 1 | 0 | -0.405916 | 0.588300  | 1.962907  |
| 41| 1 | 0 | -0.508295 | 5.346451  | 0.69370   |
| 42| 1 | 0 | 1.681156  | 0.017288  | -2.085026 |
| 43| 1 | 0 | 5.402283  | -1.82317  | 0.624642  |
| 44| 1 | 0 | 3.962622  | 0.145084  | -2.909696 |
| 45| 1 | 0 | 5.854406  | -0.748343 | -1.558707 |
| 46| 1 | 0 | -0.442924 | 4.751822  | 2.965787  |
| 47| 1 | 0 | -0.401512 | 2.358218  | 3.645625  |

|   |   |   | 5b (conformer 44) |
|---|---|---|-------------------|
| 1 | 6 | 0 | 0.104199 0.077636 0.670472 |
| 2 | 6 | 0 | -1.346107 -0.301414 0.966777 |
| 3 | 6 | 0 | -1.714233 -0.427233 2.289798 |
| 4 | 6 | 0 | -2.327120 -0.530488 -0.055727 |
| 5 | 6 | 0 | -3.023905 -0.788372 2.672755 |
| 6 | 6 | 0 | -3.660386 -0.886956 0.337368 |
| 7 | 6 | 0 | -3.978227 -1.010579 1.714564 |
| 8 | 6 | 0 | 1.000035 -1.075025 0.209454 |
| 9 | 6 | 0 | 2.420313 -0.881073 0.109279 |
| 10| 6 | 0 | 0.479508 -2.324786 -0.046527 |
| 11| 6 | 0 | 3.248708 -1.990088 -0.264227 |
| 12| 6 | 0 | 1.298799 -3.411487 -0.425932 |
| 13| 6 | 0 | 2.653750 -3.249026 -0.534839 |
| 14| 8 | 0 | 0.222248 1.136326 -0.295629 |
| 15| 1 | 0 | 0.520760 0.434971 1.623104 |
| 16| 1 | 0 | -0.973673 -0.245746 3.062336 |
| 17| 6 | 0 | -2.046344 -0.430517 -1.447982 |
| 18| 1 | 0 | -3.268052 -0.880169 3.724953 |
| 19| 6 | 0 | -4.642165 -1.118962 -0.661675 |
|    |   |   |        |        |        |        |
|----|---|---|--------|--------|--------|--------|
| 20 | 1 | 0 | -4.990612 | -1.282546 | 1.994303 |
| 21 | 6 | 0 |  3.061981  |  0.356736  |  0.384534 |
| 22 | 1 | 0 | -0.584385  | -2.492905  |  0.048874 |
| 23 | 6 | 0 |  4.654835  | -1.815461  | -0.346915 |
| 24 | 1 | 0 |  0.842348  | -4.374528  | -0.624611 |
| 25 | 1 | 0 |  3.291643  | -4.078978  | -0.820390 |
| 26 | 6 | 0 | -0.414768  |  2.373770  |  0.047735 |
| 27 | 6 | 0 | -0.432258  |  3.242593  | -1.233070 |
| 28 | 6 | 0 |  0.842348  | -4.374528  | -0.624611 |
| 29 | 1 | 0 | -1.439289  |  3.514471  | -1.552676 |
| 30 | 1 | 0 |  0.062378  |  2.680225  | -2.034239 |
| 31 | 1 | 0 |  1.011392  |  2.644657  |  1.716536 |
| 32 | 1 | 0 | -0.292558  |  3.836370  |  1.646548 |
| 33 | 1 | 0 |  2.079452  |  3.642029  | -0.284760 |
| 34 | 1 | 0 |  1.494442  |  5.097389  |  0.559479 |
| 35 | 1 | 0 | -1.421919  |  2.171321  |  0.419505 |
| 36 | 1 | 0 |  4.427827  |  0.490304  |  0.304282 |
| 37 | 1 | 0 | -3.733027  | -0.605003  | -0.066553 |
| 38 | 1 | 0 |  5.237317  | -0.605003  | -0.066553 |
| 39 | 1 | 0 |  4.333546  | -1.011424  | -1.994492 |
| 40 | 1 | 0 | -3.022570  | -0.665136  | -2.386780 |
| 41 | 1 | 0 | -1.049189  | -1.552676  | -1.761949 |
| 42 | 1 | 0 | -5.645890  | -1.387099  | -0.348542 |
| 43 | 1 | 0 |  2.459644  |  1.216527  |  0.634242 |
| 44 | 1 | 0 |  5.264900  | -2.665654  | -0.634174 |
| 45 | 1 | 0 |  4.887903  |  1.448159  |  0.520873 |
| 46 | 1 | 0 |  3.370519  | -0.556019  | -0.348542 |
| 47 | 1 | 0 |  2.106219  | -0.817966  | -0.038973 |
| 48 | 1 | 0 |  1.481746  | -0.862008  |  2.304988 |
| 49 | 1 | 0 |  3.370519  | -1.396438  |  0.315092 |

**5b (conformer 51)**

|    |   |   |        |        |        |        |
|----|---|---|--------|--------|--------|--------|
|    | 6 | 0 | -0.226176 |  0.046844 |  0.743616 |
|    | 6 | 0 | -1.265982 | -0.917851 |  0.169218 |
|    | 6 | 0 | -0.920464 | -2.179730 | -0.261104 |
|    | 6 | 0 | -2.647000 | -0.522722 |  0.128506 |
|    | 6 | 0 | -1.880655 | -3.083301 | -0.769154 |
|    | 6 | 0 | -3.618016 | -1.444356 | -0.383958 |
|    | 6 | 0 | -3.199713 | -2.722799 | -0.835155 |
|    | 6 | 0 |  1.152891 | -0.556019 |  1.001337 |
|    | 6 | 0 |  2.106219 | -0.817966 | -0.038973 |
|    | 6 | 0 |  1.481746 | -0.862008 |  2.304988 |
|    | 6 | 0 |  3.370519 | -1.396438 |  0.315092 |
|    | 6 | 0 |  2.724535 | -1.436096 |  2.649586 |
|    | 6 | 0 |  3.650548 | -1.696539 |  1.673498 |
|    | 8 | 0 | -0.194148 |  1.209187 | -0.100746 |
|    | 1 | 0 | -0.601322 |  0.366325 |  1.726385 |
|   |   |   |   |   |
|---|---|---|---|---|
|   |   |   |   |   |
| 16 | 1 | 0 | 0.111366 | -2.499308 | -0.211123 |
| 17 | 6 | 0 | -3.116007 | 0.736188 | 0.593178 |
| 18 | 1 | 0 | -1.560849 | -4.063300 | -1.104629 |
| 19 | 6 | 0 | -4.986565 | -1.070108 | -0.420790 |
| 20 | 1 | 0 | -3.944206 | -3.409577 | -1.224180 |
| 21 | 6 | 0 | 1.863728 | -0.533208 | -1.412573 |
| 22 | 1 | 0 | 0.763012 | -0.658246 | 3.092490 |
| 23 | 6 | 0 | 4.322964 | -1.664326 | -0.703434 |
| 24 | 1 | 0 | 2.940259 | -1.662469 | 3.687580 |
| 25 | 6 | 0 | 4.986565 | -1.070108 | -0.420790 |
| 26 | 1 | 0 | 3.944206 | -3.409577 | -1.224180 |
| 27 | 6 | 0 | 1.863728 | -0.533208 | -1.412573 |
| 28 | 6 | 0 | 0.591233 | 4.468094 | -0.690152 |
| 29 | 1 | 0 | 2.297694 | 1.888181 | 0.444791 |
| 30 | 1 | 0 | 1.940285 | 3.344431 | 1.390597 |
| 31 | 1 | 0 | 1.827503 | 3.091912 | -1.657519 |
| 32 | 1 | 0 | 2.632561 | 4.369289 | -0.712241 |
| 33 | 1 | 0 | -0.211885 | 2.433297 | 1.557367 |
| 34 | 6 | 0 | -0.808531 | -1.379576 | -2.018060 |
| 35 | 1 | 0 | 1.674004 | -0.312290 | 3.586460 |
| 36 | 1 | 0 | 0.165945 | 2.443685 | -0.527797 |
| 37 | 6 | 0 | -1.560849 | -4.063300 | -1.104629 |
| 38 | 1 | 0 | -2.411782 | 1.457060 | 0.981691 |
| 39 | 1 | 0 | -5.399468 | 0.155873 | 0.036945 |
| 40 | 6 | 0 | -4.450604 | 1.068287 | 0.554148 |
| 41 | 1 | 0 | -0.230213 | 0.044901 | 0.775697 |
| 42 | 6 | 0 | -1.152953 | -0.555124 | 1.017516 |
| 43 | 1 | 0 | -1.468869 | -0.922663 | 2.308644 |
| 44 | 6 | 0 | -2.120121 | -0.758704 | -0.023273 |
| 45 | 1 | 0 | -5.274346 | -2.102538 | 0.420117 |
| 46 | 1 | 0 | 2.599303 | -0.583469 | 3.411258 |
| 47 | 1 | 0 | 4.783502 | 3.685194 | -0.732664 |
| 48 | 6 | 0 | 5.399468 | 0.155873 | 0.036945 |
| 49 | 1 | 0 | -3.382884 | -1.349004 | 0.316775 |
| 50 | 1 | 0 | -3.648719 | -1.714699 | 1.661898 |
| 51 | 6 | 0 | 1.255391 | -0.900451 | 0.146574 |
| 52 | 6 | 0 | 2.642117 | -0.524498 | 0.131354 |
| 53 | 6 | 0 | 0.891139 | -2.126940 | 0.036945 |
| 54 | 6 | 0 | 3.600015 | 1.427011 | 0.436586 |

**5b (conformer 52)**

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6 | 0 | 0.230213 | 0.044901 | 0.775697 |
| 2 | 6 | 0 | -1.152953 | -0.555124 | 1.017516 |
| 3 | 6 | 0 | -1.468869 | -0.922663 | 2.308644 |
| 4 | 6 | 0 | -2.120121 | -0.758704 | -0.023273 |
| 5 | 6 | 0 | -2.710881 | -1.506678 | 2.639181 |
| 6 | 6 | 0 | -3.382884 | -1.349004 | 0.316775 |
| 7 | 6 | 0 | -3.648719 | -1.714699 | 1.661898 |
| 8 | 6 | 0 | 1.255391 | -0.900451 | 0.146574 |
| 9 | 6 | 0 | 2.642117 | -0.524498 | 0.131354 |
| 10 | 6 | 0 | 0.891139 | -2.126940 | 0.036945 |
| 11 | 6 | 0 | 3.600015 | 1.427011 | 0.436586 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 12| 6 | 0 | 1.838420 | -3.011277 | -0.926100 |   |
| 13| 6 | 0 | 3.163160 | -2.668034 | -0.967581 |   |
| 14| 8 | 0 | 0.210384 | 1.247068  | -0.011419 |   |
| 15| 1 | 0 | 0.616556 | 0.311594  | 1.770007  |   |
| 16| 1 | 0 | -0.739485| -0.763381 | 3.096683  |   |
| 17| 6 | 0 | -1.894018| -0.402399 | -1.382539 |   |
| 18| 1 | 0 | -2.916111| -1.782780 | 3.667225  |   |
| 19| 6 | 0 | -4.349018| -1.560097 | -0.701854 |   |
| 20| 1 | 0 | -4.608900| -2.159204 | 1.901934  |   |
| 21| 6 | 0 | 3.128335 | 0.697007  | 0.672160  |   |
| 22| 1 | 0 | -0.739485| -2.432189 | -0.011419 |   |
| 23| 6 | 0 | -1.894018| -0.402399 | -1.382539 |   |
| 24| 1 | 0 | -2.916111| -1.782780 | 3.667225  |   |
| 25| 6 | 0 | -4.349018| -1.560097 | -0.701854 |   |
| 26| 1 | 0 | -4.608900| -2.159204 | 1.901934  |   |
| 27| 6 | 0 | -0.158049| 2.450038  | 0.672160  |   |
| 28| 6 | 0 | -1.649581| 3.864172  | 0.556232  |   |
| 29| 8 | 0 | -1.807431| 3.568280  | 0.672160  |   |
| 30| 6 | 0 | -0.523120| 3.864172  | 0.556232  |   |
| 31| 1 | 0 | -1.959170| 3.407319  | 1.418018  |   |
| 32| 1 | 0 | -2.283250| 1.915895  | 0.50173   |   |
| 33| 1 | 0 | 1.486080 | 3.375934  | -0.432728 |   |
| 34| 1 | 0 | 0.538879 | 4.491983  | 0.580360  |   |
| 35| 1 | 0 | -0.325687| 3.199999  | -2.055077 |   |
| 36| 1 | 0 | -0.532373| 4.868655  | -1.562303 |   |
| 37| 1 | 0 | 0.162921 | 2.388112  | 1.718299  |   |
| 38| 6 | 0 | 4.467908 | 1.006357  | 0.655041  |   |
| 39| 6 | 0 | 5.404297 | 0.117341  | 0.084575  |   |
| 40| 6 | 0 | -4.092891| -1.208172 | -2.003092 |   |
| 41| 6 | 0 | -2.852793| -0.623374 | -2.341919 |   |
| 42| 1 | 0 | -0.958203| 0.064410  | -1.652294 |   |
| 43| 1 | 0 | -5.299476| -2.007065 | -0.429360 |   |
| 44| 1 | 0 | 2.433254 | 1.403774  | 1.101294  |   |
| 45| 1 | 0 | 5.683592 | -1.766486 | -0.886083 |   |
| 46| 1 | 0 | 4.808749 | 1.943958  | 1.080225  |   |
| 47| 1 | 0 | 6.457221 | 0.375243  | 0.071752  |   |
| 48| 1 | 0 | -4.839972| -1.373021 | -2.771350 |   |
| 49| 1 | 0 | -2.657659| -0.338844 | -3.369726 |   |
|   |   |   | 6b (conformer 1) |   |   |   |
| 1 | 6 | 0 | 4.386018 | -0.892904 | -0.449080 |   |
| 2 | 6 | 0 | 3.562130 | 0.214450  | 0.218523  |   |
| 3 | 6 | 0 | 3.486134 | -2.160666 | -0.553950 |   |
| 4 | 6 | 0 | 2.170976 | 0.455281  | -0.334303 |   |
| 5 | 6 | 0 | 2.090724 | -1.918520 | -1.143227 |   |
| 6 | 6 | 0 | 1.342004 | -0.837767 | -0.373496 |   |
| 7 | 6 | 0 | 5.639117 | -1.243931 | 0.424963  |   |
|    |    |   |    |    |    |    |
|----|----|---|----|----|----|----|
|  8 |  6 |  0 |  6.357791 |  0.016410 |  0.969884 |
|  9 |  6 |  0 |  4.018355 |  0.946127 |  1.238457 |
| 10 |  6 |  0 |  5.389030 |  0.831675 |  1.837368 |
| 11 |  8 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 12 |  6 |  0 |  4.792151 | -0.424367 | -1.868999 |
| 13 |  1 |  0 |  6.666327 |  0.647671 |  0.127356 |
| 14 |  1 |  0 |  5.246975 | -1.763422 |  1.312486 |
| 15 |  6 |  0 | -0.962678 |  0.831675 |  1.837368 |
| 16 |  0 |  0 |  4.792151 | -0.424367 | -1.868999 |
| 17 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 18 |  6 |  0 |  4.792151 | -0.424367 | -1.868999 |
| 19 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 20 |  6 |  0 |  4.792151 | -0.424367 | -1.868999 |
| 21 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 22 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 23 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 24 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 25 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 26 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 27 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 28 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 29 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 30 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 31 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 32 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 33 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 34 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 35 |  6 |  0 |  0.064084 | -0.691981 | -1.005131 |
| 36 |  1 |  0 |  1.188242 | -1.177027 |  0.663246 |
| 37 |  1 |  0 |  3.996328 | -2.923196 | -1.149233 |
| 38 |  1 |  0 |  3.370190 | -2.579630 |  0.453159 |
| 39 |  1 |  0 |  1.668217 |  1.219715 |  0.261908 |
| 40 |  1 |  0 |  2.226834 |  0.845002 | -1.357387 |
| 41 |  1 |  0 |  2.152073 | -1.613949 | -2.193381 |
| 42 |  1 |  0 |  1.507539 | -2.843283 | -1.121384 |
| 43 |  1 |  0 |  3.361126 |  1.695945 |  1.674908 |
| 44 |  1 |  0 |  5.313303 |  0.372151 |  2.834840 |
| 45 |  1 |  0 |  5.794243 |  1.835099 |  2.011827 |
| 46 |  1 |  0 |  5.520446 |  0.388933 | -1.822674 |
| 47 |  1 |  0 |  5.225898 | -1.240741 | -2.450995 |
| 48 |  1 |  0 |  3.932204 | -0.053746 | -2.428490 |
| 49 |  1 |  0 | -0.704866 | -0.094671 |  0.806736 |
| 50 |  1 |  0 | -0.142879 |  1.177115 | -2.502422 |
| 51 |  1 |  0 | -0.263041 |  3.572455 | -3.155739 |
| 52 |  1 |  0 | -1.241325 |  5.230744 | -1.602807 |
|   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 53| 1 | 0 | -3.056670 | 0.616212 | -1.862754 |
| 54| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 55| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 56| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 57| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 58| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 59| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 60| 1 | 0 | -4.864166 | -4.533578 | 0.367546 |
| 61| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 62| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 63| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 64| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 65| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 66| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 67| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 68| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 69| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 70| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 71| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 72| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 73| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 74| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 75| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 76| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 77| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 78| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 79| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |
| 80| 1 | 0 | -5.133078 | -0.632447 | -2.316457 |
| 81| 1 | 0 | -5.563763 | -2.788247 | -1.182162 |
| 82| 1 | 0 | -0.629212 | 0.970394 | 1.294496 |

|   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 6b (conformer 2) |   |   |   |   |   |   |   |   |   |   |   |
| 1 | 6 | 0 | 4.294549 | -1.152211 | -0.020171 |
| 2 | 6 | 0 | 3.930436 | 0.315872 | -0.270196 |
| 3 | 6 | 0 | 3.072260 | -1.840393 | 0.657135 |
| 4 | 6 | 0 | 2.581959 | 0.586880 | -0.905774 |
| 5 | 6 | 0 | 1.729029 | -1.612593 | 0.050125 |
| 6 | 6 | 0 | 1.437638 | -0.116338 | -0.174128 |
| 7 | 6 | 0 | 5.520792 | -1.248074 | 0.951109 |
| 8 | 6 | 0 | 6.648767 | -0.249842 | 0.586469 |
| 9 | 6 | 0 | 4.739843 | 1.328635 | 0.050446 |
| 10 | 6 | 0 | 6.109615 | 1.186463 | 0.646946 |
| 11 | 6 | 0 | 0.240781 | 0.195689 | -0.898653 |
| 12 | 6 | 0 | 4.586814 | -1.835066 | -1.380306 |
| 13 | 6 | 0 | 6.979855 | -0.440266 | -0.441988 |
| 14 | 6 | 0 | 5.147081 | -0.922366 | 1.933634 |
| 15 | 6 | 0 | -1.000078 | 0.033431 | -0.200225 |
| 16 | 6 | 0 | -1.891436 | 1.218747 | -0.580375 |
| 17 | 6 | 0 | -2.909855 | 1.069475 | -1.495309 |
| 18 | 6 | 0 | -1.652973 | 2.513474 | -0.007978 |
| 19 | 6 | 0 | -3.726384 | 2.154428 | -1.884919 |
| 20 | 6 | 0 | -2.492201 | 3.609476 | -0.396309 |
| 21 | 6 | 0 | -3.525555 | 3.396818 | -1.345030 |
| 22 | 6 | 0 | -1.643539 | -1.323986 | -0.473801 |
| 23 | 6 | 0 | -2.589761 | -1.885317 | 0.443451 |
| 24 | 6 | 0 | -1.319378 | -2.015945 | -1.619342 |
| 25 | 6 | 0 | -3.151598 | -3.173326 | 0.157262 |
| 26 | 6 | 0 | -1.886238 | -3.277889 | -1.904939 |
| 27 | 6 | 0 | -2.777780 | -3.848415 | -1.033425 |
| 28 | 6 | 0 | -3.009186 | -1.225680 | 1.631761 |
| 29 | 6 | 0 | -3.909425 | -1.808189 | 2.491756 |
| 30 | 6 | 0 | -4.077060 | -3.745562 | 1.068658 |
| 31 | 6 | 0 | -4.481313 | -3.083371 | 2.212293 |
| 32 | 6 | 0 | -0.622125 | 2.776289 | 0.934393 |
|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
|33 | 6 | 0 | -0.437864 | 4.030270  | 1.467480 |
|34 | 6 | 0 | -2.274895 | 4.891350  | 0.172320 |
|35 | 6 | 0 | -1.271949 | 5.102765  | 1.085142 |
|36 | 1 | 0 | 1.355017  | 0.304906  | 0.840476 |
|37 | 1 | 0 | 3.255091  | -2.915526 | 0.736328 |
|38 | 1 | 0 | 2.994184  | -1.462356 | 1.684156 |
|39 | 1 | 0 | 2.387325  | 1.661054  | -0.935356|
|40 | 1 | 0 | 2.564871  | 0.236627  | -1.945218|
|41 | 1 | 0 | 1.732433  | -2.056922 | -1.050291|
|42 | 1 | 0 | 0.934166  | -2.113353 | 0.509182 |
|43 | 1 | 0 | 4.396673  | 2.345032  | -0.133703|
|44 | 1 | 0 | 6.085352  | 1.526159  | 1.693934 |
|45 | 1 | 0 | 6.800306  | 1.869270  | 0.138422 |
|46 | 1 | 0 | 3.783762  | -1.658771 | -2.097385|
|47 | 1 | 0 | 4.688678  | -2.917302 | -1.269355|
|48 | 1 | 0 | 5.505833  | -1.448014 | -1.826320|
|49 | 1 | 0 | -0.792110 | 0.089620  | 0.874709 |
|50 | 1 | 0 | -3.097425 | 0.094683  | -1.926780|
|51 | 1 | 0 | -4.515437 | 1.991905  | -2.610451|
|52 | 1 | 0 | -4.151205 | 4.235138  | -1.633326|
|53 | 1 | 0 | -0.603529 | -1.577752 | -2.302742|
|54 | 1 | 0 | -1.605924 | -3.793423 | -2.816840|
|55 | 1 | 0 | -3.211623 | -4.820880 | -1.241667|
|56 | 1 | 0 | -2.630306 | -0.238094 | 1.861706 |
|57 | 1 | 0 | -4.213295 | -1.282298 | 3.389939 |
|58 | 1 | 0 | -4.491189 | -4.722352 | 0.840707 |
|59 | 1 | 0 | -5.156951 | -3.532047 | 2.899066 |
|60 | 1 | 0 | 0.040794  | 1.978861  | 1.240248 |
|61 | 1 | 0 | 0.357587  | 4.197892  | 2.185134 |
|62 | 1 | 0 | -2.921701 | 5.707883  | -0.131813|
|63 | 1 | 0 | -1.116580 | 6.087510  | 1.511129 |
|64 | 1 | 0 | 7.475982  | -0.378827 | 1.252786 |
|65 | 1 | 0 | 5.890283  | -2.244546 | 1.075287 |

6b (conformer 3)

|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 1 | 6 | 0 | 4.455443 | 0.223252 | -0.612389|
| 2 | 6 | 0 | 3.517139 | 0.204147 | 0.599229 |
| 3 | 6 | 0 | 3.720947 | -0.463819| -1.802168|
| 4 | 6 | 0 | 2.088036 | 0.651359 | 0.361398 |
| 5 | 6 | 0 | 2.292615 | 0.033494 | -2.055086|
| 6 | 6 | 0 | 1.428814 | -0.097786| -0.806823|
| 7 | 6 | 0 | 5.758147 | -0.589576| -0.298635|
| 8 | 6 | 0 | 6.341495 | -0.262203| 1.099079 |
| 9 | 6 | 0 | 3.911441 | -1.800688| 1.815889 |
|10 | 6 | 0 | 5.305387 | -0.597952 | 2.181919|
|11 | 8 | 0 | 0.135372 | 0.436864 | -1.134671|
|12 | 6 | 0 | 4.771132 | 1.695851 | -0.976597|
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 13 | 1 | 0 | 6.553883 | 0.812449 | 1.157408 |
| 14 | 1 | 0 | 5.445031 | -1.643423 | -0.246663 |
| 15 | 6 | 0 | -0.958694 | 0.011055 | -0.313064 |
| 16 | 6 | 0 | -2.093794 | 1.008688 | -0.548429 |
| 17 | 6 | 0 | -3.128539 | 0.699469 | -1.403369 |
| 18 | 6 | 0 | -2.078544 | 2.293114 | 0.091549 |
| 19 | 6 | 0 | -4.174881 | 1.610471 | -1.666916 |
| 20 | 6 | 0 | -3.149491 | 3.210749 | -0.169053 |
| 21 | 6 | 0 | -4.187949 | 2.838676 | -1.060717 |
| 22 | 6 | 0 | -1.352620 | -1.441338 | -0.581133 |
| 23 | 6 | 0 | -2.053513 | -2.205986 | 0.407268 |
| 24 | 6 | 0 | -3.124163 | -2.443947 | 2.584198 |
| 25 | 6 | 0 | -2.078544 | 2.293114 | 0.091549 |
| 26 | 6 | 0 | -4.174881 | 1.610471 | -1.666916 |
| 27 | 6 | 0 | -3.149491 | 3.210749 | -0.169053 |
| 28 | 6 | 0 | -4.187949 | 2.838676 | -1.060717 |
| 29 | 6 | 0 | -1.352620 | -1.441338 | -0.581133 |
| 30 | 6 | 0 | -2.053513 | -2.205986 | 0.407268 |
| 31 | 6 | 0 | -3.124163 | -2.443947 | 2.584198 |
| 32 | 6 | 0 | -2.078544 | 2.293114 | 0.091549 |
| 33 | 6 | 0 | -4.174881 | 1.610471 | -1.666916 |
| 34 | 6 | 0 | -3.149491 | 3.210749 | -0.169053 |
| 35 | 6 | 0 | -4.187949 | 2.838676 | -1.060717 |
| 36 | 1 | 0 | 1.330167 | -1.159013 | -0.543039 |
| 37 | 1 | 0 | 4.309346 | -0.337291 | 1.583586 |
| 38 | 1 | 0 | 3.684019 | -1.541809 | -1.602987 |
| 39 | 1 | 0 | 1.517341 | 0.511381 | 1.283392 |
| 40 | 1 | 0 | 2.052926 | 1.720734 | 0.119664 |
| 41 | 1 | 0 | 2.285884 | 1.082456 | -2.369123 |
| 42 | 1 | 0 | 1.842304 | -0.538182 | -2.871819 |
| 43 | 1 | 0 | 3.178198 | -0.192163 | 2.620471 |
| 44 | 1 | 0 | 5.317708 | -1.681000 | 2.378231 |
| 45 | 1 | 0 | 5.587317 | -0.129128 | 3.131963 |
| 46 | 1 | 0 | 3.859734 | 2.287001 | -1.077532 |
| 47 | 1 | 0 | 5.379041 | 2.172218 | -0.203797 |
| 48 | 1 | 0 | 5.306718 | 1.766355 | -1.926282 |
| 49 | 1 | 0 | 0.655211 | 0.076467 | 0.737335 |
| 50 | 1 | 0 | -3.148027 | -0.270088 | -1.884106 |
| 51 | 1 | 0 | -4.968622 | 1.325652 | -2.348298 |
| 52 | 1 | 0 | -4.990755 | 3.543274 | -1.251572 |
| 53 | 1 | 0 | -0.510606 | -1.436255 | -2.527076 |
| 54 | 1 | 0 | -1.089043 | -3.799950 | -3.023685 |
| 55 | 1 | 0 | -2.263779 | -5.168969 | -1.330937 |
| 56 | 1 | 0 | -2.261953 | -0.633474 | 1.893122 |
| 57 | 1 | 0 | -3.424703 | -2.010824 | 3.531664 |
|   |   |   |        |        |        |        |
|---|---|---|--------|--------|--------|--------|
| 58| 1 | 0 | -3.294924 | -5.377936 | 0.875714 |
| 59| 1 | 0 | -3.949537 | -4.393664 | 3.043316 |
| 60| 1 | 0 | -0.219014 | 2.056585  | 1.182507 |
| 61| 1 | 0 | -0.288316 | 4.239976  | 2.257264 |
| 62| 1 | 0 | -3.971953 | 5.159619  | 0.260157 |
| 63| 1 | 0 | -2.162103 | 5.816157  | 1.807752 |
| 64| 1 | 0 | 7.248813  | -0.808118 | 1.252865 |
| 65| 1 | 0 | 6.497607  | -0.525634 | -1.069356 |

**6b (conformer 4)**

|   |   |   |        |        |        |        |
|---|---|---|--------|--------|--------|--------|
| 1 | 6 | 0 | 4.475516 | -0.546611 | -0.522078 |
| 2 | 6 | 0 | 3.544333 | 0.308176  | 0.345897 |
| 3 | 6 | 0 | 3.679525 | -1.804880 | -0.985651 |
| 4 | 6 | 0 | 2.161474 | 0.585003  | -0.210491 |
| 5 | 6 | 0 | 2.90173  | -1.515649 | -1.568012 |
| 6 | 6 | 0 | 1.440896 | -0.717895 | -0.587817 |
| 7 | 6 | 0 | 5.714007 | -1.025992 | 0.311754 |
| 8 | 6 | 0 | 6.311219 | 0.092828  | 1.202035 |
| 9 | 6 | 0 | 3.899837 | 0.789474  | 1.539790 |
|10 | 6 | 0 | 5.245252 | 0.609844  | 2.178076 |
|11 | 8 | 0 | 0.164662 | -0.517029 | -1.205513 |
|12 | 6 | 0 | 4.906471 | 0.284351  | -1.756833 |
|13 | 1 | 0 | 6.619456 | 0.933005  | 0.567375 |
|14 | 1 | 0 | 5.325447 | -1.780606 | 1.012287 |
|15 | 6 | 0 | -0.887217| -0.018317 | -0.367940 |
|16 | 6 | 0 | -1.159074| 1.461157  | -0.632300 |
|17 | 6 | 0 | -0.704240| 2.047807  | -1.791902 |
|18 | 6 | 0 | -1.886173| 2.250517  | 0.317093 |
|19 | 6 | 0 | -0.931821| 3.415430  | -2.065876 |
|20 | 6 | 0 | -2.102869| 3.640444  | 0.041304 |
|21 | 6 | 0 | -1.611495| 4.196906  | -1.168237 |
|22 | 6 | 0 | -2.110499| -0.910159 | -0.593993 |
|23 | 6 | 0 | -2.287143| -2.124774 | 0.150113 |
|24 | 6 | 0 | -3.030245| -0.578924 | -1.564511 |
|25 | 6 | 0 | -3.425165| -2.951646 | -0.135386 |
|26 | 6 | 0 | -4.141396| -1.401283 | -1.850235 |
|27 | 6 | 0 | -4.337300| -2.561798 | -1.148996 |
|28 | 6 | 0 | -1.397721| -2.563964 | 1.169177 |
|29 | 6 | 0 | -1.615321| -3.731208 | 1.862435 |
|30 | 6 | 0 | -3.619764| -4.150566 | 0.598704 |
|31 | 6 | 0 | -2.738346| -4.536972 | 1.577005 |
|32 | 6 | 0 | -2.409893| 1.722552  | 1.529113 |
|33 | 6 | 0 | -3.090506| 2.519027  | 2.419253 |
|34 | 6 | 0 | -2.808939| 4.433315  | 0.982974 |
|35 | 6 | 0 | -3.291652| 3.889930  | 2.147597 |
|36 | 1 | 0 | 1.301619 | -1.313915 | 0.326969 |
|37 | 1 | 0 | 4.267594 | -2.358471 | -1.723093 |
|   | 1  |   |           |       |       |       |
|---|----|---|----------|-------|-------|-------|
| 38| 1  | 0 | 3.561690|-2.469333|-0.121048|
| 39| 1  | 0 | 1.581349| 1.153335| 0.520694|
| 40| 1  | 0 | 2.222906| 1.206217|-1.111593|
| 41| 1  | 0 | 2.364305|-0.950802|-2.503196|
| 42| 1  | 0 | 1.779222|-2.452398|-1.806886|
| 43| 1  | 0 | 3.170103| 1.366124| 2.105251|
| 44| 1  | 0 | 5.154345|-0.085533| 3.026696|
| 45| 1  | 0 | 5.568226| 1.560624| 2.617646|
| 46| 1  | 0 | 4.046774| 0.724643|-2.264082|
| 47| 1  | 0 | 5.563955| 1.107213|-1.466152|
| 48| 1  | 0 | 5.431938|-0.331940|-2.490120|
| 49| 1  | 0 | -0.572218|-0.109833| 0.676078|
| 50| 1  | 0 | -0.155408| 1.438885|-2.498223|
| 51| 1  | 0 | -0.559364| 3.841609|-2.990876|
| 52| 1  | 0 | -1.784013| 5.249308|-1.368141|
| 53| 1  | 0 | -2.902322| 0.340209|-2.122460|
| 54| 1  | 0 | -4.839155|-1.103281|-2.624677|
| 55| 1  | 0 | -5.191054|-3.198436|-1.356443|
| 56| 1  | 0 | -0.523805|-1.974508| 1.411281|
| 57| 1  | 0 | -0.917315|-4.036027| 2.634245|
| 58| 1  | 0 | -4.486795|-4.761346| 0.369041|
| 59| 1  | 0 | -2.900062|-5.455403| 2.129812|
| 60| 1  | 0 | -2.289551| 0.670748| 1.754944|
| 61| 1  | 0 | -3.481549| 2.090216| 3.335133|
| 62| 1  | 0 | -2.962921| 5.484616| 0.762293|
| 63| 1  | 0 | -3.830352| 4.507487| 2.857454|
| 64| 1  | 0 | 6.465643| -1.508281|-0.277602|
| 65| 1  | 0 | 7.162465|-0.284628| 1.729108|

|   | 6b  | 6b  |           |       |       |
|---|-----|-----|----------|-------|-------|
| 1  | 6   | 0   | 4.287243|-1.174656|-0.010342|
| 2  | 6   | 0   | 3.929385| 0.292990|-0.272702|
| 3  | 6   | 0   | 3.063100|-1.854106| 0.672208|
| 4  | 6   | 0   | 2.579103| 0.566931|-0.902455|
| 5  | 6   | 0   | 1.719169|-1.623943|-0.034244|
| 6  | 6   | 0   | 1.434479|-0.126866|-0.162857|
| 7  | 6   | 0   | 5.514432|-1.264448| 0.960792|
| 8  | 6   | 0   | 6.647798|-0.279938| 0.578853|
| 9  | 6   | 0   | 4.747314| 1.304545| 0.029268|
| 10 | 6   | 0   | 6.120344| 1.161534| 0.616366|
| 11 | 8   | 0   | 0.237986| 0.190920|-0.885057|
| 12 | 6   | 0   | 4.578614|-1.868424|-1.364810|
| 13 | 1   | 0   | 6.977101|-0.491931|-0.445840|
| 14 | 1   | 0   | 5.144580|-0.923669| 1.939735|
| 15 | 6   | 0   | -1.004591| 0.035876|-0.188044|
| 16 | 6   | 0   | -1.886508| 1.228762|-0.568396|
| 17 | 6   | 0   | -2.909987| 1.086989|-1.478769|
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 18 | 6 | 0 | -1.631800 | 2.523251 | -0.002419 |
| 19 | 6 | 0 | -3.714925 | 2.179765 | -1.871089 |
| 20 | 6 | 0 | -2.458025 | 3.627645 | -0.394550 |
| 21 | 6 | 0 | -3.496721 | 3.422715 | -1.339113 |
| 22 | 6 | 0 | -1.655071 | -1.316829 | -0.468729 |
| 23 | 6 | 0 | -2.610634 | -1.875895 | 0.440364 |
| 24 | 6 | 0 | -1.329112 | -2.006061 | -1.615476 |
| 25 | 6 | 0 | -3.177496 | -3.159735 | 0.145654 |
| 26 | 6 | 0 | -2.458025 | 3.627645 | -0.394550 |
| 27 | 6 | 0 | -3.496721 | 3.422715 | -1.339113 |
| 28 | 6 | 0 | -1.655071 | -1.316829 | -0.468729 |
| 29 | 6 | 0 | -2.610634 | -1.875895 | 0.440364 |
| 30 | 6 | 0 | -1.329112 | -2.006061 | -1.615476 |
| 31 | 6 | 0 | -3.177496 | -3.159735 | 0.145654 |
| 32 | 6 | 0 | -2.458025 | 3.627645 | -0.394550 |
| 33 | 6 | 0 | -3.496721 | 3.422715 | -1.339113 |
| 34 | 6 | 0 | -1.655071 | -1.316829 | -0.468729 |
| 35 | 6 | 0 | -2.610634 | -1.875895 | 0.440364 |
| 36 | 6 | 0 | -1.329112 | -2.006061 | -1.615476 |
| 37 | 6 | 0 | -3.177496 | -3.159735 | 0.145654 |
| 38 | 6 | 0 | -2.458025 | 3.627645 | -0.394550 |
| 39 | 6 | 0 | -3.496721 | 3.422715 | -1.339113 |
| 40 | 6 | 0 | -1.655071 | -1.316829 | -0.468729 |
| 41 | 6 | 0 | -2.610634 | -1.875895 | 0.440364 |
| 42 | 6 | 0 | -1.329112 | -2.006061 | -1.615476 |
| 43 | 6 | 0 | -3.177496 | -3.159735 | 0.145654 |
| 44 | 6 | 0 | -2.458025 | 3.627645 | -0.394550 |
| 45 | 6 | 0 | -3.496721 | 3.422715 | -1.339113 |
| 46 | 6 | 0 | -1.655071 | -1.316829 | -0.468729 |
| 47 | 6 | 0 | -2.610634 | -1.875895 | 0.440364 |
| 48 | 6 | 0 | -1.329112 | -2.006061 | -1.615476 |
| 49 | 6 | 0 | -3.177496 | -3.159735 | 0.145654 |
| 50 | 6 | 0 | -2.458025 | 3.627645 | -0.394550 |
| 51 | 6 | 0 | -3.496721 | 3.422715 | -1.339113 |
| 52 | 6 | 0 | -1.655071 | -1.316829 | -0.468729 |
| 53 | 6 | 0 | -2.610634 | -1.875895 | 0.440364 |
| 54 | 6 | 0 | -1.329112 | -2.006061 | -1.615476 |
| 55 | 6 | 0 | -3.177496 | -3.159735 | 0.145654 |
| 56 | 6 | 0 | -2.458025 | 3.627645 | -0.394550 |
| 57 | 6 | 0 | -3.496721 | 3.422715 | -1.339113 |
| 58 | 6 | 0 | -1.655071 | -1.316829 | -0.468729 |
| 59 | 6 | 0 | -2.610634 | -1.875895 | 0.440364 |
| 60 | 6 | 0 | -1.329112 | -2.006061 | -1.615476 |
| 61 | 6 | 0 | -3.177496 | -3.159735 | 0.145654 |
| 62 | 6 | 0 | -2.458025 | 3.627645 | -0.394550 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 63 | 1 | 0 | -1.044359 | 6.098173 | 1.494856 |
| 64 | 1 | 0 | 7.475109 | -0.400762 | 1.246578 |
| 65 | 1 | 0 | 5.880613 | -2.260454 | 1.097843 |

**6b (conformer 6)**

|   | 6 | 0 |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.469425 | 0.167732 | -0.616107 |
| 2 | 6 | 0 | 3.532472 | 0.192074 | 0.596909 |
| 3 | 6 | 0 | 3.728321 | -0.559417 | -1.777595 |
| 4 | 6 | 0 | 2.106168 | 0.641467 | -0.616107 |
| 5 | 6 | 0 | 2.303370 | -0.061492 | -1.044359 |
| 6 | 6 | 0 | 1.438391 | -0.139743 | -0.580241 |
| 7 | 6 | 0 | 4.469425 | -0.635294 | -0.161182 |
| 8 | 6 | 0 | 3.532472 | 0.192074 | 0.596909 |
| 9 | 6 | 0 | 3.728321 | -0.559417 | -1.777595 |
| 10 | 6 | 0 | 2.106168 | 0.641467 | -0.616107 |
| 11 | 6 | 0 | 2.303370 | -0.061492 | -1.044359 |
| 12 | 6 | 0 | 1.438391 | -0.139743 | -0.580241 |
| 13 | 6 | 0 | 4.469425 | -0.635294 | -0.161182 |
| 14 | 6 | 0 | 3.532472 | 0.192074 | 0.596909 |
| 15 | 6 | 0 | 3.728321 | -0.559417 | -1.777595 |
| 16 | 6 | 0 | 2.106168 | 0.641467 | -0.616107 |
| 17 | 6 | 0 | 2.303370 | -0.061492 | -1.044359 |
| 18 | 6 | 0 | 1.438391 | -0.139743 | -0.580241 |
| 19 | 6 | 0 | 4.469425 | -0.635294 | -0.161182 |
| 20 | 6 | 0 | 3.532472 | 0.192074 | 0.596909 |
| 21 | 6 | 0 | 3.728321 | -0.559417 | -1.777595 |
| 22 | 6 | 0 | 2.106168 | 0.641467 | -0.616107 |
| 23 | 6 | 0 | 2.303370 | -0.061492 | -1.044359 |
| 24 | 6 | 0 | 1.438391 | -0.139743 | -0.580241 |
| 25 | 6 | 0 | 4.469425 | -0.635294 | -0.161182 |
| 26 | 6 | 0 | 3.532472 | 0.192074 | 0.596909 |
| 27 | 6 | 0 | 3.728321 | -0.559417 | -1.777595 |
| 28 | 6 | 0 | 2.106168 | 0.641467 | -0.616107 |
| 29 | 6 | 0 | 2.303370 | -0.061492 | -1.044359 |
| 30 | 6 | 0 | 1.438391 | -0.139743 | -0.580241 |
| 31 | 6 | 0 | 4.469425 | -0.635294 | -0.161182 |
| 32 | 6 | 0 | 3.532472 | 0.192074 | 0.596909 |
| 33 | 6 | 0 | 3.728321 | -0.559417 | -1.777595 |
| 34 | 6 | 0 | 2.106168 | 0.641467 | -0.616107 |
| 35 | 6 | 0 | 2.303370 | -0.061492 | -1.044359 |
| 36 | 6 | 0 | 1.438391 | -0.139743 | -0.580241 |
| 37 | 6 | 0 | 4.469425 | -0.635294 | -0.161182 |
| 38 | 6 | 0 | 3.532472 | 0.192074 | 0.596909 |
| 39 | 6 | 0 | 3.728321 | -0.559417 | -1.777595 |
| 40 | 6 | 0 | 2.106168 | 0.641467 | -0.616107 |
| 41 | 6 | 0 | 2.303370 | -0.061492 | -1.044359 |
| 42 | 6 | 0 | 1.438391 | -0.139743 | -0.580241 |
|   | 1 | 0 | 3.192131 | -0.145112 | 2.628757 |
|---|---|---|-----------|------------|----------|
| 43| 1 | 0 | 5.321046 | -1.658663  | 2.420915 |
| 44| 1 | 0 | 5.600094 | -0.091624  | 3.139109 |
| 45| 1 | 0 | 5.307921 | 1.663490   | -1.991832|
| 46| 1 | 0 | 3.875473 | 2.217985   | -1.140933|
| 47| 1 | 0 | 5.406554 | 2.124669   | -0.284937|
| 48| 1 | 0 | -0.645565| 0.073942   | 0.733947 |
| 49| 1 | 0 | -3.106395| -0.229971  | 1.663490 |
| 50| 1 | 0 | -4.887423| 1.398999   | -2.434129|
| 51| 1 | 0 | -4.899230| 3.610714   | -1.325279|
| 52| 1 | 0 | -0.514578| -1.478266  | -2.509177|
| 53| 1 | 0 | -1.153328| -3.830005  | 2.988561 |
| 54| 1 | 0 | -2.376808| -5.150829  | 1.818940 |
| 55| 1 | 0 | -2.793335| -4.291850  | 3.064100 |
| 56| 1 | 0 | -3.485255| -1.918655  | 3.533577 |
| 57| 1 | 0 | -3.426011| -5.312694  | 0.909482 |
| 58| 1 | 0 | -4.067883| 4.206156   | -2.434129|
| 59| 1 | 0 | 5.817406 | 2.307953   | 1.818940 |
| 60| 1 | 0 | 2.112720 | 5.817406   | 1.818940 |
| 61| 1 | 0 | 6.513842 | -0.587493  | -1.049608|
| 62| 1 | 0 | 7.258441 | -0.821677  | 1.278430 |

**6b (conformer 7)**

|   | 1 | 0 | 4.333934 | -0.733791 | 0.634210 |
|---|---|---|-----------|------------|----------|
| 1 | 6 | 0 | 3.933687 | -0.020249 | -0.661709|
| 2 | 6 | 0 | 3.175321 | -0.549306 | 1.658179 |
| 3 | 6 | 0 | 2.538894 | -0.290901 | -1.187659|
| 4 | 6 | 0 | 1.782449 | -0.905436 | 1.120455 |
| 5 | 6 | 0 | 1.452696 | -0.087157 | -0.129406|
| 6 | 6 | 0 | 5.632219 | -0.087809 | 1.229807 |
| 7 | 6 | 0 | 6.163132 | 0.163393  | 0.152784 |
| 8 | 6 | 0 | 4.754348 | 0.803396  | -1.318473|
| 9 | 6 | 0 | 6.168333 | 1.112464  | -0.922935|
| 10| 6 | 0 | 0.214789 | -0.483576 | -0.744286|
| 11| 8 | 0 | 4.530341 | -2.241455 | 0.334238 |
| 12| 6 | 0 | 6.967957 | -0.787068 | -0.333571|
| 13| 1 | 0 | 5.332575 | 0.910031  | 1.584379 |
| 14| 1 | 0 | -0.987568| 0.011604  | -0.143225|
| 15| 6 | 0 | -1.199157| 1.501450  | -0.410544|
| 16| 6 | 0 | -0.589611| 2.097593  | -1.492402|
| 17| 6 | 0 | -2.029827| 2.290348  | 0.449863 |
| 18| 6 | 0 | -0.749973| 3.474044  | -1.766537|
| 19| 6 | 0 | -2.180960| 3.689529  | 0.175045 |
| 20| 6 | 0 | -1.523275| 4.255498  | -0.947682|
| 21| 6 | 0 | -2.125022| -0.872042 | -0.658781|
|   |   |   |   |   |
|---|---|---|---|---|
| 23 | 6 | 0 | -2.340204 | -2.177523 | -0.102771 |
| 24 | 6 | 0 | -2.937316 | -0.439575 | -1.683583 |
| 25 | 6 | 0 | -3.403180 | -2.987237 | -0.623097 |
| 26 | 6 | 0 | -3.975267 | -1.244931 | -2.201892 |
| 27 | 6 | 0 | -4.206368 | -2.490729 | -1.681508 |
| 28 | 6 | 0 | -1.552542 | -2.719877 | 0.948114  |
| 29 | 6 | 0 | -1.803612 | -3.969947 | 1.462247  |
| 30 | 6 | 0 | -3.634278 | -4.274328 | -0.071148 |
| 31 | 6 | 0 | -2.856317 | -4.758991 | 0.950287  |
| 32 | 6 | 0 | -2.728079 | 1.752470  | 1.566103  |
| 33 | 6 | 0 | -3.508408 | 2.548084  | 2.370744  |
| 34 | 6 | 0 | -2.992272 | 4.481731  | 1.028691  |
| 35 | 6 | 0 | -3.640776 | 3.928594  | 2.104578  |
| 36 | 1 | 0 | 1.403965  | 0.977103  | 0.136715  |
| 37 | 1 | 0 | 3.377110  | -1.148125 | 2.550698  |
| 38 | 1 | 0 | 3.167397  | 0.498897  | 1.980974  |
| 39 | 1 | 0 | 2.336324  | 0.350106  | -2.048729 |
| 40 | 1 | 0 | 2.449386  | -1.325691 | -1.541043 |
| 41 | 1 | 0 | 1.720175  | -1.968347 | 0.866551  |
| 42 | 1 | 0 | 1.044798  | -0.720576 | 1.908173  |
| 43 | 1 | 0 | 4.386579  | 1.294701  | -2.217430 |
| 44 | 1 | 0 | 6.223056  | 2.149874  | -0.558583 |
| 45 | 1 | 0 | 6.809684  | 1.084287  | -1.811540 |
| 46 | 1 | 0 | 3.678823  | -2.656205 | -0.207035 |
| 47 | 1 | 0 | 4.642124  | -2.821916 | 1.253290  |
| 48 | 1 | 0 | 5.414658  | -2.407584 | -0.285380 |
| 49 | 1 | 0 | -0.917583 | -0.118768 | 0.942243  |
| 50 | 1 | 0 | 0.027280  | 1.487789  | -2.140469 |
| 51 | 1 | 0 | -0.252353 | 3.907164  | -2.627120 |
| 52 | 1 | 0 | -1.645945 | 5.315036  | -1.146474 |
| 53 | 1 | 0 | -2.784031 | 0.546472  | -2.102808 |
| 54 | 1 | 0 | -4.589308 | -0.865016 | -3.010623 |
| 55 | 1 | 0 | -5.005607 | -3.114327 | -2.068389 |
| 56 | 1 | 0 | -0.728465 | -2.146423 | 1.346699  |
| 57 | 1 | 0 | -1.184440 | -4.356044 | 2.264455  |
| 58 | 1 | 0 | -4.442645 | -4.872470 | -0.475826 |
| 59 | 1 | 0 | -3.044245 | -5.743894 | 1.362679  |
| 60 | 1 | 0 | -2.663611 | 0.693858  | 1.782119  |
| 61 | 1 | 0 | -4.031822 | 2.111533  | 3.214005  |
| 62 | 1 | 0 | -3.093711 | 5.539975  | 0.810883  |
| 63 | 1 | 0 | -4.258721 | 4.545261  | 2.747449  |
| 64 | 1 | 0 | 7.595125  | 0.568599  | 0.609287  |
| 65 | 1 | 0 | 6.021645  | -0.613119 | 2.076741  |

**6b (conformer 8)**

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6 | 0 | -4.315575 | -1.591367 | -0.308812 |
| 2 | 6 | 0 | -3.658673 | -0.332644 | 0.270188  |
|   |   |   |               |               |               |
|---|---|---|---------------|---------------|---------------|
| 3 | 6 | 0 | -3.311882     | -2.236663     | -1.310163     |
| 4 | 6 | 0 | -2.235639     | -0.473361     | 0.774219      |
| 5 | 6 | 0 | -1.892362     | -2.429210     | -0.763107     |
| 6 | 6 | 0 | -1.304582     | -1.112317     | -0.264793     |
| 7 | 6 | 0 | -5.621024     | -1.213054     | -1.089812     |
| 8 | 6 | 0 | -6.498217     | -0.194039     | -0.320456     |
| 9 | 6 | 0 | -4.283735     | 0.846020      | 0.335820      |
| 10| 6 | 0 | 5.702260      | 1.097416      | -0.084520     |
| 11| 8 | 0 | -0.015957     | 1.389011      | 0.303168      |
| 12| 6 | 0 | -6.498217     | -0.194039     | -0.320456     |
| 13| 1 | 0 | -6.757561     | -0.611128     | 0.660632      |
| 14| 1 | 0 | -5.284562     | -0.686771     | 1.995786      |
| 15| 6 | 0 | 1.072681      | -0.547219     | -0.80193      |
| 16| 6 | 0 | 1.026000      | 0.785184      | 0.681866      |
| 17| 6 | 0 | 1.323667      | 0.769654      | 2.028595      |
| 18| 6 | 0 | 0.623572      | 2.017600      | 0.069699      |
| 19| 6 | 0 | 1.422264      | 1.929545      | 2.823853      |
| 20| 6 | 0 | 0.548017      | 3.200124      | 0.883765      |
| 21| 6 | 0 | 0.862266      | 3.122422      | 2.262965      |
| 22| 6 | 0 | 2.367686      | -1.321351     | 0.159731      |
| 23| 6 | 0 | 3.608400      | -0.857675     | -0.388341     |
| 24| 6 | 0 | 2.346868      | -2.487218     | 0.893116      |
| 25| 6 | 0 | 4.797985      | -1.622888     | -0.152574     |
| 26| 6 | 0 | 3.524676      | -3.231292     | 1.129826      |
| 27| 6 | 0 | 4.724477      | -2.810589     | 0.620074      |
| 28| 6 | 0 | 3.755664      | 0.323524      | -1.170668     |
| 29| 6 | 0 | 4.934922      | 0.722227      | -1.689105     |
| 30| 6 | 0 | 6.029966      | -1.180839     | -0.700873     |
| 31| 6 | 0 | 6.102397      | -0.035350     | -1.453661     |
| 32| 6 | 0 | 0.294605      | 2.152999      | -1.309644     |
| 33| 6 | 0 | -0.081463     | 3.360733      | -1.846757     |
| 34| 6 | 0 | 0.155750      | 4.431385      | 0.295060      |
| 35| 6 | 0 | -0.153400     | 4.516422      | -1.038555     |
| 36| 1 | 0 | -1.189918     | -0.425534     | -1.113195     |
| 37| 1 | 0 | -3.699993     | -3.202433     | -1.645766     |
| 38| 1 | 0 | -3.260116     | -1.596515     | -2.199745     |
| 39| 1 | 0 | -1.850994     | 0.502705      | 1.074619      |
| 40| 1 | 0 | -2.202299     | -1.112423     | 1.665343      |
| 41| 1 | 0 | -1.885109     | -3.144164     | 0.066325      |
| 42| 1 | 0 | -1.243928     | -2.846846     | -1.539337     |
| 43| 1 | 0 | -3.737714     | 1.701112      | 0.729453      |
| 44| 1 | 0 | -5.707716     | 1.704657      | -1.002686     |
| 45| 1 | 0 | -6.200798     | 1.714149      | 0.672441      |
| 46| 1 | 0 | -5.399533     | -2.204573     | 1.498448      |
| 47| 1 | 0 | -4.915589     | -3.559811     | 0.466460      |
|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 48 | 1 | 0 | -3.728234 | -2.741409 | 1.470293 |
| 49 | 1 | 0 | 1.001473 | -0.362572 | -1.156665 |
| 50 | 1 | 0 | 1.632819 | -0.162652 | 2.486245 |
| 51 | 1 | 0 | 1.485623 | 1.872192 | 3.878823 |
| 52 | 1 | 0 | 0.800144 | 4.023150 | 2.864561 |
| 53 | 1 | 0 | 1.401793 | -2.839701 | 1.281751 |
| 54 | 1 | 0 | 3.467288 | -4.142209 | 1.715468 |
| 55 | 1 | 0 | 5.632280 | -3.378810 | 0.794163 |
| 56 | 1 | 0 | 2.854043 | 0.935422 | -1.359018 |
| 57 | 1 | 0 | 4.992775 | 1.628925 | -2.280978 |
| 58 | 1 | 0 | 6.920604 | -0.362572 | -1.156665 |
| 59 | 1 | 0 | 1.485623 | 1.872192 | 3.878823 |
| 60 | 1 | 0 | 0.800144 | 4.023150 | 2.864561 |
| 61 | 1 | 0 | 1.401793 | -2.839701 | 1.281751 |
| 62 | 1 | 0 | 3.467288 | -4.142209 | 1.715468 |
| 63 | 1 | 0 | 5.632280 | -3.378810 | 0.794163 |
| 64 | 1 | 0 | 2.854043 | 0.935422 | -1.359018 |
| 65 | 1 | 0 | 4.992775 | 1.628925 | -2.280978 |

6b (conformer 9)

|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.672874 | -0.182381 | -0.666259 |
| 2 | 6 | 0 | -3.827989 | -0.936434 | 0.367416 |
| 3 | 6 | 0 | -3.862236 | 1.064701 | -1.132439 |
| 4 | 6 | 0 | -2.382322 | -1.200284 | -0.003615 |
| 5 | 6 | 0 | -2.413241 | 0.776908 | -1.544888 |
| 6 | 6 | 0 | -1.650454 | 0.083495 | -0.423860 |
| 7 | 6 | 0 | -6.014137 | 0.310750 | -0.020670 |
| 8 | 6 | 0 | -6.683644 | -0.771143 | 0.863018 |
| 9 | 6 | 0 | -4.312691 | -1.347575 | 1.541841 |
| 10 | 6 | 0 | -5.732045 | -1.177689 | 1.997239 |
| 11 | 8 | 0 | -0.334362 | -0.199603 | -0.915385 |
| 12 | 6 | 0 | -4.931884 | -1.117708 | -1.874442 |
| 13 | 1 | 0 | -6.880766 | -1.661967 | 0.253592 |
| 14 | 1 | 0 | -5.733301 | 1.121236 | 0.668626 |
| 15 | 6 | 0 | 0.683152 | -0.392761 | 0.070514 |
| 16 | 6 | 0 | 1.825181 | -1.184837 | -0.580551 |
| 17 | 6 | 0 | 1.778267 | -1.458622 | -1.930917 |
| 18 | 6 | 0 | 2.912605 | -1.707733 | 0.197077 |
| 19 | 6 | 0 | 2.792650 | -2.197006 | -2.578157 |
| 20 | 6 | 0 | 3.940414 | -2.458353 | -0.467450 |
| 21 | 6 | 0 | 3.857727 | -2.679362 | -1.865525 |
| 22 | 6 | 0 | 1.063927 | 0.942653 | 0.725626 |
| 23 | 6 | 0 | 1.634695 | 2.041740 | 0.001159 |
| 24 | 6 | 0 | 0.789797 | 1.102793 | 2.068477 |
| 25 | 6 | 0 | 1.958242 | 3.244809 | 0.713258 |
| 26 | 6 | 0 | 1.097687 | 2.291534 | 2.765550 |
| 27 | 6 | 0 | 1.682834 | 3.337121 | 2.102058 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 28 | 6 | 0 | 1.882874 | 2.013608 | -1.397918 |
| 29 | 6 | 0 | 2.439145 | 3.090842 | -2.045270 |
| 30 | 6 | 0 | 2.537819 | 4.335398 | 0.013551 |
| 31 | 6 | 0 | 3.023188 | -1.552007 | 1.606090 |
| 32 | 6 | 0 | 4.076857 | -2.085901 | 2.309371 |
| 33 | 6 | 0 | 5.019569 | -2.986571 | 0.287936 |
| 34 | 6 | 0 | 5.092438 | -2.807255 | 1.646364 |
| 35 | 6 | 0 | 3.023188 | -1.552007 | 1.606090 |
| 36 | 1 | 0 | 4.381827 | 1.546041 | -1.965638 |
| 37 | 1 | 0 | 3.852534 | 1.791189 | -0.310851 |
| 38 | 1 | 0 | 1.875120 | 1.680599 | 0.837406 |
| 39 | 1 | 0 | 2.318783 | 1.897112 | -0.848361 |
| 40 | 1 | 0 | 2.377046 | 0.140387 | -2.435652 |
| 41 | 1 | 0 | 1.905025 | 1.709714 | -1.804174 |
| 42 | 1 | 0 | 3.641253 | -1.854163 | 2.232984 |
| 43 | 1 | 0 | 5.768900 | -0.420467 | 2.795321 |
| 44 | 1 | 0 | 6.078542 | -2.107113 | 2.463729 |
| 45 | 1 | 0 | 5.092438 | -2.807255 | 1.646364 |
| 46 | 1 | 0 | 5.019569 | -2.986571 | 0.287936 |
| 47 | 1 | 0 | 5.019569 | -2.986571 | 0.287936 |
| 48 | 1 | 0 | 2.717434 | -2.378904 | -3.644524 |
| 49 | 1 | 0 | 2.643764 | -3.246087 | -2.353516 |
| 50 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 51 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 52 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 53 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 54 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 55 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 56 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 57 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 58 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 59 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 60 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 61 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 62 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 63 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 64 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |
| 65 | 1 | 0 | 2.308786 | 0.285463 | 2.614867 |

**6b (conformer 10)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.501379 | -1.363561 | 0.258425 |
| 2 | 6 | 0 | 3.994413 | -0.115301 | -0.474957 |
| 3 | 6 | 0 | 3.404899 | -1.809850 | 1.272617 |
| 4 | 6 | 0 | 2.577135 | -0.161742 | -1.009070 |
| 5 | 6 | 0 | 1.988864 | -1.907005 | 0.688455 |
| 6 | 6 | 0 | 1.568798 | -0.577108 | 0.062128 |
| 7 | 6 | 0 | 5.807812 | -1.027688 | 1.056925 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 8 | 6 | 0 | 6.814349 | -0.193046 | 0.225746 |
| 9 | 6 | 0 | 4.742456 | 0.977336 | -0.647229 |
| 10 | 6 | 0 | 6.165292 | 1.132318 | -0.197821 |
| 11 | 8 | 0 | 0.289337 | -0.666359 | -0.578379 |
| 12 | 6 | 0 | 4.736903 | -2.490262 | -0.778844 |
| 13 | 1 | 0 | 7.074970 | -0.745893 | -0.685067 |
| 14 | 1 | 0 | 5.490408 | -0.370247 | 1.880422 |
| 15 | 6 | 0 | -0.851993 | -0.530863 | 0.271943 |
| 16 | 6 | 0 | -1.012214 | 0.924728 | 0.733895 |
| 17 | 6 | 0 | -0.858701 | 1.194341 | 2.078510 |
| 18 | 6 | 0 | -1.253506 | 2.498734 | 2.605812 |
| 19 | 6 | 0 | -0.977550 | -2.490262 | -0.778844 |
| 20 | 6 | 0 | -1.428202 | 3.548545 | 1.768827 |
| 21 | 6 | 0 | -2.053189 | -1.158671 | -0.447329 |
| 22 | 6 | 0 | -3.093232 | -1.349707 | 0.220816 |
| 23 | 6 | 0 | -1.909232 | -1.615092 | -1.740282 |
| 24 | 6 | 0 | -4.388132 | -1.968484 | -0.496464 |
| 25 | 6 | 0 | -2.974658 | -2.222342 | -2.439971 |
| 26 | 6 | 0 | -4.192415 | -2.388480 | -1.836342 |
| 27 | 6 | 0 | -3.547903 | -0.985480 | 1.574399 |
| 28 | 6 | 0 | -4.764963 | -1.203276 | 2.175418 |
| 29 | 6 | 0 | -5.634801 | -2.168987 | 0.151574 |
| 30 | 6 | 0 | -5.825791 | -1.796048 | 1.458123 |
| 31 | 6 | 0 | -1.351838 | 1.861008 | -1.575518 |
| 32 | 6 | 0 | -1.593174 | 2.937257 | -2.395541 |
| 33 | 6 | 0 | -1.640810 | 4.426263 | -0.503804 |
| 34 | 6 | 0 | -1.746783 | 4.233797 | -1.858180 |
| 35 | 6 | 0 | 1.536215 | 0.201321 | 0.835439 |
| 36 | 1 | 0 | 3.680679 | -2.775386 | 1.705492 |
| 37 | 1 | 0 | 3.915800 | -1.089731 | 2.100013 |
| 38 | 1 | 0 | 2.296229 | 0.811981 | -1.416180 |
| 39 | 1 | 0 | 2.495582 | -0.884256 | -1.831220 |
| 40 | 1 | 0 | 1.929863 | -2.684288 | -0.080133 |
| 41 | 1 | 0 | 1.291995 | -2.198923 | 1.480903 |
| 42 | 1 | 0 | 4.301085 | 1.833366 | -1.154156 |
| 43 | 1 | 0 | 6.203293 | 1.844319 | 0.640899 |
| 44 | 1 | 0 | 6.750986 | 1.598747 | -0.998547 |
| 45 | 1 | 0 | 4.939138 | -3.447228 | -0.291683 |
| 46 | 1 | 0 | 3.864571 | -2.632845 | -1.418401 |
| 47 | 1 | 0 | 5.579098 | -2.253590 | -1.433260 |
| 48 | 1 | 0 | -0.689874 | -1.123866 | 1.182349 |
| 49 | 1 | 0 | -0.647930 | 0.375888 | 2.760399 |
| 50 | 1 | 0 | -0.855442 | 2.659384 | 3.670998 |
| 51 | 1 | 0 | -1.350687 | 4.555872 | 2.158663 |
| 52 | 1 | 0 | -1.350687 | 4.555872 | 2.158663 |
|   |   |   | x  | y  | z  |
|---|---|---|----|----|----|
| 53 | 1 | 0 | -0.949137 | -1.507835 | -2.225055 |
| 54 | 1 | 0 | -2.816501 | -2.556681 | -3.459356 |
| 55 | 1 | 0 | -5.018099 | -2.852255 | -2.365763 |
| 56 | 1 | 0 | -2.763080 | -0.517351 | 2.148716 |
| 57 | 1 | 0 | -4.911897 | -0.913494 | 3.210010 |
| 58 | 1 | 0 | -6.438901 | -2.632769 | -0.410515 |
| 59 | 1 | 0 | -6.783089 | -1.957459 | 1.940815 |
| 60 | 1 | 0 | -1.221631 | 0.881763 | 2.007679 |
| 61 | 1 | 0 | -2.763080 | -0.517351 | 2.148716 |
| 62 | 1 | 0 | -2.816501 | -2.556681 | -3.459356 |
| 63 | 1 | 0 | -5.018099 | -2.852255 | -2.365763 |
| 64 | 1 | 0 | -6.438901 | -2.632769 | -0.410515 |
| 65 | 1 | 0 | -6.783089 | -1.957459 | 1.940815 |

**6b (conformer 14)**

|   |   |   | x  | y  | z  |
|---|---|---|----|----|----|
| 1 | 6 | 0 | -4.682459 | -0.092140 | -0.627528 |
| 2 | 6 | 0 | -3.854470 | -0.969627 | 0.319524 |
| 3 | 6 | 0 | -3.842044 | 1.171907 | -0.981210 |
| 4 | 6 | 0 | -2.412506 | -1.222664 | -0.074435 |
| 5 | 6 | 0 | -2.401905 | 0.888389 | -1.425542 |
| 6 | 6 | 0 | -1.655460 | 0.079960 | -0.373273 |
| 7 | 6 | 0 | -6.000296 | 0.372303 | 0.082523 |
| 8 | 6 | 0 | -6.710734 | -0.782401 | 0.831187 |
| 9 | 6 | 0 | -4.355557 | -1.499879 | 1.438260 |
| 10 | 6 | 0 | -5.774311 | -1.354215 | 1.906112 |
| 11 | 8 | 0 | -0.342902 | -0.188758 | -0.882074 |
| 12 | 6 | 0 | -4.980561 | -0.896411 | -1.918215 |
| 13 | 1 | 0 | -6.936257 | -1.586846 | 0.120278 |
| 14 | 1 | 0 | -5.682950 | 1.079075 | 0.864012 |
| 15 | 6 | 0 | 0.683092 | -0.392971 | 0.092866 |
| 16 | 6 | 0 | 1.806641 | -1.204776 | -0.565907 |
| 17 | 6 | 0 | 1.723495 | -1.512729 | -1.907227 |
| 18 | 6 | 0 | 2.911388 | -1.713794 | 0.196659 |
| 19 | 6 | 0 | 2.715191 | -2.276476 | -2.560246 |
| 20 | 6 | 0 | 3.916107 | -2.489618 | -0.474005 |
| 21 | 6 | 0 | 3.794765 | -2.748472 | -1.862730 |
| 22 | 6 | 0 | 1.083163 | 0.943247 | 0.734103 |
| 23 | 6 | 0 | 1.665270 | 2.027784 | -0.003096 |
| 24 | 6 | 0 | 0.809269 | 1.122041 | 2.074696 |
| 25 | 6 | 0 | 1.994172 | 3.238374 | 0.693684 |
| 26 | 6 | 0 | 1.124200 | 2.317619 | 2.756890 |
| 27 | 6 | 0 | 1.715656 | 3.351132 | 2.080363 |
| 28 | 6 | 0 | 1.919418 | 1.978326 | -1.400533 |
| 29 | 6 | 0 | 2.483681 | 3.043495 | -2.060787 |
| 30 | 6 | 0 | 2.581866 | 4.316039 | -0.019053 |
| 31 | 6 | 0 | 2.826127 | 4.223901 | -1.366050 |
| 32 | 6 | 0 | 3.061925 | -1.518484 | 1.597051 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 33 | 6 | 0 | 4.132071 | -2.038285 | 2.285888 |
| 34 | 6 | 0 | 5.012801 | -3.003017 | 0.266151 |
| 35 | 6 | 0 | 5.124649 | -2.784957 | 1.616228 |
| 36 | 1 | 0 | -1.577183 | 0.676559 | 0.544739 |
| 37 | 1 | 0 | -4.351459 | 1.739166 | -1.764885 |
| 38 | 1 | 0 | -3.812374 | 1.820309 | -0.097111 |
| 39 | 1 | 0 | -1.912614 | -1.788670 | 0.716382 |
| 40 | 1 | 0 | -2.361378 | -1.837985 | -0.981110 |
| 41 | 1 | 0 | -2.383305 | 0.333164 | -2.369506 |
| 42 | 1 | 0 | -1.871778 | 1.828174 | -1.602834 |
| 43 | 1 | 0 | -3.698492 | -2.093755 | 2.071400 |
| 44 | 1 | 0 | -5.796306 | -0.704314 | 2.794401 |
| 45 | 1 | 0 | -6.145323 | -2.326692 | 2.250160 |
| 46 | 1 | 0 | -4.070284 | -1.321795 | -2.343308 |
| 47 | 1 | 0 | -5.659498 | -1.728318 | -1.716647 |
| 48 | 1 | 0 | -5.430775 | -0.265098 | -2.688023 |
| 49 | 1 | 0 | 0.282882 | -1.015225 | 0.905262 |
| 50 | 1 | 0 | 0.870118 | -1.159470 | -2.468532 |
| 51 | 1 | 0 | 2.611011 | -2.485616 | -3.619178 |
| 52 | 1 | 0 | 4.563747 | -3.334193 | -2.355414 |
| 53 | 1 | 0 | 0.342909 | 0.314273 | 2.630626 |
| 54 | 1 | 0 | 0.896009 | 2.408027 | 3.812867 |
| 55 | 1 | 0 | 1.970064 | 4.273959 | 2.591127 |
| 56 | 1 | 0 | 1.652980 | 1.091594 | -1.953129 |
| 57 | 1 | 0 | 2.666099 | 2.977389 | -3.127655 |
| 58 | 1 | 0 | 2.830260 | 5.221607 | 0.524805 |
| 59 | 1 | 0 | 3.274187 | 5.054835 | -1.899382 |
| 60 | 1 | 0 | 2.327822 | -0.941069 | 2.138111 |
| 61 | 1 | 0 | 4.215632 | -1.869828 | 3.353866 |
| 62 | 1 | 0 | 5.764627 | -3.581234 | -0.261119 |
| 63 | 1 | 0 | 5.967151 | -3.185094 | 2.168970 |
| 64 | 1 | 0 | -7.622515 | -0.429287 | 1.265773 |
| 65 | 1 | 0 | -6.667652 | 0.904819 | -0.562429 |

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 6b (conformer 15) |   |   |   |   |   |
| 1 | 6 | 0 | -3.905448 | -1.529786 | 0.665790 |
| 2 | 6 | 0 | -3.428644 | -0.381617 | -0.230250 |
| 3 | 6 | 0 | -2.771438 | -2.590514 | 0.732868 |
| 4 | 6 | 0 | -2.034060 | 0.157344 | 0.025430 |
| 5 | 6 | 0 | -1.377084 | -2.036935 | 1.040626 |
| 6 | 6 | 0 | -0.976912 | -0.958180 | 0.040307 |
| 7 | 6 | 0 | -5.179672 | -2.203045 | 0.050637 |
| 8 | 6 | 0 | -6.223067 | -1.169950 | -0.441561 |
| 9 | 6 | 0 | -4.187600 | 0.144493 | -1.195501 |
| 10 | 6 | 0 | -5.594296 | -0.269779 | -1.515901 |
| 11 | 8 | 0 | 0.328332 | -0.501634 | 0.419752 |
| 12 | 6 | 0 | -4.178030 | -0.973543 | 2.086020 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 13| 1 | 0 | -6.524453 | -0.532162 | 0.398524 |
| 14| 1 | 0 | -4.831140 | -2.723175 | -0.854403 |
| 15| 6 | 0 | 1.158788  | 0.051102  | -0.611261 |
| 16| 6 | 0 | 0.885723  | 1.527122  | -0.897117 |
| 17| 6 | 0 | 0.800661  | 1.912956  | -2.218614 |
| 18| 6 | 0 | 0.729280  | 2.516530  | 0.130074  |
| 19| 6 | 0 | 0.569088  | 3.253542  | -2.594557 |
| 20| 6 | 0 | 0.488462  | 3.877461  | -0.255444 |
| 21| 6 | 0 | 0.412853  | 4.215884  | -1.631196 |
| 22| 6 | 0 | 2.612405  | -0.278925 | -0.260071 |
| 23| 6 | 0 | 3.040915  | -1.650249 | -0.248081 |
| 24| 6 | 0 | 0.885723  | 1.527122  | -0.854403 |
| 25| 6 | 0 | 0.800661  | 1.912956  | -2.218614 |
| 26| 6 | 0 | 0.729280  | 2.516530  | 0.130074  |
| 27| 6 | 0 | 0.569088  | 3.253542  | -2.594557 |
| 28| 6 | 0 | 0.488462  | 3.877461  | -0.255444 |
| 29| 6 | 0 | 0.412853  | 4.215884  | -1.631196 |
| 30| 6 | 0 | 2.612405  | -0.278925 | -0.260071 |
| 31| 6 | 0 | 3.040915  | -1.650249 | -0.248081 |
| 32| 6 | 0 | 0.885723  | 1.527122  | -0.854403 |
| 33| 6 | 0 | 0.800661  | 1.912956  | -2.218614 |
| 34| 6 | 0 | 0.729280  | 2.516530  | 0.130074  |
| 35| 6 | 0 | 0.569088  | 3.253542  | -2.594557 |
| 36| 6 | 0 | 0.488462  | 3.877461  | -0.255444 |
| 37| 6 | 0 | 0.412853  | 4.215884  | -1.631196 |
| 38| 6 | 0 | 2.612405  | -0.278925 | -0.260071 |
| 39| 6 | 0 | 3.040915  | -1.650249 | -0.248081 |
| 40| 6 | 0 | 0.885723  | 1.527122  | -0.854403 |
| 41| 6 | 0 | 0.800661  | 1.912956  | -2.218614 |
| 42| 6 | 0 | 0.729280  | 2.516530  | 0.130074  |
| 43| 6 | 0 | 0.569088  | 3.253542  | -2.594557 |
| 44| 6 | 0 | 0.488462  | 3.877461  | -0.255444 |
| 45| 6 | 0 | 0.412853  | 4.215884  | -1.631196 |
| 46| 6 | 0 | 2.612405  | -0.278925 | -0.260071 |
| 47| 6 | 0 | 3.040915  | -1.650249 | -0.248081 |
| 48| 6 | 0 | 0.885723  | 1.527122  | -0.854403 |
| 49| 6 | 0 | 0.800661  | 1.912956  | -2.218614 |
| 50| 6 | 0 | 0.729280  | 2.516530  | 0.130074  |
| 51| 6 | 0 | 0.569088  | 3.253542  | -2.594557 |
| 52| 6 | 0 | 0.488462  | 3.877461  | -0.255444 |
| 53| 6 | 0 | 0.412853  | 4.215884  | -1.631196 |
| 54| 6 | 0 | 2.612405  | -0.278925 | -0.260071 |
| 55| 6 | 0 | 3.040915  | -1.650249 | -0.248081 |
| 56| 6 | 0 | 0.885723  | 1.527122  | -0.854403 |
| 57| 6 | 0 | 0.800661  | 1.912956  | -2.218614 |

S324
|   |   |   |   |   |
|---|---|---|---|---|
| 58 | 1 | 0 | 5.876914 | -3.507600 | 0.332011 |
| 59 | 1 | 0 | 4.328087 | -5.353180 | -0.214956 |
| 60 | 1 | 0 | 0.971785 | 1.198797 | 1.828188 |
| 61 | 1 | 0 | 0.725310 | 2.957713 | 3.517864 |
| 62 | 1 | 0 | 0.152886 | 5.893576 | 0.441745 |
| 63 | 1 | 0 | 0.303329 | 5.313995 | 2.837448 |
| 64 | 1 | 0 | -5.617153 | -2.946236 | 0.684022 |
| 65 | 1 | 0 | -7.083668 | -1.678632 | -0.823017 |

6b (conformer 18)

|   |   |   |   |   |
|---|---|---|---|---|
| 1  | 6 | 0 | 4.521483 | -1.342796 | 0.223850 |
| 2  | 6 | 0 | 4.014251 | -0.054069 | -0.434969 |
| 3  | 6 | 0 | 3.434084 | -1.827943 | 1.228801 |
| 4  | 6 | 0 | 2.595075 | -0.071665 | -0.965101 |
| 5  | 6 | 0 | 2.014409 | -1.900518 | 0.650201 |
| 6  | 6 | 0 | 1.587992 | -0.545979 | 0.082607 |
| 7  | 6 | 0 | 5.844027 | -1.061533 | 1.018125 |
| 8  | 6 | 0 | 6.838585 | -0.184079 | 0.217167 |
| 9  | 6 | 0 | 4.761503 | 1.047203 | -0.544729 |
| 10 | 6 | 0 | 6.189211 | 1.170738 | -0.099525 |
| 11 | 8 | 0 | 0.311346 | -0.619190 | -0.565911 |
| 12 | 6 | 0 | 4.734335 | -2.417074 | -0.873198 |
| 13 | 1 | 0 | 7.065817 | -0.675947 | -0.736749 |
| 14 | 1 | 0 | 5.547653 | -0.452387 | 1.885256 |
| 15 | 6 | 0 | -0.833197 | -0.507783 | 0.283887 |
| 16 | 6 | 0 | -1.030588 | 0.948646 | 0.726693 |
| 17 | 6 | 0 | -0.867827 | 1.242153 | 2.065139 |
| 18 | 6 | 0 | -1.313595 | 2.018576 | -0.186195 |
| 19 | 6 | 0 | -1.015793 | 2.550676 | 2.574769 |
| 20 | 6 | 0 | -1.475865 | 3.345869 | 0.334741 |
| 21 | 6 | 0 | -1.325766 | 3.579988 | 1.726138 |
| 22 | 6 | 0 | -2.017376 | -1.178537 | -0.425274 |
| 23 | 6 | 0 | -3.272787 | -1.381715 | 0.240741 |
| 24 | 6 | 0 | -1.856392 | -1.659641 | -1.707199 |
| 25 | 6 | 0 | -4.333989 | -2.039021 | -0.468408 |
| 26 | 6 | 0 | -2.904400 | -2.305251 | -2.398687 |
| 27 | 6 | 0 | -4.121784 | -2.483853 | -1.797826 |
| 28 | 6 | 0 | -3.526330 | -0.992964 | 1.584803 |
| 29 | 6 | 0 | -4.742047 | -1.222941 | 2.184008 |
| 30 | 6 | 0 | -5.579876 | -2.251246 | 0.177363 |
| 31 | 6 | 0 | -5.785954 | -1.853770 | 1.474414 |
| 32 | 6 | 0 | -1.426740 | 1.840749 | -1.591654 |
| 33 | 6 | 0 | -1.708000 | 2.897794 | -2.423837 |
| 34 | 6 | 0 | -1.771894 | 4.412701 | -0.553478 |
| 35 | 6 | 0 | -1.889947 | 4.197552 | -1.903409 |
| 36 | 1 | 0 | 1.544799 | 0.196369 | 0.890403 |
| 37 | 1 | 0 | 3.711305 | -2.809944 | 1.621952 |

5325
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 38 | 1 | 0 | 3.428829 | -1.139888 | 2.083259 |
| 39 | 1 | 0 | 2.311512 | 0.922186 | -1.317990 |
| 40 | 1 | 0 | 2.512822 | -0.747947 | -1.825359 |
| 41 | 1 | 0 | 1.952849 | -2.644732 | 1.432477 |
| 42 | 1 | 0 | 2.311512 | 0.922186 | -1.317990 |
| 43 | 1 | 0 | 2.512822 | -0.747947 | -1.825359 |
| 44 | 1 | 0 | 1.952849 | -2.644732 | 1.432477 |
| 45 | 1 | 0 | 2.311512 | 0.922186 | -1.317990 |
| 46 | 1 | 0 | 2.512822 | -0.747947 | -1.825359 |
| 47 | 1 | 0 | 1.952849 | -2.644732 | 1.432477 |
| 48 | 1 | 0 | 2.311512 | 0.922186 | -1.317990 |
| 49 | 1 | 0 | 2.512822 | -0.747947 | -1.825359 |

**6b (conformer 24)**

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.518305 | -1.340879 | 0.226891 |
| 2 | 6 | 0 | 4.020349 | -0.050405 | -0.435708 |
| 3 | 6 | 0 | 3.430857 | -1.807953 | 1.240004 |
| 4 | 6 | 0 | 2.599343 | -0.057747 | -0.961801 |
| 5 | 6 | 0 | 2.009538 | -1.875181 | 0.665177 |
| 6 | 6 | 0 | 1.589590 | -0.522576 | 0.087998 |
| 7 | 6 | 0 | 5.848076 | -1.071288 | 1.012336 |
| 8 | 6 | 0 | 6.847229 | -0.200468 | 0.209675 |
| 9 | 6 | 0 | 4.777701 | 1.043164 | -0.554317 |
| 10 | 6 | 0 | 6.207360 | 1.157017 | -0.113026 |
| 11 | 8 | 0 | 0.314344 | -0.595953 | -0.563117 |
| 12 | 6 | 0 | 4.710038 | -2.424331 | -0.864499 |
| 13 | 1 | 0 | 7.076080 | -0.697921 | -0.741091 |
| 14 | 1 | 0 | 5.561745 | -0.462761 | 1.883319 |
| 15 | 6 | 0 | -0.833051 | -0.494561 | 0.283953 |
| 16 | 6 | 0 | -1.041098 | 0.959864 | 0.728586 |
| 17 | 6 | 0 | -0.880438 | 1.252384 | 2.067602 |

5326
|    |    |    |   |   |   |   |
|----|----|----|---|---|---|---|
| 18 | 6  | 0  | -1.328406 | 2.029654 | -0.183069 |
| 19 | 6  | 0  | -1.032527 | 2.559944 | 2.578500  |
| 20 | 6  | 0  | -1.493860 | 3.356001 | 0.339047  |
| 21 | 6  | 0  | -1.344475 | 3.589304 | 1.730681  |
| 22 | 6  | 0  | -2.009596 | -1.175139 | -0.428526 |
| 23 | 6  | 0  | -3.263183 | -1.393204 | 0.235997  |
| 24 | 6  | 0  | -1.841997 | -1.652714 | -1.710985 |
| 25 | 6  | 0  | -4.315322 | -2.064157 | -0.474063 |
| 26 | 6  | 0  | -1.493860 | 3.356001 | 0.339047  |
| 27 | 6  | 0  | -1.344475 | 3.589304 | 1.730681  |
| 28 | 6  | 0  | -2.009596 | -1.175139 | -0.428526 |
| 29 | 6  | 0  | -3.263183 | -1.393204 | 0.235997  |
| 30 | 6  | 0  | -1.841997 | -1.652714 | -1.710985 |
| 31 | 6  | 0  | -4.315322 | -2.064157 | -0.474063 |
| 32 | 6  | 0  | -1.493860 | 3.356001 | 0.339047  |
| 33 | 6  | 0  | -1.344475 | 3.589304 | 1.730681  |
| 34 | 6  | 0  | -2.009596 | -1.175139 | -0.428526 |
| 35 | 6  | 0  | -3.263183 | -1.393204 | 0.235997  |
| 36 | 6  | 0  | -1.841997 | -1.652714 | -1.710985 |
| 37 | 6  | 0  | -4.315322 | -2.064157 | -0.474063 |
| 38 | 6  | 0  | -1.493860 | 3.356001 | 0.339047  |
| 39 | 6  | 0  | -1.344475 | 3.589304 | 1.730681  |
| 40 | 6  | 0  | -2.009596 | -1.175139 | -0.428526 |
| 41 | 6  | 0  | -3.263183 | -1.393204 | 0.235997  |
| 42 | 6  | 0  | -1.841997 | -1.652714 | -1.710985 |
| 43 | 6  | 0  | -4.315322 | -2.064157 | -0.474063 |
| 44 | 6  | 0  | -1.493860 | 3.356001 | 0.339047  |
| 45 | 6  | 0  | -1.344475 | 3.589304 | 1.730681  |
| 46 | 6  | 0  | -2.009596 | -1.175139 | -0.428526 |
| 47 | 6  | 0  | -3.263183 | -1.393204 | 0.235997  |
| 48 | 6  | 0  | -1.841997 | -1.652714 | -1.710985 |
| 49 | 6  | 0  | -4.315322 | -2.064157 | -0.474063 |
| 50 | 6  | 0  | -1.493860 | 3.356001 | 0.339047  |
| 51 | 6  | 0  | -1.344475 | 3.589304 | 1.730681  |
| 52 | 6  | 0  | -2.009596 | -1.175139 | -0.428526 |
| 53 | 6  | 0  | -3.263183 | -1.393204 | 0.235997  |
| 54 | 6  | 0  | -1.841997 | -1.652714 | -1.710985 |
| 55 | 6  | 0  | -4.315322 | -2.064157 | -0.474063 |
| 56 | 6  | 0  | -1.493860 | 3.356001 | 0.339047  |
| 57 | 6  | 0  | -1.344475 | 3.589304 | 1.730681  |
| 58 | 6  | 0  | -2.009596 | -1.175139 | -0.428526 |
| 59 | 6  | 0  | -3.263183 | -1.393204 | 0.235997  |
| 60 | 6  | 0  | -1.841997 | -1.652714 | -1.710985 |
| 61 | 6  | 0  | -4.315322 | -2.064157 | -0.474063 |
| 62 | 6  | 0  | -1.493860 | 3.356001 | 0.339047  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 63 | 1 | 0 | -2.138678 | 5.031609 | -2.565849 |
| 64 | 1 | 0 | 7.751342 | -0.077302 | 0.768521 |
| 65 | 1 | 0 | 6.305623 | -1.960717 | 1.392425 |
| **6b (conformer 32)** |   |   |   |   |   |
|   |   |   |   |   |   |
| 1 | 6 | 0 | -4.123046 | -0.526886 | -0.855647 |
| 2 | 6 | 0 | -3.423049 | -0.839583 | 0.472413 |
| 3 | 6 | 0 | -3.265824 | 0.527662 | -1.616998 |
| 4 | 6 | 0 | -1.934239 | -1.118873 | 0.407739 |
| 5 | 6 | 0 | -1.771103 | 0.198072 | -1.715649 |
| 6 | 6 | 0 | -1.166677 | -0.012607 | -0.333402 |
| 7 | 6 | 0 | -5.541081 | 0.084372 | -0.585058 |
| 8 | 6 | 0 | -6.324363 | -0.691616 | 0.503325 |
| 9 | 6 | 0 | -4.067810 | -0.872560 | 1.641646 |
| 10 | 6 | 0 | -5.541879 | -0.658517 | 1.824152 |
| 11 | 8 | 0 | 0.219788 | -0.345284 | -0.515709 |
| 12 | 6 | 0 | -4.210225 | -1.825875 | -1.696309 |
| 13 | 1 | 0 | -6.422837 | -1.740891 | 0.198427 |
| 14 | 1 | 0 | -5.356957 | 1.082499 | -0.160108 |
| 15 | 6 | 0 | 1.089761 | -0.073672 | 0.595585 |
| 16 | 6 | 0 | 2.445757 | -0.717884 | 0.293192 |
| 17 | 6 | 0 | 3.594563 | 0.038273 | 0.208716 |
| 18 | 6 | 0 | 2.544053 | -2.144955 | 0.155590 |
| 19 | 6 | 0 | 4.856883 | -0.545710 | -0.039814 |
| 20 | 6 | 0 | 3.828140 | -2.733533 | -0.090452 |
| 21 | 6 | 0 | 4.972412 | -1.901355 | -0.191739 |
| 22 | 6 | 0 | 1.141193 | 1.410475 | 0.957424 |
| 23 | 6 | 0 | 1.321669 | 2.452175 | -0.013873 |
| 24 | 6 | 0 | 1.002213 | 1.751100 | 2.286502 |
| 25 | 6 | 0 | 1.352392 | 3.814770 | 0.434386 |
| 26 | 6 | 0 | 1.042465 | 3.092118 | 2.725502 |
| 27 | 6 | 0 | 1.210529 | 4.103576 | 1.816242 |
| 28 | 6 | 0 | 1.486711 | 2.204423 | -1.406228 |
| 29 | 6 | 0 | 1.665963 | 3.238221 | -2.294365 |
| 30 | 6 | 0 | 1.534569 | 4.855980 | -0.513786 |
| 31 | 6 | 0 | 1.687989 | 4.578395 | -1.848717 |
| 32 | 6 | 0 | 1.430222 | -3.019458 | 0.274153 |
| 33 | 6 | 0 | 1.573053 | -4.381917 | 0.159290 |
| 34 | 6 | 0 | 3.938473 | -4.143066 | -0.215839 |
| 35 | 6 | 0 | 2.838543 | -4.954353 | -0.092946 |
| 36 | 1 | 0 | -1.244860 | 0.920921 | 0.238336 |
| 37 | 1 | 0 | -3.668227 | 0.664752 | -2.624435 |
| 38 | 1 | 0 | -3.374654 | 1.491313 | -1.104569 |
| 39 | 1 | 0 | -1.549306 | -1.248328 | 1.422892 |
| 40 | 1 | 0 | -1.748469 | -2.057643 | -0.128465 |
| 41 | 1 | 0 | -1.601669 | -0.704982 | -2.311691 |
| 42 | 1 | 0 | -1.245487 | 1.012732 | -2.220360 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 43 | 1 | 0 | -3.495332 | -1.075284 | 2.545231 |
| 44 | 1 | 0 | -5.708624 | 0.307301 | 2.325311 |
| 45 | 1 | 0 | -5.934892 | -1.413989 | 2.514540 |
| 46 | 1 | 0 | -4.563350 | -2.309638 | -1.788661 |
| 47 | 1 | 0 | -4.563350 | -1.620482 | -2.709578 |
| 48 | 1 | 0 | -4.887364 | -2.549857 | -1.237482 |
| 49 | 1 | 0 | -5.937729 | 0.091925 | -0.106680 |
| 50 | 1 | 0 | -4.887364 | -2.549857 | -1.237482 |
| 51 | 1 | 0 | -3.236642 | -2.309638 | -1.788661 |
| 52 | 1 | 0 | -4.563350 | -1.620482 | -2.709578 |
| 53 | 1 | 0 | -3.236642 | -2.309638 | -1.788661 |
| 54 | 1 | 0 | -0.691611 | 0.585731 | 1.482789 |
| 55 | 1 | 0 | 3.542269 | 1.110457 | 0.338423 |
| 56 | 1 | 0 | 5.731148 | 0.091925 | -0.106680 |
| 57 | 1 | 0 | 5.937729 | 0.091925 | -0.106680 |
| 58 | 1 | 0 | 3.891126 | -1.637132 | 0.352468 |
| 59 | 1 | 0 | 3.444692 | -0.624066 | -0.708331 |
| 60 | 1 | 0 | 3.789079 | -0.267052 | 0.624050 |
| 61 | 1 | 0 | 3.891126 | -1.637132 | 0.352468 |
| 62 | 1 | 0 | 3.444692 | -0.624066 | -0.708331 |
| 63 | 1 | 0 | 3.891126 | -1.637132 | 0.352468 |
| 64 | 1 | 0 | 3.891126 | -1.637132 | 0.352468 |

### 6b (conformer 44)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.891126 | -1.637132 | 0.352468 |
| 2 | 6 | 0 | 3.444692 | -0.624066 | -0.708331 |
| 3 | 6 | 0 | 2.930764 | -1.509994 | 1.571922 |
| 4 | 6 | 0 | 1.964901 | -0.579421 | -1.033037 |
| 5 | 6 | 0 | 1.437497 | -1.545977 | 1.216924 |
| 6 | 6 | 0 | 1.096221 | -0.438505 | 0.217792 |
| 7 | 6 | 0 | 5.347834 | -1.315587 | 0.831670 |
| 8 | 6 | 0 | 6.035523 | -0.998324 | -0.346397 |
| 9 | 6 | 0 | 4.295951 | 0.195410 | -1.330344 |
| 10 | 6 | 0 | 5.782109 | 0.218159 | -1.124765 |
| 11 | 8 | 0 | 0.270204 | -0.481335 | -0.225395 |
| 12 | 6 | 0 | 3.789079 | -3.063723 | -0.244778 |
| 13 | 1 | 0 | 6.322636 | -1.853284 | -1.033716 |
| 14 | 1 | 0 | 5.272728 | -0.382142 | 1.409683 |
| 15 | 6 | 0 | 1.251635 | 0.037382 | 0.677904 |
| 16 | 6 | 0 | 1.036873 | 1.514264 | 1.018618 |
| 17 | 6 | 0 | 1.089138 | 1.885057 | 2.345950 |
| 18 | 6 | 0 | 0.784138 | 2.518026 | 0.024069 |
| 19 | 6 | 0 | -0.913165 | 3.223549 | 2.758422 |
| 20 | 6 | 0 | -0.595020 | 3.875812 | 0.447387 |
| 21 | 6 | 0 | -0.667140 | 4.198422 | 1.821755 |
| 22 | 6 | 0 | -2.634820 | -0.311534 | 0.130476 |

5329
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 23| 6 | 0 | -3.021672 | -1.688448 | -0.009025 |
| 24| 6 | 0 | -3.550237 | 0.670715  | -0.178639 |
| 25| 6 | 0 | -4.339560 | -1.996177 | -0.482619 |
| 26| 6 | 0 | -4.845211 | 0.362571  | -0.652540 |
| 27| 6 | 0 | -5.231955 | -0.941751 | -0.805244 |
| 28| 6 | 0 | -2.169267 | -2.776240 | 0.322139  |
| 29| 6 | 0 | -2.589004 | -4.079288 | 0.197391  |
| 30| 6 | 0 | -4.737092 | -3.352768 | -0.609889 |
| 31| 6 | 0 | -3.885211 | -4.375760 | -0.805244 |
| 32| 6 | 0 | -0.722041 | 2.239546  | -1.370726 |
| 33| 6 | 0 | -0.484977 | 3.239436  | -2.283763 |
| 34| 6 | 0 | -0.347534 | 4.880444  | -0.525026 |
| 35| 6 | 0 | -0.292763 | 4.573500  | -0.805244 |
| 36| 1 | 0 | 1.295874  | 0.536150  | 0.681432  |
| 37| 1 | 0 | 3.147099  | -2.304273 | 2.291740  |
| 38| 1 | 0 | 3.145490  | 0.561772  | 2.079513  |
| 39| 1 | 0 | 1.758449  | 0.248355  | -1.714331 |
| 40| 1 | 0 | 1.650056  | -1.497363 | -1.545482 |
| 41| 1 | 0 | 1.168810  | -2.512328 | 0.777174  |
| 42| 1 | 0 | 0.850028  | -1.438088 | 2.134390  |
| 43| 1 | 0 | 3.897660  | 0.909077  | -2.049026 |
| 44| 1 | 0 | 6.059045  | 1.141159  | -0.592641 |
| 45| 1 | 0 | 6.282632  | 0.284697  | -2.097855 |
| 46| 1 | 0 | 2.821078  | -3.230904 | -0.719292 |
| 47| 1 | 0 | 3.909031  | -3.830184 | 0.524896  |
| 48| 1 | 0 | 4.552000  | -3.224540 | -1.009872 |
| 49| 1 | 0 | -1.156642 | -0.499795 | 1.640872  |
| 50| 1 | 0 | -1.273384 | 1.124988  | 3.098728  |
| 51| 1 | 0 | -0.966326 | 3.470261  | 3.812767  |
| 52| 1 | 0 | -0.523438 | 5.230163  | 2.130611  |
| 53| 1 | 0 | -3.283581 | 1.711119  | -0.053179 |
| 54| 1 | 0 | -5.528173 | 1.170394  | -0.889983 |
| 55| 1 | 0 | -6.225318 | -1.188236 | -1.165498 |
| 56| 1 | 0 | -1.164532 | -2.573117 | 0.659373  |
| 57| 1 | 0 | -1.916059 | -4.888298 | 0.459789  |
| 58| 1 | 0 | -5.736773 | -3.566233 | -0.974156 |
| 59| 1 | 0 | -4.202520 | -5.407755 | -0.376143 |
| 60| 1 | 0 | -0.855624 | 1.221493  | -1.705602 |
| 61| 1 | 0 | -0.445510 | 3.001260  | -3.340936 |
| 62| 1 | 0 | -0.205108 | 5.902240  | -0.188602 |
| 63| 1 | 0 | -0.104826 | 5.350553  | -2.593716 |
| 64| 1 | 0 | 7.291532  | -0.822684 | 0.024937  |
| 65| 1 | 0 | 5.753825  | -2.055823 | 1.489029  |

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 6b (conformer 51) | 1 | 6 | 0 | -4.114710 | -0.608384 | -0.852888 |
| 2 | 6 | 0 | -3.398503 | -0.868510 | 0.478165  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 3 | 6 | 0 | -3.270343 | 0.415471 | -1.669638 |
| 4 | 6 | 0 | -1.908085 | -1.137525 | 0.409941 |
| 5 | 6 | 0 | -1.772007 | 0.097217 | -1.760697 |
| 6 | 6 | 0 | -1.161544 | -0.046484 | -0.372892 |
| 7 | 6 | 0 | -5.529644 | 0.011387 | -0.585857 |
| 8 | 6 | 0 | -6.298602 | -0.732847 | 0.534559 |
| 9 | 6 | 0 | -4.029823 | -0.864813 | 1.654977 |
| 10 | 6 | 0 | -5.502849 | -0.653324 | 1.845629 |
| 11 | 8 | 0 | 0.231538 | -0.354463 | -0.544418 |
| 12 | 6 | 0 | -4.210830 | -1.941345 | -1.637531 |
| 13 | 1 | 0 | -6.395413 | -1.791593 | 0.264427 |
| 14 | 1 | 0 | -5.340459 | 1.021180 | -0.191629 |
| 15 | 6 | 0 | 1.086579 | -0.065381 | 0.574304 |
| 16 | 6 | 0 | 2.458987 | -0.680577 | 0.286170 |
| 17 | 6 | 0 | 3.592661 | 0.099693 | 0.218000 |
| 18 | 6 | 0 | 2.589650 | -2.105510 | 0.153418 |
| 19 | 6 | 0 | 4.871690 | -0.458256 | -0.003702 |
| 20 | 6 | 0 | 3.890764 | -2.667773 | -0.063081 |
| 21 | 6 | 0 | 5.019053 | -1.811963 | -0.144693 |
| 22 | 6 | 0 | 1.101994 | 1.418744 | 0.941202 |
| 23 | 6 | 0 | 1.267337 | 2.468382 | -0.023949 |
| 24 | 6 | 0 | 0.941560 | 1.750355 | 2.270156 |
| 25 | 6 | 0 | 1.259747 | 3.829518 | 0.429706 |
| 26 | 6 | 0 | 0.944965 | 3.090116 | 2.714776 |
| 27 | 6 | 0 | 1.096761 | 4.109179 | 1.811105 |
| 28 | 6 | 0 | 1.452272 | 2.230057 | -1.415348 |
| 29 | 6 | 0 | 1.617238 | 3.271327 | -2.297536 |
| 30 | 6 | 0 | 1.426370 | 4.878527 | -0.512668 |
| 31 | 6 | 0 | 1.601988 | 4.609957 | -1.846704 |
| 32 | 6 | 0 | 1.491571 | -3.002409 | 0.248757 |
| 33 | 6 | 0 | 1.664922 | -4.361850 | 0.141188 |
| 34 | 6 | 0 | 4.033048 | -4.075124 | -0.180146 |
| 35 | 6 | 0 | 2.947589 | -4.908639 | -0.079073 |
| 36 | 1 | 0 | -1.259605 | 0.906268 | 0.162742 |
| 37 | 1 | 0 | -3.679284 | 0.499203 | -2.680278 |
| 38 | 1 | 0 | -3.385519 | 1.401943 | -1.204420 |
| 39 | 1 | 0 | -1.514542 | -1.230148 | 1.425736 |
| 40 | 1 | 0 | -1.717277 | -2.091564 | -0.097080 |
| 41 | 1 | 0 | -1.594864 | -0.828948 | -2.317860 |
| 42 | 1 | 0 | -1.257103 | 0.894926 | -2.302304 |
| 43 | 1 | 0 | -3.445962 | -1.032048 | 2.558472 |
| 44 | 1 | 0 | -5.669178 | 0.327655 | 2.316845 |
| 45 | 1 | 0 | -5.886028 | -1.387556 | 2.563869 |
| 46 | 1 | 0 | -4.574770 | -1.779206 | -2.654776 |
| 47 | 1 | 0 | -3.237555 | -2.427961 | -1.719092 |
|   |    |   |          |          |          |
|---|----|---|----------|----------|----------|
| 48|  1 |  0 | -4.882102 | -2.645912 | -1.141084 |
| 49|  1 |  0 |  0.691907  | -0.587258 |  1.457174 |
| 50|  1 |  0 |  3.514963  |  1.711013 |  0.342247 |
| 51|  1 |  0 |  5.733331  |  0.197591 | -0.056979 |
| 52|  1 |  0 |  5.997588  | -2.249992 | -0.311762 |
| 53|  1 |  0 |  0.808676  |  0.957004 |  2.998903 |
| 54|  1 |  0 |  0.818401  |  3.304358 |  3.769945 |
| 55|  1 |  0 |  3.514963  |  1.171013 |  0.342247 |
| 56|  1 |  0 |  5.733331  |  0.197591 | -0.056979 |
| 57|  1 |  0 |  5.997588  | -2.249992 | -0.311762 |
| 58|  1 |  0 |  0.808676  |  0.957004 |  2.998903 |
| 59|  1 |  0 |  0.818401  |  3.304358 |  3.769945 |
| 60|  1 |  0 |  3.514963  |  1.171013 |  0.342247 |
| 61|  1 |  0 |  5.733331  |  0.197591 | -0.056979 |
| 62|  1 |  0 |  5.997588  | -2.249992 | -0.311762 |
| 63|  1 |  0 |  0.808676  |  0.957004 |  2.998903 |

| 6b (conformer 60) |   |    |          |          |          |
|-------------------|----|---|----------|----------|----------|
| 1                 |  6 |  0 |  3.883202 | -1.665164 |  0.329588 |
| 2                 |  6 |  0 |  3.439118 | -0.626032 | -0.706628 |
| 3                 |  6 |  0 |  2.923602 | -1.562057 |  1.552631 |
| 4                 |  6 |  0 |  1.960206 | -0.574872 | -1.033325 |
| 5                 |  6 |  0 |  1.429888 | -1.582855 |  1.198398 |
| 6                 |  6 |  0 |  1.092209 | -0.455545 |  0.220499 |
| 7                 |  6 |  0 |  5.340942 | -1.359082 |  0.817740 |
| 8                 |  6 |  0 |  6.297315 | -1.003681 | -0.347604 |
| 9                 |  6 |  0 |  4.290166 |  0.212885 | -1.302657 |
| 10                |  6 |  0 |  5.775023 |  0.235734 | -1.087968 |
| 11                |  8 |  0 | -0.275612 | -0.487119 | -0.219829 |
| 12                |  6 |  0 |  3.777476 | -3.077600 | -0.299703 |
| 13                |  6 |  0 |  6.319350 | -1.836226 | -1.061621 |
| 14                |  6 |  0 |  5.265804 | -0.445012 |  1.425706 |
| 15                |  6 |  0 | -1.250350 |  0.039000 |  0.695651 |
| 16                |  6 |  0 | -1.020084 |  1.513593 |  1.024761 |
| 17                |  6 |  0 | -1.054763 |  1.886501 |  2.351997 |
| 18                |  6 |  0 | -0.768279 |  2.513650 |  0.026212 |
| 19                |  6 |  0 | -0.861538 |  3.223763 |  2.760921 |
| 20                |  6 |  0 | -0.562837 |  3.870227 |  0.445670 |
| 21                |  6 |  0 | -0.616727 |  4.195196 |  1.825756 |
| 22                |  6 |  0 | -2.637875 | -0.297147 |  0.141998 |
| 23                |  6 |  0 | -3.035692 | -1.670601 | -0.001464 |
| 24                |  6 |  0 | -3.545860 |  0.693136 | -0.163532 |
| 25                |  6 |  0 | -4.354735 | -1.966552 | -0.479320 |
| 26                |  6 |  0 | -4.842115 |  0.396531 | -0.641172 |
| 27                |  6 |  0 | -5.238144 | -0.904216 | -0.800684 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 28| 6 | 0 | -2.193203 | -2.766217 | 0.329611 |   |
| 29| 6 | 0 | -2.623603 | -4.065494 | 0.200947 |   |
| 30| 6 | 0 | -4.762984 | -3.319536 | -0.611391 |   |
| 31| 6 | 0 | -3.920594 | -4.350303 | -0.278139 |   |
| 32| 6 | 0 | -0.723617 | 2.232354 | 1.368705 |   |
| 33| 6 | 0 | -0.487697 | 3.228763 | -0.530996 |   |
| 34| 6 | 0 | -0.317094 | 4.871182 | -0.278139 |   |
| 35| 6 | 0 | -0.279570 | 4.561714 | -0.431360 |   |
| 36| 1 | 0 | 1.296182 | 0.509667 | 0.701740 |   |
| 37| 1 | 0 | 3.136463 | -2.374168 | 2.253213 |   |
| 38| 1 | 0 | 3.143157 | -0.626969 | 2.082046 |   |
| 39| 1 | 0 | 1.754707 | 0.266169 | 1.698435 |   |
| 40| 1 | 0 | 1.644849 | -1.482671 | -1.562923 |   |
| 41| 1 | 0 | 1.155032 | -2.539065 | 0.740996 |   |
| 42| 1 | 0 | 0.844315 | -1.488802 | 2.118658 |   |
| 43| 1 | 0 | 3.892180 | 0.944422 | 0.200947 |   |
| 44| 1 | 0 | 6.044291 | 1.140922 | -0.522379 |   |
| 45| 1 | 0 | 6.281172 | 0.337447 | -2.054983 |   |
| 46| 1 | 0 | 3.900414 | -3.861460 | 0.451798 |   |
| 47| 1 | 0 | 2.807402 | -3.233994 | -0.773557 |   |
| 48| 1 | 0 | 4.537117 | -3.221557 | -0.773557 |   |
| 49| 1 | 0 | -1.157650 | -0.499438 | 1.649003 |   |
| 50| 1 | 0 | -1.237606 | 1.128905 | 3.107587 |   |
| 51| 1 | 0 | -0.900773 | 3.472092 | 3.815495 |   |
| 52| 1 | 0 | -0.459937 | 5.225955 | 2.126046 |   |
| 53| 1 | 0 | -3.272077 | 1.731151 | -0.033785 |   |
| 54| 1 | 0 | -5.518506 | 1.210411 | -0.876726 |   |
| 55| 1 | 0 | -6.232354 | -1.141763 | -1.164653 |   |
| 56| 1 | 0 | -1.187844 | -2.572840 | 0.670727 |   |
| 57| 1 | 0 | -1.958261 | -4.880544 | 0.464042 |   |
| 58| 1 | 0 | -5.765350 | -3.523748 | -0.978590 |   |
| 59| 1 | 0 | -4.245985 | -5.379446 | -0.380888 |   |
| 60| 1 | 0 | -0.869248 | 1.214716 | -1.699739 |   |
| 61| 1 | 0 | -0.461108 | 2.988790 | -3.342959 |   |
| 62| 1 | 0 | -0.161921 | 5.892269 | -0.199012 |   |
| 63| 1 | 0 | -0.092695 | 5.336025 | -2.602887 |   |
| 64| 1 | 0 | 7.284324 | -0.838068 | 0.030927 |   |
| 65| 1 | 0 | 5.746907 | -2.119867 | 1.451221 |   |

| 6b (conformer 70) |   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6 | 0 | -4.053598 | -0.931797 | -0.820510 |   |
| 2 | 6 | 0 | -3.364770 | -0.838967 | 0.546303 |   |
| 3 | 6 | 0 | -3.234248 | -0.076001 | -1.833028 |   |
| 4 | 6 | 0 | -1.863551 | -1.052289 | 0.569347 |   |
| 5 | 6 | 0 | -1.722644 | -0.333298 | -1.824855 |   |
| 6 | 6 | 0 | -1.139455 | -0.137828 | -0.431360 |   |
| 7 | 6 | 0 | -5.504611 | -0.344874 | -0.737109 |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 8 | 6 | 0 | -6.271309 | -0.823430 | 0.520657 |
| 9 | 6 | 0 | -4.027690 | -0.585048 | 1.677288 |
| 10 | 6 | 0 | -5.512034 | -0.397316 | 1.785885 |
| 11 | 8 | 0 | 0.265967 | -0.415121 | 0.520657 |
| 12 | 6 | 0 | -4.060321 | -2.412456 | -1.276546 |
| 13 | 1 | 0 | -6.327184 | -1.919132 | 0.513064 |
| 14 | 1 | 0 | -5.378217 | 0.740803 | 0.513064 |
| 15 | 6 | 0 | 1.085922 | -0.033796 | 0.585300 |
| 16 | 6 | 0 | 2.498303 | -0.563619 | 0.320572 |
| 17 | 6 | 0 | 3.581183 | 0.286136 | 0.261535 |
| 18 | 6 | 0 | 2.719212 | -1.978413 | 0.198379 |
| 19 | 6 | 0 | 4.895089 | -0.191300 | 0.056369 |
| 20 | 6 | 0 | 4.055306 | -2.458397 | -0.002647 |
| 21 | 6 | 0 | 5.128392 | -1.533610 | -0.077539 |
| 22 | 6 | 0 | 1.000446 | 1.456307 | 0.912625 |
| 23 | 6 | 0 | 1.110723 | 2.489381 | -0.077709 |
| 24 | 6 | 0 | 0.807322 | 1.810648 | 2.231233 |
| 25 | 6 | 0 | 1.017971 | 3.858656 | 0.340636 |
| 26 | 6 | 0 | 0.726596 | 3.158941 | 2.641404 |
| 27 | 6 | 0 | 0.826956 | 4.162320 | -0.077709 |
| 28 | 6 | 0 | 1.317832 | 2.227255 | -1.461581 |
| 29 | 6 | 0 | 1.421442 | 3.253652 | -2.370100 |
| 30 | 6 | 0 | 1.126777 | 4.891350 | 1.713388 |
| 31 | 6 | 0 | 1.323449 | 4.599856 | -1.954015 |
| 32 | 6 | 0 | 1.678727 | -2.942548 | 0.288734 |
| 33 | 6 | 0 | 1.939006 | -4.288726 | 0.190077 |
| 34 | 6 | 0 | 4.287206 | -3.854427 | -0.111813 |
| 35 | 6 | 0 | 3.255637 | -4.754339 | -0.016154 |
| 36 | 1 | 0 | -1.282350 | 0.905802 | -0.122149 |
| 37 | 1 | 0 | -3.618806 | -0.240858 | -2.843416 |
| 38 | 1 | 0 | -3.407181 | 0.982289 | -1.603044 |
| 39 | 1 | 0 | -1.497187 | -0.889344 | 1.585891 |
| 40 | 1 | 0 | -1.624625 | -2.090184 | 0.304515 |
| 41 | 1 | 0 | -1.490757 | -1.349995 | -2.159394 |
| 42 | 1 | 0 | -1.227258 | 0.347579 | -2.522262 |
| 43 | 1 | 0 | -3.463185 | -0.508104 | 2.604842 |
| 44 | 1 | 0 | -5.727196 | 0.660157 | 2.003164 |
| 45 | 1 | 0 | -5.886423 | -0.952101 | 2.654152 |
| 46 | 1 | 0 | -4.719598 | -3.016061 | -0.648245 |
| 47 | 1 | 0 | -4.391083 | -2.509153 | -2.313153 |
| 48 | 1 | 0 | -3.064596 | -2.854350 | -1.215139 |
| 49 | 1 | 0 | 0.721251 | -0.558707 | 1.478751 |
| 50 | 1 | 0 | 3.434239 | 1.351038 | 0.378796 |
| 51 | 1 | 0 | 5.714430 | 0.517087 | 0.008707 |
| 52 | 1 | 0 | 6.134059 | -1.910023 | -0.233454 |
|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 53 | 1 | 0 | 0.717135 | 1.029041 | 2.978980 |
| 54 | 1 | 0 | 0.578291 | 3.391636 | 3.689816 |
| 55 | 1 | 0 | 0.760436 | 5.202736 | 2.014065 |
| 56 | 1 | 0 | 1.384045 | 1.201643 | -1.794128 |
| 57 | 1 | 0 | 1.580888 | 3.027186 | -3.418508 |
| 58 | 1 | 0 | 1.053237 | 5.921859 | -0.295686 |
| 59 | 1 | 0 | 1.405685 | 5.398228 | -2.683048 |
| 60 | 1 | 0 | 0.660639 | -2.606852 | 0.414307 |
| 61 | 1 | 0 | 1.124181 | -5.000528 | 0.264765 |
| 62 | 1 | 0 | 5.304389 | -4.198510 | -0.268627 |
| 63 | 1 | 0 | 3.446960 | -5.818398 | -0.098444 |
| 64 | 1 | 0 | -7.262244 | -0.419781 | 0.516721 |
| 65 | 1 | 0 | -6.075322 | -0.486571 | -1.631039 |

7b (conformer 1)

|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 1  | 6 | 0 | 5.395958 | -0.606925 | -0.534047 |
| 2  | 6 | 0 | 6.224609 | -0.300630 | 0.716571 |
| 3  | 6 | 0 | 5.840154 | 0.318554 | -1.696885 |
| 4  | 6 | 0 | 7.366563 | 0.412100 | 0.683005 |
| 5  | 6 | 0 | 7.357178 | 0.457886 | -1.845292 |
| 6  | 6 | 0 | 8.011412 | 0.896514 | -0.548092 |
| 7  | 6 | 0 | 3.877352 | -0.322470 | -0.221380 |
| 8  | 6 | 0 | 3.370673 | -0.984374 | 1.091157 |
| 9  | 6 | 0 | 5.726835 | -0.871940 | 2.019495 |
| 10 | 6 | 0 | 4.247737 | -0.554742 | 2.272980 |
| 11 | 6 | 0 | 2.944036 | -0.618760 | -1.418807 |
| 12 | 6 | 0 | 1.463867 | -0.296583 | -1.134763 |
| 13 | 6 | 0 | 1.902425 | -0.598707 | 1.304024 |
| 14 | 6 | 0 | 0.970992 | -1.001700 | 0.135697 |
| 15 | 6 | 0 | 1.154138 | -1.078905 | 2.562660 |
| 16 | 6 | 0 | -0.346652 | -0.873474 | 2.202710 |
| 17 | 6 | 0 | -0.373324 | -0.485738 | 0.693195 |
| 18 | 8 | 0 | -1.473151 | -1.031663 | -0.027209 |
| 19 | 6 | 0 | 0.891707 | -2.526647 | -0.085799 |
| 20 | 6 | 0 | 5.638873 | -2.088728 | -0.923441 |
| 21 | 6 | 0 | 9.030453 | 1.562913 | -0.522258 |
| 22 | 1 | 0 | 3.822156 | 0.761755 | -0.040070 |
| 23 | 1 | 0 | 3.440374 | -2.076198 | 0.999478 |
| 24 | 1 | 0 | 1.881041 | 0.502232 | 1.333477 |
| 25 | 1 | 0 | -0.381471 | 0.606248 | 0.590923 |
| 26 | 1 | 0 | 5.418334 | 1.315472 | -1.523588 |
| 27 | 1 | 0 | 5.415173 | -0.041429 | -2.636767 |
| 28 | 1 | 0 | 7.910577 | 0.625755 | 1.598803 |
| 29 | 1 | 0 | 7.622447 | 1.174531 | -2.625456 |
| 30 | 1 | 0 | 7.811467 | -0.499273 | -2.130231 |
| 31 | 1 | 0 | 6.349811 | -0.510949 | 2.841580 |
| 32 | 1 | 0 | 5.850381 | -1.963140 | 1.991926 |
|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
|33 |1  |0  |3.921351 |-1.051045 |3.191657 |
|34 |1  |0  |4.130608 |0.524041  |2.437088 |
|35 |1  |0  |3.032569 |-1.669765 |-1.707917 |
|36 |1  |0  |3.263623 |-0.038258 |2.287468 |
|37 |1  |0  |0.851233 |-1.669765 |-1.707917 |
|38 |1  |0  |1.348058 |0.786974  |-1.007986 |
|39 |1  |0  |1.442922 |-0.520332 |3.455132 |
|40 |1  |0  |1.366464 |0.524041  |2.437088 |
|41 |1  |0  |0.851233 |-0.520332 |3.455132 |
|42 |1  |0  |1.860629 |-2.953722 |-0.347593 |
|43 |1  |0  |0.526251 |-3.056967 |0.795575 |
|44 |1  |0  |0.199695 |-2.741186 |-0.901872 |
|45 |1  |0  |5.132798 |-2.335195 |-1.859132 |
|46 |1  |0  |5.280440 |-2.779543 |0.165014 |
|47 |1  |0  |6.70512  |-2.820797 |-1.062224 |
|48 |1  |0  |2.732515 |-0.379485 |0.165014 |
|49 |1  |0  |1.366464 |-2.133164 |2.763873 |
|50 |6  |0  |-2.764463 |0.942443  |-0.622626 |
|51 |6  |0  |-2.832670 |0.870599  |-1.998641 |
|52 |6  |0  |-2.809633 |2.023738  |-2.807475 |
|53 |6  |0  |-2.719446 |3.265699  |-2.231550 |
|54 |6  |0  |-2.644748 |3.401184  |-0.823713 |
|55 |6  |0  |-2.661784 |2.227006  |0.004963 |
|56 |6  |0  |-2.548364 |4.682687  |-0.219252 |
|57 |6  |0  |-2.473202 |4.823447  |1.142889 |
|58 |6  |0  |-2.490871 |3.675605  |1.965699 |
|59 |6  |0  |-2.581752 |2.420246  |1.414153 |
|60 |6  |0  |-5.205878 |-1.070767 |0.078906 |
|61 |6  |0  |-6.213374 |2.010696  |-0.317630 |
|62 |6  |0  |-5.838264 |-3.181372 |-1.026157 |
|63 |6  |0  |-4.522194 |-3.419961 |-1.321421 |
|64 |6  |0  |-3.523177 |-2.501741 |-0.926160 |
|65 |6  |0  |-5.623504 |0.086834  |0.790451 |
|66 |6  |0  |-6.947014 |0.302067  |1.094122 |
|67 |6  |0  |-7.934367 |-0.626805 |0.700847 |
|68 |6  |0  |-7.570424 |1.755628  |0.009792 |
|69 |6  |0  |-2.863368 |0.174468  |1.232065 |
|70 |6  |0  |-2.916081 |0.174468  |1.232065 |
|71 |6  |0  |-2.869071 |1.921691  |3.885190 |
|72 |6  |0  |-2.706348 |4.161085  |-2.844065 |
|73 |6  |0  |-2.535575 |5.556195  |-0.862897 |
|74 |6  |0  |-2.400861 |5.808291  |1.589960 |
|75 |6  |0  |-2.432012 |3.786270  |3.042725 |
|76 |6  |0  |-2.590299 |1.565429  |2.077535 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 78| 1 | 0 | -6.610452 | -3.883186 | -1.323453 |
| 79| 1 | 0 | -4.234849 | -4.318111 | -1.856880 |
| 80| 1 | 0 | -2.486009 | -2.710930 | -1.146702 |
| 81| 1 | 0 | -4.894899 | 0.825918  | 1.093922  |
| 82| 1 | 0 | -7.235186 | 1.195278  | 1.637086  |
| 83| 1 | 0 | -8.975092 | -0.445314 | 0.944556  |
| 84| 1 | 0 | -8.320529 | -2.476779 | -0.298302 |

| 7b (conformer 2) |
|---|---|---|---|---|---|---|
| 1 | 6 | 0 | -5.497715 | -0.300995 | 0.569740 |
| 2 | 6 | 0 | -6.282317 | -0.409567 | -0.740722 |
| 3 | 6 | 0 | -6.037271 | 0.888688  | 1.406334  |
| 4 | 6 | 0 | -7.456626 | 0.216653  | -0.945786 |
| 5 | 6 | 0 | -7.564451 | 0.974595  | 1.464112  |
| 6 | 6 | 0 | -8.178661 | 0.990879  | 0.076702  |
| 7 | 6 | 0 | -3.981175 | -0.030142 | 0.569740  |
| 8 | 6 | 0 | -3.848888 | -1.001805 | -0.821172 |
| 9 | 6 | 0 | -5.699271 | -1.293670 | -1.813319 |
| 10| 6 | 0 | -4.227452 | -0.973153 | -2.101507 |
| 11| 6 | 0 | -3.089128 | 0.070942  | 1.493894  |
| 12| 6 | 0 | -1.611340 | 0.380663  | 1.178785  |
| 13| 6 | 0 | -1.930098 | -0.601122 | -1.091140 |
| 14| 6 | 0 | -1.029751 | -0.616410 | 0.167069  |
| 15| 6 | 0 | -1.111741 | -1.359545 | -2.154647 |
| 16| 6 | 0 | 0.367515  | -1.024368 | -1.802817 |
| 17| 6 | 0 | 0.313467  | -0.205872 | -0.478838 |
| 18| 8 | 0 | 1.400547  | -0.443931 | 0.414842  |
| 19| 6 | 0 | -0.884171 | -2.013122 | 0.806692  |
| 20| 6 | 0 | -5.690354 | -1.622521 | 1.358965  |
| 21| 8 | 0 | -9.225237 | 1.563334  | -0.168545 |
| 22| 1 | 0 | -3.966897 | 0.961605  | -0.242247 |
| 23| 1 | 0 | -3.401352 | -2.026332 | -0.426819 |
| 24| 1 | 0 | -1.963871 | 0.449829  | -1.419172 |
| 25| 1 | 0 | 0.270976  | 0.865821  | -0.713495 |
| 26| 1 | 0 | -5.656967 | 1.818489  | 0.967560  |
| 27| 1 | 0 | -5.637936 | 0.836128  | 2.422015  |
| 28| 1 | 0 | -7.967751 | 0.131590  | -1.900630 |
| 29| 1 | 0 | -7.898994 | 1.864913  | 2.000736  |
| 30| 1 | 0 | -7.984370 | 0.111115  | 1.994928  |
| 31| 1 | 0 | -6.301083 | -1.214389 | -2.722007 |
| 32| 1 | 0 | -5.771419 | -2.338832 | -1.483100 |
| 33| 1 | 0 | -3.835787 | -1.686007 | -2.833116 |
| 34| 1 | 0 | -4.155743 | 0.021765  | -2.559393 |
| 35| 1 | 0 | -3.145141 | -0.861390 | 2.062288  |
| 36| 1 | 0 | -3.470953 | 0.852134  | 2.155709  |
| 37| 1 | 0 | -1.033688 | 0.373781  | 2.109068  |
| 38| 1 | 0 | -1.535406 | 1.394049  | 0.765304  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 39 | 1 | 0 | -1.372269 | -1.052923 | -3.169524 |
| 40 | 1 | 0 | -1.291015 | -2.436925 | -2.092332 |
| 41 | 1 | 0 | 0.855762  | -0.464898 | -2.603854 |
| 42 | 1 | 0 | 0.948018  | -1.933720 | -1.635609 |
| 43 | 6 | 0 | 2.669879  | 0.095654  | 0.020096  |
| 44 | 1 | 0 | -1.821933 | -2.365074 | 1.238341  |
| 45 | 1 | 0 | -0.550822 | -2.765979 | 0.089682  |
| 46 | 1 | 0 | -0.136734 | -1.971120 | 1.600125  |
| 47 | 1 | 0 | -5.205395 | -1.569316 | 2.335821  |
| 48 | 1 | 0 | -5.279423 | -2.483446 | 0.828701  |
| 49 | 1 | 0 | -6.751755 | -1.820356 | 1.525607  |
| 50 | 6 | 0 | 3.729486  | -0.705397 | 0.775840  |
| 51 | 6 | 0 | 2.764128  | 1.603273  | 0.020096  |
| 52 | 6 | 0 | 1.907733  | 2.221739  | 1.138360  |
| 53 | 6 | 0 | 1.959231  | 3.615499  | 1.366296  |
| 54 | 6 | 0 | 2.872092  | 4.390737  | 0.700038  |
| 55 | 6 | 0 | 3.782933  | 3.802470  | -0.215489 |
| 56 | 6 | 0 | 3.740827  | 2.387365  | -0.441896 |
| 57 | 6 | 0 | 4.740095  | 4.588525  | -0.908328 |
| 58 | 6 | 0 | 5.629491  | 4.015265  | -1.782778 |
| 59 | 6 | 0 | 5.601586  | 2.620254  | -1.999159 |
| 60 | 6 | 0 | 4.685876  | 1.829613  | -1.346383 |
| 61 | 6 | 0 | 4.290619  | -1.904102 | 0.221794  |
| 62 | 6 | 0 | 5.241390  | -2.645740 | 1.000337  |
| 63 | 6 | 0 | 5.595247  | -2.188366 | 2.294884  |
| 64 | 6 | 0 | 5.040505  | -1.043022 | 2.802939  |
| 65 | 6 | 0 | 4.112766  | -0.305437 | 2.037212  |
| 66 | 6 | 0 | 3.966231  | -2.406416 | -1.068559 |
| 67 | 6 | 0 | 4.538781  | -3.556187 | -1.558818 |
| 68 | 6 | 0 | 5.473384  | -4.279395 | -0.786739 |
| 69 | 6 | 0 | 5.813278  | -3.829073 | 0.464024  |
| 70 | 1 | 0 | 2.798361  | -0.070836 | -1.052553 |
| 71 | 1 | 0 | 1.176865  | 1.618916  | 1.661581  |
| 72 | 1 | 0 | 1.267338  | 4.065876  | 2.069340  |
| 73 | 1 | 0 | 2.913991  | 5.462448  | 0.863740  |
| 74 | 1 | 0 | 4.758218  | 5.658690  | -0.729512 |
| 75 | 1 | 0 | 6.356665  | 4.627774  | -2.303730 |
| 76 | 1 | 0 | 6.312599  | 2.168517  | -2.681776 |
| 77 | 1 | 0 | 4.703481  | 0.760929  | -1.516592 |
| 78 | 1 | 0 | 6.313935  | -2.760107 | 2.872621  |
| 79 | 1 | 0 | 5.312849  | -0.692788 | 3.792129  |
| 80 | 1 | 0 | 3.696725  | 0.603742  | 2.452764  |
| 81 | 1 | 0 | 3.249518  | -1.881831 | -1.684937 |
| 82 | 1 | 0 | 4.269231  | -3.911644 | -2.547176 |
| 83 | 1 | 0 | 5.918166  | -5.184796 | -1.183747 |
|    |  84 |  1 |  0 |       |       |       |
|----|-----|----|----|-------|-------|-------|

| Conformer |  1 |  6 |  0 |  -5.012330 |  -0.841672 |  0.554093 |
|-----------|----|----|----|------------|------------|----------|
| 7b (conformer 3) |  2 |  6 |  0 |  -6.056235  |  -0.055696  |  -0.243876 |
|            |  3 |  6 |  0 |  -5.179668  |  -0.548985  |  2.067925  |
|            |  4 |  6 |  0 |  -7.135155  |  0.516548   |  0.323292  |
|            |  5 |  6 |  0 |  -6.630802  |  -0.560455  |  2.554629  |
|            |  6 |  6 |  0 |  -7.503903  |  0.377152   |  1.741274  |
|            |  7 |  6 |  0 |  -3.574725  |  -0.372958  |  0.110134  |
|            |  8 |  6 |  0 |  -3.361360  |  -0.360395  |  -1.429067 |
|            |  9 |  6 |  0 |  -5.848379  |  0.031181   |  -1.734192 |
|            | 10 |  6 |  0 |  -4.435624  |  0.500400   |  -2.103756 |
|            | 11 |  6 |  0 |  -2.438785  |  -1.125268  |  0.840308  |
|            | 12 |  6 |  0 |  -1.030435  |  -0.634075  |  0.450640  |
|            | 13 |  6 |  0 |  -1.949398  |  0.156831   |  -1.728340 |
|            | 14 |  6 |  0 |  -0.818022  |  -0.671673  |  -1.070255 |
|            | 15 |  6 |  0 |  -1.492825  |  0.332338   |  -3.191180 |
|            | 16 |  6 |  0 |   0.056706  |  0.399241   |  -3.092717 |
|            | 17 |  6 |  0 |   0.408916  |  0.115492   |  -1.611384 |
|            | 18 |  8 |  0 |  1.657872   |  -0.568569  |  -1.540275 |
|            | 19 |  6 |  0 |  -0.748892  |  -2.128306  |  -1.570202 |
|            | 20 |  6 |  0 |  -5.234921  |  -2.353482  |  0.287733  |
|            | 21 |  8 |  0 |  -8.475474  |  0.939908   |  2.212950  |
|            | 22 |  1 |  0 |  -3.508858  |  0.680635   |  0.422369  |
|            | 23 |  1 |  0 |  -3.452536  |  -1.383493  |  -1.816830 |
|            | 24 |  1 |  0 |  -1.891942  |  1.155492   |  -1.266349 |
|            | 25 |  1 |  0 |  0.480692   |  1.063684   |  -1.067111 |
|            | 26 |  1 |  0 |  -4.755811  |  0.440461   |  2.275981  |
|            | 27 |  1 |  0 |  -4.596334  |  -1.267193  |  2.649022  |
|            | 28 |  1 |  0 |  -7.837023  |  1.087317   |  -0.278238 |
|            | 29 |  1 |  0 |  -6.706117  |  -0.276927  |  3.606554  |
|            | 30 |  1 |  0 |  -7.065176  |  -1.564396  |  2.468161  |
|            | 31 |  1 |  0 |  -6.604136  |  0.687115   |  -2.173302 |
|            | 32 |  1 |  0 |  -6.011331  |  -0.964549  |  -2.168733 |
|            | 33 |  1 |  0 |  -4.316850  |  0.477409   |  -3.190926 |
|            | 34 |  1 |  0 |  -4.307942  |  1.545414   |  -1.793593 |
|            | 35 |  1 |  0 |  -2.512195  |  -2.196837  |  0.634936  |
|            | 36 |  1 |  0 |  -2.555409  |  -1.014825  |  1.921221  |
|            | 37 |  1 |  0 |  -0.282869  |  -1.245725  |  0.968268  |
|            | 38 |  1 |  0 |  -0.901631  |  0.397277   |  0.802919  |
|            | 39 |  1 |  0 |  -1.915625  |  1.229252   |  -3.648130 |
|            | 40 |  1 |  0 |  -1.810754  |  -0.516267  |  -3.804332 |
|            | 41 |  1 |  0 |  0.456209   |  1.365485   |  -3.406173 |
|            | 42 |  1 |  0 |  0.536583   |  -0.358811  |  -3.714940 |
|            | 43 |  6 |  0 |  2.505910   |  -0.260519  |  -0.426578 |
|            | 44 |  1 |  0 |  -1.634765  |  -2.702485  |  -1.295060 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|45 | 1  | 0 | -0.644877 | -2.189403 | -2.655302 |
|46 | 1  | 0 | 0.122758  | -2.622673 | -1.136720 |
|47 | 1  | 0 | -4.560270 | -2.959544 |  0.895837 |
|48 | 1  | 0 | -5.069241 | -2.617850 | -0.758350 |
|49 | 1  | 0 | -6.258026 | -2.644043 |  0.537014 |
|50 | 6  | 0 |  3.117684 |  1.138750 | -0.596770 |
|51 | 6  | 0 |  3.562797 | -1.359695 | -0.336445 |
|52 | 6  | 0 |  3.753120 | -2.219089 | -1.396834 |
|53 | 6  | 0 |  4.723009 | -3.245742 | -1.351023 |
|54 | 6  | 0 |  5.495999 | -3.419032 | -0.233602 |
|55 | 6  | 0 |  5.331724 | -2.569043 |  0.890274 |
|56 | 6  | 0 |  4.356971 | -1.517975 |  0.846703 |
|57 | 6  | 0 |  6.114220 | -2.744265 |  2.061087 |
|58 | 6  | 0 |  5.954631 | -1.925975 |  3.151545 |
|59 | 6  | 0 |  4.999156 | -0.887728 |  3.113590 |
|60 | 6  | 0 |  4.225981 | -0.689319 |  1.994180 |
|61 | 6  | 0 |  2.763411 |  2.253600 |  0.231646 |
|62 | 6  | 0 |  3.364102 |  3.531595 | -0.036799 |
|63 | 6  | 0 |  4.275500 |  3.665098 | -1.112322 |
|64 | 6  | 0 |  4.587989 |  2.584486 | -1.898076 |
|65 | 6  | 0 |  4.007507 |  1.328767 | -1.634005 |
|66 | 6  | 0 |  1.846739 |  2.178797 |  1.319886 |
|67 | 6  | 0 |  1.546663 |  3.278488 |  2.087375 |
|68 | 6  | 0 |  2.144138 |  4.529458 |  1.817141 |
|69 | 6  | 0 |  3.030416 |  4.646642 |  0.777270 |
|70 | 1  | 0 |  1.913124 | -0.297993 |  0.490185 |
|71 | 1  | 0 |  3.133889 | -2.105987 | -2.275670 |
|72 | 1  | 0 |  4.844180 | -3.898901 | -2.208099 |
|73 | 1  | 0 |  6.239206 | -4.208200 | -0.188534 |
|74 | 1  | 0 |  6.846571 | -3.544897 |  2.077769 |
|75 | 1  | 0 |  6.559553 | -2.071883 |  4.039348 |
|76 | 1  | 0 |  4.877221 | -0.237576 |  3.972723 |
|77 | 1  | 0 |  3.515727 |  0.125460 |  1.992297 |
|78 | 1  | 0 |  4.721016 |  4.635906 | -1.302209 |
|79 | 1  | 0 |  5.285779 |  2.687966 | -2.721333 |
|80 | 1  | 0 |  4.272301 |  0.483703 | -2.258357 |
|81 | 1  | 0 |  1.365387 |  1.239311 |  1.556639 |
|82 | 1  | 0 |  0.844666 |  3.185108 |  2.908477 |
|83 | 1  | 0 |  1.899766 |  5.389364 |  2.430209 |
|84 | 1  | 0 |  3.494905 |  5.602268 |  0.557142 |

**7b (conformer 4)**

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1 | 6  | 0 | -5.421494 | -0.848070 |  0.047214 |
| 2 | 6  | 0 | -6.280173 |  0.412717 | -0.093880 |
| 3 | 6  | 0 | -5.870100 | -1.585375 |  1.361752 |
| 4 | 6  | 0 | -7.390280 |  0.629051 |  0.636919 |
| 5 | 6  | 0 | -7.291002 | -1.697340 |  1.623108 |
|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 6 | 6 | 0  | -7.972485 | -0.342129 | 1.576933 |
| 7 | 6 | 0  | -3.903706  | -0.425984 | 0.112949 |
| 8 | 6 | 0  | -3.475406  | 0.548084  | -1.021092|
| 9 | 6 | 0  | -5.852092  | 1.417680  | -1.132831|
|10 | 6 | 0  | -4.369975  | 1.792276  | -1.012550|
|11 | 6 | 0  | -2.942072  | -1.631238 | 0.243122 |
|12 | 6 | 0  | -1.457540  | 0.548084  | -1.021092|
|13 | 6 | 0  | -1.997729  | 0.909634  | -0.834205|
|14 | 6 | 0  | -1.051949  | -0.313432 | -0.827897|
|15 | 6 | 0  | -1.321762  | 1.905359  | -1.798348|
|16 | 6 | 0  | -1.053108  | -1.098482 | -2.156160|
|17 | 6 | 0  | -1.053108  | -1.098482 | -2.156160|
|18 | 6 | 0  | -5.712176  | -1.768431 | -1.167245|
|19 | 6 | 0  | -8.964944  | -0.086482 | 2.234923 |
|20 | 6 | 0  | -3.808341  | 0.153123  | 1.044336 |
|21 | 6 | 0  | -3.595498  | 0.052461  | -1.993114|
|22 | 6 | 0  | -1.920393  | 1.351030  | 0.172320 |
|23 | 6 | 0  | 0.383575   | 0.743966  | 0.381708 |
|24 | 6 | 0  | -5.332290  | -1.042210 | 2.198395 |
|25 | 6 | 0  | -5.343189  | -2.583725 | 1.359377 |
|26 | 6 | 0  | -7.956261  | 1.549092  | 0.521173 |
|27 | 6 | 0  | -7.773751  | -2.329200 | 0.867055 |
|28 | 6 | 0  | -6.486116  | 2.305442  | -1.068517|
|29 | 6 | 0  | -6.023345  | 0.985661  | -2.128261|
|30 | 6 | 0  | -4.096092  | 2.465150  | -1.830425|
|31 | 6 | 0  | -4.209055  | 2.346369  | -0.078985|
|32 | 6 | 0  | -3.074405  | -2.306673 | -0.606618|
|33 | 6 | 0  | -3.198190  | -2.211879 | 1.132692 |
|34 | 6 | 0  | -0.830487  | -2.122834 | 0.367081 |
|35 | 6 | 0  | -1.290448  | -0.691235 | 1.281145 |
|36 | 6 | 0  | -1.595789  | 2.939569  | -1.580812|
|37 | 6 | 0  | -1.619916  | 1.708233  | -2.832703|
|38 | 6 | 0  | 0.713259   | 2.511221  | -1.175608|
|39 | 6 | 0  | 0.698271   | 1.412447  | -2.541120|
|40 | 6 | 0  | 2.573039   | -0.318153 | -0.144499|
|41 | 6 | 0  | -2.025650  | -1.543788 | -2.369249|
|42 | 6 | 0  | -0.786188  | -0.471180 | -3.008875|
|43 | 6 | 0  | -0.318718  | -1.903756 | -2.101377|
|44 | 6 | 0  | -5.177106  | -2.715954 | -1.077085|
|45 | 6 | 0  | -5.418810  | -1.308264 | -2.112557|
|46 | 6 | 0  | -6.778655  | -1.994510 | -1.233986|
|47 | 6 | 0  | 3.304959   | 0.998918  | -0.439228|
|    |   |   |         |         |         |         |         |         |         |
|----|---|---|--------|--------|--------|--------|--------|--------|--------|
| 51 | 6 | 0 | 3.443829 | -1.547130 | -0.390166 |
| 52 | 6 | 0 | 3.200940 | -2.358235 | -1.476962 |
| 53 | 6 | 0 | 3.984162 | -3.049412 | 0.250488 |
| 54 | 6 | 0 | 5.007735 | -3.847292 | -0.887137 |
| 55 | 6 | 0 | 5.294589 | -2.623559 | 2.241701 |
| 56 | 6 | 0 | 5.858210 | -1.466150 | 2.499248 |
| 57 | 6 | 0 | 4.833487 | -1.103693 | 1.657376 |
| 58 | 6 | 0 | 3.271042 | 2.120105 | 0.454192 |
| 59 | 6 | 0 | 3.929132 | 3.335928 | 0.060736 |
| 60 | 6 | 0 | 4.586685 | 3.402968 | -1.192307 |
| 61 | 6 | 0 | 4.605391 | 2.315019 | -2.027526 |
| 62 | 6 | 0 | 3.966431 | 1.119464 | -1.643605 |
| 63 | 6 | 0 | 2.626022 | 2.109298 | 1.724421 |
| 64 | 6 | 0 | 2.627489 | 3.21628 | 2.543998 |
| 65 | 6 | 0 | 3.762754 | 4.118071 | -2.598935 |
| 66 | 6 | 0 | 5.610592 | 4.730189 | -1.072223 |
| 67 | 6 | 0 | 6.928413 | 4.284332 | 0.931077 |
| 68 | 6 | 0 | 7.430083 | 2.89702 | 2.912694 |
| 69 | 6 | 0 | 6.082460 | -0.855259 | 3.366547 |
| 70 | 1 | 0 | 4.277179 | -0.202121 | 1.875134 |
| 71 | 1 | 0 | 5.078158 | 4.327769 | -1.475495 |
| 72 | 1 | 0 | 5.114125 | 2.365741 | -2.983576 |
| 73 | 1 | 0 | 3.999889 | 0.266826 | -2.311151 |
| 74 | 1 | 0 | 2.118626 | 1.216952 | 2.065821 |
| 75 | 1 | 0 | 2.127132 | 3.168357 | 3.504914 |
| 76 | 1 | 0 | 3.269769 | 5.266207 | 2.802901 |
| 77 | 1 | 0 | 4.412669 | 5.364516 | 0.615495 |

**7b (conformer 5)**

|    |   |   |         |         |         |         |         |         |         |
|----|---|---|--------|--------|--------|--------|--------|--------|--------|
| 1  | 6 | 0 | -5.373780 | -0.184741 | 0.688116 |
| 2  | 6 | 0 | -6.268688 | -0.654418 | -0.461557 |
| 3  | 6 | 0 | -5.779134 | 1.250147 | 1.116171 |
| 4  | 6 | 0 | -7.419119 | -0.038825 | -0.794257 |
| 5  | 6 | 0 | -7.289588 | 1.468623 | 1.231472 |
| 6  | 6 | 0 | -8.012409 | 1.080605 | -0.045003 |
| 7  | 6 | 0 | -3.879482 | -0.153017 | 0.187800 |
| 8  | 6 | 0 | -3.421357 | -1.464878 | -0.510642 |
| 9  | 6 | 0 | -5.825118 | -1.885696 | -1.210322 |
| 10 | 6 | 0 | -4.365476 | -1.798108 | -1.673525 |
| 11 | 6 | 0 | -2.882111 | 0.304827 | 1.277772 |
|   |   |   |            |            |            |            |
|---|---|---|------------|------------|------------|------------|
| 12| 6 | 0 | -1.424776  | 0.379270   | 0.782300   |
| 13| 6 | 0 | -1.975446  | -1.293971  | -0.984616  |
| 14| 6 | 0 | -0.980581  | -0.945328  | 0.148303   |
| 15| 6 | 0 | -1.279842  | -2.430520  | -1.760462  |
| 16| 6 | 0 | 0.235035   | -2.084590  | -1.653097  |
| 17| 6 | 0 | 0.322359   | -0.874697  | -0.676157  |
| 18| 8 | 0 | 1.466780   | -0.880342  | 0.171349   |
| 19| 6 | 0 | -0.863450  | -2.048976  | 1.220447   |
| 20| 6 | 0 | -5.566455  | -1.157825  | 1.880401   |
| 21| 8 | 0 | -9.042612  | 1.621873   | -0.404022  |
| 22| 1 | 0 | -3.859062  | 0.616512   | -0.598764  |
| 23| 1 | 0 | -3.462899  | -2.294141  | 0.207411   |
| 24| 1 | 0 | -1.978995  | -0.419613  | -1.654261  |
| 25| 1 | 0 | 0.308881   | 0.060245   | -1.249506  |
| 26| 1 | 0 | -5.385128  | 1.954662   | 0.374475   |
| 27| 1 | 0 | -5.302447  | 1.498471   | 2.067286   |
| 28| 1 | 0 | -8.010239  | -0.391285  | -1.634945  |
| 29| 1 | 0 | -7.530728  | 2.508301   | 1.462749   |
| 30| 1 | 0 | -7.711809  | 0.860426   | 2.041178   |
| 31| 1 | 0 | -6.493407  | -2.060763  | -2.056957  |
| 32| 1 | 0 | -5.930168  | -2.754755  | -0.546624  |
| 33| 1 | 0 | -4.074794  | -2.742722  | -2.142623  |
| 34| 1 | 0 | -4.275774  | -1.021261  | -2.443625  |
| 35| 1 | 0 | -2.935649  | -0.368752  | 2.137720   |
| 36| 1 | 0 | -3.170289  | 1.291390   | 1.648605   |
| 37| 1 | 0 | -0.766114  | 0.657069   | 1.610935   |
| 38| 1 | 0 | -1.337839  | 1.177634   | 0.035029   |
| 39| 1 | 0 | -1.615305  | -2.488359  | -2.797767  |
| 40| 1 | 0 | -1.490850  | -3.402064  | -1.303719  |
| 41| 1 | 0 | 0.661306   | -1.843384  | -2.629337  |
| 42| 1 | 0 | 0.811265   | -2.919530  | -1.246925  |
| 43| 6 | 0 | 2.716654   | -0.591152  | -0.464089  |
| 44| 1 | 0 | -1.807681  | -2.217753  | 1.740129   |
| 45| 1 | 0 | -0.543563  | -3.004740  | 0.801007   |
| 46| 1 | 0 | -0.120041  | -1.757374  | 1.964244   |
| 47| 1 | 0 | -4.993036  | -0.828914  | 2.749397   |
| 48| 1 | 0 | -5.252048  | -2.174439  | 1.638011   |
| 49| 1 | 0 | -6.617716  | -1.204378  | 2.174042   |
| 50| 6 | 0 | 3.837951   | -1.011478  | 0.494776   |
| 51| 6 | 0 | 2.757135   | 0.858264   | -0.969300  |
| 52| 6 | 0 | 2.814913   | 1.061358   | -2.333129  |
| 53| 6 | 0 | 2.848159   | 2.352060   | -2.904174  |
| 54| 6 | 0 | 2.815656   | 3.455408   | -2.093071  |
| 55| 6 | 0 | 2.726367   | 3.311097   | -0.684544  |
| 56| 6 | 0 | 2.681925   | 1.999403   | -0.103472  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 57 | 6 | 0 | 2.667444  | 4.450720  | 0.159686 |
| 58 | 6 | 0 | 2.554840  | 4.318274  | 1.520610 |
| 59 | 6 | 0 | 2.490035  | 3.030456  | 2.095877 |
| 60 | 6 | 0 | 2.549618  | 1.905358  | 1.308597 |
| 61 | 6 | 0 | 5.212423  | -1.020546 | 0.079904 |
| 62 | 6 | 0 | 6.215415  | -1.439519 | 1.017854 |
| 63 | 6 | 0 | 5.833276  | -1.850428 | 2.319843 |
| 64 | 6 | 0 | 4.511876  | -1.866335 | 2.678028 |
| 65 | 6 | 0 | 5.20680   | -1.452796 | 0.623943 |
| 66 | 6 | 0 | 6.215415  | -1.439519 | 1.017854 |
| 67 | 6 | 0 | 5.833276  | -1.850428 | 2.319843 |
| 68 | 6 | 0 | 4.511876  | -1.866335 | 2.678028 |
| 69 | 6 | 0 | 5.20680   | -1.452796 | 0.623943 |
| 70 | 1 | 0 | 2.810070  | -1.227438 | -1.354797 |
| 71 | 1 | 0 | 2.845138  | 0.200154  | -2.994002 |
| 72 | 1 | 0 | 2.901126  | 2.460421  | -3.981545 |
| 73 | 1 | 0 | 2.847578  | 4.454450  | -2.514919 |
| 74 | 1 | 0 | 2.708832  | 5.434643  | -0.295892 |
| 75 | 1 | 0 | 2.510228  | 5.196769  | 2.154457 |
| 76 | 1 | 0 | 2.391604  | 2.928156  | 3.170911 |
| 77 | 1 | 0 | 2.487063  | 0.931565  | 1.767732 |
| 78 | 1 | 0 | 6.603334  | -2.161826 | 3.017782 |
| 79 | 1 | 0 | 4.214816  | -2.196072 | 3.667413 |
| 80 | 1 | 0 | 2.481392  | -1.483704 | 2.055600 |
| 81 | 1 | 0 | 4.924461  | -0.345828 | -1.962278 |
| 82 | 1 | 0 | 7.271280  | -0.418001 | -2.582983 |
| 83 | 1 | 0 | 9.002467  | -1.108812 | -0.931173 |
| 84 | 1 | 0 | 8.321592  | -1.766789 | 1.350565 |

**7b (conformer 6)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 1  | 6 | 0 | 5.141065  | 0.519786  | 0.101361 |
| 2  | 6 | 0 | 6.102530  | -0.669021 | 0.022916 |
| 3  | 6 | 0 | 5.353786  | 1.278533  | 1.437472 |
| 4  | 6 | 0 | 7.169045  | -0.804037 | 0.833728 |
| 5  | 6 | 0 | 6.822279  | 1.504673  | 1.804915 |
| 6  | 6 | 0 | 7.605279  | 0.204710  | 1.812690 |
| 7  | 6 | 0 | 3.661465  | -0.021142 | 0.062787 |
| 8  | 6 | 0 | 3.386593  | -1.014417 | -1.100645 |
| 9  | 6 | 0 | 5.829589  | -1.696091 | -1.046564 |
| 10 | 6 | 0 | 4.375624  | -2.184677 | -1.036872 |
| 11 | 6 | 0 | 2.603056  | 1.103150  | 0.129175 |
| 12 | 6 | 0 | 1.151572  | 0.583951  | 0.124511 |
| 13 | 6 | 0 | 1.932943  | -1.493150 | -1.011560 |
| 14 | 6 | 0 | 0.889521  | -0.351350 | -1.063256 |
| 15 | 6 | 0 | 1.407288  | -2.534555 | -2.020299 |
| 16 | 6 | 0 | -0.138585 | -2.395662 | -1.929473 |
| 17 | 6 | 0 | -0.412227 | -1.193262 | -0.986317 |
|   |   |   | 18          8          0        -1.594513   0.486304   -1.376002  |
|---|---|---|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| 19| 6 | 0 | 0.902992              | 0.439544               | -2.386934              |                          |                          |                          |                          |
| 20| 6 | 0 | 5.441617              | 1.465778               | -1.090628              |                          |                          |                          |                          |
| 21| 8 | 0 | 8.562392              | 0.022029               | 2.543234               |                          |                          |                          |                          |
| 22| 1 | 0 | 3.549966              | -0.614026              | 0.983520               |                          |                          |                          |                          |
| 23| 1 | 0 | 3.528616              | -0.501117              | -2.060436              |                          |                          |                          |                          |
| 24| 1 | 0 | 1.826281              | -1.948307              | -0.013727              |                          |                          |                          |                          |
| 25| 1 | 0 | -0.534507             | -1.554307              | 0.042362               |                          |                          |                          |                          |
| 26| 1 | 0 | 4.884364              | 0.698399               | 2.240576               |                          |                          |                          |                          |
| 27| 1 | 0 | 4.835613              | 2.239814               | 1.402075               |                          |                          |                          |                          |
| 28| 1 | 0 | 7.810683              | -1.677666              | 0.760105               |                          |                          |                          |                          |
| 29| 1 | 0 | 6.925556              | 1.975902               | 2.784653               |                          |                          |                          |                          |
| 30| 1 | 0 | 7.308165              | 2.172178               | 1.082297               |                          |                          |                          |                          |
| 31| 1 | 0 | 6.523222              | -2.533330              | -0.937090              |                          |                          |                          |                          |
| 32| 1 | 0 | 6.040286              | -1.243946              | -2.025283              |                          |                          |                          |                          |
| 33| 1 | 0 | 4.215275              | -2.867219              | -1.876617              |                          |                          |                          |                          |
| 34| 1 | 0 | 4.192217              | -2.761395              | -0.121301              |                          |                          |                          |                          |
| 35| 1 | 0 | 2.736842              | 1.790755               | -0.710343              |                          |                          |                          |                          |
| 36| 1 | 0 | 2.753637              | 1.697635               | 1.033612               |                          |                          |                          |                          |
| 37| 1 | 0 | 0.466295              | 1.437342               | 0.108577               |                          |                          |                          |                          |
| 38| 1 | 0 | 0.963500              | 0.036716               | 1.058006               |                          |                          |                          |                          |
| 39| 1 | 0 | 1.744109              | -3.545054              | -1.780566              |                          |                          |                          |                          |
| 40| 1 | 0 | 1.761546              | -2.312995              | -3.031565              |                          |                          |                          |                          |
| 41| 1 | 0 | -0.615791             | -3.302924              | -1.555538              |                          |                          |                          |                          |
| 42| 1 | 0 | -0.580221             | -2.177805              | -2.904243              |                          |                          |                          |                          |
| 43| 6 | 0 | -2.548767             | -0.204609              | -0.343821              |                          |                          |                          |                          |
| 44| 1 | 0 | 1.828878              | 1.000115               | -2.522350              |                          |                          |                          |                          |
| 45| 1 | 0 | 0.782888              | -0.207307              | -3.258199              |                          |                          |                          |                          |
| 46| 1 | 0 | 0.071810              | 1.146594               | -2.394676              |                          |                          |                          |                          |
| 47| 1 | 0 | 4.835745              | 2.372424               | -1.033310              |                          |                          |                          |                          |
| 48| 1 | 0 | 5.242143              | 0.992038               | -2.053451              |                          |                          |                          |                          |
| 49| 1 | 0 | 6.491353              | 1.767773               | -1.088925              |                          |                          |                          |                          |
| 50| 6 | 0 | -3.449755             | -1.407755              | -0.051539              |                          |                          |                          |                          |
| 51| 6 | 0 | -3.331639             | 1.026981               | -0.799170              |                          |                          |                          |                          |
| 52| 6 | 0 | -4.258539             | 0.880364               | -1.809133              |                          |                          |                          |                          |
| 53| 6 | 0 | -4.973895             | 1.977742               | -2.329705              |                          |                          |                          |                          |
| 54| 6 | 0 | -4.767583             | 3.235004               | -1.823508              |                          |                          |                          |                          |
| 55| 6 | 0 | -3.833759             | 3.444500               | -0.778584              |                          |                          |                          |                          |
| 56| 6 | 0 | -3.091907             | 2.331476               | -0.254434              |                          |                          |                          |                          |
| 57| 6 | 0 | -3.619660             | 4.742359               | -0.244115              |                          |                          |                          |                          |
| 58| 6 | 0 | -2.717267             | 4.956472               | 0.766558               |                          |                          |                          |                          |
| 59| 6 | 0 | -1.983851             | 3.868809               | 1.288475               |                          |                          |                          |                          |
| 60| 6 | 0 | -2.160007             | 2.599682               | 0.792841               |                          |                          |                          |                          |
| 61| 6 | 0 | -4.180117             | -1.495635              | 1.179179               |                          |                          |                          |                          |
| 62| 6 | 0 | -4.990459             | -2.653341              | 1.422970               |                          |                          |                          |                          |
|    |   |   |   |   |   |   |
|----|---|---|---|---|---|---|
| 63 |  6 |   0 | -5.069323 | -3.672050 |  0.438247 |
| 64 |  6 |   0 | -4.375677 | -3.554853 | -0.737474 |
| 65 |  6 |   0 | -3.563471 | -2.423113 | -0.975371 |
| 66 |  6 |   0 | -4.147629 | -0.486047 |  2.179744 |
| 67 |  6 |   0 | -4.853965 | -0.618101 |  3.351931 |
| 68 |  6 |   0 | -5.638367 | -1.766756 |  3.592373 |
| 69 |  6 |   0 | -5.704077 | -2.758076 |  2.645041 |
| 70 |  1 |   0 | -2.004629 |  0.027572 |  0.573793 |
| 71 |  1 |   0 | -4.446765 | -1.067022 | -2.213055 |
| 72 |  1 |   0 | -5.690231 |  1.817618 | -3.127532 |
| 73 |  1 |   0 | -5.317032 |  4.086309 | -2.211377 |
| 74 |  1 |   0 | -4.190422 |  5.569002 | -0.654410 |
| 75 |  1 |   0 | -2.563590 |  5.952899 |  1.165498 |
| 76 |  1 |   0 | -1.270444 |  4.036081 |  2.087755 |
| 77 |  1 |   0 | -1.582457 |  1.793424 |  1.216204 |
| 78 |  1 |   0 | -5.688650 | -4.541261 |  0.633134 |
| 79 |  1 |   0 | -4.439306 | -4.331650 | -1.491430 |
| 80 |  1 |   0 | -3.008607 | -2.348765 |  4.095873 |
| 81 |  1 |   0 | -3.573290 |  0.416074 |  2.018593 |
| 82 |  1 |   0 | -4.812921 |  1.695865 |  4.095873 |
| 83 |  1 |   0 | -6.190254 | -1.859296 |  4.520930 |
| 84 |  1 |   0 | -6.310045 | -3.641865 |  2.816115 |

**7b (conformer 7)**

|    |   |   |   |   |   |   |
|----|---|---|---|---|---|---|
|  1 |  6 |   0 |  5.023868 | -0.615512 | -0.684855 |
|  2 |  6 |   0 |  5.948323 | -0.556135 |  0.534434 |
|  3 |  6 |   0 |  5.496308 |  0.406909 | -1.751742 |
|  4 |  6 |   0 |  7.152668 |  0.045594 |  0.512521 |
|  5 |  6 |   0 |  7.009034 |  0.417530 | -1.984563 |
|  6 |  6 |   0 |  7.774642 |  0.622398 | -0.690276 |
|  7 |  6 |   0 |  3.563989 | -0.228403 | -0.234194 |
|  8 |  6 |   0 |  3.064198 | -1.009259 |  1.013639 |
|  9 |  6 |   0 |  5.467742 | -1.243041 |  1.787505 |
| 10 |  6 |   0 |  4.044628 | -0.825246 |  2.177922 |
| 11 |  6 |   0 |  2.539219 | -0.264643 | -1.392292 |
| 12 |  6 |   0 |  1.115703 |  0.148133 | -0.969530 |
| 13 |  6 |   0 |  1.657663 | -0.516925 |  1.373079 |
| 14 |  6 |   0 |  0.626653 | -0.674820 |  0.229723 |
| 15 |  6 |   0 |  0.939333 | -1.086154 |  2.613004 |
| 16 |  6 |   0 | -0.562515 | -0.748577 |  2.371799 |
| 17 |  6 |   0 | -0.626245 | -1.241977 |  0.946993 |
| 18 |  8 |   0 | -1.805759 | -0.409036 |  0.195334 |
| 19 |  6 |   0 |  0.385918 | -2.141750 | -0.182993 |
| 20 |  6 |   0 |  5.088682 | -2.049372 | -1.272781 |
| 21 |  8 |   0 |  8.855736 |  1.181793 | -0.651217 |
| 22 |  1 |   0 |  3.634084 |  0.821277 |  0.089686 |
| 23 |  1 |   0 |  3.012991 | -2.080337 |  0.778598 |

S346
|   |  |  | X   | Y   | Z   |
|---|---|---|----|----|----|
| 24| 1 | 0 | 1.752507 | 0.567500 | 1.539331 |
| 25| 1 | 0 | -0.517907 | 0.964240 | 1.033171 |
| 26| 1 | 0 | 5.191513  | -1.426800 | 2.697467 |
| 27| 1 | 0 | 4.983759  | 0.964240  | 1.033171 |
| 28| 1 | 0 | 2.506964  | -1.267374 | 1.827422 |
| 29| 1 | 0 | 7.345217  | -0.535048 | 2.417943 |
| 30| 1 | 0 | 6.168557  | -1.051163 | 2.603772 |
| 31| 1 | 0 | 5.479149  | -2.328175 | 1.616865 |
| 32| 1 | 0 | 3.720161  | -1.405440 | 3.046851 |
| 33| 1 | 0 | 4.047008  | 0.228747  | 2.484027 |
| 34| 1 | 0 | 2.506964  | -1.267374 | 1.827422 |
| 35| 1 | 0 | 0.435587  | 0.038968  | -1.820037|
| 36| 1 | 0 | 1.272876  | -2.591688 | -0.630415|
| 37| 1 | 0 | 1.110171  | 1.210818  | -0.698669|
| 38| 1 | 0 | 1.312073  | -0.649857 | 3.541707 |
| 39| 1 | 0 | 1.087526  | -2.167488 | 2.688832 |
| 40| 1 | 0 | -0.949198 | -0.058812 | 3.124559 |
| 41| 1 | 0 | -1.177754 | -1.650347 | 2.417943 |
| 42| 1 | 0 | -3.044559 | 0.075130  | 0.743646 |
| 43| 1 | 0 | -0.422530 | -2.186805 | -0.914050|
| 44| 1 | 0 | 4.493426  | -2.124559 | -2.185066|
| 45| 1 | 0 | 4.720905  | -2.800617 | -0.571649|
| 46| 1 | 0 | 6.117570  | -2.316519 | 1.524387 |
| 47| 1 | 0 | -4.180075 | -0.454842 | -0.136748|
| 48| 1 | 0 | -3.053644 | 1.584600  | 0.982509 |
| 49| 1 | 0 | -3.482230 | 2.030003  | 2.215491 |
| 50| 1 | 0 | -3.541266 | 3.402876  | 2.538736 |
| 51| 1 | 0 | -3.151108 | 4.338723  | 1.616736 |
| 52| 1 | 0 | -2.694394 | 3.940149  | 0.333949 |
| 53| 1 | 0 | -2.642152 | 2.545807  | -0.000478|
| 54| 1 | 0 | -2.945040 | 4.902580  | -0.630299|
| 55| 1 | 0 | -1.865344 | 4.519645  | -1.876047|
| 56| 1 | 0 | -1.816831 | 3.148380  | -2.211640|
| 57| 1 | 0 | -2.192132 | 2.188221  | -1.302367|
| 58| 1 | 0 | -4.385917 | -1.871708 | -0.263181|
| 59| 1 | 0 | -5.482544 | -2.347283 | -1.055392|
| 60| 1 | 0 | -6.339429 | -1.416263 | -1.696523|
| 61| 1 | 0 | -6.133103 | -0.071108 | -1.548631|
| 62| 1 | 0 | -5.058139 | 0.402422  | -0.763580 |
| 63| 1 | 0 | -3.569183 | -2.841521 | 0.379162 |
| 64| 1 | 0 | -3.817646 | -4.187552 | 0.250498 |
| 65| 1 | 0 | -4.893752 | -4.648897 | -0.537898|
|    |   |   |   |   |   |
|----|---|---|---|---|---|
| 69 | 6 | 0 | -5.704078 | -3.744009 | -1.176373 |
| 70 | 1 | 0 | -3.176170 | -0.383194 | 1.733512 |
| 71 | 1 | 0 | -3.788600 | 1.302868 | 2.960813 |
| 72 | 1 | 0 | -3.889698 | 3.707521 | 3.519052 |
| 73 | 1 | 0 | -3.185264 | 5.396987 | 1.853488 |
| 74 | 1 | 0 | -2.338264 | 5.953096 | -0.362165 |
| 75 | 1 | 0 | -1.564851 | 5.264869 | -2.603986 |
| 76 | 1 | 0 | -1.479756 | 2.850160 | -3.198157 |
| 77 | 1 | 0 | -3.185264 | 5.396987 | 1.853488 |
| 78 | 1 | 0 | -2.338264 | 5.953096 | -0.362165 |
| 79 | 1 | 0 | -1.564851 | 5.264869 | -2.603986 |
| 80 | 1 | 0 | -1.479756 | 2.850160 | -3.198157 |
| 81 | 1 | 0 | -3.185264 | 5.396987 | 1.853488 |
| 82 | 1 | 0 | -2.338264 | 5.953096 | -0.362165 |
| 83 | 1 | 0 | -1.564851 | 5.264869 | -2.603986 |
| 84 | 1 | 0 | -6.536409 | -4.084031 | -1.783987 |

| 7b (conformer 9) |
|------------------|
| 1 | 6 | 0 | -5.481185 | -0.332663 | 0.543078 |
| 2 | 6 | 0 | -6.372241 | -0.065501 | 0.673073 |
| 3 | 6 | 0 | -5.912941 | 0.581096 | 1.719856 |
| 4 | 6 | 0 | -7.539252 | 0.601522 | -0.594419 |
| 5 | 6 | 0 | -7.426759 | 0.661169 | 1.931320 |
| 6 | 6 | 0 | -8.151792 | 1.065438 | 0.660870 |
| 7 | 6 | 0 | -3.988993 | 0.009024 | 0.166821 |
| 8 | 6 | 0 | -3.511667 | -0.634841 | -1.164528 |
| 9 | 6 | 0 | -5.906112 | -0.621427 | -1.994241 |
| 10 | 6 | 0 | -4.453170 | -0.244562 | -2.309471 |
| 11 | 6 | 0 | -2.996363 | -0.253355 | 1.322962 |
| 12 | 6 | 0 | -1.539477 | 0.115794 | 0.979853 |
| 13 | 6 | 0 | -2.069371 | -0.192296 | -1.438339 |
| 14 | 6 | 0 | -1.073647 | -0.567385 | -0.313792 |
| 15 | 6 | 0 | -1.362906 | -0.641455 | -2.731776 |
| 16 | 6 | 0 | 0.146690 | -0.404602 | -2.435692 |
| 17 | 6 | 0 | 0.229226 | -0.009895 | -0.929421 |
| 18 | 8 | 0 | 1.374078 | -0.521080 | -0.250051 |
| 19 | 6 | 0 | -0.931951 | -2.089660 | -0.102810 |
| 20 | 6 | 0 | -5.650130 | -1.820712 | 0.947870 |
| 21 | 8 | 0 | -9.197583 | 1.689270 | 0.675175 |
| 22 | 1 | 0 | -3.982615 | 1.094342 | -0.015849 |
| 23 | 1 | 0 | -3.531684 | -1.728237 | -1.068296 |
| 24 | 1 | 0 | -2.090330 | 0.908903 | -1.462638 |
| 25 | 1 | 0 | 0.215948 | 1.084701 | -0.833810 |
| 26 | 1 | 0 | -5.538509 | 1.592857 | 1.525054 |
| 27 | 1 | 0 | -5.435121 | 0.243396 | 2.642562 |
| 28 | 1 | 0 | -8.128720 | 0.788839 | -1.487522 |
| 29 | 1 | 0 | -7.687417 | 1.371541 | 2.718708 |
|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 30 | 1 | 0 | -7.830160 | -0.311432 | 2.239542 |
| 31 | 1 | 0 | -6.576856 | -0.289521 | -2.790540 |
| 32 | 1 | 0 | -5.983384 | -1.716621 | -1.959238 |
| 33 | 1 | 0 | -4.144842 | -0.729858 | -2.479692 |
| 34 | 1 | 0 | -4.387360 | 0.837698 | -2.479692 |
| 35 | 1 | 0 | -3.038221 | -1.306096 | 0.857769 |
| 36 | 1 | 0 | -1.702827 | -0.080861 | -3.604649 |
| 37 | 1 | 0 | -1.558989 | -1.698261 | -2.935577 |
| 38 | 1 | 0 | 0.561576 | -0.374783 | -3.078358 |
| 39 | 1 | 0 | 0.736119 | -1.309173 | -2.600444 |
| 40 | 1 | 0 | 2.626964 | 0.062969 | -0.627207 |
| 41 | 1 | 0 | -1.865004 | -2.545032 | 0.231731 |
| 42 | 1 | 0 | -0.622441 | -2.607506 | -1.012497 |
| 43 | 1 | 0 | -1.680666 | -2.285631 | 0.650933 |
| 44 | 1 | 0 | -5.095277 | -2.043387 | 1.861540 |
| 45 | 1 | 0 | -5.299295 | -2.501566 | 0.170326 |
| 46 | 1 | 0 | -6.701208 | -2.053164 | 1.135853 |
| 47 | 1 | 0 | 3.675681 | -1.053268 | -0.640179 |
| 48 | 1 | 0 | 2.955657 | 1.301076 | 0.227160 |
| 49 | 1 | 0 | 2.201598 | 1.578853 | 1.346232 |
| 50 | 6 | 0 | 2.441625 | 2.715391 | 2.148929 |
| 51 | 6 | 0 | 3.442054 | 3.591212 | 1.821248 |
| 52 | 6 | 0 | 4.235279 | 3.370893 | 0.666643 |
| 53 | 6 | 0 | 3.995085 | 2.216108 | -0.151503 |
| 54 | 6 | 0 | 5.256579 | 4.286010 | 0.301036 |
| 55 | 6 | 0 | 6.013111 | 4.093042 | -0.827480 |
| 56 | 6 | 0 | 5.775759 | 2.965836 | -1.642627 |
| 57 | 6 | 0 | 4.799715 | 2.055764 | -1.312462 |
| 58 | 6 | 0 | 4.055416 | -1.800750 | 0.523191 |
| 59 | 6 | 0 | 5.060091 | -2.817602 | 0.393357 |
| 60 | 6 | 0 | 5.636484 | -3.081026 | -0.875549 |
| 61 | 6 | 0 | 5.229122 | -2.382743 | -1.981057 |
| 62 | 6 | 0 | 4.247241 | -1.376788 | -1.853464 |
| 63 | 6 | 0 | 3.471939 | -1.609242 | 1.804374 |
| 64 | 6 | 0 | 3.870028 | -2.351767 | 2.890020 |
| 65 | 6 | 0 | 4.875909 | -3.334147 | 2.761472 |
| 66 | 6 | 0 | 5.452613 | -3.560653 | 1.537410 |
| 67 | 6 | 0 | 2.550215 | 0.407449 | -1.664100 |
| 68 | 6 | 0 | 1.398445 | 0.905134 | 1.612198 |
| 69 | 6 | 0 | 1.825888 | 2.887090 | 3.024804 |
| 70 | 6 | 0 | 3.636322 | 4.467318 | 2.430888 |
| 71 | 6 | 0 | 5.425510 | 5.150504 | 0.934790 |
| 72 | 6 | 0 | 5.425510 | 5.150504 | 0.934790 |
| 73 | 6 | 0 | 5.425510 | 5.150504 | 0.934790 |
| 74 | 6 | 0 | 5.425510 | 5.150504 | 0.934790 |
|   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 75 | 1 | 0 | 6.788993 | 4.801258 | -1.095361 |
| 76 | 1 | 0 | 6.372100 | 2.813798 | -2.535395 |
| 77 | 1 | 0 | 4.655557 | 1.195327 | -1.948170 |
| 78 | 1 | 0 | 6.395361 | -3.852268 | -0.955260 |
| 79 | 1 | 0 | 5.655203 | -2.593935 | -2.955296 |
| 80 | 1 | 0 | 3.936952 | -0.841171 | -2.745194 |
| 81 | 1 | 0 | 2.690025 | -0.876589 | 1.920894 |
| 82 | 1 | 0 | 3.405116 | -2.183564 | 3.855152 |
| 83 | 1 | 0 | 5.183509 | -3.910238 | 3.626960 |
| 84 | 1 | 0 | 6.218140 | -4.321016 | 1.422180 |

7b (conformer 11)

|   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 6 | 0 | -5.543676 | -0.624326 | 0.687745 |
| 2 | 6 | 0 | -6.275700 | -0.551460 | -0.650339 |
| 3 | 6 | 0 | -6.207153 | 0.341489 | 1.702523 |
| 4 | 6 | 0 | -7.176613 | 0.404017 | -0.948424 |
| 5 | 6 | 0 | -6.582111 | 1.709434 | 1.132159 |
| 6 | 6 | 0 | -7.475995 | 1.561273 | -0.087430 |
| 7 | 6 | 0 | -4.040473 | -0.263328 | 0.372870 |
| 8 | 6 | 0 | -3.441736 | -1.180634 | -0.738308 |
| 9 | 6 | 0 | -5.792917 | -1.510473 | -1.703060 |
| 10 | 6 | 0 | -4.313168 | -1.184666 | -2.004646 |
| 11 | 6 | 0 | -3.127393 | -0.211554 | 1.617380 |
| 12 | 6 | 0 | -1.667875 | 0.161669 | 1.284119 |
| 13 | 6 | 0 | -2.010096 | -0.716154 | -1.030498 |
| 14 | 6 | 0 | -1.079076 | -0.758474 | 0.205802 |
| 15 | 6 | 0 | -1.190275 | -1.398230 | -2.144059 |
| 16 | 6 | 0 | 0.284893 | -1.028347 | -1.807936 |
| 17 | 6 | 0 | 0.230820 | -0.266366 | -0.451327 |
| 18 | 8 | 0 | 1.345346 | -0.492789 | 0.410572 |
| 19 | 6 | 0 | -0.865067 | -2.178306 | 0.771518 |
| 20 | 6 | 0 | -5.672521 | -2.045242 | 1.293440 |
| 21 | 8 | 0 | -8.333119 | 2.376803 | -0.374778 |
| 22 | 1 | 0 | -4.055572 | 0.750444 | -0.052484 |
| 23 | 1 | 0 | -3.399112 | -2.209708 | -0.361800 |
| 24 | 1 | 0 | -2.087242 | 0.346262 | -1.310171 |
| 25 | 1 | 0 | 0.138348 | 0.810803 | -0.641849 |
| 26 | 1 | 0 | -5.573538 | 0.453101 | 2.584802 |
| 27 | 1 | 0 | -7.127581 | -0.138339 | 2.054533 |
| 28 | 1 | 0 | -7.678747 | 0.407087 | -1.911921 |
| 29 | 1 | 0 | -5.689641 | 2.265424 | 0.817966 |
| 30 | 1 | 0 | -7.099167 | 2.328931 | 1.867867 |
| 31 | 1 | 0 | -6.394117 | -1.415262 | -2.610338 |
| 32 | 1 | 0 | -5.876197 | -2.548264 | -1.364201 |
| 33 | 1 | 0 | -3.919849 | -1.905215 | -2.728020 |
| 34 | 1 | 0 | -4.264535 | -0.197474 | -2.480720 |
| 35 | 1 | 0 | -3.149479 | -1.174912 | 2.135387 |

S350
|   |   |   | 3.512878 | 0.523037 | 2.328913 |
|---|---|---|-----------|-----------|-----------|
| 36| 1 | 0 | -1.065156 | 0.125105 | 2.197536 |
| 37| 1 | 0 | -1.637521 | 1.197853 | 0.924464 |
| 38| 1 | 0 | -1.331454 | -2.482884 | -2.127231 |
| 39| 1 | 0 | 0.738582  | -0.421997 | -2.594975 |
| 40| 1 | 0 | -1.065156 | -0.125105 | -1.688673 |
| 41| 1 | 0 | -1.483722 | -1.197853 | -0.924464 |
| 42| 1 | 0 | -1.331454 | -2.482884 | -2.127231 |
| 43| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 44| 1 | 0 | -1.777181 | -2.585576 | 1.209246 |
| 45| 1 | 0 | -0.523441 | -2.883904 | 0.011717 |
| 46| 1 | 0 | -0.099003 | -1.245601 | 2.317873 |
| 47| 1 | 0 | -1.637521 | 1.197853 | 0.924464 |
| 48| 1 | 0 | -1.483722 | -2.482884 | -2.127231 |
| 49| 1 | 0 | -1.331454 | -2.482884 | -2.127231 |
| 50| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 51| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 52| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 53| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 54| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 55| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 56| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 57| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 58| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 59| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 60| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 61| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 62| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 63| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 64| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 65| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 66| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 67| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 68| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 69| 6 | 0 | 2.587353  | 0.102868 | 0.009263 |
| 70| 1 | 0 | -2.708255 | 0.040700 | 1.067713 |
| 71| 1 | 0 | -2.708255 | 0.040700 | 1.067713 |
| 72| 1 | 0 | -2.708255 | 0.040700 | 1.067713 |
| 73| 1 | 0 | -2.708255 | 0.040700 | 1.067713 |
| 74| 1 | 0 | -2.708255 | 0.040700 | 1.067713 |
| 75| 1 | 0 | -2.708255 | 0.040700 | 1.067713 |
| 76| 1 | 0 | -2.708255 | 0.040700 | 1.067713 |
| 77| 1 | 0 | 0.161651  | 1.995121 | 0.161651 |
| 78| 1 | 0 | 0.161651  | 1.995121 | 0.161651 |
| 79| 1 | 0 | 0.161651  | 1.995121 | 0.161651 |
| 80| 1 | 0 | 0.161651  | 1.995121 | 0.161651 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 81 | 1 | 0 | 3.191461 | -1.841008 | -1.721404 |
| 82 | 1 | 0 | 4.258829 | -3.829027 | -2.623731 |
| 83 | 1 | 0 | 5.978971 | -5.057111 | -1.307868 |
| 84 | 1 | 0 | 6.612943 | -4.246308 | 0.937582 |

**7b (conformer 12)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 5.373736 | -0.184595 | -0.688121 |
| 2 | 6 | 0 | 6.268661 | -0.654513 | 0.461432 |
| 3 | 6 | 0 | 5.779064 | 1.250404 | -1.115853 |
| 4 | 6 | 0 | 7.419087 | -0.038983 | 0.794248 |
| 5 | 6 | 0 | 7.289507 | 1.468923 | -1.231147 |
| 6 | 6 | 0 | 8.012350 | 1.080657 | 0.045253 |
| 7 | 6 | 0 | 3.879445 | 0.152997 | -0.187802 |
| 8 | 6 | 0 | 3.423143 | 1.464973 | 0.510437 |
| 9 | 6 | 0 | 5.825117 | 1.885965 | 1.209934 |
| 10 | 6 | 0 | 4.365496 | -1.798448 | 1.673216 |
| 11 | 6 | 0 | 2.882064 | 0.304937 | -1.277723 |
| 12 | 6 | 0 | 1.424729 | 0.379308 | -0.782234 |
| 13 | 6 | 0 | 1.975456 | -1.294101 | 0.984502 |
| 14 | 6 | 0 | 0.980547 | -0.945354 | -0.148345 |
| 15 | 6 | 0 | 1.279866 | -2.430682 | 1.760320 |
| 16 | 6 | 0 | -0.235019 | -2.084749 | 1.653017 |
| 17 | 6 | 0 | -0.322358 | -0.874795 | 0.676163 |
| 18 | 8 | 0 | -1.466791 | -0.880376 | -0.171324 |
| 19 | 6 | 0 | 0.863363 | -2.048882 | -1.220603 |
| 20 | 6 | 0 | 5.566404 | -1.157411 | -1.880628 |
| 21 | 8 | 0 | 9.042507 | 1.621893 | 0.404422 |
| 22 | 1 | 0 | 3.859001 | 0.616419 | 0.598873 |
| 23 | 1 | 0 | 3.462828 | -2.294108 | -0.207773 |
| 24 | 1 | 0 | 1.979067 | -0.419791 | 1.654209 |
| 25 | 1 | 0 | -0.308852 | 0.060101 | 1.249591 |
| 26 | 1 | 0 | 5.385073 | 1.954743 | -0.373984 |
| 27 | 1 | 0 | 5.302345 | 1.498943 | -2.066898 |
| 28 | 1 | 0 | 8.010242 | -0.391618 | 1.634839 |
| 29 | 1 | 0 | 7.530639 | 2.508650 | -1.462222 |
| 30 | 1 | 0 | 7.711714 | 0.860882 | -2.040975 |
| 31 | 1 | 0 | 6.493434 | -2.061238 | 2.056506 |
| 32 | 1 | 0 | 5.930115 | -2.754875 | 0.546031 |
| 33 | 1 | 0 | 4.074816 | -2.743148 | 2.142147 |
| 34 | 1 | 0 | 4.275843 | -1.021743 | 2.443466 |
| 35 | 1 | 0 | 2.935630 | -0.368580 | -2.137720 |
| 36 | 1 | 0 | 3.170217 | 1.291536 | -1.648484 |
| 37 | 1 | 0 | 0.766055 | 0.657169 | -1.610839 |
| 38 | 1 | 0 | 1.337787 | 1.177611 | -0.034897 |
| 39 | 1 | 0 | 1.615358 | -2.488555 | 2.797613 |
| 40 | 1 | 0 | 1.490849 | -3.402216 | 1.303542 |
| 41 | 1 | 0 | -0.661280 | -1.843626 | 2.629282 |
|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 42 | 1 | 0 | -0.811232 | -2.919674 | 1.246789 |
| 43 | 6 | 0 | -2.716644 | -0.591189 | 0.464194 |
| 44 | 1 | 0 | 1.807522 | -2.217463 | -1.740478 |
| 45 | 1 | 0 | 0.543685  | -3.004745  | -0.801228 |
| 46 | 1 | 0 | 0.119777  | -1.757274  | -1.964224 |
| 47 | 1 | 0 | 4.993001  | -0.828286  | -2.749556 |
| 48 | 1 | 0 | 5.251956  | -2.174069  | -1.638466 |
| 49 | 6 | 0 | -3.837961 | -1.011600  | -0.494595 |
| 50 | 6 | 0 | -2.757076  | 0.858256    | 0.969308 |
| 51 | 6 | 0 | -2.716644 | 0.200312    | 2.994067 |
| 52 | 6 | 0 | -2.847909  | 3.252208    | 2.904060 |
| 53 | 6 | 0 | -2.815370  | 3.455488    | 2.092870 |
| 54 | 6 | 0 | -2.726189  | 3.311062    | 0.684351 |
| 55 | 6 | 0 | -2.681857  | 1.999323    | 0.103380 |
| 56 | 6 | 0 | -2.667290  | 4.450616    | -0.159976 |
| 57 | 6 | 0 | -2.554823  | 4.318054    | -1.520897 |
| 58 | 6 | 0 | -2.490104  | 3.030187    | -2.096068 |
| 59 | 6 | 0 | -2.549650  | 1.905158    | -1.308693 |
| 60 | 6 | 0 | -5.212443  | -1.020457   | -0.079743 |
| 61 | 6 | 0 | -6.215452  | -1.439497   | -1.017642 |
| 62 | 6 | 0 | -5.833323  | -1.850700   | -2.319539 |
| 63 | 6 | 0 | -4.511922  | -1.867999   | -2.677698 |
| 64 | 6 | 0 | -3.520705  | -1.453166   | -1.761342 |
| 65 | 6 | 0 | -5.647101  | -0.661706   | 1.225692 |
| 66 | 6 | 0 | -6.975376  | -0.697201   | 1.578044 |
| 67 | 6 | 0 | -7.957273  | -1.090381   | 0.644033 |
| 68 | 6 | 0 | -7.578863  | -1.453742   | -0.623767 |
| 69 | 1 | 0 | -2.809979  | -1.227445   | 1.354933 |
| 70 | 1 | 0 | -2.845014  | 0.200312    | 2.994067 |
| 71 | 1 | 0 | -2.900793  | 2.460660    | 3.981427 |
| 72 | 1 | 0 | -2.847171  | 4.454564    | 2.514647 |
| 73 | 1 | 0 | -2.708599  | 5.434580    | 0.295522 |
| 74 | 1 | 0 | -2.510238  | 5.196495    | -2.154821 |
| 75 | 1 | 0 | -2.391779  | 2.927811    | -3.171103 |
| 76 | 1 | 0 | -2.487141  | 0.931325    | -1.767741 |
| 77 | 1 | 0 | -6.603394  | -2.162169   | -3.017435 |
| 78 | 1 | 0 | -4.214877  | -2.196759   | -3.667015 |
| 79 | 1 | 0 | -2.481414  | -1.484203   | -2.055308 |
| 80 | 1 | 0 | -4.924451  | -0.345448   | 1.962335 |
| 81 | 1 | 0 | -7.271304  | -0.417221   | 2.582983 |
| 82 | 1 | 0 | -9.002521  | -1.108091   | 0.931240 |
| 83 | 1 | 0 | -8.321657  | -1.766585   | -1.350352 |
| 84 | 1 | 0 | -5.189456  | 0.097304    | 0.570261 |
| 85 | 2 | 0 | -6.001053  | -1.033198   | -0.069192 |

**7b (conformer 13)**
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 3 | 6 | 0 | -5.803824 | 1.468039 | 0.182707 |   |
| 4 | 6 | 0 | -7.229977 | -0.849804 | -0.588234 |   |
| 5 | 6 | 0 | -7.330199 | 1.522510 | 0.281412 |   |
| 6 | 6 | 0 | -7.984800 | 0.411584 | -0.518932 |   |
| 7 | 6 | 0 | -3.712908 | 0.036081 | 0.021598 |   |
| 8 | 6 | 0 | -3.688444 | -1.374966 | 0.112843 |   |
| 9 | 6 | 0 | -5.378378 | -2.406113 | -0.065141 |   |
|10 | 6 | 0 | -3.945018 | -2.403652 | -0.611034 |   |
|11 | 6 | 0 | -2.791665 | 1.132928 | 0.615079 |   |
|12 | 6 | 0 | -1.358812 | 1.100440 | 0.063063 |   |
|13 | 6 | 0 | -1.656187 | -1.314381 | -0.479038 |   |
|14 | 6 | 0 | -0.729116 | -0.289690 | 0.217757 |   |
|15 | 6 | 0 | -0.807294 | -2.597182 | 0.565148 |   |
|16 | 6 | 0 | -3.945018 | -2.403652 | -0.611034 |   |
|17 | 6 | 0 | -2.791665 | 1.132928 | 0.615079 |   |
|18 | 6 | 0 | -1.358812 | 1.100440 | 0.063063 |   |
|19 | 6 | 0 | -1.656187 | -1.314381 | -0.479038 |   |
|20 | 6 | 0 | -0.729116 | -0.289690 | 0.217757 |   |
|21 | 6 | 0 | -0.807294 | -2.597182 | 0.565148 |   |
|22 | 6 | 0 | -3.945018 | -2.403652 | -0.611034 |   |
|23 | 6 | 0 | -2.791665 | 1.132928 | 0.615079 |   |
|24 | 6 | 0 | -1.358812 | 1.100440 | 0.063063 |   |
|25 | 6 | 0 | -1.656187 | -1.314381 | -0.479038 |   |
|26 | 6 | 0 | -0.729116 | -0.289690 | 0.217757 |   |
|27 | 6 | 0 | -0.807294 | -2.597182 | 0.565148 |   |
|28 | 6 | 0 | -3.945018 | -2.403652 | -0.611034 |   |
|29 | 6 | 0 | -2.791665 | 1.132928 | 0.615079 |   |
|30 | 6 | 0 | -1.358812 | 1.100440 | 0.063063 |   |
|31 | 6 | 0 | -1.656187 | -1.314381 | -0.479038 |   |
|32 | 6 | 0 | -0.729116 | -0.289690 | 0.217757 |   |
|33 | 6 | 0 | -0.807294 | -2.597182 | 0.565148 |   |
|34 | 6 | 0 | -3.945018 | -2.403652 | -0.611034 |   |
|35 | 6 | 0 | -2.791665 | 1.132928 | 0.615079 |   |
|36 | 6 | 0 | -1.358812 | 1.100440 | 0.063063 |   |
|37 | 6 | 0 | -1.656187 | -1.314381 | -0.479038 |   |
|38 | 6 | 0 | -0.729116 | -0.289690 | 0.217757 |   |
|39 | 6 | 0 | -0.807294 | -2.597182 | 0.565148 |   |
|40 | 6 | 0 | -3.945018 | -2.403652 | -0.611034 |   |
|41 | 6 | 0 | -2.791665 | 1.132928 | 0.615079 |   |
|42 | 6 | 0 | -1.358812 | 1.100440 | 0.063063 |   |
|43 | 6 | 0 | -1.656187 | -1.314381 | -0.479038 |   |
|44 | 6 | 0 | -0.729116 | -0.289690 | 0.217757 |   |
|45 | 6 | 0 | -0.807294 | -2.597182 | 0.565148 |   |
|46 | 6 | 0 | -3.945018 | -2.403652 | -0.611034 |   |
|47 | 6 | 0 | -2.791665 | 1.132928 | 0.615079 |   |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 48 | 1 | 0 | -4.770906 | -1.011243 | 2.433279 |
| 49 | 1 | 0 | -6.276620 | -0.102679 | 2.460336 |
| 50 | 6 | 0 | 3.694176 | -0.951042 | -0.973246 |
| 51 | 6 | 0 | 3.611300 | 1.511158 | -0.209669 |
| 52 | 6 | 0 | 4.883202 | 1.384475 | 0.304272 |
| 53 | 6 | 0 | 5.598570 | 2.492973 | 0.810168 |
| 54 | 6 | 0 | 5.040294 | 3.742800 | 0.788820 |
| 55 | 6 | 0 | 3.744058 | 3.939226 | 0.246953 |
| 56 | 6 | 0 | 3.013070 | 2.816297 | -0.263104 |
| 57 | 6 | 0 | 3.165926 | 5.234138 | 0.190017 |
| 58 | 6 | 0 | 1.923001 | 5.432774 | -0.356712 |
| 59 | 6 | 0 | 1.203043 | 4.332394 | -0.872197 |
| 60 | 6 | 0 | 1.730411 | 3.064546 | -0.821601 |
| 61 | 6 | 0 | 4.080960 | -1.824692 | 0.097178 |
| 62 | 6 | 0 | 4.882402 | -2.975009 | -0.207310 |
| 63 | 6 | 0 | 5.276727 | -3.222493 | -1.547385 |
| 64 | 6 | 0 | 4.899090 | -2.371091 | -2.552833 |
| 65 | 6 | 0 | 4.105218 | -1.242123 | -2.257163 |
| 66 | 6 | 0 | 3.715307 | -1.608029 | 1.456109 |
| 67 | 6 | 0 | 4.118441 | -2.471759 | 2.446342 |
| 68 | 6 | 0 | 4.905126 | -3.604696 | 2.140595 |
| 69 | 6 | 0 | 5.275491 | -3.847392 | 0.842108 |
| 70 | 1 | 0 | 2.498798 | 0.593089 | -1.774245 |
| 71 | 1 | 0 | 5.359768 | 4.143337 | 0.323482 |
| 72 | 1 | 0 | 6.593649 | 2.341739 | 1.212933 |
| 73 | 1 | 0 | 5.581994 | 4.600141 | 1.174484 |
| 74 | 1 | 0 | 3.732903 | 6.070875 | 0.584820 |
| 75 | 1 | 0 | 1.494093 | 6.427630 | 0.309700 |
| 76 | 1 | 0 | 0.222933 | 4.491059 | -1.308655 |
| 77 | 1 | 0 | 1.149903 | 2.240605 | -1.208143 |
| 78 | 1 | 0 | 5.882449 | -0.969727 | -1.760720 |
| 79 | 1 | 0 | 5.200385 | -2.560464 | -3.576863 |
| 80 | 1 | 0 | 3.810083 | -0.583226 | -3.067815 |
| 81 | 1 | 0 | 3.101881 | -0.753849 | 1.702015 |
| 82 | 1 | 0 | 3.828463 | -2.282154 | 3.473873 |
| 83 | 1 | 0 | 5.214141 | -4.277759 | 2.932489 |
| 84 | 1 | 0 | 5.881229 | -4.713294 | 0.595528 |
| 7b (conformer 14) |   |   |   |   |   |   |
| 1 | 6 | 0 | 5.313552 | 0.756014 | -0.082513 |
| 2 | 6 | 0 | 6.280159 | -0.430315 | -0.123444 |
| 3 | 6 | 0 | 5.596981 | 1.620811 | 1.173961 |
| 4 | 6 | 0 | 7.393506 | -0.495445 | 0.630945 |
| 5 | 6 | 0 | 7.082439 | 1.881883 | 1.434734 |
| 6 | 6 | 0 | 7.876062 | 0.589948 | 1.500170 |
| 7 | 6 | 0 | 3.839439 | 0.207098 | 0.011601 |
| 8 | 6 | 0 | 3.503465 | -0.884483 | -1.041601 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 9 | 6 | 0 | 5.952953 | -1.540871 | -1.088861 |
| 10 | 6 | 0 | 4.509223 | -2.038105 | -0.944181 |
| 11 | 6 | 0 | 2.775575 | 1.327900 | 0.040129 |
| 12 | 6 | 0 | 1.333015 | 0.801807 | 0.179010 |
| 13 | 6 | 0 | 2.065322 | -1.365349 | -0.815594 |
| 14 | 6 | 0 | 1.001877 | -0.241842 | -0.899022 |
| 15 | 6 | 0 | 1.491450 | -2.499822 | -1.688587 |
| 16 | 6 | 0 | -0.045506 | 2.038105 | 0.944181 |
| 17 | 6 | 0 | 2.775575 | -1.365349 | -0.815594 |
| 18 | 6 | 0 | 1.001877 | -0.241842 | -0.899022 |
| 19 | 6 | 0 | 5.536280 | 1.605220 | 0.040129 |
| 20 | 6 | 0 | 8.875117 | 0.470159 | 2.186145 |
| 21 | 6 | 0 | 3.786852 | -0.303307 | 0.985431 |
| 22 | 6 | 0 | 3.576279 | -0.454250 | -2.048678 |
| 23 | 6 | 0 | 2.030627 | -1.729693 | 0.223742 |
| 24 | 6 | 0 | -0.322897 | -1.355395 | 0.405834 |
| 25 | 6 | 0 | 5.180700 | 1.104859 | 2.047036 |
| 26 | 6 | 0 | 5.069082 | 2.574015 | 1.092859 |
| 27 | 6 | 0 | 8.038191 | -1.368882 | 0.588971 |
| 28 | 6 | 0 | 7.238847 | 2.431113 | 2.365344 |
| 29 | 6 | 0 | 7.518915 | 2.490593 | 0.633024 |
| 30 | 6 | 0 | 6.630900 | -2.361373 | -0.959828 |
| 31 | 6 | 0 | 6.093098 | -1.166523 | -2.112004 |
| 32 | 6 | 0 | 4.304179 | -2.790301 | -1.711397 |
| 33 | 6 | 0 | 4.393098 | -2.536374 | 0.026798 |
| 34 | 6 | 0 | 2.847541 | 1.931912 | -0.868668 |
| 35 | 6 | 0 | 2.976102 | 2.007495 | 0.871860 |
| 36 | 6 | 0 | 0.640398 | 1.649380 | 0.134123 |
| 37 | 6 | 0 | 1.212208 | 0.342968 | 1.168935 |
| 38 | 6 | 0 | 1.868253 | -3.479656 | -1.388750 |
| 39 | 6 | 0 | 1.766148 | -2.361971 | -2.738809 |
| 40 | 6 | 0 | -0.474817 | -3.247214 | -0.992340 |
| 41 | 6 | 0 | -0.569026 | -2.273412 | -2.446215 |
| 42 | 6 | 0 | -2.238132 | 0.196642 | -0.025181 |
| 43 | 6 | 0 | 1.839292 | 0.942495 | -2.552883 |
| 44 | 6 | 0 | 0.709856 | -0.299731 | -3.079025 |
| 45 | 6 | 0 | 0.105081 | 1.151957 | -2.296474 |
| 46 | 6 | 0 | 4.922834 | 2.508482 | -1.344260 |
| 47 | 6 | 0 | 5.292527 | 1.053555 | -2.270970 |
| 48 | 6 | 0 | 6.580664 | 1.915737 | -1.440076 |
| 49 | 6 | 0 | -2.853627 | -0.801891 | 0.965757 |
| 50 | 6 | 0 | -3.212183 | 1.162251 | -0.712359 |
| 51 | 6 | 0 | -3.350502 | 1.130309 | -2.083889 |
| 52 | 6 | 0 | -4.223270 | 2.006052 | -2.766793 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 54 | 6 | 0 | -4.954406 | 2.931794 | -2.072629 |
| 55 | 6 | 0 | -4.826580 | 3.033095 | -0.664223 |
| 56 | 6 | 0 | -3.940721 | 2.146906 | 0.036464 |
| 57 | 6 | 0 | -5.552546 | 4.013379 | 0.061164 |
| 58 | 6 | 0 | -5.412128 | 4.142100 | 1.419987 |
| 59 | 6 | 0 | -4.529120 | 3.287251 | 2.113332 |
| 60 | 6 | 0 | -3.819018 | 2.319996 | 1.442501 |
| 61 | 6 | 0 | -3.824591 | 1.790175 | 0.592154 |
| 62 | 6 | 0 | -4.333813 | 2.673654 | 1.602173 |
| 63 | 6 | 0 | -2.896575 | 1.650316 | 3.260036 |
| 64 | 6 | 0 | -2.403052 | 0.812269 | 0.555849 |
| 65 | 6 | 0 | -1.540204 | 0.812269 | 0.555849 |
| 66 | 6 | 0 | -2.770388 | 0.413874 | 2.648069 |
| 67 | 6 | 0 | -4.305165 | 1.936669 | 3.845745 |
| 68 | 6 | 0 | -5.630393 | 3.606815 | -2.586884 |
| 69 | 6 | 0 | -6.221966 | 4.668842 | -0.486365 |
| 70 | 6 | 0 | -5.971565 | 4.897246 | 1.960477 |
| 71 | 6 | 0 | -4.411921 | 3.391877 | 3.186258 |
| 72 | 6 | 0 | -3.162430 | 1.674748 | 2.006095 |
| 73 | 6 | 0 | -4.247833 | 3.251890 | 3.683294 |
| 74 | 6 | 0 | -2.516582 | 1.583446 | 4.273153 |
| 75 | 6 | 0 | -1.648899 | -0.044190 | 2.551885 |
| 76 | 6 | 0 | -3.916120 | -1.326199 | -1.518486 |
| 77 | 6 | 0 | -5.591762 | -3.016534 | -2.061068 |
| 78 | 6 | 0 | -6.500354 | -4.512407 | -0.291788 |
| 79 | 6 | 0 | -5.685471 | -4.301343 | 2.030698 |

**7b (conformer 16)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | 5.279493 | -0.403756 | -0.579896 |
| 2  | 6 | 0 | 6.268146 | 0.112334 | 0.469434 |
| 3  | 6 | 0 | 5.572676 | 0.261632 | -1.950123 |
| 4  | 6 | 0 | 7.398323 | 0.771000 | 0.150368 |
| 5  | 6 | 0 | 7.057959 | 0.322304 | -2.314711 |
| 6  | 6 | 0 | 7.877401 | 0.987578 | -1.224340 |
| 7  | 6 | 0 | 3.819238 | -0.012046 | -0.135941 |
| 8  | 6 | 0 | 3.485207 | -0.399830 | 1.331100 |
| 9  | 6 | 0 | 5.944497 | -0.181974 | 1.912079 |
| 10 | 6 | 0 | 4.512136 | 0.218376 | 2.287164 |
| 11 | 6 | 0 | 2.733390 | -0.496120 | -1.123944 |
| 12 | 6 | 0 | 1.302993 | -0.090639 | -0.715334 |
| 13 | 6 | 0 | 2.059593 | 0.060074 | 1.656048 |
| 14 | 6 | 0 | 0.976827 | -0.530476 | 0.720125 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 15 | 6 | 0 | 1.496011 | -0.156194 | 3.075064 |
| 16 | 6 | 0 | -0.041434 | -0.026462 | 2.889139 |
| 17 | 6 | 0 | -0.283382 | 0.111673 | 1.364580 |
| 18 | 8 | 0 | -1.527875 | -0.494952 | 1.012559 |
| 19 | 6 | 0 | 0.858686 | -2.065653 | 0.801682 |
| 20 | 6 | 0 | 5.456513 | -1.940666 | -0.696459 |
| 21 | 8 | 0 | 8.892453 | 1.617296 | -1.461296 |
| 22 | 1 | 0 | 3.799531 | 1.088196 | -0.158414 |
| 23 | 1 | 0 | 3.533632 | -1.491262 | 1.440454 |
| 24 | 1 | 0 | 2.044121 | 1.147690 | 1.479380 |
| 25 | 1 | 0 | -0.313759 | 1.174161 | 1.091028 |
| 26 | 1 | 0 | 5.182594 | -1.940666 | -0.696459 |
| 27 | 1 | 0 | 8.892453 | 1.617296 | -1.461296 |
| 28 | 1 | 0 | 3.799531 | 1.088196 | -0.158414 |
| 29 | 1 | 0 | 3.533632 | -1.491262 | 1.440454 |
| 30 | 1 | 0 | 2.044121 | 1.147690 | 1.479380 |
| 31 | 1 | 0 | 8.058931 | 1.142201 | 0.928858 |
| 32 | 1 | 0 | 7.222773 | 0.862733 | -3.249227 |
| 33 | 1 | 0 | 4.421022 | 1.311647 | 2.256609 |
| 34 | 1 | 0 | 2.779865 | -1.583878 | -1.222866 |
| 35 | 1 | 0 | 2.933893 | -0.93143 | -2.119600 |
| 36 | 1 | 0 | 0.592183 | -0.522682 | -1.427869 |
| 37 | 1 | 0 | 1.204677 | 1.000534 | -0.786702 |
| 38 | 1 | 0 | 1.887305 | 0.572082 | 3.788145 |
| 39 | 1 | 0 | 1.762683 | -1.147187 | 3.454089 |
| 40 | 1 | 0 | -0.453746 | 0.828644 | 3.428093 |
| 41 | 1 | 0 | -0.567944 | -0.914752 | 3.244321 |
| 42 | 1 | 0 | -2.268833 | 0.135237 | -0.038518 |
| 43 | 1 | 0 | 1.754226 | 1.254864 | 0.434450 |
| 44 | 1 | 0 | 0.683725 | -2.414679 | 1.821177 |
| 45 | 1 | 0 | 0.010788 | -2.398781 | 0.200722 |
| 46 | 1 | 0 | 4.823390 | -2.348894 | -1.486997 |
| 47 | 1 | 0 | 5.203927 | -2.455484 | 0.232102 |
| 48 | 1 | 0 | 6.491841 | -2.192633 | -0.937030 |
| 49 | 1 | 0 | -3.199996 | 1.230791 | 0.515261 |
| 50 | 1 | 0 | -2.941188 | -0.963815 | -0.868610 |
| 51 | 1 | 0 | -2.573742 | -1.081756 | -2.191535 |
| 52 | 1 | 0 | -3.140692 | -2.048472 | -3.049770 |
| 53 | 1 | 0 | -4.086402 | -2.914632 | -2.569348 |
| 54 | 1 | 0 | -4.480717 | -2.864731 | -1.207784 |
| 55 | 1 | 0 | -3.896842 | -1.889874 | -0.331053 |
| 56 | 1 | 0 | -5.436245 | -3.780825 | -0.695130 |
| 57 | 1 | 0 | -5.797832 | -3.760706 | 0.628123 |
| 58 | 1 | 0 | -5.206243 | -2.821775 | 1.500787 |
| 59 | 1 | 0 | -5.206243 | -2.821775 | 1.500787 |
|    |   |   |   |   |
|----|---|---|---|---|
| 60 | 6 | 0 | -4.283536 | -1.915978 | 1.035705 |
| 61 | 6 | 0 | -3.812426 | 2.200840 | -0.348290 |
| 62 | 6 | 0 | -4.648270 | 3.215033 | 0.229410 |
| 63 | 6 | 0 | -4.846959 | 3.246533 | 1.633113 |
| 64 | 6 | 0 | -4.233073 | 2.324477 | 2.437945 |
| 65 | 6 | 0 | -3.408641 | 1.326471 | 1.873990 |
| 66 | 6 | 0 | -3.623164 | 2.231873 | -1.756953 |
| 67 | 6 | 0 | -4.219190 | 3.189685 | -2.542644 |
| 68 | 6 | 0 | -5.049043 | 4.176053 | -1.968524 |
| 69 | 6 | 0 | -5.255271 | 4.183319 | -0.611866 |
| 70 | 6 | 0 | -1.562641 | 0.629722 | -0.713904 |
| 71 | 1 | 0 | -1.825487 | -0.408318 | -2.596859 |
| 72 | 1 | 0 | -2.824684 | -2.095243 | -4.085742 |
| 73 | 1 | 0 | -4.538712 | -3.657545 | -3.217863 |
| 74 | 1 | 0 | -5.872700 | -4.506369 | -1.373766 |
| 75 | 1 | 0 | -6.527593 | -4.467240 | 1.007385 |
| 76 | 1 | 0 | -5.479558 | -2.818684 | 2.550156 |
| 77 | 1 | 0 | -3.824438 | -1.224812 | 1.723264 |
| 78 | 1 | 0 | -5.483661 | 4.017107 | 2.054774 |
| 79 | 1 | 0 | -4.373385 | 2.352949 | 3.512777 |
| 80 | 1 | 0 | -2.921106 | 0.616136 | 2.527737 |
| 81 | 1 | 0 | -3.007128 | 1.482918 | -2.231072 |
| 82 | 1 | 0 | -4.053433 | 3.184685 | -3.614230 |
| 83 | 1 | 0 | -5.518058 | 4.923171 | -2.598705 |
| 84 | 1 | 0 | -5.887695 | 4.938412 | -0.156492 |

8b (conformer 1)

|    |   |   |   |   |
|----|---|---|---|---|
| 1  | 6 | 0 | 0.792749 | -3.710698 | -1.422503 |
| 2  | 8 | 0 | 1.063780 | -2.310417 | -1.207296 |
| 3  | 6 | 0 | 1.746177 | -2.004653 | -0.093400 |
| 4  | 6 | 0 | 1.905412 | -0.481500 | 0.052594 |
| 5  | 6 | 0 | 3.197591 | -0.138340 | 0.781480 |
| 6  | 6 | 0 | 4.426207 | -0.490923 | -0.023024 |
| 7  | 8 | 0 | 5.548606 | -0.274033 | 0.687407 |
| 8  | 6 | 0 | 6.789873 | -0.571060 | 0.018660 |
| 9  | 8 | 0 | 2.153806 | -2.816156 | 0.700644 |
| 10 | 8 | 0 | 4.423051 | -0.902331 | -1.159669 |
| 11 | 8 | 0 | 0.852345 | 0.075478 | 0.839512 |
| 12 | 6 | 0 | -0.445564 | 0.197771 | 0.218010 |
| 13 | 6 | 0 | -1.357951 | -0.968472 | 0.584579 |
| 14 | 6 | 0 | -1.076561 | -1.748704 | 1.683761 |
| 15 | 6 | 0 | -2.512834 | -1.261335 | -0.212153 |
| 16 | 6 | 0 | -1.898198 | -2.842839 | 2.040962 |
| 17 | 6 | 0 | -3.338040 | -2.376207 | 0.149552 |
| 18 | 6 | 0 | -3.003155 | -3.152305 | 1.290417 |
| 19 | 6 | 0 | -0.992564 | 1.565082 | 0.622941 |
| 20 | 6 | 0 | -1.861658 | 1.680743 | 1.685387 |
|     |     |     |     |     |
|-----|-----|-----|-----|-----|
| 21  | 6   | 0   | -0.568172 | 2.749798 | -0.067708 |
| 22  | 6   | 0   | -2.345950 | 2.935698 | 2.116438 |
| 23  | 6   | 0   | -1.070556 | 4.021219 | 0.366965 |
| 24  | 6   | 0   | -1.960871 | 4.081461 | 1.470186 |
| 25  | 6   | 0   | 0.328254  | 2.739452 | -1.171194 |
| 26  | 6   | 0   | 0.701273  | 3.901142 | -1.806709 |
| 27  | 6   | 0   | -0.665277 | 5.201483 | -0.309831 |
| 28  | 6   | 0   | -2.345950 | 2.935698 | -1.171194 |
| 29  | 6   | 0   | -4.032111 | -0.497222 | -1.351391 |
| 30  | 6   | 0   | -1.070556 | 4.021219 | 0.366965 |
| 31  | 6   | 0   | 0.328254  | 2.739452 | -1.171194 |
| 32  | 6   | 0   | 0.701273  | 3.901142 | -1.806709 |
| 33  | 1   | 0   | 1.903790  | -0.045413 | -0.950776 |
| 34  | 1   | 0   | 0.242703  | -3.758469 | -2.359221 |
| 35  | 1   | 0   | 1.728230  | -4.266418 | -1.494308 |
| 36  | 1   | 0   | 0.193089  | -4.106681 | -0.602410 |
| 37  | 1   | 0   | 3.210129  | 0.933812  | 0.094886 |
| 38  | 1   | 0   | 3.237064  | -0.657936 | 1.740944 |
| 39  | 1   | 0   | 6.896280  | 0.041691  | -0.877440 |
| 40  | 1   | 0   | 7.569485  | -0.335605 | 0.739472 |
| 41  | 1   | 0   | 6.828293  | -1.625003 | -0.259144 |
| 42  | 1   | 0   | -0.302412 | 0.175273  | -0.865774 |
| 43  | 1   | 0   | -0.199040 | -1.525167 | 2.276284 |
| 44  | 1   | 0   | -1.642145 | -3.436643 | 2.911191 |
| 45  | 1   | 0   | -3.636082 | -3.992615 | 1.556294 |
| 46  | 1   | 0   | -2.186783 | 0.788335  | 2.05357 |
| 47  | 1   | 0   | -3.026045 | 2.982906  | 2.959361 |
| 48  | 1   | 0   | -2.330697 | 5.049659  | 1.791305 |
| 49  | 1   | 0   | 0.734037  | 1.802348  | -1.528240 |
| 50  | 1   | 0   | 1.385125  | 3.858437  | -2.647086 |
| 51  | 1   | 0   | -1.055168 | 6.154070  | 0.032746 |
| 52  | 1   | 0   | 0.503083  | 6.057937  | 1.880990 |
| 53  | 1   | 0   | -2.301734 | 0.366100  | -1.640203 |
| 54  | 1   | 0   | -4.262403 | -0.221023 | -2.958273 |
| 55  | 1   | 0   | -5.092342 | -3.530517 | -0.355162 |
| 56  | 1   | 0   | -5.677089 | -2.171502 | -2.323464 |

**8b (conformer 2)**

|     |     |     |     |     |
|-----|-----|-----|-----|-----|
| 1   | 6   | 0   | 3.784585 | 2.202039 | -2.612898 |
| 2   | 6   | 0   | 3.364739 | 1.790317 | -1.297350 |
| 3   | 6   | 0   | 2.366066 | 0.889727 | -1.252752 |
| 4   | 6   | 0   | 2.034993 | 0.529394 | 0.205008 |
| 5   | 6   | 0   | 3.266236 | 0.116612 | 1.020832 |
| 6   | 6   | 0   | 3.955747 | -1.106443 | 0.448844 |
| 7   | 6   | 0   | 4.215075 | -2.022342 | 1.402446 |
| 8   | 8   | 0   | 4.894912 | -3.214188 | 0.960418 |
| 9   | 8   | 0   | 1.772415 | 0.488904  | -2.220657 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 10| 8 | 0 | 4.264356 | -1.242934 | -0.709803 |
| 11| 8 | 0 | 1.111356 | -0.530873 | 0.298500 |
| 12| 6 | 0 | -0.268086 | -0.263623 | -0.035619 |
| 13| 6 | 0 | -1.007869 | -1.594857 | 0.033191 |
| 14| 6 | 0 | -0.427013 | -2.687877 | 0.638174 |
| 15| 6 | 0 | -2.315962 | -1.720460 | -0.540538 |
| 16| 6 | 0 | -1.097416 | -3.929873 | 0.717370 |
| 17| 6 | 0 | -2.988418 | -2.984145 | -0.459808 |
| 18| 6 | 0 | -2.350667 | -4.077056 | 0.182624 |
| 19| 6 | 0 | -0.854076 | 0.796303 | 0.905001 |
| 20| 6 | 0 | -1.103305 | 0.446262 | 2.216611 |
| 21| 6 | 0 | -1.106371 | 2.142754 | 0.479842 |
| 22| 6 | 0 | -1.602362 | 1.374139 | 3.153116 |
| 23| 6 | 0 | -1.625192 | 3.082349 | 1.435484 |
| 24| 6 | 0 | -1.862791 | 2.666124 | 2.768974 |
| 25| 6 | 0 | -0.873548 | 4.182811 | 1.030995 |
| 26| 6 | 0 | -1.139606 | 3.913432 | -1.201604 |
| 27| 6 | 0 | -1.888548 | 4.418281 | 1.030995 |
| 28| 6 | 0 | -1.654238 | 4.829646 | -0.257197 |
| 29| 6 | 0 | -2.988334 | -0.652547 | -1.195716 |
| 30| 6 | 0 | -4.240879 | -0.820637 | -1.738863 |
| 31| 6 | 0 | -4.281216 | -3.122546 | -1.029584 |
| 32| 6 | 0 | -4.898072 | -2.067751 | -1.656514 |
| 33| 1 | 0 | 1.631646 | 1.443806 | 0.660918 |
| 34| 1 | 0 | 4.582918 | 2.922662 | -2.450458 |
| 35| 1 | 0 | 4.150600 | 1.340741 | -3.172402 |
| 36| 1 | 0 | 2.955008 | 2.661497 | -3.151671 |
| 37| 1 | 0 | 3.989740 | 0.935413 | 1.013368 |
| 38| 1 | 0 | 2.961576 | -0.071019 | 2.049648 |
| 39| 1 | 0 | 5.004893 | -3.831097 | 1.849409 |
| 40| 1 | 0 | 4.302092 | -3.728887 | 0.203563 |
| 41| 1 | 0 | 5.870947 | -2.963162 | 0.542983 |
| 42| 1 | 0 | -0.298834 | 0.078876 | -1.068649 |
| 43| 1 | 0 | 0.568584 | -2.592891 | 1.048828 |
| 44| 1 | 0 | -0.607152 | -4.767069 | 1.201925 |
| 45| 1 | 0 | -2.869903 | -5.028246 | 0.237146 |
| 46| 1 | 0 | -0.919249 | -0.574100 | 2.532434 |
| 47| 1 | 0 | -1.787665 | 1.057101 | 4.173235 |
| 48| 1 | 0 | -2.255654 | 3.386068 | 3.479349 |
| 49| 1 | 0 | -0.472496 | 1.943277 | -1.595722 |
| 50| 1 | 0 | -0.952543 | 4.239268 | -2.218774 |
| 51| 1 | 0 | -2.282002 | 5.112598 | 1.766323 |
| 52| 1 | 0 | -1.861070 | 5.851999 | -0.552617 |
| 53| 1 | 0 | -2.516966 | 0.317979 | -1.269951 |
| 54| 1 | 0 | -4.727982 | 0.012225 | -2.233624 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 55 | 1 | 0 | -4.776069 | -4.086004 | -0.961649 |
| 56 | 1 | 0 | -5.885359 | -2.188340 | -2.088062 |
| **8b (conformer 3)** |   |   |   |   |   |
| 1 | 6 | 0 | -2.844895 | -3.127956 | 2.530384 |
| 2 | 8 | 0 | -2.726752 | -2.396210 | 1.293530 |
| 3 | 6 | 0 | -1.992289 | -1.274568 | 1.339715 |
| 4 | 6 | 0 | -1.859408 | -0.589098 | -0.026442 |
| 5 | 6 | 0 | -2.957555 | -0.925704 | -1.027335 |
| 6 | 6 | 0 | -4.324083 | -0.474983 | -0.567976 |
| 7 | 8 | 0 | -5.277545 | -0.858653 | -1.439227 |
| 8 | 6 | 0 | -6.625867 | -0.466785 | -1.115417 |
| 9 | 8 | 0 | -1.431860 | -0.878901 | 2.335315 |
| 10 | 8 | 0 | -4.551712 | 0.156484 | 0.436334 |
| 11 | 8 | 0 | -0.630254 | -1.018535 | -0.613675 |
| 12 | 6 | 0 | 0.571636 | -0.364840 | -0.144087 |
| 13 | 6 | 0 | 1.750342 | -1.253721 | -0.523876 |
| 14 | 6 | 0 | 1.591687 | -2.277895 | -1.432005 |
| 15 | 6 | 0 | 3.036017 | -1.033685 | 0.071877 |
| 16 | 6 | 0 | 2.672611 | -3.112124 | -1.798710 |
| 17 | 6 | 0 | 4.126040 | -1.887728 | -0.299635 |
| 18 | 6 | 0 | 3.912784 | -2.922897 | -1.246815 |
| 19 | 6 | 0 | 0.665991 | 1.049074 | -0.728515 |
| 20 | 6 | 0 | 0.985272 | 1.187079 | -2.064267 |
| 21 | 6 | 0 | 0.404360 | 2.221593 | 0.055862 |
| 22 | 6 | 0 | 1.066484 | 2.450737 | -2.682984 |
| 23 | 6 | 0 | 0.507500 | 3.508438 | -0.575868 |
| 24 | 6 | 0 | 0.839029 | 3.589620 | -1.951013 |
| 25 | 6 | 0 | 0.046666 | 2.190521 | 1.435184 |
| 26 | 6 | 0 | -0.178700 | 3.348949 | 2.140829 |
| 27 | 6 | 0 | 0.269076 | 4.683065 | 0.186434 |
| 28 | 6 | 0 | -0.062716 | 4.610754 | 1.516036 |
| 29 | 6 | 0 | 3.290442 | -0.009631 | 1.025074 |
| 30 | 6 | 0 | 4.538190 | 0.157839 | 1.579248 |
| 31 | 6 | 0 | 5.401089 | -1.686122 | 0.290889 |
| 32 | 6 | 0 | 5.607718 | -0.687318 | 1.210635 |
| 33 | 1 | 0 | -1.848407 | 0.486866 | 0.163546 |
| 34 | 1 | 0 | -3.312547 | -2.503737 | 3.292432 |
| 35 | 1 | 0 | -3.469348 | -3.987921 | 2.299569 |
| 36 | 1 | 0 | -1.861030 | -3.446820 | 2.875989 |
| 37 | 1 | 0 | -2.727958 | -0.428752 | -1.974188 |
| 38 | 1 | 0 | -2.981512 | -1.997638 | -1.231180 |
| 39 | 1 | 0 | -6.926966 | -0.894807 | -0.158457 |
| 40 | 1 | 0 | -6.704825 | 0.619833 | -1.063471 |
| 41 | 1 | 0 | -7.241986 | -0.858238 | -1.921661 |
| 42 | 1 | 0 | 0.530384 | -0.319271 | 0.944233 |
| 43 | 1 | 0 | 0.614898 | -2.452082 | -1.861979 |

S362
|    |     |    |            |            |            |            |
|----|-----|----|------------|------------|------------|------------|
| 44 | 1   | 0  | 2.508688   | -3.907143  | -2.517791  |
| 45 | 1   | 0  | 4.745667   | -3.561925  | -1.521186  |
| 46 | 1   | 0  | 1.191081   | 0.299490   | -2.651234  |
| 47 | 1   | 0  | 1.322364   | 2.516009   | -3.734554  |
| 48 | 1   | 0  | 0.911937   | 4.568257   | -2.414045  |
| 49 | 1   | 0  | -0.082990  | 1.245166   | 1.945933   |
| 50 | 1   | 0  | -0.457791  | 3.290622   | 3.186837   |
| 51 | 1   | 0  | 0.353198   | 5.645507   | -0.307851  |
| 52 | 1   | 0  | -0.243163  | 5.15168    | 2.085997   |
| 53 | 1   | 0  | 2.496554   | 0.661566   | 1.323724   |
| 54 | 1   | 0  | 4.701977   | 0.947566   | 2.303892   |
| 55 | 1   | 0  | 6.215301   | -2.342045  | 0.00149    |
| 56 | 1   | 0  | 6.586918   | -0.544837  | 1.653757   |
| 8b |     |    |            |            |            |            |
| 1  | 6   | 0  | -3.635628  | -0.918596  | 3.178964   |
| 2  | 8   | 0  | -3.235776  | -0.872038  | 1.793896   |
| 3  | 6   | 0  | -1.946146  | -1.154537  | 1.533670   |
| 4  | 6   | 0  | -1.682074  | -1.094745  | 0.021873   |
| 5  | 6   | 0  | -2.591288  | -2.068789  | -0.751851  |
| 6  | 6   | 0  | -4.055382  | -1.688216  | -0.829559  |
| 7  | 8   | 0  | -4.210232  | -0.414443  | -1.426269  |
| 8  | 6   | 0  | -5.566669  | 0.049415   | -1.373745  |
| 9  | 8   | 0  | -1.127482  | -1.406327  | 2.381082   |
| 10 | 8   | 0  | -4.975959  | -2.433932  | -0.605185  |
| 11 | 8   | 0  | -0.359097  | -1.470689  | -0.288985  |
| 12 | 6   | 0  | 0.696275   | -0.537777  | 0.029900   |
| 13 | 6   | 0  | 2.016982   | -1.241009  | -0.264199  |
| 14 | 6   | 0  | 2.040214   | -2.415241  | -0.984385  |
| 15 | 6   | 0  | 3.248204   | -0.690414  | 0.223009   |
| 16 | 6   | 0  | 3.252988   | -3.085438  | -1.264598  |
| 17 | 6   | 0  | 4.473845   | -1.378474  | -0.059798  |
| 18 | 6   | 0  | 4.444492   | -2.580165  | -0.814141  |
| 19 | 6   | 0  | 0.516966   | 0.765448   | -0.756979  |
| 20 | 6   | 0  | 0.769099   | 0.753819   | -2.113572  |
| 21 | 6   | 0  | 0.051314   | 1.974264   | -0.141306  |
| 22 | 6   | 0  | 0.580625   | 1.897470   | -2.915739  |
| 23 | 6   | 0  | 0.132391   | 3.139668   | -0.961813  |
| 24 | 6   | 0  | 0.140749   | 3.068469   | -2.350446  |
| 25 | 6   | 0  | 0.239488   | 2.096341   | 1.248369   |
| 26 | 6   | 0  | 0.679606   | 3.282032   | 1.788201   |
| 27 | 6   | 0  | -0.589169  | 4.347189   | -0.369550  |
| 28 | 6   | 0  | -0.857698  | 4.422976   | 0.974228   |
| 29 | 6   | 0  | 3.322009   | 0.508827   | 0.983373   |
| 30 | 6   | 0  | 4.525155   | 0.995284   | 1.439326   |
| 31 | 6   | 0  | 5.698143   | -0.847913  | 0.424633   |
| 32 | 6   | 0  | 5.728832   | 0.312504   | 1.158572   |
|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 33| 1 | 0 | -1.8970| 95 | -0.0731| 81 | -0.3109| 33 |
| 34| 1 | 0 | -4.7| 019| 91 | -0.70192| 99 | 3.1801| 83 |
| 35| 1 | 0 | -3.4| 4422| 5 | -1.9082| 43 | 3.5942| 73 |
| 36| 1 | 0 | -3.0| 8881| 5 | -0.1712| 33 | 3.7551| 29 |
| 37| 1 | 0 | -2.2| 0396| 1 | -2.1018| 60 | -1.7742| 03 |
| 38| 1 | 0 | -2.5| 2484| 0 | -3.0739| 13 | -0.3354| 19 |
| 39| 1 | 0 | -6.0| 7863| 4 | -0.0092| 85 | -0.4123| 96 |
| 40| 1 | 0 | -5.4| 9041| 6 | 1.0825| 96 | -1.7051| 75 |
| 41| 1 | 0 | -6.1| 0780| 9 | -0.5510| 81 | -2.1061| 86 |
| 42| 1 | 0 | 0.6| 5989| 1 | -0.3466| 89 | 1.1017| 47 |
| 43| 1 | 0 | 1.1| 0698| 5 | -2.8389| 75 | -1.3281| 18 |
| 44| 1 | 0 | 3.2| 2940| 0 | -4.0072| 55 | -1.8352| 07 |
| 45| 1 | 0 | 5.3| 7863| 0 | -3.0915| 08 | -1.0219| 26 |
| 46| 1 | 0 | 1.1| 2987| 6 | -0.1593| 15 | -2.5728| 59 |
| 47| 1 | 0 | 0.7| 9286| 2 | 1.8467| 80 | -3.9776| 98 |
| 48| 1 | 0 | -0.0| 0059| 1 | 3.9565| 71 | -2.9573| 27 |
| 49| 1 | 0 | -0.1| 1605| 0 | 1.2451| 83 | 1.9051| 74 |
| 50| 1 | 0 | -0.8| 9000| 5 | 3.3421| 83 | 2.8502| 42 |
| 51| 1 | 0 | -0.7| 2107| 0 | 5.2164| 74 | -1.0055| 59 |
| 52| 1 | 0 | -1.2| 0363| 8 | 5.3519| 32 | 1.4130| 57 |
| 53| 1 | 0 | 2.4| 2047| 5 | 1.0619| 19 | 1.2086| 51 |
| 54| 1 | 0 | 4.5| 4940| 5 | 1.9119| 57 | 2.0179| 80 |
| 55| 1 | 0 | 6.6| 1663| 8 | -1.3816| 26 | 0.2027| 90 |
| 56| 1 | 0 | 6.6| 7132| 8 | 0.7055| 83 | 1.5228| 04 |

|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 8b (conformer 6) |   |   |   |   |   |   |   |
| 1  | 6 | 0 | 4.1| 0422| 4 | 1.8153| 31 | -2.3369| 59 |
| 2  | 8 | 0 | 3.5| 8972| 9 | 1.4535| 33 | -1.0409| 66 |
| 3  | 6 | 0 | 2.5| 3605| 5 | 0.6152| 82 | -1.0344| 42 |
| 4  | 6 | 0 | 2.0| 7408| 3 | 0.3485| 55 | 0.4065| 70 |
| 5  | 6 | 0 | 3.2| 0117| 1 | -0.1247| 43 | 1.3378| 84 |
| 6  | 6 | 0 | 3.6| 8546| 7 | -1.5317| 07 | 1.0435| 40 |
| 7  | 8 | 0 | 4.0| 7937| 7 | -1.6555| 35 | -0.2400| 97 |
| 8  | 6 | 0 | 4.5| 0526| 1 | -2.9681| 81 | -0.6530| 57 |
| 9  | 8 | 0 | 2.0| 0088| 1 | 0.1979| 20 | -2.0296| 27 |
| 10 | 8 | 0 | 3.7| 3858| 6 | -2.4274| 10 | 1.8487| 21 |
| 11 | 8 | 0 | 1.0| 6081| 4 | -0.6267| 36 | 0.4702| 05 |
| 12 | 6 | 0 | -0.2| 6819| 2 | -0.2659| 73 | 0.0349| 33 |
| 13 | 6 | 0 | -1.1| 2339| 0 | -1.5240| 00 | 0.1402| 53 |
| 14 | 6 | 0 | -0.6| 8147| 6 | -2.6124| 19 | 0.8607| 02 |
| 15 | 6 | 0 | -2.3| 9711| 4 | -1.5833| 10 | -0.5154| 11 |
| 16 | 6 | 0 | -1.4| 6320| 2 | -3.7845| 51 | 0.9782| 85 |
| 17 | 6 | 0 | -3.1| 8257| 9 | -2.7767| 78 | -0.3946| 08 |
| 18 | 6 | 0 | -2.6| 8712| 3 | -3.8668| 77 | 0.3670| 93 |
| 19 | 6 | 0 | -0.8| 1387| 8 | 0.8988| 30 | 0.8694| 02 |
| 20 | 6 | 0 | 1.1| 6578| 9 | 0.6576| 18 | 2.1820| 18 |
| 21 | 6 | 0 | -0.9| 2930| 8 | 2.2293| 76 | 0.3461| 61 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 22 | 6 | 0 | -1.639205 | 1.682326 | 3.026222 |
| 23 | 6 | 0 | -1.423530 | 3.268460 | 1.207515 |
| 24 | 6 | 0 | -1.769800 | 2.962038 | 2.547041 |
| 25 | 6 | 0 | -1.423530 | 3.268460 | 1.207515 |
| 26 | 6 | 0 | -1.769800 | 2.962038 | 2.547041 |
| 27 | 6 | 0 | -1.553539 | 4.590686 | 0.705187 |
| 28 | 6 | 0 | -1.213791 | 4.895983 | -0.988429 |
| 29 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 30 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 31 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 32 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 33 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 34 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 35 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 36 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 37 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 38 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 39 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 40 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 41 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 42 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 43 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 44 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 45 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 46 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 47 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 48 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 49 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 50 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 51 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 52 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 53 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 54 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 55 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |
| 56 | 6 | 0 | -1.553539 | 4.590686 | -0.988429 |

| 8b (conformer 7) |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.381591 | -4.013716 | 2.653709 |
| 2 | 6 | 0 | 1.144739 | -3.570123 | 1.302441 |
| 3 | 6 | 0 | 0.988747 | -2.244504 | 1.136237 |
| 4 | 6 | 0 | 0.749886 | -1.926287 | -0.348393 |
| 5 | 6 | 0 | 1.854088 | -2.478635 | -1.258634 |
| 6 | 6 | 0 | 3.215273 | -1.899219 | -0.926063 |
| 7 | 8 | 0 | 3.872925 | -1.508068 | -2.031647 |
| 8 | 6 | 0 | 5.184526 | -0.948277 | -1.819104 |
| 9 | 8 | 0 | 0.966739 | -1.451657 | 2.043284 |
| 10 | 8 | 0 | 3.672370 | -1.825504 | 0.189073 |
|    |    |    |        |        |        |
|----|----|----|--------|--------|--------|
| 11 | 8  | 0  | 0.660699 | -0.543337 | -0.628792 |
| 12 | 6  | 0  | -0.483411 | 0.190289  | -0.121508 |
| 13 | 6  | 0  | -0.209447 | 1.664326  | -0.420378 |
| 14 | 6  | 0  | -0.916912 | 2.332756  | -1.396213 |
| 15 | 6  | 0  | 0.794418  | 2.372627  | 0.324679  |
| 16 | 6  | 0  | -0.677724 | 3.694674  | -1.688322 |
| 17 | 6  | 0  | 1.027521  | 3.756605  | 0.029201  |
| 18 | 6  | 0  | -0.483411 | 0.190289  | -0.121508 |
| 19 | 6  | 0  | -1.795425 | -0.330005 | -0.697475 |
| 20 | 6  | 0  | -1.826209 | -0.865648 | -1.968229 |
| 21 | 6  | 0  | -3.008524 | -0.259667 | -0.062975 |
| 22 | 6  | 0  | -0.677724 | 3.694674  | -1.688322 |
| 23 | 6  | 0  | 1.027521  | 3.756605  | 0.029201  |
| 24 | 6  | 0  | -0.419043 | -1.324405 | -1.820845 |
| 25 | 6  | 0  | -3.083252 | 0.311219  | 1.364372  |
| 26 | 6  | 0  | -4.270671 | 0.358383  | 2.055818  |
| 27 | 6  | 0  | -5.425937 | -0.709804 | 0.229807  |
| 28 | 6  | 0  | -5.455864 | -0.159444 | 1.487261  |
| 29 | 6  | 0  | 1.572239  | 1.769856  | 1.350517  |
| 30 | 6  | 0  | 2.513784  | 2.494235  | 2.045028  |
| 31 | 6  | 0  | 2.009344  | 4.471656  | 0.764254  |
| 32 | 6  | 0  | 2.737977  | 3.857758  | 1.753325  |
| 33 | 1  | 0  | -0.184278 | -2.439389 | -0.612117 |
| 34 | 1  | 0  | 0.546494  | -3.734711 | 3.297198  |
| 35 | 1  | 0  | 1.474315  | -5.095554 | 2.591165  |
| 36 | 1  | 0  | 2.301158  | -3.569229 | 3.035405  |
| 37 | 1  | 0  | 1.915418  | -3.562234 | -1.131373 |
| 38 | 1  | 0  | 1.600556  | -2.263750 | -2.295986 |
| 39 | 1  | 0  | 5.115907  | -0.058664 | -1.192437 |
| 40 | 1  | 0  | 5.837236  | -1.679098 | -1.339882 |
| 41 | 1  | 0  | 5.553702  | -0.693313 | -2.809783 |
| 42 | 1  | 0  | -0.499753 | 0.054999  | 0.960055  |
| 43 | 1  | 0  | -1.683065 | 1.811711  | -1.955361 |
| 44 | 1  | 0  | -1.257090 | 4.181049  | -2.465109 |
| 45 | 1  | 0  | 0.459998  | 5.439769  | -1.204338 |
| 46 | 1  | 0  | -0.908342 | -0.897352 | -2.543758 |
| 47 | 1  | 0  | -3.002331 | -1.781268 | -3.355962 |
| 48 | 1  | 0  | -5.111595 | -1.708813 | -2.246203 |
| 49 | 1  | 0  | -2.196220 | 0.728452  | 1.822489  |
| 50 | 1  | 0  | -4.298509 | 0.800129  | 3.045531  |
| 51 | 1  | 0  | -6.331770 | -1.104453 | -0.218871 |
| 52 | 1  | 0  | -6.385199 | -0.116569 | 2.043915  |
| 53 | 1  | 0  | 1.436855  | 0.723658  | 1.585747  |
| 54 | 1  | 0  | 3.093447  | 2.008255  | 2.821976  |
| 55 | 1  | 0  | 2.172678  | 5.518415  | 0.528647  |
|     |      |      |            |            |            |
|-----|------|------|-----------|-----------|-----------|
| 56  | 1    | 0    | 3.484517  | 4.414685  | 2.308800  |
| 8b  | (conformer 10) |      |            |            |            |
| 1   | 6    | 0    | -0.928788 | -4.413733 | -2.528365 |
| 2   | 8    | 0    | -0.341459 | -3.728544 | -1.404109 |
| 3   | 6    | 0    | -0.609799 | -2.413705 | -1.309754 |
| 4   | 6    | 0    | 0.066976  | -1.822353 | -0.063930 |
| 5   | 6    | 0    | -0.319782 | -2.549620 | 1.230176  |
| 6   | 6    | 0    | -1.809648 | -2.498777 | 1.502291  |
| 7   | 8    | 0    | -2.069918 | -2.181311 | 2.783523  |
| 8   | 6    | 0    | -3.463547 | -2.124309 | 3.148229  |
| 9   | 8    | 0    | -1.233045 | -1.791386 | -2.131927 |
| 10  | 8    | 0    | -2.664413 | -2.744484 | 0.685415  |
| 11  | 8    | 0    | -0.235544 | -0.456515 | 0.131600  |
| 12  | 6    | 0    | 0.338402  | 0.502619  | -0.797106 |
| 13  | 6    | 0    | -0.207479 | 1.875752  | -0.407081 |
| 14  | 6    | 0    | 0.633513  | 2.901753  | -0.033622 |
| 15  | 6    | 0    | -1.621390 | 2.124810  | -0.485660 |
| 16  | 6    | 0    | 0.140965  | 4.180889  | 0.311034  |
| 17  | 6    | 0    | -2.115665 | 3.422894  | -0.127895 |
| 18  | 6    | 0    | -1.205002 | 4.433690  | 0.275423  |
| 19  | 6    | 0    | 1.856486  | 0.386527  | -0.887710 |
| 20  | 6    | 0    | 2.409203  | 0.310882  | -2.150101 |
| 21  | 6    | 0    | 2.721813  | 0.329690  | 0.257014  |
| 22  | 6    | 0    | 3.801916  | 0.196811  | -2.353339 |
| 23  | 6    | 0    | 4.135237  | 0.196348  | 0.046919  |
| 24  | 6    | 0    | 4.647122  | 0.135779  | -1.275307 |
| 25  | 6    | 0    | 2.251998  | 0.403330  | 1.599361  |
| 26  | 6    | 0    | 3.123227  | 0.341999  | 2.661791  |
| 27  | 6    | 0    | 5.004017  | 0.134083  | 1.168857  |
| 28  | 6    | 0    | 4.513300  | 0.203357  | 2.449168  |
| 29  | 6    | 0    | -2.561494 | 1.152253  | -0.925336 |
| 30  | 6    | 0    | -3.904431 | 1.443786  | -0.993191 |
| 31  | 6    | 0    | -3.509416 | 3.683628  | -0.198640 |
| 32  | 6    | 0    | -4.388947 | 2.717017  | -0.620354 |
| 33  | 1    | 0    | 1.145542  | -1.966505 | -0.210517 |
| 34  | 1    | 0    | -0.579880 | -3.976922 | -3.464787 |
| 35  | 1    | 0    | -0.601740 | -5.447336 | -2.440961 |
| 36  | 1    | 0    | -2.015979 | -4.347469 | -2.478077 |
| 37  | 1    | 0    | -0.037124 | -3.602042 | 1.145049  |
| 38  | 1    | 0    | 0.230073  | -2.110370 | 2.061205  |
| 39  | 1    | 0    | -3.939275 | -3.092438 | 2.986202  |
| 40  | 1    | 0    | -3.475372 | -1.861613 | 4.203540  |
| 41  | 1    | 0    | -3.976697 | -1.365676 | 2.556610  |
| 42  | 1    | 0    | -0.052869 | 0.267522  | -1.790565 |
| 43  | 1    | 0    | 1.702053  | 2.737887  | -0.001667 |
| 44  | 1    | 0    | 0.839025  | 4.956692  | 0.604922  |
|   |   |   | 1.592566 | 5.411442 | 0.542797 |
|---|---|---|-----------|-----------|-----------|
| 45| 1 | 0 | -1.753311 | 0.340002 | -3.014237 |
| 46| 1 | 0 | 4.193227  | 0.148420  | -3.363164 |
| 47| 1 | 0 | 5.187520  | 0.039286  | -1.417048 |
| 48| 1 | 0 | 1.92067   | 0.511530  | 1.779153  |
| 49| 1 | 0 | 2.739637  | 0.404447  | 3.674183  |
| 50| 1 | 0 | 6.070088  | 0.033147  | -1.210820 |
| 51| 1 | 0 | -2.222061 | 0.167026  | -1.210820 |
| 52| 1 | 0 | -4.597545 | 0.683739  | -1.336397 |
| 53| 1 | 0 | -3.866714 | 4.669340  | 0.081707  |
| 54| 1 | 0 | -5.451091 | 2.929337  | -0.673668 |

**8b (conformer 11)**

|   |   |   | 3.095515 | -3.291315 | -1.463948 |
|---|---|---|-----------|-----------|-----------|
| 1 | 6 | 0 | 2.921010  | -2.237888 | -0.494738 |
| 2 | 6 | 0 | 2.128553  | -1.218256 | -0.857326 |
| 3 | 6 | 0 | 1.939400  | -0.184866 | 0.259886  |
| 4 | 6 | 0 | 3.004367  | -0.228188 | 1.352920  |
| 5 | 6 | 0 | 4.432727  | 0.008046  | 0.909504  |
| 6 | 6 | 0 | 4.496088  | 0.621730  | -0.293409 |
| 7 | 6 | 0 | 5.817295  | 0.916247  | -0.787770 |
| 8 | 6 | 0 | 1.577948  | -1.143766 | -1.931605 |
| 9 | 6 | 0 | 5.405419  | -0.281418 | 1.559273  |
| 10| 6 | 0 | 0.685613  | -0.447278 | 0.903652  |
| 11| 6 | 0 | -0.488192 | 0.101654  | 0.255553  |
| 12| 6 | 0 | -1.678840 | -0.673950 | 0.811849  |
| 13| 6 | 0 | -2.322218 | -0.222024 | 1.943816  |
| 14| 6 | 0 | -2.113948 | -1.896590 | 0.198379  |
| 15| 6 | 0 | -3.393863 | -0.933425 | 2.525219  |
| 16| 6 | 0 | -3.212309 | -2.609386 | 0.786452  |
| 17| 6 | 0 | -3.830861 | -2.102404 | 1.957948  |
| 18| 6 | 0 | -0.586777 | 1.612022  | 0.451659  |
| 19| 6 | 0 | 0.047294  | 2.220702  | 1.513118  |
| 20| 6 | 0 | -1.349100 | 2.411689  | -0.462141 |
| 21| 6 | 0 | -0.023568 | 3.617310  | 1.718213  |
| 22| 6 | 0 | -1.413315 | 3.829028  | -0.254273 |
| 23| 6 | 0 | -0.734901 | 4.405852  | 0.851011  |
| 24| 6 | 0 | -2.059175 | 1.867870  | -1.568078 |
| 25| 6 | 0 | -2.773753 | 2.674259  | -2.422749 |
| 26| 6 | 0 | -2.158697 | 4.631573  | -1.157229 |
| 27| 6 | 0 | -2.824391 | 4.071125  | -2.219663 |
| 28| 6 | 0 | -1.523110 | -2.444600 | -0.974006 |
| 29| 6 | 0 | -1.989495 | -3.613650 | -1.529818 |
| 30| 6 | 0 | -3.665223 | -3.814208 | 0.187431  |
| 31| 6 | 0 | -3.071183 | -4.309663 | -0.946790 |
| 32| 6 | 0 | 1.923430  | 0.795931  | -0.221613 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 34 | 1 | 0 | 3.790556 | -3.991686 | -1.007063 |
| 35 | 1 | 0 | 2.139972 | -3.775330 | -1.668012 |
| 36 | 1 | 0 | 3.503659 | -2.888111 | -2.391289 |
| 37 | 1 | 0 | 2.768925 | 0.545842 | 2.089665 |
| 38 | 1 | 0 | 2.974283 | -1.183112 | 1.877325 |
| 39 | 1 | 0 | 6.337233 | 1.586884 | -0.102739 |
| 40 | 1 | 0 | 6.394475 | 0.586892 | -0.897560 |
| 41 | 1 | 0 | 5.665769 | 1.394093 | -1.752938 |
| 42 | 1 | 0 | -0.398940 | 0.090973 | -0.813636 |
| 43 | 1 | 0 | -2.004175 | 0.706519 | 2.400681 |
| 44 | 1 | 0 | -3.870054 | -0.544355 | 3.418091 |
| 45 | 1 | 0 | -4.657820 | -2.654081 | 2.392981 |
| 46 | 1 | 0 | 0.609668 | 1.608969 | 2.207486 |
| 47 | 1 | 0 | 2.974283 | -1.183112 | 1.877325 |
| 48 | 1 | 0 | 6.337233 | 1.586884 | -0.102739 |
| 49 | 1 | 0 | 6.394475 | 0.586892 | -0.897560 |
| 50 | 1 | 0 | 5.665769 | 1.394093 | -1.752938 |
| 51 | 1 | 0 | -0.398940 | 0.090973 | -0.813636 |
| 52 | 1 | 0 | -2.004175 | 0.706519 | 2.400681 |
| 53 | 1 | 0 | -3.870054 | -0.544355 | 3.418091 |
| 54 | 1 | 0 | -4.657820 | -2.654081 | 2.392981 |
| 55 | 1 | 0 | -0.398940 | 0.090973 | -0.813636 |
| 56 | 1 | 0 | -2.004175 | 0.706519 | 2.400681 |

8b (conformer 12)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | -2.071475 | 0.099938 | 3.736416 |
| 2  | 8 | 0 | -1.713375 | 0.081461 | 2.339816 |
| 3  | 6 | 0 | -2.342390 | 0.973899 | 1.566020 |
| 4  | 6 | 0 | -1.974236 | 0.863401 | 0.075864 |
| 5  | 6 | 0 | -3.240473 | 0.843471 | -0.783874 |
| 6  | 6 | 0 | -4.115988 | -0.365180 | -0.521821 |
| 7  | 8 | 0 | -4.793741 | -0.721803 | -1.632125 |
| 8  | 6 | 0 | -5.715413 | -1.819052 | -1.481978 |
| 9  | 8 | 0 | -3.087075 | 1.830433 | 1.977848 |
| 10 | 8 | 0 | -4.234991 | -0.924091 | 0.540359 |
| 11 | 8 | 0 | -1.201344 | -0.264155 | -0.277159 |
| 12 | 6 | 0 | 0.212283 | -0.209573 | -0.002965 |
| 13 | 6 | 0 | 0.769431 | -1.613638 | -0.207773 |
| 14 | 6 | 0 | 0.017123 | -2.579694 | -0.838943 |
| 15 | 6 | 0 | 2.080786 | -1.943217 | 0.269697 |
| 16 | 6 | 0 | 0.515319 | -3.887348 | -1.040151 |
| 17 | 6 | 0 | 2.577856 | -3.272624 | 0.066346 |
| 18 | 6 | 0 | 1.767836 | -4.228191 | -0.600503 |
| 19 | 6 | 0 | 0.888382 | 0.843534 | -0.889372 |
| 20 | 6 | 0 | 1.044558 | 0.568892 | -2.232798 |
| 21 | 6 | 0 | 1.316156 | 2.114506 | -0.380566 |
| 22 | 6 | 0 | 1.614820 | 1.501915 | -3.122099 |
| 23 | 6 | 0 | 1.904471 | 3.059628 | -1.289470 |
| 24 | 6 | 0 | 2.040061 | 2.722246 | -2.658897 |
| 25 | 6 | 0 | 1.194721 | 2.505691 | -0.584247 |
| 26 | 6 | 0 | 1.622643 | 3.737104 | -1.420664 |
| 27 | 6 | 0 | 2.336652 | 4.322358 | -0.803241 |
| 28 | 6 | 0 | 2.022222 | 4.658813 | 0.520390  |
| 29 | 6 | 0 | 2.922191 | -1.018094| 0.946688  |
| 30 | 6 | 0 | 4.170796 | -1.380686| 1.395965  |
| 31 | 6 | 0 | 3.872073 | -3.612545| 0.540328  |
| 32 | 6 | 0 | 4.655028 | -2.691378| 1.191984  |
| 33 | 1 | 0 | 1.439102 | 1.791786 | -0.160359 |
| 34 | 1 | 0 | 1.469506 | -0.678652| 4.199182  |
| 35 | 1 | 0 | 1.851744 | -1.074157| 4.175091  |
| 36 | 1 | 0 | -3.133847| -0.117957| 3.848273  |
| 37 | 1 | 0 | -3.836999| 1.731870 | -0.556454 |
| 38 | 1 | 0 | -2.965985| 0.881901 | -1.837817 |
| 39 | 1 | 0 | -5.186204| -2.719792| -1.168730 |
| 40 | 1 | 0 | -6.479137| -1.575880| -0.742030 |
| 41 | 1 | 0 | -6.162679| -1.957904| -2.463675 |
| 42 | 1 | 0 | 0.343677 | 0.039783 | 1.050123  |
| 43 | 1 | 0 | -0.980634| -2.332343| -1.173530 |
| 44 | 1 | 0 | -0.106974| -4.619983| -1.542059 |
| 45 | 1 | 0 | 2.155173 | -5.230692| -0.749736 |
| 46 | 1 | 0 | 0.726957 | -0.395442| -2.612301 |
| 47 | 1 | 0 | 1.721871 | 1.245431 | -4.170027 |
| 48 | 1 | 0 | 2.486810 | 3.445040 | -3.33579  |
| 49 | 1 | 0 | 0.753088 | 1.829053 | 1.704365  |
| 50 | 1 | 0 | 1.511725 | 4.004532 | 2.465492  |
| 51 | 1 | 0 | 2.777929 | 5.022161 | -1.505424 |
| 52 | 1 | 0 | 2.535399 | 5.626619 | 0.877236  |
| 53 | 1 | 0 | 2.587311 | -0.002810| 1.110209  |
| 54 | 1 | 0 | 4.789701 | -0.652607| 1.908432  |
| 55 | 1 | 0 | 4.233371 | -4.622812| 0.377481  |
| 56 | 1 | 0 | 5.641408 | -2.965285| 1.548981  |

8b (conformer 14)

| 1  | 6 | 0 | -1.767093 | 3.273737 | -3.583245 |
| 2  | 8 | 0 | -1.730190 | 2.772925 | -2.231123 |
| 3  | 6 | 0 | -0.586594 | 2.179092 | -1.847199 |
| 4  | 6 | 0 | -0.673364 | 1.756476 | -0.376309 |
| 5  | 6 | 0 | -0.315206 | 2.978829 | 0.480654  |
| 6  | 6 | 0 | -0.523852 | 2.728114 | 1.961333  |
| 7  | 8 | 0 | 0.482923 | 3.253188 | 2.685747  |
| 8  | 6 | 0 | 0.372943 | 3.113647 | 4.115439  |
| 9  | 8 | 0 | 0.374454 | 2.039581 | -2.563878 |
| 10 | 8 | 0 | -1.478469| 2.171600 | 2.444150  |
| 11 | 8 | 0 | 0.247189 | 0.742566 | -0.024704 |
|   |   |   |      |      |      |
|---|---|---|------|------|------|
| 12| 6 | 0 | 0.251639 | -0.486806 | -0.800445 |
| 13| 6 | 0 | 1.366603 | -1.353492 | -0.218952 |
| 14| 6 | 0 | 1.106665 | -2.574143 | 0.364587 |
| 15| 6 | 0 | 2.728602 | -0.908089 | -0.331883 |
| 16| 6 | 0 | 2.141084 | -3.384146 | 0.885701 |
| 17| 6 | 0 | 3.773364 | -1.732797 | 0.200813 |
| 18| 6 | 0 | 3.445093 | -2.969581 | 0.814296 |
| 19| 6 | 0 | -1.116180 | -1.147474 | -0.938064 |
| 20| 6 | 0 | -1.495840 | -1.518205 | -2.213122 |
| 21| 6 | 0 | -2.003832 | -1.414556 | 0.158201 |
| 22| 6 | 0 | -2.718916 | -2.173983 | 0.218952 |
| 23| 6 | 0 | -2.574143 | -2.076700 | -0.109128 |
| 24| 6 | 0 | -3.578388 | -2.447216 | -1.438673 |
| 25| 6 | 0 | -1.713735 | -1.058902 | 1.504150 |
| 26| 6 | 0 | -2.595136 | -1.343165 | 2.519962 |
| 27| 6 | 0 | -4.133603 | -2.357051 | 0.965807 |
| 28| 6 | 0 | -3.815891 | -2.001261 | 2.253461 |
| 29| 6 | 0 | 3.101070 | 0.305912 | -0.973108 |
| 30| 6 | 0 | 4.420800 | 0.681662 | -1.071257 |
| 31| 6 | 0 | 5.123492 | -1.307018 | 0.092642 |
| 32| 6 | 0 | 5.445057 | -0.125464 | -0.528599 |
| 33| 1 | 0 | -1.702983 | 1.449956 | -0.165660 |
| 34| 1 | 0 | -1.627319 | 2.456885 | -4.291934 |
| 35| 1 | 0 | -2.752671 | 3.718068 | -3.69653 |
| 36| 1 | 0 | -0.986224 | 4.020161 | -3.734252 |
| 37| 1 | 0 | 0.719304 | 3.269534 | 0.296398 |
| 38| 1 | 0 | -0.965825 | 3.814358 | 0.203484 |
| 39| 1 | 0 | 1.251984 | 3.607894 | 4.522591 |
| 40| 1 | 0 | -0.540014 | 3.589387 | 4.475885 |
| 41| 1 | 0 | 0.363637 | 2.058801 | 4.392339 |
| 42| 1 | 0 | 0.557439 | -0.220347 | -1.815692 |
| 43| 1 | 0 | 0.089436 | -2.935276 | 0.428806 |
| 44| 1 | 0 | 1.890757 | -4.335308 | 1.341933 |
| 45| 1 | 0 | 4.244846 | -3.584539 | 1.214148 |
| 46| 1 | 0 | -0.828791 | -1.308248 | -3.043157 |
| 47| 1 | 0 | -2.971783 | -2.455049 | -3.487665 |
| 48| 1 | 0 | -4.522882 | -2.948717 | -1.622760 |
| 49| 1 | 0 | -0.792066 | -0.541101 | 1.724860 |
| 50| 1 | 0 | -2.354738 | -1.046729 | 3.534329 |
| 51| 1 | 0 | -5.070662 | -2.859316 | 0.748436 |
| 52| 1 | 0 | -4.501159 | -2.217998 | 3.065334 |
| 53| 1 | 0 | 2.337963 | 0.948346 | -1.389780 |
| 54| 1 | 0 | 4.677166 | 1.609407 | -1.570943 |
| 55| 1 | 0 | 5.901104 | -1.940671 | 0.506893 |
| 56| 1 | 0 | 6.480318 | 0.187095 | -0.608496 |
|   |   |   | x  | y  | z    |
|---|---|---|----|----|------|
| 1 | 6 | 0 | 1.805647 | -3.895972 | 2.589944 |
| 2 | 8 | 0 | 1.446922 | -3.503077 | 1.250260 |
| 3 | 6 | 0 | 1.236516 | -2.188000 | 1.054027 |
| 4 | 6 | 0 | 0.810536 | -1.933724 | -0.399474 |
| 5 | 6 | 0 | 1.779519 | -2.525366 | -1.433708 |
| 6 | 6 | 0 | 3.113037 | -1.808739 | -1.534772 |
| 7 | 8 | 0 | 3.663582 | -1.616410 | -0.319625 |
| 8 | 6 | 0 | 4.912018 | -0.897608 | -0.292878 |
| 9 | 8 | 0 | 1.306560 | -1.363130 | 1.930026 |
|10 | 8 | 0 | 3.639039 | -1.482052 | -2.568467 |
|11 | 8 | 0 | 0.666171 | -0.563769 | -0.714845 |
|12 | 6 | 0 | -0.463050 | 0.150292 | -0.151854 |
|13 | 6 | 0 | -0.255106 | 1.624255 | -0.501652 |
|14 | 6 | 0 | -0.989161 | 2.221561 | -1.503610 |
|15 | 6 | 0 | 0.714507 | 2.405307 | 0.214907 |
|16 | 6 | 0 | -0.811170 | 3.788014 | -0.128678 |
|17 | 6 | 0 | 0.101308 | 4.348251 | -1.173839 |
|18 | 6 | 0 | -1.794225 | -0.418389 | -0.631237 |
|19 | 6 | 0 | -1.886988 | -1.003387 | -1.876982 |
|20 | 6 | 0 | -2.962849 | -0.340133 | 0.194983 |
|21 | 6 | 0 | -3.100922 | -1.545672 | -2.353986 |
|22 | 6 | 0 | -4.193042 | -0.895341 | -0.291548 |
|23 | 6 | 0 | -4.229665 | -1.497208 | -1.575811 |
|24 | 6 | 0 | -2.973961 | 0.279206 | 1.476213 |
|25 | 6 | 0 | -4.120398 | 0.331306 | 2.233582 |
|26 | 6 | 0 | -5.357051 | -0.826346 | 0.518764 |
|27 | 6 | 0 | -5.325699 | -0.228824 | 1.754541 |
|28 | 6 | 0 | 1.521052 | 1.878114 | 1.260080 |
|29 | 6 | 0 | 2.419995 | 2.673475 | 1.933265 |
|30 | 6 | 0 | 1.821182 | 4.576738 | 0.583988 |
|31 | 6 | 0 | 2.574556 | 4.036443 | 1.596953 |
|32 | 6 | 0 | -0.145684 | -2.462237 | -0.512678 |
|33 | 6 | 0 | 2.739629 | -3.416940 | 2.885316 |
|34 | 1 | 0 | 1.018036 | -3.617533 | 3.290998 |
|35 | 1 | 0 | 1.923276 | -4.976516 | 2.553225 |
|36 | 1 | 0 | 1.967783 | -3.573934 | -1.190408 |
|37 | 1 | 0 | 1.319713 | -2.478662 | -2.420078 |
|38 | 1 | 0 | 5.674661 | -1.439881 | -0.853286 |
|39 | 1 | 0 | 4.781691 | 0.095673 | -0.723041 |
|40 | 1 | 0 | 5.183032 | -0.825911 | 0.757938 |
|41 | 1 | 0 | -0.408967 | 0.040280 | 0.931800 |
|42 | 1 | 0 | -1.729438 | 1.644418 | -2.041901 |
|43 | 1 | 0 | -1.407750 | 4.008541 | -2.645830 |
|44 | 1 | 0 | 0.239500 | 5.394488 | -1.426584 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 46 | 1 | 0 | -1.003852 | -1.041866 | -2.504066 |
| 47 | 1 | 0 | -3.132665 | -1.998425 | -3.386979 |
| 48 | 1 | 0 | -5.165987 | -1.913481 | -1.932436 |
| 49 | 1 | 0 | -2.071478 | 0.732175  | 2.504066  |
| 50 | 1 | 0 | -4.100664 | 0.811057  | 3.205657  |
| 51 | 1 | 0 | -6.279193 | -1.253544 | 0.138381  |
| 52 | 1 | 0 | -6.222300 | -0.180637 | 2.362104  |
| 53 | 1 | 0 | 1.443037  | 0.833093  | 1.525004  |
| 54 | 1 | 0 | 3.019169  | 2.245824  | 2.729790  |
| 55 | 1 | 0 | 1.932996  | 5.621356  | 0.311893  |
| 56 | 1 | 0 | 3.287777  | 4.650275  | 2.135855  |

8b (conformer 16)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6  | 0 | 3.601604 | -0.240938 | 3.392607 |
| 2  | 8  | 0 | 2.618876 | 0.240802  | 2.454339 |
| 3  | 6  | 0 | 3.095345 | 0.639475  | 1.271941 |
| 4  | 6  | 0 | 2.013028 | 1.133879  | 0.293155 |
| 5  | 6  | 0 | 2.348763 | 2.536866  | -0.168773|
| 6  | 6  | 0 | 1.543504 | 2.942605  | -1.383481|
| 7  | 8  | 0 | 1.498263 | 4.279914  | -1.510441|
| 8  | 6  | 0 | 0.791229 | 4.786884  | -2.660595|
| 9  | 8  | 0 | 4.267839 | 0.636554  | 0.975255 |
| 10 | 8  | 0 | 1.023859 | 2.181403  | -2.167172|
| 11 | 8  | 0 | 0.712804 | 1.094830  | 0.847738 |
| 12 | 6  | 0 | -0.265200| 0.241489  | 0.212682 |
| 13 | 6  | 0 | 0.105770 | -1.240101 | 0.346960 |
| 14 | 6  | 0 | -0.043349| -1.851130 | 1.575080 |
| 15 | 6  | 0 | 0.627828 | -1.997309 | -0.754675|
| 16 | 6  | 0 | 0.301655 | -3.201621 | 1.781347 |
| 17 | 6  | 0 | 0.965740 | -3.378074 | -0.541765|
| 18 | 6  | 0 | 0.792278 | -3.952599 | 0.741858 |
| 19 | 6  | 0 | -1.614503| 0.573519  | 0.837623 |
| 20 | 6  | 0 | -1.680030| 1.244464  | 2.039736 |
| 21 | 6  | 0 | -2.828120| 0.188747  | 0.178540 |
| 22 | 6  | 0 | -2.919745| 1.554191  | 2.644080 |
| 23 | 6  | 0 | -4.082135| 0.510702  | 0.794975 |
| 24 | 6  | 0 | -4.095747| 1.195420  | 2.038008 |
| 25 | 6  | 0 | -2.858052| -0.497037 | -1.067071|
| 26 | 6  | 0 | -4.047467| -0.837770 | -1.668009|
| 27 | 6  | 0 | -5.290928| 0.142287  | 0.148128 |
| 28 | 6  | 0 | -5.279463| -0.516613 | -1.056866|
| 29 | 6  | 0 | 0.833660 | -1.463682 | -2.060740|
| 30 | 6  | 0 | 1.328947 | -2.240835 | -3.081548|
| 31 | 6  | 0 | 1.474325 | -4.149210 | -1.620797|
| 32 | 6  | 0 | 1.651710 | -3.599055 | -2.865357|
| 33 | 1  | 0 | 2.090392 | 0.444394  | -0.567720|
| 34 | 1  | 0 | 4.328394 | 0.540644  | 3.617357|
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 35| 1 | 0 | 3.040057 | -0.512751 | 4.283354 |
| 36| 1 | 0 | 4.120787 | -1.108702 | 2.984431 |
| 37| 1 | 0 | 2.170432 | 3.250543 | 0.638256 |
| 38| 1 | 0 | 3.490911 | 2.598252 | -0.433330 |
| 39| 1 | 0 | 1.258387 | 4.432408 | -3.580184 |
| 40| 1 | 0 | -0.250241 | 4.464677 | -2.636596 |
| 41| 1 | 0 | 0.860434 | 2.598252 | -0.433330 |
| 42| 1 | 0 | -0.305782 | 0.519599 | -0.840625 |
| 43| 1 | 0 | -0.441753 | -1.277206 | 2.403041 |
| 44| 1 | 0 | 0.166883 | -3.644275 | 2.761977 |
| 45| 1 | 0 | 1.258387 | -4.995819 | 0.886892 |
| 46| 1 | 0 | -0.250241 | 1.432160 | 2.495358 |
| 47| 1 | 0 | 1.051974 | -4.995819 | 0.886892 |
| 48| 1 | 0 | -0.759913 | 1.546342 | 2.521176 |
| 49| 1 | 0 | 0.616723 | -0.423623 | -2.267229 |
| 50| 1 | 0 | 1.477607 | -1.802774 | -4.062188 |
| 51| 1 | 0 | 1.723427 | -5.189740 | -1.439295 |
| 52| 1 | 0 | 0.616723 | -0.423623 | -2.267229 |
| 53| 1 | 0 | 1.477607 | -1.802774 | -4.062188 |
| 54| 1 | 0 | 1.723427 | -5.189740 | -1.439295 |
| 55| 1 | 0 | 2.041497 | -4.199026 | -3.679852 |
| 56| 1 | 0 | 2.041497 | -4.199026 | -3.679852 |

**8b (conformer 19)**

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.138205 | -2.873467 | 3.246006 |
| 2 | 8 | 0 | -1.243246 | -1.803239 | 2.284479 |
| 3 | 6 | 0 | -1.159263 | -0.916246 | 0.992239 |
| 4 | 6 | 0 | -1.303700 | -0.948643 | 0.057783 |
| 5 | 6 | 0 | -2.059462 | -1.330559 | -1.208862 |
| 6 | 6 | 0 | -3.482619 | -1.752293 | -0.932470 |
| 7 | 8 | 0 | -4.136595 | -2.027770 | -2.076673 |
| 8 | 6 | 0 | -5.504659 | -2.457911 | -1.937055 |
| 9 | 8 | 0 | -0.950160 | -3.290850 | 0.618778 |
| 10| 8 | 0 | -3.986822 | -1.836839 | 0.162768 |
| 11| 8 | 0 | -0.014809 | -0.506689 | -0.375016 |
| 12| 6 | 0 | 0.756607 | 0.253470 | 0.585907 |
| 13| 6 | 0 | 2.171774 | 0.411760 | 0.027878 |
| 14| 6 | 0 | 2.727044 | 1.662369 | -0.139211 |
| 15| 6 | 0 | 2.976330 | -0.749350 | -0.242952 |
| 16| 6 | 0 | 4.054931 | 1.836889 | -0.589496 |
| 17| 6 | 0 | 4.326311 | -0.565529 | -0.692719 |
| 18| 6 | 0 | 4.837794 | 0.746896 | -0.863427 |
| 19| 6 | 0 | 0.053934 | 1.546747 | 0.988523 |
| 20| 6 | 0 | -0.064065 | 1.817990 | 2.335483 |
| 21| 6 | 0 | -0.498574 | 2.469748 | 0.037636 |
| 22| 6 | 0 | -0.701730 | 2.984423 | 2.811129 |
| 23| 6 | 0 | -1.160974 | 3.645602 | 0.525334 |

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|   |    |          |       |       |
|---|----|----------|-------|-------|
| 24| 6  | 0        | -1.244231 | 3.877125 | 1.922962 |
| 25| 6  | 0        | -0.417923 | 2.288120 | -1.372380 |
| 26| 6  | 0        | -0.965755 | 3.204161 | -2.239782 |
| 27| 6  | 0        | -1.718232 | 4.567295 | -0.400612 |
| 28| 6  | 0        | -1.626901 | 4.354409 | -1.753681 |
| 29| 6  | 0        | 2.515739  | -2.083474 | -0.070689 |
| 30| 6  | 0        | 3.332453  | -3.161541 | -0.322314 |
| 31| 6  | 0        | 5.139150  | -2.973451 | -0.769877 |
| 32| 6  | 0        | 4.658168  | -2.973451 | -0.769877 |
| 33| 1  | 0        | -1.825061 | -0.154476 | 0.597258  |
| 34| 1  | 0        | -1.252277 | -2.401152 | 4.218964  |
| 35| 1  | 0        | -1.929258 | -3.604791 | 3.077978  |
| 36| 1  | 0        | -0.167461 | -3.364407 | 3.165675  |
| 37| 1  | 0        | -2.065331 | -0.479977 | -1.894161 |
| 38| 1  | 0        | -1.541866 | -2.148949 | -1.715890 |
| 39| 1  | 0        | -5.857435 | -2.631847 | -2.951029 |
| 40| 1  | 0        | -5.562110 | -3.375166 | -1.349187 |
| 41| 1  | 0        | -6.099429 | -1.684148 | -1.449986 |
| 42| 1  | 0        | 0.842397  | -0.347108 | 1.500156  |
| 43| 1  | 0        | 2.141544  | 2.543440  | 0.085509  |
| 44| 1  | 0        | 4.460343  | 2.840622  | -0.711501 |
| 45| 1  | 0        | 5.859920  | 0.869895  | -1.206285 |
| 46| 1  | 0        | 0.338369  | 1.110676  | 3.052987  |
| 47| 1  | 0        | -0.769199 | 3.160283  | 3.878665  |
| 48| 1  | 0        | -1.746961 | 4.771724  | 2.275398  |
| 49| 1  | 0        | 0.082662  | 1.413756  | -1.762274 |
| 50| 1  | 0        | -0.886817 | 3.043448  | -3.309343 |
| 51| 1  | 0        | -2.218372 | 5.449803  | -0.015232 |
| 52| 1  | 0        | -2.055735 | 5.066302  | -2.449986 |
| 53| 1  | 0        | 1.496987  | -2.265256 | 0.234699  |
| 54| 1  | 0        | 2.947429  | -4.165754 | -0.184649 |
| 55| 1  | 0        | 6.155999  | -1.540098 | -1.294988 |
| 56| 1  | 0        | 5.289480  | -3.831843 | -0.970368 |

8b (conformer 20)

|   |    |          |       |       |
|---|----|----------|-------|-------|
| 1 | 6  | 0        | 0.907333 | 4.566318 | 2.375797 |
| 2 | 8  | 0        | 1.219413 | 3.517438 | 1.436135 |
| 3 | 6  | 0        | 0.174867 | 2.817570 | 0.956627 |
| 4 | 6  | 0        | 0.659952 | 1.779570 | -0.066313 |
| 5 | 6  | 0        | 0.911930 | 2.491297 | -1.408285 |
| 6 | 6  | 0        | 1.789055 | 1.710062 | -2.367005 |
| 7 | 8  | 0        | 3.006177 | 1.486644 | -1.828448 |
| 8 | 6  | 0        | 3.957289 | 0.801127 | -2.665154 |
| 9 | 8  | 0        | -0.969435 | 3.010849 | 1.284948 |
| 10| 8  | 0        | 1.476288 | 1.370868 | -3.480308 |
| 11| 8  | 0        | -0.289585 | 0.763121 | -0.315538 |
| 12| 6  | 0        | -0.616484 | -0.115159 | 0.793874 |
|   |   |   |   |   |
|---|---|---|---|---|
| 13 | 6 | 0 | -1.766104 | -1.021378 | 0.345995 |
| 14 | 6 | 0 | -1.644971 | -2.393955 | 0.393411 |
| 15 | 6 | 0 | -3.021486 | -0.447755 | -0.059559 |
| 16 | 6 | 0 | -2.700969 | -3.251778 | 0.012444 |
| 17 | 6 | 0 | -4.086320 | -1.324280 | -0.454881 |
| 18 | 6 | 0 | -3.924204 | -2.728991 | -0.415483 |
| 19 | 6 | 0 | 0.615314  | 0.825786  | 1.344537  |
| 20 | 6 | 0 | 0.852697  | -0.734824 | 2.700589  |
| 21 | 6 | 0 | 1.529544  | -1.568252 | 0.523207  |
| 22 | 6 | 0 | 1.963749  | -1.358616 | 3.310016  |
| 23 | 6 | 0 | 2.657315  | -2.201615 | 1.145478  |
| 24 | 6 | 0 | 2.849926  | -2.073297 | 2.545968  |
| 25 | 6 | 0 | 1.363708  | -1.731688 | -0.881140 |
| 26 | 6 | 0 | 2.247969  | -2.485043 | 0.161763  |
| 27 | 6 | 0 | 3.556993  | -2.959649 | 0.351016  |
| 28 | 6 | 0 | 3.357204  | -3.105991 | -0.062672 |
| 29 | 6 | 0 | 3.320376  | -0.775022 | -0.862750 |
| 30 | 6 | 0 | 5.382825  | 0.582007  | -0.863981 |
| 31 | 1 | 0 | 1.601675  | 1.368821  | 0.311235  |
| 32 | 1 | 0 | 0.416726  | 4.150912  | 3.256636  |
| 33 | 1 | 0 | 1.863906  | 5.009613  | 2.642026  |
| 34 | 1 | 0 | 0.253246  | 5.307718  | 1.915196  |
| 35 | 1 | 0 | -0.043229 | 2.681071  | -1.897259 |
| 36 | 1 | 0 | 1.413492  | 3.443477  | -1.215408 |
| 37 | 1 | 0 | 4.872527  | 0.748597  | -2.079871 |
| 38 | 1 | 0 | 3.598940  | -0.200153 | -2.902855 |
| 39 | 1 | 0 | 4.120056  | 1.359400  | 3.588117  |
| 40 | 1 | 0 | 1.005580  | 0.513264  | 1.602618  |
| 41 | 1 | 0 | -0.720632 | -2.841794 | 0.730747  |
| 42 | 1 | 0 | -2.555145 | -4.325086 | 0.058900  |
| 43 | 1 | 0 | -4.707161 | -3.379039 | -0.717423 |
| 44 | 1 | 0 | 0.162008  | -0.172057 | 3.320614  |
| 45 | 1 | 0 | 2.110293  | -1.264959 | 4.380054  |
| 46 | 1 | 0 | 3.708360  | -2.556000 | 3.001349  |
| 47 | 1 | 0 | 0.526413  | -1.258288 | -1.373715 |
| 48 | 1 | 0 | 2.088817  | -2.605562 | -2.683082 |
| 49 | 1 | 0 | 4.404267  | -3.432873 | 0.836568  |
| 50 | 1 | 0 | 4.045109  | -3.698022 | -1.592876 |
| 51 | 1 | 0 | -2.505943 | 1.638760  | 0.244560  |
| 52 | 1 | 0 | -6.120261 | -1.453822 | -1.167773 |
| 53 | 1 | 0 | -6.493834 | 0.989615  | -1.174898 |

8b (conformer 22) | 1 | 6 | 0 | -2.371980 | 0.350811 | 3.466581 |
| 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|
| 2 | 8 | 0 | -1.953553 | 0.230844 | 2.091967 |
| 3 | 6 | 0 | -2.466137 | 1.136989 | 1.246422 |
| 4 | 6 | 0 | -1.991772 | 0.959041 | -0.206315 |
| 5 | 6 | 0 | -3.184276 | 0.935436 | -1.175121 |
| 6 | 6 | 0 | -3.949896 | -0.373545 | -1.169483 |
| 7 | 8 | 0 | -4.360986 | -0.701204 | 0.072678 |
| 8 | 6 | 0 | -5.077544 | -1.943668 | 0.197198 |
| 9 | 8 | 0 | -3.191542 | 2.041317 | 1.580825 |
| 10 | 8 | 0 | -4.189866 | -1.036916 | -2.147534 |
| 11 | 8 | 0 | -1.229890 | -0.201775 | -0.455759 |
| 12 | 6 | 0 | 0.160765 | -0.192401 | -0.075693 |
| 13 | 6 | 0 | 0.688785 | -1.607032 | -0.284796 |
| 14 | 6 | 0 | -0.016407 | 2.509060 | 1.051606 |
| 15 | 6 | 0 | 1.921072 | -2.012119 | 0.325592 |
| 16 | 6 | 0 | 0.453448 | -3.826576 | -1.256531 |
| 17 | 6 | 0 | 2.385759 | -3.353313 | 0.122141 |
| 18 | 6 | 0 | 1.626747 | -4.242181 | -0.682679 |
| 19 | 6 | 0 | 0.933435 | 0.864464 | -0.873119 |
| 20 | 6 | 0 | 1.166188 | 0.635522 | -2.214146 |
| 21 | 6 | 0 | 1.378717 | 2.094466 | -0.284912 |
| 22 | 6 | 0 | 1.834347 | 1.575406 | -3.024552 |
| 23 | 6 | 0 | 2.068749 | 3.045075 | -1.112893 |
| 24 | 6 | 0 | 2.281488 | 2.755020 | -2.483318 |
| 25 | 6 | 0 | 1.177188 | 2.440678 | 1.082465 |
| 26 | 6 | 0 | 1.626616 | 3.633997 | 1.596401 |
| 27 | 6 | 0 | 2.521217 | 4.267005 | -0.547515 |
| 28 | 6 | 0 | 2.309104 | 4.559907 | 0.776292 |
| 29 | 6 | 0 | 2.714562 | -1.151497 | 1.133170 |
| 30 | 6 | 0 | 3.884309 | -1.587874 | 1.710787 |
| 31 | 6 | 0 | 3.597774 | -3.770486 | 0.732242 |
| 32 | 6 | 0 | 4.333627 | -2.911754 | 1.511617 |
| 33 | 1 | 0 | -1.413912 | 1.865041 | -0.428483 |
| 34 | 1 | 0 | -2.083411 | 1.322303 | 3.869956 |
| 35 | 1 | 0 | -3.454171 | 0.239301 | 3.540275 |
| 36 | 1 | 0 | -1.865239 | -0.453665 | 3.994604 |
| 37 | 1 | 0 | -3.866033 | 1.747646 | -0.910043 |
| 38 | 1 | 0 | -2.823518 | 1.091921 | -2.190526 |
| 39 | 1 | 0 | -4.443549 | -2.777532 | -0.106741 |
| 40 | 1 | 0 | -5.337813 | -2.025542 | 1.250152 |
| 41 | 1 | 0 | -5.976131 | -1.928597 | -0.420667 |
| 42 | 1 | 0 | 0.216080 | 0.022457 | 0.991242 |
| 43 | 1 | 0 | -0.954392 | -2.204142 | -1.495012 |
| 44 | 1 | 0 | -0.128078 | -4.506391 | -1.869275 |
| 45 | 1 | 0 | 1.990193 | 5.233497 | 0.832441 |
| 46 | 1 | 0 | 0.833093 | -0.297008 | -2.654474 |
|   |   |   |     |     |     |
|---|---|---|-----|-----|-----|
| 47 | 1 | 0 | 1.998539 | 1.355748 | -4.073372 |
| 48 | 1 | 0 | 2.803644 | 3.482045 | -3.096444 |
| 49 | 1 | 0 | 0.655039 | 1.759815 | 1.742124 |
| 50 | 1 | 0 | 1.453219 | 3.868142 | 2.640749 |
| 51 | 1 | 0 | 3.040810 | 4.971286 | -1.188962 |
| 52 | 1 | 0 | 2.658610 | 5.497158 | 1.193851 |
| 53 | 1 | 0 | 2.407784 | -0.127011 | 1.295124 |
| 54 | 1 | 0 | 4.468598 | -0.907922 | 2.320764 |
| 55 | 1 | 0 | 3.934469 | -4.789218 | 0.569533 |
| 56 | 1 | 0 | 5.257554 | -3.244151 | 1.971265 |

| 8b (conformer 25) |
|---|---|---|-----|-----|-----|
| 1 | 6 | 0 | -1.423730 | -2.315785 | 3.276665 |
| 2 | 8 | 0 | -1.341944 | -1.492944 | 2.093816 |
| 3 | 6 | 0 | -2.059153 | -1.914848 | 1.030951 |
| 4 | 6 | 0 | -1.804952 | -1.023322 | -0.192066 |
| 5 | 6 | 0 | -2.764926 | -1.351529 | -1.330667 |
| 6 | 6 | 0 | -4.234468 | -1.099628 | -1.066250 |
| 7 | 8 | 0 | -4.429991 | -0.255345 | -0.028097 |
| 8 | 6 | 0 | -5.802472 | 0.047959 | 0.288012 |
| 9 | 8 | 0 | -2.771930 | -2.885782 | 1.048952 |
| 10 | 8 | 0 | -5.131677 | -1.560728 | -1.724603 |
| 11 | 8 | 0 | -0.483986 | -1.283729 | -0.671195 |
| 12 | 6 | 0 | 0.571711 | -0.432592 | -0.177389 |
| 13 | 6 | 0 | 1.894982 | -1.110574 | -0.514889 |
| 14 | 6 | 0 | 1.936951 | -2.151795 | -1.416492 |
| 15 | 6 | 0 | 3.107378 | -0.675030 | 0.115140 |
| 16 | 6 | 0 | 3.152707 | -2.794473 | -1.744589 |
| 17 | 6 | 0 | 4.335524 | -1.336079 | -0.217438 |
| 18 | 6 | 0 | 4.326930 | -2.396495 | -1.160551 |
| 19 | 6 | 0 | 0.442665 | 0.973492 | -0.774944 |
| 20 | 6 | 0 | 0.749651 | 1.148159 | -2.109194 |
| 21 | 6 | 0 | -0.015824 | 2.095671 | -0.008490 |
| 22 | 6 | 0 | 0.630175 | 2.401236 | -2.742658 |
| 23 | 6 | 0 | -0.118691 | 3.375391 | -0.654726 |
| 24 | 6 | 0 | 0.210887 | 3.495452 | -2.027488 |
| 25 | 6 | 0 | -0.377285 | 2.024352 | 1.368216 |
| 26 | 6 | 0 | -0.796979 | 3.136809 | 2.058693 |
| 27 | 6 | 0 | -0.555328 | 4.502939 | 0.090767 |
| 28 | 6 | 0 | -0.884875 | 4.393215 | 1.418307 |
| 29 | 6 | 0 | 3.159535 | 0.381623 | 1.065451 |
| 30 | 6 | 0 | 4.344841 | 0.758425 | 1.653244 |
| 31 | 6 | 0 | 5.540981 | -0.920579 | 0.406600 |
| 32 | 6 | 0 | 5.550891 | 0.102336 | 1.323027 |
| 33 | 1 | 0 | -1.915245 | 0.021541 | 0.105106 |
| 34 | 1 | 0 | -2.452761 | -2.361865 | 3.634508 |
| 35 | 1 | 0 | -1.070901 | -3.324466 | 3.059772 |
|   |    |    |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 36| 1 | 0 | -0.781826 | -1.834698 |  4.011158 |
| 37| 1 | 0 | -2.483149 | -0.742431 | -2.194775 |
| 38| 1 | 0 | -2.662325 | -2.396508 | -1.625141 |
| 39| 1 | 0 | -5.761614 |  0.734147 |  1.131066 |
| 40| 1 | 0 | -6.294475 |  0.515581 | -0.565576 |
| 41| 1 | 0 | -6.337446 | -0.863434 |  0.557384 |
| 42| 1 | 0 |  0.492287 | -0.389431 |  0.908843 |
| 43| 1 | 0 |  1.016221 | -2.490544 | -1.871228 |
| 44| 1 | 0 |  3.144939 |  0.734147 |  1.131066 |
| 45| 1 | 0 |  6.294475 |  0.515581 | -0.565576 |
| 46| 1 | 0 |  6.337446 | -0.863434 |  0.557384 |
| 47| 1 | 0 |  0.492287 | -0.389431 |  0.908843 |
| 48| 1 | 0 |  1.016221 | -2.490544 | -1.871228 |
| 49| 1 | 0 |  3.144939 |  0.734147 |  1.131066 |
| 50| 1 | 0 |  6.294475 |  0.515581 | -0.565576 |
| 51| 1 | 0 |  6.337446 | -0.863434 |  0.557384 |
| 52| 1 | 0 |  0.492287 | -0.389431 |  0.908843 |
| 53| 1 | 0 |  1.016221 | -2.490544 | -1.871228 |
| 54| 1 | 0 |  3.144939 |  0.734147 |  1.131066 |
| 55| 1 | 0 |  6.294475 |  0.515581 | -0.565576 |
| 56| 1 | 0 |  6.337446 | -0.863434 |  0.557384 |

|   |    |    |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 8b (conformer 27) |   |    |   |   |   |   |   |
| 1 | 6 | 0 | -1.172250 | -4.471241 | -2.278564 |
| 2 | 8 | 0 | -0.501044 | -3.770748 | -1.212666 |
| 3 | 6 | 0 | -0.754061 | -2.452027 | -1.117839 |
| 4 | 6 | 0 |  0.059944 | -1.835316 |  0.028934 |
| 5 | 6 | 0 | -0.151630 | -2.534830 |  1.380465 |
| 6 | 6 | 0 | -1.508442 | -2.289781 |  2.011853 |
| 7 | 8 | 0 | -2.509700 | -2.543816 |  1.447747 |
| 8 | 6 | 0 | -3.845036 | -2.295691 |  1.625990 |
| 9 | 8 | 0 | -1.469247 | -1.850227 | -1.878893 |
|10 | 8 | 0 | -1.683041 | -1.945052 |  3.153316 |
|11 | 8 | 0 | -0.220312 | -0.465097 |  0.22507 |
|12 | 6 | 0 |  0.300283 |  0.473794 | -0.756051 |
|13 | 6 | 0 | -0.211324 |  1.857823 | -0.357671 |
|14 | 6 | 0 |  0.656058 |  2.868891 | -0.004486 |
|15 | 6 | 0 | -1.621425 |  2.132733 | -0.403677 |
|16 | 6 | 0 |  0.194715 |  4.157147 |  0.348540 |
|17 | 6 | 0 | -2.083791 |  3.441652 | -0.043665 |
|18 | 6 | 0 | -1.146499 |  4.435962 |  0.338400 |
|19 | 6 | 0 |  1.809521 |  0.350721 | -0.943212 |
|20 | 6 | 0 |  2.278066 |  0.280081 | -2.239592 |
|21 | 6 | 0 |  2.748473 |  0.292125 |  0.142175 |
|22 | 6 | 0 |  3.654495 |  0.171440 | -2.534942 |
|23 | 6 | 0 |  4.145571 |  0.164515 | -0.161959 |
|24 | 6 | 0 |  4.569192 |  0.110172 | -1.515219 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 25 | 6 | 0 | 2.369419 | 0.359430 | 1.513436 |   |
| 26 | 6 | 0 | 3.309820 | 0.295823 | 2.515091 |   |
| 27 | 6 | 0 | 5.087407 | 0.101277 | 0.899305 |   |
| 28 | 6 | 0 | 4.682987 | 0.162967 | 2.209761 |   |
| 29 | 6 | 0 | -2.588736 | 1.175254 | -0.815990 |   |
| 30 | 6 | 0 | -3.926490 | 1.494005 | -0.863442 |   |
| 31 | 6 | 0 | 4.682987 | 0.162967 | 2.209761 |   |
| 32 | 6 | 0 | -2.588736 | 1.175254 | -0.815990 |   |
| 33 | 6 | 0 | -3.926490 | 1.494005 | -0.863442 |   |
| 34 | 6 | 0 | 4.682987 | 0.162967 | 2.209761 |   |
| 35 | 6 | 0 | -2.588736 | 1.175254 | -0.815990 |   |
| 36 | 6 | 0 | -3.926490 | 1.494005 | -0.863442 |   |
| 37 | 6 | 0 | 4.682987 | 0.162967 | 2.209761 |   |
| 38 | 6 | 0 | -2.588736 | 1.175254 | -0.815990 |   |
| 39 | 6 | 0 | -3.926490 | 1.494005 | -0.863442 |   |
| 40 | 6 | 0 | 4.682987 | 0.162967 | 2.209761 |   |
| 41 | 6 | 0 | -2.588736 | 1.175254 | -0.815990 |   |
| 42 | 6 | 0 | -3.926490 | 1.494005 | -0.863442 |   |
| 43 | 1 | 0 | 1.721769 | 2.686084 | 0.003985 |   |
| 44 | 1 | 0 | -1.509831 | 5.421611 | 0.610448 |   |
| 45 | 1 | 0 | 1.566945 | 0.311316 | -3.058901 |   |
| 46 | 1 | 0 | 3.978418 | 0.127675 | -3.568567 |   |
| 47 | 1 | 0 | 5.629212 | 0.017724 | -1.727515 |   |
| 48 | 1 | 0 | 1.324241 | 0.464860 | 1.766168 |   |
| 49 | 1 | 0 | 2.993241 | 0.351795 | 3.550671 |   |
| 50 | 1 | 0 | 6.139662 | 0.004734 | 0.652499 |   |
| 51 | 1 | 0 | 5.412350 | 0.114174 | 3.010474 |   |
| 52 | 1 | 0 | -2.273434 | 0.180539 | -1.097172 |   |
| 53 | 1 | 0 | -4.641827 | 0.748012 | -1.192484 |   |
| 54 | 1 | 0 | -3.805704 | 4.723395 | 0.191443 |   |
| 55 | 1 | 0 | -5.437614 | 3.012880 | -0.528684 |   |
| 56 | 1 | 0 | 1.019327 | 0.864050 | -0.815990 |   |

**8b (conformer 31)**

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.104912 | -4.425177 | 1.752236 |   |
| 2 | 6 | 0 | -3.037528 | -3.095580 | 1.197637 |   |
| 3 | 6 | 0 | -1.939828 | -2.811157 | 0.466755 |   |
| 4 | 6 | 0 | -2.021588 | -1.374063 | -0.071183 |   |
| 5 | 6 | 0 | -3.133505 | -1.275065 | -1.126003 |   |
| 6 | 6 | 0 | -3.374741 | 0.143066 | -1.606071 |   |
| 7 | 6 | 0 | -3.632369 | 0.968847 | -0.572972 |   |
| 8 | 6 | 0 | -3.877125 | 2.349978 | -0.905866 |   |
| 9 | 6 | 0 | -1.037471 | -3.584862 | 0.278282 |   |
| 10 | 6 | 0 | -3.375127 | 0.490659 | -2.760541 |   |
| 11 | 6 | 0 | -0.825058 | -0.978735 | -0.700719 |   |
| 12 | 6 | 0 | 0.318240 | -0.759372 | 0.148995 |   |
| 13 | 6 | 0 | 1.560645 | -0.757019 | -0.746809 |   |
|     |   |   |            |            |            |
|-----|---|---|------------|------------|------------|
| 14  | 6 | 0 | 1.422014   | -0.861548  | -2.114498  |
| 15  | 6 | 0 | 2.878628   | -0.718688  | -0.179620  |
| 16  | 6 | 0 | 2.541237   | -0.885817  | -2.975400  |
| 17  | 6 | 0 | 4.011177   | -0.740185  | -1.061458  |
| 18  | 6 | 0 | 3.810006   | -0.816152  | -2.463148  |
| 19  | 6 | 0 | 0.099033   | 0.466013   | 1.043544   |
| 20  | 6 | 0 | -0.069700  | 0.242194   | 2.395295   |
| 21  | 6 | 0 | 0.114158   | 2.147608   | 3.314382   |
| 22  | 6 | 0 | -0.280829  | 0.885817   | 2.975400   |
| 23  | 6 | 0 | -0.182579  | 2.879399   | 1.486122   |
| 24  | 6 | 0 | -0.325691  | 2.588232   | 2.867928   |
| 25  | 6 | 0 | 0.114158   | 2.147608   | 3.314382   |
| 26  | 6 | 0 | -0.244362  | 4.217880   | 1.016357   |
| 27  | 6 | 0 | 0.045872   | 3.455005   | -1.250441  |
| 28  | 6 | 0 | -0.128451  | 4.504731   | 2.300473   |
| 29  | 6 | 0 | 3.137480   | -0.686428  | 1.218603   |
| 30  | 6 | 0 | 4.420689   | -0.662045  | 1.713390   |
| 31  | 6 | 0 | 5.321968   | -0.703694  | -0.517391  |
| 32  | 6 | 0 | 5.529054   | -0.664040  | 0.839201   |
| 33  | 1 | 0 | -2.267540  | -0.717302  | 0.770567   |
| 34  | 1 | 0 | -4.043334  | -4.463215  | 2.300473   |
| 35  | 1 | 0 | -3.093462  | -5.169934  | 0.955591   |
| 36  | 1 | 0 | -2.261046  | -4.600776  | 2.420434   |
| 37  | 1 | 0 | -2.875281  | -1.879948  | 1.995639   |
| 38  | 1 | 0 | -4.063931  | -1.652163  | 0.694242   |
| 39  | 1 | 0 | -4.106233  | 2.838474   | 0.038359   |
| 40  | 1 | 0 | -2.987429  | 2.789968   | -1.356470  |
| 41  | 1 | 0 | -4.716849  | 2.430151   | -1.597194  |
| 42  | 1 | 0 | 0.415857   | -1.624435  | 0.813721   |
| 43  | 1 | 0 | 0.429950   | -0.928936  | -2.538345  |
| 44  | 1 | 0 | 2.383917   | -0.961280  | -4.045551  |
| 45  | 1 | 0 | 4.675734   | -0.831685  | -3.117002  |
| 46  | 1 | 0 | -0.022189  | -0.775420  | 2.771800   |
| 47  | 1 | 0 | -0.400546  | 1.068634   | 4.368145   |
| 48  | 1 | 0 | -0.476554  | 3.408238   | 3.562304   |
| 49  | 1 | 0 | 0.237770   | 1.362683   | -1.558324  |
| 50  | 1 | 0 | 0.125486   | 3.681093   | -2.307954  |
| 51  | 1 | 0 | -0.386904  | 5.014376   | 1.739484   |
| 52  | 1 | 0 | -0.174401  | 5.531339   | -0.667413  |
| 53  | 1 | 0 | 2.313409   | -0.675373  | 1.916262   |
| 54  | 1 | 0 | 4.581904   | -0.639955  | 2.785530   |
| 55  | 1 | 0 | 6.164409   | -0.714824  | -1.201369  |
| 56  | 1 | 0 | 6.536061   | -0.639709  | 1.240141   |

**8b (conformer 42)**

|     |   |   |            |            |
|-----|---|---|------------|------------|
| 1   | 6 | 0 | -1.964722  | -2.328237  | -3.271418  |
| 2   | 8 | 0 | -1.284557  | -1.732618  | -2.148262  |
|   |   |   |                  |                  |                  |
|---|---|---|------------------|------------------|------------------|
| 3 | 6 | 0 | 0.538581        | -2.567669        | -1.409653        |
| 4 | 6 | 0 | 0.116733        | -1.911439        | -0.181898        |
| 5 | 6 | 0 | -0.242267       | -2.697748        | 1.086592         |
| 6 | 8 | 0 | -1.719353       | -2.609611        | 1.415451         |
| 7 | 8 | 0 | -1.925742       | -2.480364        | 2.738649         |
| 8 | 6 | 0 | -3.02319        | -2.415083        | 3.159215         |
| 9 | 8 | 0 | -0.339824       | -3.725957        | -1.688979        |
| 10| 8 | 0 | -2.612343       | -2.682364        | 0.603141         |
| 11| 8 | 0 | -0.206017       | -0.557330        | 0.075512         |
| 12| 6 | 0 | 0.356362        | 0.457367         | -0.793637        |
| 13| 6 | 0 | -0.173917       | 1.813243         | -0.318241        |
| 14| 6 | 0 | 0.695229        | 2.834739         | 0.003114         |
| 15| 6 | 0 | -1.589693       | 2.066732         | -0.282007        |
| 16| 6 | 0 | 0.236487        | 4.110112         | 0.402663         |
| 17| 6 | 0 | -2.048813       | 3.363331         | 0.128929         |
| 18| 6 | 0 | -1.107150       | 4.367247         | 0.473212         |
| 19| 6 | 0 | 1.873035        | 0.341909         | -0.905937        |
| 20| 6 | 0 | 2.419175        | 0.319504         | -2.172885        |
| 21| 6 | 0 | 2.742937        | 0.230195         | 0.231869         |
| 22| 6 | 0 | 3.810426        | 0.205472         | -2.387929        |
| 23| 6 | 0 | 4.154711        | 0.099613         | 0.009205         |
| 24| 6 | 0 | 4.659814        | 0.093462         | -1.317256        |
| 25| 6 | 0 | 2.278901        | 0.246582         | 1.577842         |
| 26| 6 | 0 | 3.155083        | 0.134782         | 2.632579         |
| 27| 6 | 0 | 5.028255        | -0.015895        | 1.122864         |
| 28| 6 | 0 | 4.543367        | -0.003070        | 2.407576         |
| 29| 6 | 0 | -2.570473       | 1.106310         | -0.656097        |
| 30| 6 | 0 | -3.913213       | 1.405815         | -0.614035        |
| 31| 6 | 0 | -3.442193       | 3.632644         | 0.170555         |
| 32| 6 | 0 | -4.359649       | 2.677247         | -0.192033        |
| 33| 1 | 0 | 1.195333        | -2.025961        | -0.345157        |
| 34| 1 | 0 | -1.247803       | -2.789108        | -3.952232        |
| 35| 1 | 0 | -2.668504       | -3.083498        | -2.919276        |
| 36| 1 | 0 | -2.491472       | -1.510541        | -3.759155        |
| 37| 1 | 0 | 0.002900        | -3.751692        | 0.927106         |
| 38| 1 | 0 | 0.349828        | -2.328029        | 1.922955         |
| 39| 1 | 0 | -3.795385       | -1.554588        | 2.704833         |
| 40| 1 | 0 | -3.832057       | -3.325658        | 2.874575         |
| 41| 1 | 0 | -3.270634       | -2.312073        | 4.241982         |
| 42| 1 | 0 | -0.045655       | 0.290483         | -1.798461        |
| 43| 1 | 0 | 1.762704        | 2.666808         | -0.047814        |
| 44| 1 | 0 | 0.958787        | 4.879163         | 0.653791         |
| 45| 1 | 0 | -1.470589       | 5.342726         | 0.780938         |
| 46| 1 | 0 | 1.759787        | 0.392679         | -3.032288        |
| 47| 1 | 0 | 4.197187        | 0.197296         | -3.400930        |
|      |      |      |       |       |       |
|------|------|------|-------|-------|-------|
| 48   | 1    | 0    | 5.730243 | -0.003652 | -1.468273 |
| 49   | 1    | 0    | 1.219865 | 0.348715  | 1.767417  |
| 50   | 1    | 0    | 2.776008 | 0.153418  | 3.648776  |
| 51   | 1    | 0    | 6.093237 | -0.115195 | 0.937774  |
| 52   | 1    | 0    | 5.221568 | -0.088515 | 3.249307  |
| 53   | 1    | 0    | -2.260232 | 0.119806 | -0.965162 |
| 54   | 1    | 0    | -4.636035 | 0.650618 | -0.904186 |
| 55   | 1    | 0    | -3.768741 | 4.617420 | 0.490258  |
| 56   | 1    | 0    | -5.421517 | 2.896550 | -0.159102 |
| **9b** (conformer 1) | | | | | |
| 1    | 6    | 0    | 2.029895 | 0.386649  | 1.748722  |
| 2    | 6    | 0    | 2.840791 | 0.624583  | 2.833008  |
| 3    | 6    | 0    | 2.534368 | -0.230966 | 0.571384  |
| 4    | 6    | 0    | 3.923406 | -0.585076 | 0.541719  |
| 5    | 6    | 0    | 4.730781 | -0.326147 | 1.679748  |
| 6    | 6    | 0    | 4.205211 | 0.262806  | 3.249307  |
| 7    | 6    | 0    | 1.724201 | -0.507503 | -0.577953 |
| 8    | 6    | 0    | 2.301392 | -1.089139 | -1.685370 |
| 9    | 6    | 0    | 3.673205 | -1.426955 | -1.714465 |
| 10   | 6    | 0    | 4.467005 | -1.184885 | -0.623873 |
| 11   | 6    | 0    | 0.232892 | -0.165978 | -0.580198 |
| 12   | 8    | 0    | -0.482819 | -0.901945 | -1.583766 |
| 13   | 6    | 0    | -0.041933 | 1.314609 | -0.839270 |
| 14   | 6    | 0    | 0.684308 | 1.970830  | -1.809532 |
| 15   | 6    | 0    | -1.066702 | 2.026481 | -0.131611 |
| 16   | 6    | 0    | -1.287114 | 3.410568 | -0.444943 |
| 17   | 6    | 0    | -0.512051 | 4.032354 | -1.455705 |
| 18   | 6    | 0    | 0.450083 | 3.324685  | -2.128150 |
| 19   | 6    | 0    | -1.882824 | 1.444081 | 0.877596  |
| 20   | 6    | 0    | -2.839114 | 2.176902 | 1.539828  |
| 21   | 6    | 0    | -3.042054 | 3.540008 | 1.233739  |
| 22   | 6    | 0    | -2.282154 | 4.137329 | 0.260010  |
| 23   | 6    | 0    | -0.751221 | -2.275132 | -1.254639 |
| 24   | 6    | 0    | -1.080217 | -2.972450 | -2.573452 |
| 25   | 6    | 0    | -1.878778 | -2.415230 | -0.242508 |
| 26   | 6    | 0    | -3.074418 | -1.707066 | -0.406085 |
| 27   | 6    | 0    | -4.125782 | -1.877848 | 0.489893  |
| 28   | 6    | 0    | -3.996967 | -2.757782 | 1.564707  |
| 29   | 6    | 0    | -2.808165 | -3.461108 | 1.740584  |
| 30   | 6    | 0    | -1.756172 | -3.287305 | 0.841787  |
| 31   | 1    | 0    | 0.992931 | 0.692185  | 1.795957  |
| 32   | 1    | 0    | 2.430381 | 1.098890  | 3.717404  |
| 33   | 1    | 0    | 5.779545 | -0.602630 | 1.644125  |
| 34   | 1    | 0    | 4.833922 | 0.455655  | 3.664792  |
| 35   | 1    | 0    | 1.680065 | -1.291754 | -2.548676 |
| 36   | 1    | 0    | 4.090238 | -1.883320 | -2.605385 |

S383
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 37 | 1 | 0 | 5.519818 | -1.446873 | -0.635009 |
| 38 | 1 | 0 | -0.167535 | -0.442585 | 0.398113 |
| 39 | 1 | 0 | 1.464508 | 1.436718 | -2.337314 |
| 40 | 1 | 0 | -0.693403 | 5.077387 | -1.684394 |
| 41 | 1 | 0 | 1.042966 | 3.800777 | -2.900976 |
| 42 | 1 | 0 | -1.772731 | 0.397470 | 1.124931 |
| 43 | 1 | 0 | -3.446231 | 4.107433 | 1.764766 |
| 44 | 1 | 0 | -0.167535 | -0.442585 | 0.398113 |
| 45 | 1 | 0 | 1.464508 | 1.436718 | -2.337314 |
| 46 | 1 | 0 | -0.693403 | 5.077387 | -1.684394 |
| 47 | 1 | 0 | 1.042966 | 3.800777 | -2.900976 |
| 48 | 1 | 0 | -1.772731 | 0.397470 | 1.124931 |
| 49 | 1 | 0 | -3.446231 | 4.107433 | 1.764766 |
| 50 | 1 | 0 | -0.167535 | -0.442585 | 0.398113 |
| 51 | 1 | 0 | 1.464508 | 1.436718 | -2.337314 |
| 52 | 1 | 0 | -0.693403 | 5.077387 | -1.684394 |
| 53 | 1 | 0 | 1.042966 | 3.800777 | -2.900976 |
| 54 | 1 | 0 | -1.772731 | 0.397470 | 1.124931 |

**9b (conformer 3)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | -1.363974 | 1.714243 | -1.156361 |
| 2  | 6 | 0 | -2.046432 | 2.625584 | -1.926152 |
| 3  | 6 | 0 | -0.627072 | 2.115261 | -0.004932 |
| 4  | 6 | 0 | -0.630286 | 3.513305 | 0.328599 |
| 5  | 6 | 0 | -1.345127 | 4.426295 | -0.491353 |
| 6  | 6 | 0 | -2.037361 | 3.998743 | -1.595536 |
| 7  | 6 | 0 | 0.110078 | 1.210388 | 0.827571 |
| 8  | 6 | 0 | 0.772697 | 1.702225 | 1.933187 |
| 9  | 6 | 0 | 0.756536 | 3.071681 | 2.263306 |
| 10 | 6 | 0 | 0.073358 | 3.961373 | 1.473287 |
| 11 | 6 | 0 | 0.150088 | -0.303206 | 0.576364 |
| 12 | 8 | 0 | -0.632402 | -0.990998 | 1.562312 |
| 13 | 6 | 0 | 1.562876 | -0.878856 | 0.626775 |
| 14 | 6 | 0 | 1.948008 | -1.671370 | 1.686121 |
| 15 | 6 | 0 | 2.495535 | -0.615713 | -0.429625 |
| 16 | 6 | 0 | 3.808518 | -1.186760 | -0.351466 |
| 17 | 6 | 0 | 4.157756 | -1.988996 | 0.765442 |
| 18 | 6 | 0 | 3.246403 | -2.224556 | 1.760548 |
| 19 | 6 | 0 | 2.185451 | 0.180279 | -1.565838 |
| 20 | 6 | 0 | 3.108339 | 0.396277 | -2.561648 |
| 21 | 6 | 0 | 4.399158 | -0.169197 | -2.479659 |
| 22 | 6 | 0 | 4.736669 | -0.942041 | -1.396659 |
| 23 | 6 | 0 | -2.051842 | -0.887471 | 1.426320 |
| 24 | 6 | 0 | -2.635081 | -1.359883 | 2.757979 |
| 25 | 6 | 0 | -2.579987 | -1.705652 | 0.254724 |
| 26 | 6 | 0 | -3.700527 | -1.273046 | -0.459983 |
| 27 | 6 | 0 | -4.227448 | -2.044604 | -1.494153 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 28 | 6 | 0 | -3.631055 | -3.257187 | -1.833047 |
| 29 | 6 | 0 | -2.506884 | -3.691265 | -1.132486 |
| 30 | 6 | 0 | -1.986314 | -2.922565 | -0.094310 |
| 31 | 1 | 0 | -1.407295 | 0.669884 | -1.435316 |
| 32 | 1 | 0 | -2.599576 | 2.285413 | -2.794463 |
| 33 | 1 | 0 | -1.333311 | 5.477800 | -0.223497 |
| 34 | 1 | 0 | -2.578122 | 4.707277 | -2.212606 |
| 35 | 1 | 0 | 1.330653 | 1.015285 | 2.558514 |
| 36 | 1 | 0 | 1.294396 | 3.416444 | 3.139270 |
| 37 | 1 | 0 | 0.621199 | 5.019585 | 1.712471 |
| 38 | 1 | 0 | -0.259757 | -0.530488 | -0.411035 |
| 39 | 1 | 0 | 1.231056 | 1.879988 | 2.468095 |
| 40 | 1 | 0 | 5.155236 | 2.413228 | 0.813470 |
| 41 | 1 | 0 | 3.511643 | -2.841440 | 2.612064 |
| 42 | 1 | 0 | 1.209641 | 0.637749 | -1.654049 |
| 43 | 1 | 0 | 2.843179 | 1.009061 | -3.415955 |
| 44 | 1 | 0 | 5.118758 | 0.009557 | -3.270698 |
| 45 | 1 | 0 | 5.726114 | -1.381536 | -1.322510 |
| 46 | 1 | 0 | -2.330723 | 0.162720 | 1.274246 |
| 47 | 1 | 0 | -4.161514 | -0.322952 | -0.207801 |
| 48 | 1 | 0 | -5.098033 | -1.695484 | -2.038564 |
| 49 | 1 | 0 | -4.035550 | -3.856732 | -2.640825 |
| 50 | 1 | 0 | -2.033198 | -4.630601 | -1.395922 |
| 51 | 1 | 0 | -1.106896 | -3.254784 | 0.444969 |
| 52 | 1 | 0 | -2.348263 | -2.396923 | 2.947948 |
| 53 | 1 | 0 | -2.258286 | -0.736587 | 3.571682 |
| 54 | 1 | 0 | -3.725552 | -1.301746 | 2.739921 |

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 9b (conformer 5) | 1 | 6 | 0 | -1.082152 | -2.690709 | -1.261124 |
| 2 | 6 | 0 | -1.457766 | -3.918896 | -1.751406 |
| 3 | 6 | 0 | -1.502812 | -2.243814 | 0.020476 |
| 4 | 6 | 0 | -2.323273 | -3.126902 | 0.797383 |
| 5 | 6 | 0 | -2.691748 | -4.388501 | 0.261921 |
| 6 | 6 | 0 | -2.273048 | -4.779833 | -0.985086 |
| 7 | 6 | 0 | -1.150186 | -0.964424 | 0.566356 |
| 8 | 6 | 0 | -1.594719 | -0.628093 | 1.825914 |
| 9 | 6 | 0 | -2.391155 | -1.506174 | 2.593425 |
| 10 | 6 | 0 | -2.752023 | -2.727490 | 2.089230 |
| 11 | 6 | 0 | -0.266994 | -0.000681 | -0.227372 |
| 12 | 8 | 0 | 1.074914 | -0.488134 | -0.104418 |
| 13 | 6 | 0 | -0.394790 | 1.456891 | 0.213863 |
| 14 | 6 | 0 | 0.537747 | 1.999666 | 1.070695 |
| 15 | 6 | 0 | -1.478104 | 2.270136 | -0.252800 |
| 16 | 6 | 0 | -1.545753 | 3.640064 | 0.165040 |
| 17 | 6 | 0 | -0.554396 | 4.152336 | 1.041388 |
| 18 | 6 | 0 | 0.460861 | 3.347052 | 1.488552 |
|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 19| 6 | 0 | -2.506118 | 1.783210 | -1.106427 |
| 20| 6 | 0 | -3.523014 | 2.601626 | -1.537250 |
| 21| 6 | 0 | -3.575452 | 3.954502 | -1.135812 |
| 22| 6 | 0 | -2.608502 | 4.457080 | -0.301240 |
| 23| 6 | 0 | 2.036868  | 0.041881 | -1.030848 |
| 24| 6 | 0 | 1.979731  | -0.690956| -2.378444 |
| 25| 6 | 0 | 3.410261  | -0.082123| -0.395495 |
| 26| 6 | 0 | 3.687088  | -1.083167| 0.539394 |
| 27| 6 | 0 | 4.965201  | -1.207794| 1.080257 |
| 28| 6 | 0 | 5.981854  | -0.337031| 0.694257 |
| 29| 6 | 0 | 5.711879  | 0.666213 | -0.234427 |
| 30| 6 | 0 | 2.036868  | 0.041881 | -1.030848 |
| 31| 1 | 0 | -0.441112 | -2.061357| -1.861008 |
| 32| 1 | 0 | -1.120356 | -4.232446| -2.733158 |
| 33| 1 | 0 | -3.314844 | -5.042943| 0.862732 |
| 34| 1 | 0 | -2.561685 | -5.746477| -1.382105|
| 35| 1 | 0 | -1.334681 | 0.337226 | 2.240404 |
| 36| 1 | 0 | -2.717887 | -1.201131| 3.581099 |
| 37| 1 | 0 | -3.369854 | -3.406157| 2.668062 |
| 38| 1 | 0 | -0.562864 | -0.052608| -1.281530|
| 39| 1 | 0 | 1.350841  | 1.376163 | 1.421364 |
| 40| 1 | 0 | -0.616699 | 5.190056 | 1.351964 |
| 41| 1 | 0 | 1.215927  | 3.738259 | 2.161176 |
| 42| 1 | 0 | -2.505064 | 0.744896 | -1.412032|
| 43| 1 | 0 | -4.295631 | 2.204148 | -2.185842|
| 44| 1 | 0 | -4.382726 | 4.589416 | -1.483044|
| 45| 1 | 0 | -2.644595 | 5.492871 | 0.020308 |
| 46| 1 | 0 | 1.830112  | 1.105816 | -1.195756|
| 47| 1 | 0 | 2.891808  | -1.749087| 0.848689 |
| 48| 1 | 0 | 5.165811  | -1.987015| 1.807509 |
| 49| 1 | 0 | 6.975226  | -0.434984| 1.117706 |
| 50| 1 | 0 | 6.493556  | 1.355719 | -0.533862|
| 51| 1 | 0 | 4.228099  | 1.583004 | -1.488013|
| 52| 1 | 0 | 2.747208  | -0.301242| -3.051709|
| 53| 1 | 0 | 2.159255  | -1.758621| -2.233863|
| 54| 1 | 0 | 1.011491  | -0.554856| -2.868231|

**9b (conformer 9)**

|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.560898 | -0.656876| 1.352681 |
| 2 | 6 | 0 | 3.702751 | -0.893159| 2.080585 |
| 3 | 6 | 0 | 2.628850 | -0.178306| 0.013070 |
| 4 | 6 | 0 | 3.927513 | 0.047720 | -0.554426|
| 5 | 6 | 0 | 5.083765 | -0.204119| 0.230448|
| 6 | 6 | 0 | 4.974842 | -0.664167| 1.518722|
| 7 | 6 | 0 | 1.469326 | 0.077303 | -0.793644|
| 8 | 6 | 0 | 1.639828 | 0.533702 | -2.084204|
| 9 | 6 | 0 | 2.918735 | 0.744138 | -2.643158|

S386
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 10| 6 | 0 | 4.040297 | 0.509336 | -1.891076 |
| 11| 6 | 0 | 0.034205 | -0.129533 | -0.307293 |
| 12| 8 | 0 | -0.204474 | 0.406462 | 1.007913  |
| 13| 6 | 0 | -0.442053 | -1.583934 | -0.300148 |
| 14| 6 | 0 | 0.439605  | -2.630640 | -0.462322 |
| 15| 6 | 0 | -1.842821 | -1.873274 | -0.167104 |
| 16| 6 | 0 | -2.276776 | -3.239575 | -0.178400 |
| 17| 6 | 0 | -1.319837 | -4.276299 | -0.323545 |
| 18| 6 | 0 | 0.008189  | -3.975913 | -0.468252 |
| 19| 6 | 0 | -2.836412 | -0.865247 | -0.048348 |
| 20| 6 | 0 | -4.169893 | -1.183414 |  0.053990 |
| 21| 6 | 0 | -4.590873 | -2.531028 |  0.054138 |
| 22| 6 | 0 | -3.660286 | -3.533405 | -0.059213 |
| 23| 6 | 0 | 0.037540  |  1.818573 |  1.167370 |
| 24| 6 | 0 | 0.122717  |  2.060055 |  2.671792 |
| 25| 6 | 0 | -1.022054 |  2.673754 |  0.485877 |
| 26| 6 | 0 | -2.359135 |  2.640243 |  0.901726 |
| 27| 6 | 0 | -3.316505 |  3.438482 |  0.282866 |
| 28| 6 | 0 | -2.953350 |  4.286419 | -0.763735 |
| 29| 6 | 0 | -1.628004 |  4.328958 | -1.185872 |
| 30| 6 | 0 | -0.671776 |  3.525954 | -0.564287 |
| 31| 1 | 0 | 1.590373  | -0.827016 |  1.795466 |
| 32| 1 | 0 | 3.623507  | -1.260392 |  3.097822 |
| 33| 1 | 0 | 6.058399  | -0.027694 | -0.212799 |
| 34| 1 | 0 | 5.869600  | -0.854339 |  2.106319 |
| 35| 1 | 0 | 0.762758  |  0.736476 | -2.690266 |
| 36| 1 | 0 | 3.004760  |  1.098085 | -3.664282 |
| 37| 1 | 0 | 5.029545  |  0.673154 | -2.305498 |
| 38| 1 | 0 | -0.602786 |  0.416385 | -1.015810 |
| 39| 1 | 0 | 1.493794  | -2.430540 | -0.594360 |
| 40| 1 | 0 | -1.660175 | -5.306647 | -0.328155 |
| 41| 1 | 0 | 0.740480  | -4.765973 | -0.590786 |
| 42| 1 | 0 | -2.539680 |  0.172551 | -0.029725 |
| 43| 1 | 0 | -4.905521 | -0.390829 |  0.136560 |
| 44| 1 | 0 | -5.645003 | -2.769132 |  0.140476 |
| 45| 1 | 0 | -3.970326 | -4.573379 | -0.065957 |
| 46| 1 | 0 | 1.005603  |  2.064437 |  0.716778 |
| 47| 1 | 0 | -2.651621 |  1.983972 |  1.713599 |
| 48| 1 | 0 | -4.346944 |  3.403405 |  0.619272 |
| 49| 1 | 0 | -3.699580 |  4.909053 | -1.244381 |
| 50| 1 | 0 | -1.336566 |  4.984515 | -1.999082 |
| 51| 1 | 0 | 0.360560  |  3.561650 | -0.897376 |
| 52| 1 | 0 | 0.287751  |  3.120087 |  2.877943 |
| 53| 1 | 0 | -0.800215 |  1.749803 |  3.166486 |
| 54| 1 | 0 | 0.949056  |  1.486189 |  3.095024 |
|    |    |    | 1      | 6      | 0  | 1.365757 | -1.815672 | -1.747420 |
|----|----|----|--------|--------|----|----------|------------|------------|
| 2  | 6  | 0  | -2.084805 | -2.589739 | -2.626838 |
| 3  | 6  | 0  | -1.572444 | -1.898314 | -0.343358 |
| 4  | 6  | 0  | -2.558848 | -2.828681 | 0.127847 |
| 5  | 6  | 0  | -3.289242 | -3.606136 | -0.808228 |
| 6  | 6  | 0  | -3.061796 | -3.493198 | -2.156795 |
| 7  | 6  | 0  | -0.838527 | -1.119656 | 0.613627 |
| 8  | 6  | 0  | -1.081716 | -1.316397 | 1.955759 |
| 9  | 6  | 0  | -2.052042 | -2.233404 | 2.415482 |
| 10 | 6  | 0  | -2.782092 | -2.969908 | 1.521104 |
| 11 | 6  | 0  | 0.250253  | -0.125308 | 0.170673 |
| 12 | 8  | 0  | 1.057854  | 0.292907  | 1.278931 |
| 13 | 6  | 0  | -0.237413 | 1.130056  | 0.557480 |
| 14 | 6  | 0  | 0.204133  | 1.327650  | -1.849674 |
| 15 | 6  | 0  | 1.517241  | 3.232350  | -0.754714 |
| 16 | 6  | 0  | 1.093400  | 2.113923  | 0.038739 |
| 17 | 6  | 0  | 1.517241  | 3.232350  | -0.754714 |
| 18 | 6  | 0  | -0.201923 | 2.436102  | 2.623378 |
| 19 | 6  | 0  | -1.530383 | 2.059036  | 1.389420 |
| 20 | 6  | 0  | -2.357277 | 3.023385  | 1.913236 |
| 21 | 6  | 0  | -2.796250 | 4.105091  | 1.119009 |
| 22 | 6  | 0  | -2.378435 | 4.205808  | 0.183869 |
| 23 | 6  | 0  | 2.161766  | -0.570818 | 1.584382 |
| 24 | 6  | 0  | 2.658702  | -0.153225 | 2.967359 |
| 25 | 6  | 0  | 3.264183  | -0.484500 | 0.537530 |
| 26 | 6  | 0  | 3.981622  | -1.625409 | 0.170099 |
| 27 | 6  | 0  | 5.029168  | -1.543906 | 0.745897 |
| 28 | 6  | 0  | 5.365773  | -0.316616 | -1.311553 |
| 29 | 6  | 0  | 4.648565  | 0.825813  | -0.957595 |
| 30 | 6  | 0  | 3.606125  | 0.743243  | -0.038460 |
| 31 | 1  | 0  | -0.636332 | -1.124051 | 2.141147 |
| 32 | 1  | 0  | -1.902195 | 2.502535  | -3.692117 |
| 33 | 1  | 0  | -4.034278 | -4.300051 | 0.432828 |
| 34 | 1  | 0  | -3.626350 | -4.094491 | 2.860454 |
| 35 | 1  | 0  | -0.507968 | -0.750660 | 2.678023 |
| 36 | 1  | 0  | -2.212556 | -2.347295 | 3.481814 |
| 37 | 1  | 0  | -3.532063 | -3.675482 | 1.862655 |
| 38 | 1  | 0  | 0.895243  | -0.652192 | 0.541472 |
| 39 | 1  | 0  | 0.887728  | 0.609771  | -2.290961 |
| 40 | 1  | 0  | -1.389275 | 4.213915  | 2.676177 |
| 41 | 1  | 0  | 0.165556  | 2.543302  | 3.637684 |
| 42 | 1  | 0  | -1.186134 | 1.254852  | 2.019046 |
| 43 | 1  | 0  | 2.672358  | 2.955910  | 2.948642 |
| 44 | 1  | 0  | -3.452516 | 4.856705  | 1.543326 |
| 45 | 1  | 0  | -2.695688 | 5.040496  | -0.800473 |
|   |   |   |          |          |          |          |
|---|---|---|----------|----------|----------|----------|
| 46| 1 | 0 | 1.806303 | -1.608971| 1.630459 |
| 47| 1 | 0 | 3.717102 | -2.586390| 0.601092 |
| 48| 1 | 0 | 5.575618 | -2.438908| -1.022248|
| 49| 1 | 0 | 4.901426 | 1.783480 | -1.399313|
| 50| 1 | 0 | 3.037587 | 1.626814 | 0.226470 |
| 51| 1 | 0 | 6.177510 | 0.250856 | -2.027381|
| 52| 1 | 0 | 4.901426 | 1.783480 | -1.399313|
| 53| 1 | 0 | 3.037587 | 1.626814 | 0.226470 |
| 54| 1 | 0 | 2.969509 | 0.893862 | 2.953316 |

9b (conformer 17)

|   |   |   |          |          |          |          |
|---|---|---|----------|----------|----------|----------|
| 1 | 6 | 0 | 1.743284 | -1.859005| -1.328039|
| 2 | 6 | 0 | 2.659065 | -2.742321| -1.847737|
| 3 | 6 | 0 | 1.321571 | -1.945250| 0.026527 |
| 4 | 6 | 0 | 1.867872 | -3.001206| 0.830505 |
| 5 | 6 | 0 | 2.816538 | -3.891222| 0.262409 |
| 6 | 6 | 0 | 3.208281 | -3.766993| -1.046621|
| 7 | 6 | 0 | 0.369437 | -1.049459| 0.617702 |
| 8 | 6 | 0 | -0.027180| -1.266213| 1.921720 |
| 9 | 6 | 0 | 0.507575 | -2.308669| 2.709619 |
|10 | 6 | 0 | 1.445016 | -3.153047| 2.176183 |
|11 | 6 | 0 | -0.290511| 0.108444 | -0.144338|
|12 | 6 | -0.106532| -0.379319| -1.246327|
|13 | 6 | 0 | 0.644954 | 1.197972 | -0.682078|
|14 | 6 | 0 | 0.719431 | 1.425387 | -2.040044|
|15 | 6 | 0 | 1.396938 | 2.039408 | 0.205177 |
|16 | 6 | 0 | 2.235454 | 3.061498 | -0.354361|
|17 | 6 | 0 | 2.296435 | 3.229426 | -1.760873|
|18 | 6 | 0 | 1.545949 | 2.432762 | -2.583709|
|19 | 6 | 0 | 1.341708 | 1.941048 | 1.622487 |
|20 | 6 | 0 | 2.070169 | 2.780342 | 2.431483 |
|21 | 6 | 0 | 2.905849 | 3.771153 | 1.873496 |
|22 | 6 | 0 | 2.981785 | 3.904279 | 0.510006 |
|23 | 6 | 0 | -2.231308| -1.136995| -0.904823 |
|24 | 6 | 0 | -2.698709| -1.793657| -2.202705|
|25 | 6 | 0 | -3.316448| -0.273801| -0.276091|
|26 | 6 | 0 | -4.103567| -0.775318| 0.763469 |
|27 | 6 | 0 | -5.135944| -0.013201| 1.308043 |
|28 | 6 | 0 | -5.386091| 1.268279 | 0.823355 |
|29 | 6 | 0 | -4.598673| 1.781378 | -0.206667 |
|30 | 6 | 0 | -3.572995| 1.015385 | -0.753984|
|31 | 6 | 0 | 1.327105 | -1.091386| -1.960499|
|32 | 6 | 0 | 2.962287 | -2.652105| -2.884931|
|33 | 6 | 0 | 3.224369 | -4.679780| 0.886383 |
|34 | 6 | 0 | 3.932546 | -4.454423| -1.469084|
|35 | 6 | 0 | -0.775630| -0.613786| 2.360698 |
|36 | 6 | 0 | 0.171433 | -2.433104| 3.732798 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 37 |  1  |  0 |  1.869604 | -3.955919 |  2.769787 |
| 38 |  1  |  0 | -0.970726 |  0.596486 |  0.565767 |
| 39 |  1  |  0 |  0.120799 |  0.816330 | -2.702819 |
| 40 |  1  |  0 |  2.936729 |  4.004644 | -2.168525 |
| 41 |  1  |  0 |  1.578294 |  2.568535 | -3.659082 |
| 42 |  1  |  0 |  0.720434 |  1.187682 |  2.082245 |
| 43 |  1  |  0 |  2.003571 |  2.678200 |  3.508983 |
| 44 |  1  |  0 |  3.479943 |  4.423719 |  2.521590 |
| 45 |  1  |  0 |  3.614630 |  4.666173 |  0.066614 |
| 46 |  1  |  0 | -1.955964 | -1.922648 | -0.190805 |
| 47 |  1  |  0 | -3.905699 | -1.770161 |  1.151219 |
| 48 |  1  |  0 | -5.738218 | -0.417203 |  2.114354 |
| 49 |  1  |  0 | -6.184548 |  1.865936 |  1.248591 |
| 50 |  1  |  0 | -4.783506 |  2.781375 | -0.583484 |
| 51 |  1  |  0 | -2.954585 |  1.418535 | -1.547746 |
| 52 |  1  |  0 | -3.580255 | -2.412062 | -2.019884 |
| 53 |  1  |  0 | -2.960294 | -1.032083 | -2.941296 |
| 54 |  1  |  0 | -1.903366 | -2.420815 | -2.610927 |

**10b (conformer 1)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  |  6  |  0 | -1.987038 | -0.516155 | -0.496772 |
| 2  |  6  |  0 | -2.964752 | -1.109623 | -1.518035 |
| 3  |  8  |  0 | -0.708861 | -0.992774 | -0.859600 |
| 4  |  8  |  0 | -2.784763 | -2.102341 | -2.168720 |
| 5  |  6  |  0 |  0.410005 | -0.328652 | -0.251540 |
| 6  |  6  |  0 |  1.632104 | -1.208075 | -0.499886 |
| 7  |  6  |  0 |  1.562189 | -2.241891 | -1.408672 |
| 8  |  6  |  0 |  2.852005 | -0.976962 |  0.215562 |
| 9  |  6  |  0 |  2.676952 | -3.072691 | -1.662626 |
| 10 |  6  |  0 |  3.975866 | -1.828952 | -0.043310 |
| 11 |  6  |  0 |  3.857899 | -2.871864 | -0.998059 |
| 12 |  6  |  0 |  0.558268 |  1.088258 | -0.820353 |
| 13 |  6  |  0 |  0.959061 |  1.219587 | -2.133971 |
| 14 |  6  |  0 |  0.246036 |  2.264473 | -0.062754 |
| 15 |  6  |  0 |  1.083476 |  2.479615 | -2.751584 |
| 16 |  6  |  0 |  0.385992 |  3.548175 | -0.693759 |
| 17 |  6  |  0 |  0.808101 |  3.622203 | -2.043740 |
| 18 |  6  |  0 | -0.197875 |  2.243572 |  1.290761 |
| 19 |  6  |  0 | -0.474897 |  3.403559 |  1.973862 |
| 20 |  6  |  0 |  0.092237 |  4.725436 |  0.043914 |
| 21 |  6  |  0 | -0.326967 |  4.661157 |  1.348289 |
| 22 |  6  |  0 |  3.009115 |  0.052301 |  1.183309 |
| 23 |  6  |  0 |  4.196200 |  0.228723 |  1.854054 |
| 24 |  6  |  0 |  5.186884 | -1.616585 |  0.665289 |
| 25 |  6  |  0 |  5.299724 | -0.612396 |  1.594350 |
| 26 |  1  |  0 |  0.243917 | -0.286594 |  0.828016 |
| 27 |  1  |  0 |  0.628492 | -2.422658 | -1.923815 |
|   |   |   | x1   | y1   | z1   |
|---|---|---|------|------|------|
| 28| 1 | 0 | 2.584375 | -3.874691 | -2.386462 |
| 29| 1 | 0 | 4.716461 | -3.508089 | -1.186133 |
| 30| 1 | 0 | 1.193180 | 0.327355  | -2.702487 |
| 31| 1 | 0 | 1.405375 | 2.538179  | -3.785127 |
| 32| 1 | 0 | 0.909045 | 4.598330  | -2.506475 |
| 33| 1 | 0 | -0.335280 | 1.299973  | 1.801615  |
| 34| 1 | 0 | -0.812568 | 3.351544  | 0.302871  |
| 35| 1 | 0 | 0.206094 | 5.684999  | -0.449828 |
| 36| 1 | 0 | 0.909045 | 4.598330  | -2.506475 |
| 37| 1 | 0 | 2.187149 | 0.721693  | 1.397573  |
| 38| 1 | 0 | 4.286368 | 1.023146  | 2.586493  |
| 39| 1 | 0 | 6.028168 | -2.269911 | 0.457817  |
| 40| 1 | 0 | 6.231172 | -0.462400 | 2.128574  |
| 41| 1 | 0 | -2.409972 | -0.939233 | 0.907495  |
| 42| 6 | 0 | -3.198161 | -0.100876 | 1.699272  |
| 43| 6 | 0 | -2.035597 | -2.193434 | 1.397914  |
| 44| 6 | 0 | -3.605749 | -0.509043 | 2.967568  |
| 45| 6 | 0 | -2.438534 | -2.597289 | 2.668150  |
| 46| 6 | 0 | -3.225274 | -1.757740 | 3.455101  |
| 47| 1 | 0 | -3.491581 | 0.872695  | 1.321976  |
| 48| 1 | 0 | -1.423236 | -2.840421 | 0.781391  |
| 49| 1 | 0 | -4.215185 | 0.149966  | 3.576000  |
| 50| 1 | 0 | -2.139612 | -3.569842 | 3.042932  |
| 51| 1 | 0 | -3.538033 | -2.074057 | 4.443890  |
| 52| 8 | 0 | -4.086369 | -0.363822 | -1.558169 |
| 53| 6 | 0 | -5.134015 | -0.859010 | -2.413145 |
| 54| 6 | 0 | -4.789349 | -0.911189 | -3.446765 |
| 55| 1 | 0 | -5.450278 | -1.852260 | -2.091039 |
| 56| 1 | 0 | -5.949684 | -0.146387 | -2.315724 |
| 57| 6 | 0 | -1.976431 | -0.156035 | -0.109790 |
| 58| 6 | 0 | -2.113594 | 0.409824  | -1.534455 |
| 59| 8 | 0 | -0.847434 | -0.991161 | 0.021200  |
| 60| 8 | 0 | -1.512410 | 0.023257  | -2.504436 |
| 61| 6 | 0 | 0.456201 | -0.394369 | -0.124149 |
| 62| 6 | 0 | 0.654922 | 0.741044  | 0.887099  |
| 63| 6 | 0 | 0.743122 | 0.414719  | 2.224741  |
| 64| 6 | 0 | 0.697460 | 2.120869  | 0.499286  |
| 65| 6 | 0 | 0.880017 | 1.398770  | 3.223877  |
| 66| 6 | 0 | 0.848700 | 3.120038  | 1.520987  |
| 67| 6 | 0 | 0.935641 | 2.725463  | 2.878712  |
| 68| 6 | 0 | 1.472522 | -1.520820 | 0.039680  |
| 69| 6 | 0 | 1.089037 | -2.728765 | 0.580201  |
| 70| 6 | 0 | 2.831550 | -1.336774 | -0.377621 |
| 71| 6 | 0 | 2.008547 | -3.789428 | 0.742095  |

**10b (conformer 2)**

|   |   |   | x1   | y1   | z1   |
|---|---|---|------|------|------|
| 1 | 6 | 0 | -1.976431 | -0.156035 | -0.109790 |
| 2 | 6 | 0 | -2.113594 | 0.409824  | -1.534455 |
| 3 | 8 | 0 | -0.847434 | -0.991161 | 0.021200  |
| 4 | 8 | 0 | -1.512410 | 0.023257  | -2.504436 |
| 5 | 6 | 0 | 0.456201 | -0.394369 | -0.124149 |
| 6 | 6 | 0 | 0.654922 | 0.741044  | 0.887099  |
| 7 | 6 | 0 | 0.743122 | 0.414719  | 2.224741  |
| 8 | 6 | 0 | 0.697460 | 2.120869  | 0.499286  |
| 9 | 6 | 0 | 0.880017 | 1.398770  | 3.223877  |
| 10| 6 | 0 | 0.848700 | 3.120038  | 1.520987  |
| 11| 6 | 0 | 0.935641 | 2.725463  | 2.878712  |
| 12| 6 | 0 | 1.472522 | -1.520820 | 0.039680  |
| 13| 6 | 0 | 1.089037 | -2.728765 | 0.580201  |
| 14| 6 | 0 | 2.831550 | -1.336774 | -0.377621 |
| 15| 6 | 0 | 2.008547 | -3.789428 | 0.742095  |
|   |   |   |            |            |            |
|---|---|---|------------|------------|------------|
| 16| 6 | 0 | 3.757471   | -2.419627  | -0.215380  |
| 17| 6 | 0 | 3.313740   | -3.640690  | 0.354471   |
| 18| 6 | 0 | 3.316591   | -0.132117  | -0.955624  |
| 19| 6 | 0 | 4.627374   | -0.003633  | -1.349498  |
| 20| 6 | 0 | 5.103635   | -2.252162  | -0.631762  |
| 21| 6 | 0 | 5.534219   | -1.073049  | -1.187063  |
| 22| 6 | 0 | 0.601795   | 2.570395   | -0.849382  |
| 23| 6 | 0 | 0.661689   | 3.906612   | -1.166240  |
| 24| 6 | 0 | 3.313740   | -3.640690  | 0.354471   |
| 25| 6 | 0 | 3.316591   | -0.132117  | -0.955624  |
| 26| 6 | 0 | 4.627374   | -0.003633  | -1.349498  |
| 27| 6 | 0 | 5.103635   | -2.252162  | -0.631762  |
| 28| 6 | 0 | 5.534219   | -1.073049  | -1.187063  |
| 29| 6 | 0 | 0.601795   | 2.570395   | -0.849382  |
| 30| 6 | 0 | 0.661689   | 3.906612   | -1.166240  |
| 31| 6 | 0 | 3.313740   | -3.640690  | 0.354471   |
| 32| 6 | 0 | 3.316591   | -0.132117  | -0.955624  |
| 33| 6 | 0 | 4.627374   | -0.003633  | -1.349498  |
| 34| 6 | 0 | 5.103635   | -2.252162  | -0.631762  |
| 35| 6 | 0 | 5.534219   | -1.073049  | -1.187063  |
| 36| 6 | 0 | 0.601795   | 2.570395   | -0.849382  |
| 37| 6 | 0 | 0.661689   | 3.906612   | -1.166240  |
| 38| 6 | 0 | 3.313740   | -3.640690  | 0.354471   |
| 39| 6 | 0 | 3.316591   | -0.132117  | -0.955624  |
| 40| 6 | 0 | 4.627374   | -0.003633  | -1.349498  |
| 41| 6 | 0 | 5.103635   | -2.252162  | -0.631762  |
| 42| 6 | 0 | 5.534219   | -1.073049  | -1.187063  |
| 43| 6 | 0 | 0.601795   | 2.570395   | -0.849382  |
| 44| 6 | 0 | 0.661689   | 3.906612   | -1.166240  |
| 45| 6 | 0 | 3.313740   | -3.640690  | 0.354471   |
| 46| 6 | 0 | 3.316591   | -0.132117  | -0.955624  |
| 47| 6 | 0 | 4.627374   | -0.003633  | -1.349498  |
| 48| 6 | 0 | 5.103635   | -2.252162  | -0.631762  |
| 49| 6 | 0 | 5.534219   | -1.073049  | -1.187063  |
| 50| 6 | 0 | 0.601795   | 2.570395   | -0.849382  |
| 51| 6 | 0 | 0.661689   | 3.906612   | -1.166240  |
| 52| 6 | 0 | 3.313740   | -3.640690  | 0.354471   |
| 53| 6 | 0 | 3.316591   | -0.132117  | -0.955624  |
| 54| 6 | 0 | 4.627374   | -0.003633  | -1.349498  |
| 55| 6 | 0 | 5.103635   | -2.252162  | -0.631762  |
| 56| 6 | 0 | 5.534219   | -1.073049  | -1.187063  |
| 57| 6 | 0 | 0.601795   | 2.570395   | -0.849382  |
| **10b** (conformer 4) | 1 | 6 | 0 | 1.333332 | -1.472840 | -0.086899 |
|   | 2 | 6 | 0 | 1.654198 | -2.644811 | -1.029320 |
|   | 3 | 8 | 0 | 0.664221 | -0.471059 | -0.830883 |
| 4 | 8 | 0 | 1.567573 | -2.631210 | -2.227378 |
|---|---|---|----------|-----------|-----------|
| 5 | 6 | 0 | -0.483012 | 0.103389  | -0.178598 |
| 6 | 6 | 0 | -0.705287 | 1.478350  | -0.800852 |
| 7 | 6 | 0 | -1.599035 | 1.632573  | -1.837541 |
| 8 | 6 | 0 | 0.034206  | 2.617476  | -0.336854 |
| 9 | 6 | 0 | -1.811597 | 2.883992  | -2.455313 |
| 10| 6 | 0 | -0.199342 | 3.890643  | -0.955398 |
| 11| 6 | 0 | -1.131388 | 3.990617  | -2.019901 |
| 12| 6 | 0 | -0.693384 | -0.823186 | -0.263396 |
| 13| 6 | 0 | -1.749857 | -1.788458 | -1.245457 |
| 14| 6 | 0 | -2.771834 | -0.701519 | 0.672191 |
| 15| 6 | 0 | -2.840911 | -2.672936 | -1.343232 |
| 16| 6 | 0 | -3.876115 | -1.610544 | 0.575472 |
| 17| 6 | 0 | -3.884789 | -2.591315 | -0.450410 |
| 18| 6 | 0 | -2.808883 | 0.286033  | 1.694734 |
| 19| 6 | 0 | -3.859601 | 0.358218  | 2.578252 |
| 20| 6 | 0 | -4.942740 | -1.508557 | 1.505930 |
| 21| 6 | 0 | -4.937478 | -0.549503 | 2.488191 |
| 22| 6 | 0 | 0.992982  | 2.559420  | 0.711150 |
| 23| 6 | 0 | 1.663395  | 3.683672  | 1.131967 |
| 24| 6 | 0 | 0.508981  | 5.031027  | -0.495285 |
| 25| 6 | 0 | 1.419142  | 4.935641  | 0.527564 |
| 26| 1 | 0 | -0.24036  | 0.236641  | 0.880824 |
| 27| 1 | 0 | -2.159692 | 0.774994  | -2.186911 |
| 28| 1 | 0 | -2.521863 | 2.961069  | -3.270657 |
| 29| 1 | 0 | -1.294941 | 4.958873  | -2.481567 |
| 30| 1 | 0 | -0.930913 | -1.866358 | -1.949804 |
| 31| 1 | 0 | -2.859077 | -3.419169 | -2.129780 |
| 32| 1 | 0 | -4.727386 | -3.271889 | -0.515111 |
| 33| 1 | 0 | -2.007256 | 1.009003  | 1.774326 |
| 34| 1 | 0 | -3.864238 | 1.122329  | 3.347448 |
| 35| 1 | 0 | -5.770201 | -2.205764 | 1.423320 |
| 36| 1 | 0 | -5.759834 | -0.482045 | 3.191450 |
| 37| 1 | 0 | 1.225200  | 1.612591  | 1.178790 |
| 38| 1 | 0 | 2.392524  | 3.604734  | 1.930408 |
| 39| 1 | 0 | 0.316395  | 5.986314  | -0.972671 |
| 40| 1 | 0 | 1.953766  | 5.814741  | 0.869364 |
| 41| 1 | 0 | 0.698356  | -1.876919 | 0.704582 |
| 42| 6 | 0 | 2.627690  | -0.943695 | 0.530046 |
| 43| 6 | 0 | 3.434882  | -0.069103 | -0.202965 |
| 44| 6 | 0 | 3.028175  | -1.338499 | 1.807830 |
| 45| 6 | 0 | 4.627107  | 0.402520  | 0.338609 |
| 46| 6 | 0 | 4.221394  | -0.864396 | 2.349698 |
| 47| 6 | 0 | 5.024024  | 0.005677  | 1.615153 |
| 48| 1 | 0 | 3.111501  | 0.247843  | -1.186911 |
|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
| 49| 1 | 0 | 2.407869 | -2.020797 | 2.379316 |
| 50| 1 | 0 | 5.245680 | 1.083128  | -0.235555 |
| 51| 1 | 0 | 4.521216 | -1.172137 | 3.345306 |
| 52| 1 | 0 | 5.952268 | 0.375482  | 2.036258 |
| 53| 8 | 0 | 2.059958 | -3.708139 | -0.235555 |
| 54| 6 | 0 | 2.450104 | -4.867132 | -1.069251 |
| 55| 1 | 0 | 3.280541 | -4.624176 | -1.733696 |
| 56| 6 | 0 | 2.751970 | -5.608982 | -0.333649 |
| 57| 1 | 0 | 1.611480 | -5.232755 | -1.663503 |

**10b (conformer 5)**

|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
| 1 | 6 | 0 | -1.543375 | -1.074006 | 0.024250 |
| 2 | 6 | 0 | -1.623894 | -1.148184 | 1.559821 |
| 3 | 8 | 0 | -0.855494 | 0.071195  | -0.436867 |
| 4 | 8 | 0 | -1.504314 | -0.224908 | 2.325485 |
| 5 | 6 | 0 | 0.541183  | 0.198407  | -0.085453 |
| 6 | 6 | 0 | 1.377751  | -0.937782 | -0.663544 |
| 7 | 6 | 0 | 0.999760  | -1.502070 | -1.855167 |
| 8 | 6 | 0 | 2.557272  | -1.402577 | 0.002881 |
| 9 | 6 | 0 | 1.735584  | -2.580226 | -2.427242 |
|10 | 6 | 0 | 3.297455  | -2.485668 | -0.578061 |
|11 | 6 | 0 | 2.857301  | -3.057557 | -1.799198 |
|12 | 6 | 0 | 0.975294  | 1.590001  | -0.550472 |
|13 | 6 | 0 | 1.855751  | 1.739542  | -1.599778 |
|14 | 6 | 0 | 0.469646  | 2.761543  | 0.109990 |
|15 | 6 | 0 | 2.272373  | 3.013179  | -2.046820 |
|16 | 6 | 0 | 0.901204  | 4.051510  | -0.344486 |
|17 | 6 | 0 | 1.806391  | 4.144780  | -1.432788 |
|18 | 6 | 0 | -0.439563 | 2.709623  | 1.201374 |
|19 | 6 | 0 | -0.885334 | 3.861284  | 1.807473 |
|20 | 6 | 0 | 0.416929  | 5.217490  | 0.303507 |
|21 | 6 | 0 | -0.456677 | 5.129065  | 1.358314 |
|22 | 6 | 0 | 3.048519  | -0.834149 | 1.211174 |
|23 | 6 | 0 | 4.184261  | -1.316657 | 1.815917 |
|24 | 6 | 0 | 4.463723  | -2.960990 | 0.076856 |
|25 | 6 | 0 | 4.899573  | -2.394135 | 1.248070 |
|26 | 1 | 0 | 0.609358  | 0.165287  | 1.005241 |
|27 | 1 | 0 | 0.112780  | -1.150720 | -2.356323 |
|28 | 1 | 0 | 1.404588  | -3.013990 | -3.364134 |
|29 | 1 | 0 | 3.426379  | -3.875724 | -2.228083 |
|30 | 1 | 0 | 2.248290  | 0.863096  | -2.097741 |
|31 | 1 | 0 | 2.965583  | 3.083444  | -2.877467 |
|32 | 1 | 0 | 2.123333  | 5.127489  | -1.766596 |
|33 | 1 | 0 | -0.802830 | 1.755326  | 1.555972 |
|34 | 1 | 0 | -1.578309 | 3.792225  | 2.638802 |
|35 | 1 | 0 | 0.753604  | 6.185455  | -0.053506 |
|36 | 1 | 0 | -0.819437 | 6.027371  | 1.845516 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 37 | 1 | 0 | 2.533205 | 0.004989 | 1.659964 |
| 38 | 1 | 0 | 4.537986 | -0.862774 | 2.734820 |
| 39 | 1 | 0 | 5.010319 | -3.783801 | -0.372221 |
| 40 | 1 | 0 | 5.793418 | -2.765270 | 1.736545 |
| 41 | 1 | 0 | -1.050098 | -1.993820 | -0.305732 |
| 42 | 6 | 0 | -2.956610 | -1.039982 | -0.541690 |
| 43 | 6 | 0 | -3.581148 | 0.808959 | -0.810700 |
| 44 | 6 | 0 | -3.646637 | -2.232022 | -0.775833 |
| 45 | 6 | 0 | -4.879893 | 0.202404 | -1.313720 |
| 46 | 6 | 0 | -4.946604 | -2.205978 | -1.274878 |
| 47 | 6 | 0 | -5.562524 | -0.987689 | -1.543542 |
| 48 | 1 | 0 | -3.038803 | 1.101037 | -0.642008 |
| 49 | 1 | 0 | -3.166121 | -3.181171 | -0.565735 |
| 50 | 1 | 0 | -5.355350 | 1.153498 | -1.526146 |
| 51 | 1 | 0 | -5.470422 | -3.136860 | -1.458785 |
| 52 | 1 | 0 | -6.576747 | -0.967655 | -1.937931 |
| 53 | 8 | 0 | -1.870243 | -2.411794 | 1.944761 |
| 54 | 1 | 0 | -1.153061 | -2.330727 | 3.903938 |
| 55 | 1 | 0 | -2.896034 | -2.024855 | 3.722188 |
| 56 | 1 | 0 | -2.252576 | -3.678935 | 3.475770 |

**10b (conformer 7)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.533781 | -1.534559 | -0.053068 |
| 2 | 6 | 0 | 2.381660 | -2.435039 | -0.957078 |
| 3 | 8 | 0 | 0.815765 | -0.605787 | -0.860518 |
| 4 | 8 | 0 | 2.600475 | -3.593800 | -0.707894 |
| 5 | 6 | 0 | -0.384193 | -0.095625 | -0.248278 |
| 6 | 6 | 0 | -0.716185 | 1.209934 | -0.966548 |
| 7 | 6 | 0 | -1.408012 | 1.164638 | -2.157565 |
| 8 | 6 | 0 | -0.278966 | 2.478056 | -0.457723 |
| 9 | 6 | 0 | -1.699845 | 2.331718 | -2.893907 |
| 10 | 6 | 0 | -0.593881 | 3.664588 | -1.202459 |
| 11 | 6 | 0 | -1.304928 | 3.557112 | -2.424162 |
| 12 | 6 | 0 | -1.518346 | -1.119649 | -0.292064 |
| 13 | 6 | 0 | -1.475244 | -2.159914 | -1.194091 |
| 14 | 6 | 0 | -2.633503 | -1.008981 | 0.601066 |
| 15 | 6 | 0 | -2.501715 | -3.128978 | -1.255353 |
| 16 | 6 | 0 | -3.667567 | -2.00248 | 0.541985 |
| 17 | 6 | 0 | -3.572614 | -3.054129 | -0.403748 |
| 18 | 6 | 0 | -2.772612 | 0.043871 | 1.546479 |
| 19 | 6 | 0 | -3.855019 | 0.104435 | 2.391791 |
| 20 | 6 | 0 | -4.769961 | -1.907018 | 1.430581 |
| 21 | 6 | 0 | -4.864284 | -0.881498 | 2.338225 |
| 22 | 6 | 0 | 0.449731 | 2.636971 | 0.753613 |
| 23 | 6 | 0 | 0.832235 | 3.878416 | 1.203792 |
| 24 | 6 | 0 | -0.184342 | 4.930235 | -0.707369 |
|   |   |   | 10b (conformer 9) |
|---|---|---|---|
|   |   |   |   |
|25| 6| 0| 0.511416 5.040929 0.470062 |
|26| 1| 0| -0.167531 0.114287 0.802046 |
|27| 1| 0| -1.744508 0.208272 -2.537634 |
|28| 1| 0| -2.443444 2.250511 -3.827819 |
|29| 1| 0| -1.531711 4.462438 -2.977540 |
|30| 1| 0| -0.629626 -2.231639 -1.866761 |
|31| 1| 0| -2.429773 -3.934544 -1.977324 |
|32| 1| 0| -4.361933 -3.797662 -0.438599 |
|33| 1| 0| -2.025378 0.824923 1.597371 |
|34| 1| 0| -3.937498 0.919305 3.102222 |
|35| 1| 0| -5.543565 -2.666087 1.377162 |
|36| 1| 0| -5.712563 -0.822234 3.010750 |
|37| 1| 0| 0.732828 1.769046 1.332825 |
|38| 1| 0| 1.390628 3.963386 2.129256 |
|39| 1| 0| -0.433927 5.815215 -1.283612 |
|40| 1| 0| 0.817960 6.014038 0.836770 |
|41| 1| 0| 0.849603 -2.213708 0.463776 |
|42| 6| 0| 2.442198 -0.858616 0.966699 |
|43| 6| 0| 3.179370 0.273835 0.607365 |
|44| 6| 0| 2.582140 -1.389285 2.250843 |
|45| 6| 0| 4.038891 0.868877 1.526303 |
|46| 6| 0| 3.445974 -0.794856 3.168857 |
|47| 6| 0| 4.175529 0.335553 2.807926 |
|48| 1| 0| 3.062944 0.684046 -0.388162 |
|49| 1| 0| 2.017082 -2.271925 2.531180 |
|50| 1| 0| 4.603203 1.749926 1.241680 |
|51| 1| 0| 3.545602 -1.212596 4.164404 |
|52| 1| 0| 4.846875 0.799983 3.521601 |
|53| 8| 0| 2.881287 -1.779133 -2.013175 |
|54| 6| 0| 3.739395 -2.551801 -2.873811 |
|55| 1| 0| 4.617127 -2.896699 -2.325119 |
|56| 1| 0| 3.204331 -3.415818 -3.269960 |
|57| 1| 0| 4.027363 -1.876529 -3.675983 |

|   |   |   |   |
|---|---|---|---|
|1  | 6| 0| -1.953796 -0.432802 0.471759 |
|2  | 6| 0| -2.092641 0.273440 1.832445 |
|3  | 8| 0| -0.999573 0.148020 -0.399055 |
|4  | 8| 0| -2.415825 -0.306127 2.839003 |
|5  | 6| 0| 0.380004 -0.111383 -0.083392 |
|6  | 6| 0| 0.765213 -1.568664 -0.335971 |
|7  | 6| 0| 0.012500 -2.347500 -1.187815 |
|8  | 6| 0| 1.913398 -2.136275 0.306428 |
|9  | 6| 0| 0.338124 -3.700255 -1.434170 |
|10 | 6| 0| 2.233223 -3.512078 0.061470 |
|11 | 6| 0| 1.421107 -4.272311 -0.819429 |
|12 | 6| 0| 1.203531 0.880046 -0.904853 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 13 | 6 | 0 | 1.568116 | 0.549731 | -2.192287 |
| 14 | 6 | 0 | 1.577727 | 2.161292 | -0.379433 |
| 15 | 6 | 0 | 2.302580 | 1.434822 | -3.009121 |
| 16 | 6 | 0 | 2.346865 | 3.048132 | -1.205587 |
| 17 | 6 | 0 | 2.690606 | 2.656118 | -2.523748 |
| 18 | 6 | 0 | 1.237992 | 2.608870 | 0.926451  |
| 19 | 6 | 0 | 1.645705 | 3.835919 | 1.393137  |
| 20 | 6 | 0 | 2.749246 | 4.308930 | -0.692427 |
| 21 | 6 | 0 | 4.131669 | 4.697629 | 0.579605  |
| 22 | 6 | 0 | 2.765381 | -1.398777 | 1.173560  |
| 23 | 6 | 0 | 3.852092 | -1.987173 | 1.775607  |
| 24 | 6 | 0 | 2.302580 | -4.087534 | 0.701663  |
| 25 | 6 | 0 | 4.153831 | -1.910655 | 1.542623  |
| 26 | 1 | 0 | 0.532627 | 0.090829 | -0.981104 |
| 27 | 1 | 0 | -0.852135 | -1.910655 | -1.672596 |
| 28 | 1 | 0 | -0.280345 | -4.281009 | -2.109184 |
| 29 | 1 | 0 | 1.674158 | -5.312170 | -0.997446 |
| 30 | 1 | 0 | 1.295420 | -0.420460 | -2.587565 |
| 31 | 1 | 0 | 2.565351 | 1.135083  | -4.017245 |
| 32 | 1 | 0 | 3.267161 | 3.339468  | -3.138432 |
| 33 | 1 | 0 | 0.622253 | 1.987689  | 1.560061  |
| 34 | 1 | 0 | 1.372204 | 4.148017  | 2.395107  |
| 35 | 1 | 0 | 3.332121 | 4.964188  | -1.331406 |
| 36 | 1 | 0 | 2.728670 | 5.662515  | 0.960057  |
| 37 | 1 | 0 | 2.572623 | -0.349624 | 1.356285  |
| 38 | 1 | 0 | 4.486374 | -1.401258 | 2.431242  |
| 39 | 1 | 0 | 3.588962 | -5.131073 | 0.510057  |
| 40 | 1 | 0 | 5.013145 | -3.798910 | 2.024629  |
| 41 | 1 | 0 | -1.690937 | -1.467602 | 0.711302  |
| 42 | 6 | 0 | -3.315977 | -0.409424 | -0.208821 |
| 43 | 6 | 0 | -3.590362 | 0.509507  | -1.223719 |
| 44 | 6 | 0 | -4.312889 | -1.296666 | 0.206002  |
| 45 | 6 | 0 | -4.847415 | 0.529127  | -1.824377 |
| 46 | 6 | 0 | -5.569184 | -1.270631 | -0.393368 |
| 47 | 6 | 0 | -5.838983 | -0.358253 | -1.411843 |
| 48 | 1 | 0 | -2.813628 | 1.191999  | -1.541991 |
| 49 | 1 | 0 | -4.105210 | -2.002647 | 1.002597  |
| 50 | 1 | 0 | -5.051553 | 1.241083  | -2.616485 |
| 51 | 1 | 0 | -6.334865 | -1.966015 | -0.068120 |
| 52 | 1 | 0 | -6.815905 | -0.340787 | -1.881969 |
| 53 | 8 | 0 | -1.878806 | 1.595928  | 1.757033  |
| 54 | 6 | 0 | -2.116318 | 2.334273  | 2.971879  |
| 55 | 1 | 0 | -3.160921 | 2.239386  | 3.271217  |
| 56 | 1 | 0 | -1.480465 | 1.962858  | 3.776796  |
| 57 | 1 | 0 | -1.877124 | 3.367589  | 2.732529  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.180446 | -1.105002 | 0.332634 |
| 2 | 6 | 0 | 1.038311 | -1.817079 | 1.689769 |
| 3 | 8 | 0 | -0.034203 | -0.525693 | -0.096805 |
| 4 | 8 | 0 | 0.008665 | -2.217242 | 2.172465 |
| 5 | 6 | 0 | -0.562230 | 0.560125 | 0.702621 |
| 6 | 6 | 0 | 0.433740 | 1.701030 | 0.890810 |
| 7 | 6 | 0 | 0.596206 | 2.191528 | 2.169907 |
| 8 | 6 | 0 | 1.196269 | 2.278034 | -0.180357 |
| 9 | 6 | 0 | 1.475371 | 3.257373 | 2.457959 |
|10 | 6 | 0 | 2.097671 | 3.353968 | 0.118572 |
|11 | 6 | 0 | 2.212698 | 3.825100 | 1.451829 |
|12 | 6 | 0 | -1.906097 | 0.948474 | 0.086009 |
|13 | 6 | 0 | -2.122814 | 2.211584 | 0.419602 |
|14 | 6 | 0 | -3.366457 | 2.588344 | -0.973957 |
|15 | 6 | 0 | -4.243529 | 0.386408 | -0.487155 |
|16 | 6 | 0 | -4.402416 | 1.693976 | -1.013789 |
|17 | 6 | 0 | -2.873785 | -1.311811 | 0.621367 |
|18 | 6 | 0 | -3.941393 | -2.178999 | 0.602010 |
|19 | 6 | 0 | -5.319027 | -0.539560 | -0.498335 |
|20 | 6 | 0 | -5.175774 | -1.796387 | 0.033727 |
|21 | 6 | 0 | 1.103263 | 1.841571 | -1.532277 |
|22 | 6 | 0 | 1.854378 | 2.431430 | -2.520799 |
|23 | 6 | 0 | 2.857472 | 3.936965 | -0.929442 |
|24 | 6 | 0 | 2.741294 | 3.488889 | -2.221148 |
|25 | 1 | 0 | -0.770484 | 0.162404 | 1.702259 |
|26 | 1 | 0 | 0.025873 | 1.748458 | 2.979991 |
|27 | 1 | 0 | 1.565964 | 3.616128 | 3.476910 |
|28 | 1 | 0 | 2.896508 | 4.641477 | 1.659688 |
|29 | 1 | 0 | -1.328171 | 2.944561 | -0.394582 |
|30 | 1 | 0 | -3.489731 | 3.591495 | -1.366232 |
|31 | 1 | 0 | -5.360855 | 1.973725 | -1.438876 |
|32 | 1 | 0 | -1.938761 | -1.638695 | 1.054175 |
|33 | 1 | 0 | -3.831012 | -3.169878 | 1.028741 |
|34 | 1 | 0 | -6.263824 | -0.229718 | -0.933199 |
|35 | 1 | 0 | -6.006060 | -2.493830 | 0.022214 |
|36 | 1 | 0 | 0.436614 | 1.027054 | -1.775197 |
|37 | 1 | 0 | 1.765314 | 2.079174 | -3.542307 |
|38 | 1 | 0 | 3.534221 | 4.749974 | -0.687558 |
|39 | 1 | 0 | 3.326867 | 3.943359 | -3.012447 |
|40 | 1 | 0 | 1.963900 | -0.349135 | 0.448525 |
|41 | 1 | 0 | 1.620955 | -2.123220 | -0.708498 |
|42 | 6 | 0 | 2.979875 | -2.350236 | -0.937365 |
|43 | 6 | 0 | 0.671246 | -2.858157 | -1.422554 |
|44 | 6 | 0 | 3.386978 | -3.301134 | -1.869605 |
|45 | 6 | 0 | 3.386978 | -3.301134 | -1.869605 |
|      |      |      |    |    |            |    |            |    |            |    |
|------|------|------|----|----|------------|----|------------|----|------------|----|
| 46   | 6    | 0    | 1.081523 | -3.805346 | -2.357597 |
| 47   | 6    | 0    | 2.438061 | -4.031262 | -2.582316 |
| 48   | 1    | 0    | 3.719961 | -1.780451 | -0.386482 |
| 49   | 1    | 0    | -0.381333 | -2.671794 | -1.253537 |
| 50   | 1    | 0    | 4.444446 | -3.465314 | -2.044376 |
| 51   | 1    | 0    | 0.338374 | -4.367293 | -2.912341 |
| 52   | 1    | 0    | 2.754082 | -4.768695 | -3.311704 |
| 53   | 8    | 0    | 2.242802 | -1.957249 | 2.268235  |
| 54   | 6    | 0    | 2.66077 | -2.694857 | 3.506315  |
| 55   | 1    | 0    | 1.653182 | -2.195159 | 4.257493  |
| 56   | 1    | 0    | 1.890143 | -3.707024 | 3.351646  |
| 57   | 1    | 0    | 3.309252 | -2.714844 | 3.812226  |

10b (conformer 13)

|      |      |      |    |    |            |    |            |    |            |    |
|------|------|------|----|----|------------|----|------------|----|------------|----|
| 1    | 6    | 0    | -2.078625 | -0.248033 | -0.470115 |
| 2    | 6    | 0    | -3.150843 | -0.762522 | -1.436336 |
| 3    | 8    | 0    | -0.862822 | -0.918545 | -0.746906 |
| 4    | 8    | 0    | -4.046313 | -0.068928 | -1.850857 |
| 5    | 6    | 0    | 0.321381 | -0.316135 | -0.196798 |
| 6    | 6    | 0    | 1.438972 | -1.348725 | -0.310600 |
| 7    | 6    | 0    | 1.261370 | -2.473247 | -1.087105 |
| 8    | 6    | 0    | 2.671857 | -1.167922 | 0.397661  |
| 9    | 6    | 0    | 2.275557 | -3.449678 | -1.211112 |
| 10   | 6    | 0    | 3.692907 | -2.166822 | 0.272179  |
| 11   | 6    | 0    | 3.465180 | -3.301719 | -0.548304 |
| 12   | 6    | 0    | 0.634960 | 0.997897 | -0.922188 |
| 13   | 6    | 0    | 1.050377 | 0.927812 | -2.235824 |
| 14   | 6    | 0    | 0.461655 | 2.282146 | -0.309252 |
| 15   | 6    | 0    | 1.322934 | 2.084274 | -2.924040 |
| 16   | 6    | 0    | 0.756085 | 3.458468 | -1.080598 |
| 17   | 6    | 0    | 1.185162 | 3.325233 | -2.423884 |
| 18   | 6    | 0    | 0.013651 | 2.470688 | 1.029960  |
| 19   | 6    | 0    | -0.121548 | 3.726479 | 1.571794  |
| 20   | 6    | 0    | 0.605828 | 4.739471 | -0.486822 |
| 21   | 6    | 0    | 0.180113 | 4.876623 | 0.809776  |
| 22   | 6    | 0    | 2.938613 | -0.048045 | 1.231540  |
| 23   | 6    | 0    | 4.133196 | 0.077388 | 1.900447  |
| 24   | 6    | 0    | 4.914770 | -2.004102 | 0.975260  |
| 25   | 6    | 0    | 5.134830 | -0.909101 | 1.773125  |
| 26   | 1    | 0    | 0.150367 | -0.128062 | 0.866131  |
| 27   | 1    | 0    | 0.318281 | -2.610265 | -1.598190 |
| 28   | 1    | 0    | 2.099539 | -4.319718 | -1.833922 |
| 29   | 1    | 0    | 4.247239 | -4.048642 | -0.636262 |
| 30   | 1    | 0    | 1.178703 | -0.045922 | -2.693711 |
| 31   | 1    | 0    | 1.649450 | 1.985261 | -4.021371 |
| 32   | 1    | 0    | 1.401601 | 4.222410 | -2.994257 |
| 33   | 1    | 0    | -0.241118 | 1.616102 | 1.642653  |
\begin{tabular}{|c|c|c|c|c|c|}
\hline
34 & 1 & 0 & -0.467075 & 3.834247 & 2.593817 \\
35 & 1 & 0 & 0.835240 & 5.615051 & -1.085260 \\
36 & 1 & 0 & 0.070480 & 0.943489 & 2.528789 \\
37 & 1 & 0 & 4.308344 & 0.943489 & 2.528789 \\
38 & 1 & 0 & 5.677641 & -2.768574 & 0.869419 \\
39 & 1 & 0 & 6.073319 & -0.798176 & 2.304529 \\
40 & 1 & 0 & -1.996524 & 0.823072 & 0.961972 \\
41 & 1 & 0 & -2.310469 & -1.650822 & 1.631673 \\
42 & 6 & 0 & -3.313195 & 0.543886 & 1.597472 \\
43 & 6 & 0 & -2.785492 & -1.844313 & 2.926321 \\
44 & 6 & 0 & -3.795197 & 0.345015 & 2.889314 \\
45 & 6 & 0 & -3.529964 & -0.848818 & 3.557223 \\
46 & 1 & 0 & -2.132824 & -2.420564 & 1.134427 \\
47 & 1 & 0 & -3.518451 & 1.473537 & 1.077989 \\
48 & 1 & 0 & -2.576357 & -2.774882 & 3.442224 \\
49 & 1 & 0 & -4.373243 & 1.123396 & 3.374095 \\
50 & 1 & 0 & -3.899904 & -1.002307 & 4.564788 \\
51 & 8 & 0 & -3.009910 & -2.065625 & -1.717106 \\
52 & 6 & 0 & -4.020861 & -2.625639 & -2.576444 \\
53 & 1 & 0 & -3.755275 & -3.673996 & 2.926321 \\
54 & 1 & 0 & -5.006750 & -2.524169 & -2.121025 \\
55 & 1 & 0 & -4.020776 & -2.120718 & -3.543809 \\
\hline
\textbf{10b (conformer 26)} & & & & & \\
1 & 6 & 0 & -2.138767 & 0.092588 & -0.212208 \\
2 & 6 & 0 & -3.056820 & 0.585688 & -1.335786 \\
3 & 8 & 0 & -0.885518 & -0.150724 & -0.816659 \\
4 & 8 & 0 & -2.906038 & 0.377223 & -2.508897 \\
5 & 6 & 0 & 0.212212 & -0.380794 & 0.077692 \\
6 & 6 & 0 & 1.366932 & -0.926310 & -0.771416 \\
7 & 6 & 0 & 1.232785 & -0.985075 & -2.143009 \\
8 & 6 & 0 & -2.561705 & -1.439303 & -0.164127 \\
9 & 6 & 0 & -2.259406 & -1.490453 & -2.968057 \\
10 & 6 & 0 & -1.801843 & -1.951120 & -1.010754 \\
11 & 6 & 0 & -3.424353 & -1.957313 & -2.417370 \\
12 & 6 & 0 & -0.050485 & -0.865396 & -1.920734 \\
13 & 6 & 0 & -0.323809 & 0.771813 & -2.869799 \\
14 & 6 & 0 & -0.906845 & -1.222854 & -0.860123 \\
15 & 6 & 0 & 0.574348 & 1.855918 & 3.156035 \\
16 & 6 & 0 & 1.171455 & 3.220406 & 1.246323 \\
17 & 6 & 0 & 1.002910 & -1.052546 & 2.645071 \\
18 & 6 & 0 & 1.038229 & 2.351120 & -1.036603 \\
19 & 6 & 0 & 1.433325 & -3.574190 & -1.523443 \\
20 & 6 & 0 & 1.585226 & 4.466837 & 0.708240 \\
21 & 6 & 0 & 1.718461 & 4.642946 & -0.646044 \\
\hline
\end{tabular}
|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 22 | 6 | 0 | 2.771961 | -1.498434 | 1.240728 |
| 23 | 6 | 0 | 3.930888 | -2.009996 | 1.774351 |
| 24 | 6 | 0 | 4.790078 | -2.461973 | -0.426582 |
| 25 | 6 | 0 | 4.957651 | -2.492237 | 0.934943 |
| 26 | 1 | 0 | -0.075019 | -1.172931 | 0.781444 |
| 27 | 1 | 0 | 0.313859 | -0.636126 | -2.593957 |
| 28 | 1 | 0 | 2.113031 | -1.512865 | 4.223105 |
| 29 | 1 | 0 | 0.313859 | -0.636126 | -2.593957 |
| 30 | 1 | 0 | -0.015925 | -0.168292 | 2.710575 |
| 31 | 1 | 0 | 0.428502 | 1.731970 | 4.223105 |
| 32 | 1 | 0 | 1.208536 | 3.892509 | 3.30371 |
| 33 | 1 | 0 | 0.807184 | 1.554101 | -1.725323 |
| 34 | 1 | 0 | 1.523760 | 3.720580 | -2.593972 |
| 35 | 1 | 0 | 1.789350 | 5.283787 | 1.392606 |
| 36 | 1 | 0 | 2.033834 | 5.600529 | -1.044990 |
| 37 | 1 | 0 | 2.010735 | -1.129646 | 1.911275 |
| 38 | 1 | 0 | 2.010735 | -1.129646 | 1.911275 |
| 39 | 1 | 0 | 2.010735 | -1.129646 | 1.911275 |
| 40 | 1 | 0 | 4.057891 | -2.041107 | 2.850826 |
| 41 | 1 | 0 | 5.567295 | -2.837331 | -1.084332 |
| 42 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 43 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 44 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 45 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 46 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 47 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 48 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 49 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 50 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 51 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 52 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 53 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 54 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 55 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 56 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |
| 57 | 1 | 0 | 5.869898 | -2.887910 | 1.367028 |

**10b (conformer 53)**

|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 1  | 6 | 0 | -0.871697 | 1.420645 | 0.419251 |
| 2  | 6 | 0 | -0.572693 | 2.029689 | 1.802170 |
| 3  | 8 | 0 | 0.106116 | 0.520664 | -0.065040 |
| 4  | 8 | 0 | -1.436784 | 2.374112 | 2.567266 |
| 5  | 6 | 0 | 0.306979 | -0.691512 | 0.697589 |
| 6  | 6 | 0 | -0.985487 | -1.466994 | 0.934966 |
| 7  | 6 | 0 | -1.251871 | -1.877187 | 2.224227 |
| 8  | 6 | 0 | -1.920066 | -1.784456 | -0.107777 |
| 9  | 6 | 0 | -2.408107 | -2.617842 | 2.550765 |
|   |   |   |                      |                      |                      |
|---|---|---|----------------------|----------------------|----------------------|
| 10| 6 | 0 | -3.098489            | -2.530094            | 0.229712             |
| 11| 6 | 0 | -3.313112            | -2.935885            | 1.572246             |
| 12| 6 | 0 | 1.430947             | -1.477835            | 0.017644             |
| 13| 6 | 0 | 1.228846             | -2.771881            | -0.410822            |
| 14| 6 | 0 | 2.740009             | -0.897797            | -0.114439            |
| 15| 6 | 0 | 2.262103             | -3.533619            | -1.000246            |
| 16| 6 | 0 | 3.786252             | -1.678571            | -0.708850            |
| 17| 6 | 0 | 3.513004             | -2.998380            | -1.150675            |
| 18| 6 | 0 | 3.064966             | 0.412113             | 0.333913             |
| 19| 6 | 0 | 4.338696             | 0.914241             | 0.201099             |
| 20| 6 | 0 | 5.086618             | -1.124029            | -0.836084            |
| 21| 6 | 0 | 5.362744             | 0.144273             | 0.333913             |
| 22| 6 | 0 | -1.739724            | -1.399367            | -1.466093            |
| 23| 6 | 0 | -2.665655            | -1.731933            | -2.425904            |
| 24| 6 | 0 | -4.031916            | -2.854669            | -0.789360            |
| 25| 6 | 0 | -3.823557            | -2.468649            | -2.089002            |
| 26| 1 | 0 | 0.678767             | -0.398060            | 1.688115             |
| 27| 1 | 0 | -0.550534            | -1.625290            | 3.013156             |
| 28| 1 | 0 | -2.576190            | -2.923151            | 3.577103             |
| 29| 1 | 0 | -4.209425            | -3.499107            | 1.809978             |
| 30| 1 | 0 | 0.256613             | -3.230102            | -0.294010            |
| 31| 1 | 0 | 2.052678             | -4.545211            | -1.328980            |
| 32| 1 | 0 | 4.313797             | -3.576049            | -1.600542            |
| 33| 1 | 0 | 2.294570             | 1.030876             | 0.768648             |
| 34| 1 | 0 | 4.557102             | 1.917765             | 0.549976             |
| 35| 1 | 0 | 5.863835             | -1.729055            | -1.291598            |
| 36| 1 | 0 | 6.360689             | 0.555864             | -0.493119            |
| 37| 1 | 0 | -0.864703            | -0.827358            | -1.738484            |
| 38| 1 | 0 | -2.505934            | -1.423981            | -3.453089            |
| 39| 1 | 0 | -4.918268            | -3.419061            | -0.518747            |
| 40| 1 | 0 | -4.544689            | -2.720879            | -2.857724            |
| 41| 1 | 0 | -1.838176            | 0.921512             | 0.538668             |
| 42| 6 | 0 | -1.021948            | 2.562245             | -0.579192            |
| 43| 6 | 0 | -0.024701            | 2.835755             | -1.516741            |
| 44| 6 | 0 | -2.168707            | 3.361027             | -0.541688            |
| 45| 6 | 0 | -0.179829            | 3.892862             | -2.411896            |
| 46| 6 | 0 | -2.317283            | 4.418908             | -1.433645            |
| 47| 6 | 0 | -1.322963            | 4.687096             | -2.373100            |
| 48| 1 | 0 | 0.858768             | 2.212494             | -1.549607            |
| 49| 1 | 0 | -2.941530            | 3.156185             | 0.190961             |
| 50| 1 | 0 | 0.597020             | 4.094342             | -3.141248            |
| 51| 1 | 0 | -3.212439            | 5.029723             | -1.398375            |
| 52| 1 | 0 | -1.440770            | 5.508303             | -3.071270            |
| 53| 8 | 0 | 0.743135             | 2.180671             | 2.038091             |
| 54| 6 | 0 | 1.085092             | 2.820331             | 3.284555             |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 55 | 1 | 0 | 0.712758 | 3.845447 | 3.294651 |
| 56 | 1 | 0 | 0.654192 | 2.274361 | 4.124302 |
| 57 | 1 | 0 | 2.171416 | 2.805144 | 3.330076 |

**10b (conformer 74)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.996604 | -0.248294 | 0.447552 |
| 2 | 6 | 0 | 2.187271 | -0.937024 | 1.810090 |
| 3 | 8 | 0 | 0.836248 | -0.703950 | -0.216682 |
| 4 | 8 | 0 | 1.682589 | -1.976663 | 2.147959 |
| 5 | 6 | 0 | -0.429006 | -0.703950 | -0.216682 |
| 6 | 6 | 0 | -0.626710 | 1.060285 | 0.674746 |
| 7 | 6 | 0 | -0.725230 | 1.472225 | 1.988305 |
| 8 | 6 | 0 | -0.666817 | 2.048921 | -0.364604 |
| 9 | 6 | 0 | -0.917542 | 2.825166 | 2.342668 |
| 10 | 6 | 0 | -0.873451 | 3.422560 | -0.003356 |
| 11 | 6 | 0 | -1.002862 | 3.779452 | 1.363689 |
| 12 | 6 | 0 | -1.503729 | -1.127974 | -0.433858 |
| 13 | 6 | 0 | -1.170047 | -1.678647 | -1.652821 |
| 14 | 6 | 0 | -2.848305 | -1.269030 | 0.048220 |
| 15 | 6 | 0 | -2.124126 | -2.335427 | -2.460018 |
| 16 | 6 | 0 | -3.813922 | -1.934382 | -0.779779 |
| 17 | 6 | 0 | -3.422121 | -2.452047 | -2.040018 |
| 18 | 6 | 0 | -3.283163 | -0.811624 | 1.322097 |
| 19 | 6 | 0 | -4.580053 | -0.981681 | 1.744658 |
| 20 | 6 | 0 | -5.147516 | -2.082689 | -0.317188 |
| 21 | 6 | 0 | -5.528828 | -1.617749 | 0.916051 |
| 22 | 6 | 0 | -0.488647 | 1.745264 | -1.741520 |
| 23 | 6 | 0 | -0.541271 | 2.728514 | -2.700433 |
| 24 | 6 | 0 | -0.930243 | 4.410195 | -1.021042 |
| 25 | 6 | 0 | -0.772279 | 4.074368 | -2.342116 |
| 26 | 1 | 0 | -0.427242 | -0.933332 | 1.391712 |
| 27 | 1 | 0 | -0.662281 | 0.731544 | 2.779601 |
| 28 | 1 | 0 | -0.999257 | 3.098572 | 3.388504 |
| 29 | 1 | 0 | -1.159154 | 4.822365 | 1.618716 |
| 30 | 1 | 0 | -0.146924 | -1.610823 | -1.994685 |
| 31 | 1 | 0 | -1.816420 | -2.746255 | -3.415161 |
| 32 | 1 | 0 | -4.163767 | -2.951421 | -2.654580 |
| 33 | 1 | 0 | -2.585364 | -0.314516 | 1.978342 |
| 34 | 1 | 0 | -4.876851 | -0.622734 | 2.723912 |
| 35 | 1 | 0 | -5.863495 | -2.582497 | -0.961522 |
| 36 | 1 | 0 | -6.550358 | -1.741453 | 1.257526 |
| 37 | 1 | 0 | -0.294900 | 0.725944 | -2.034655 |
| 38 | 1 | 0 | -0.401509 | 2.467796 | -3.743572 |
| 39 | 1 | 0 | -1.096097 | 5.442693 | -0.731487 |
| 40 | 1 | 0 | -0.816550 | 4.838396 | -3.110135 |
| 41 | 1 | 0 | 1.957233 | 0.830648 | 0.627682 |
| 42 | 6 | 0 | 3.191872 | -0.568645 | -0.433071 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 43|   6|0  |3.329174 | -1.848122 | -0.980245 |
| 44|   6|0  |4.166833 | 0.395638  | -0.689073 |
| 45|   6|0  |4.426747 | -2.152151 | -1.779975 |
| 46|   6|0  |5.267696 | 0.088388  | -1.486223 |
| 47|   6|0  |5.398924 | -1.185312 | -2.034062 |
| 48|   1|0  |2.570641 | -2.594479 | -0.777810 |
| 49|   1|0  |4.062213 | 1.390193  | -0.269398 |
| 50|   1|0  |4.524755 | -3.145351 | -2.203879 |
| 51|   1|0  |6.017639 | 0.845990  | -1.684360 |
| 52|   1|0  |6.253276 | -1.423554 | -2.657753 |
| 53|   8|0  |3.028924 | -0.218743 | 2.575266  |
| 54|   6|0  |3.377648 | -0.802571 | 3.845226  |
| 55|   1|0  |3.864559 | -1.767640 | 3.698177  |
| 56|   1|0  |4.059678 | -0.096051 | 4.312214  |
| 57|   1|0  |2.486680 | -0.941723 | 4.459069  |
Table S34. Cartesian coordinates of each conformer of 1e calculated at IEFPCM/B3LYP/6-311++G(d,p) level with the use of an IEFPCM model of cyclohexane.

| 1e (conformer 1) |  |  |  |  |  |  |
|------------------|---|---|------------------|------------------|---|---|
|                  | 1 | 6 | 0               | 4.197565 -2.409854 -0.658824 |
|                  | 2 | 6 | 0               | 4.659268 -1.237229 -0.113886 |
|                  | 3 | 6 | 0               | 3.788769 -0.138495 0.109999 |
|                  | 4 | 6 | 0               | 2.402371 -0.257399 -0.237227 |
|                  | 5 | 6 | 0               | 1.963494 -1.488116 -0.798143 |
|                  | 6 | 6 | 0               | 2.834096 -2.532428 -1.004381 |
|                  | 7 | 6 | 0               | 4.269778 1.074903 0.667261  |
|                  | 8 | 6 | 0               | 3.419009 2.130516 0.864573  |
|                  | 9 | 6 | 0               | 2.052852 2.022452 0.517939  |
|                  | 10| 6| 0               | 1.534410 0.862566 -0.014779 |
|                  | 11| 6| 0               | 0.053540 0.783236 -0.381037 |
|                  | 12| 6| 0               | -0.739598 -0.158523 0.536654 |
|                  | 13| 6| 0               | -1.656453 -1.140007 0.034523 |
|                  | 14| 6| 0               | -0.596626 -0.008780 1.900669 |
|                  | 15| 6| 0               | -1.321215 -0.795633 2.817831 |
|                  | 16| 6| 0               | -2.196552 -1.749814 2.363554 |
|                  | 17| 6| 0               | -2.385527 -1.948106 0.973507 |
|                  | 18| 6| 0               | -1.889348 -1.376463 -1.351232 |
|                  | 19| 6| 0               | -2.772021 -2.338919 -1.779810 |
|                  | 20| 6| 0               | -3.482473 -3.129499 -0.849250 |
|                  | 21| 6| 0               | -3.290383 -2.932926 0.494793 |
|                  | 22| 8| 0               | -0.485324 2.107160 -0.319627 |
|                  | 23| 6| 0               | -1.704759 2.344283 -1.044188 |
|                  | 24| 6| 0               | -2.359923 3.574908 -0.414961 |
|                  | 25| 6| 0               | -1.419248 2.550309 -2.532747 |
|                  | 26| 6| 0               | -2.776735 3.384613 1.044646 |
|                  | 27| 1| 0               | 4.873901 -3.240923 -0.824117 |
|                  | 28| 1| 0               | 5.705058 -1.131278 0.155702 |
|                  | 29| 1| 0               | 0.923368 -1.620184 -1.062718 |
|                  | 30| 1| 0               | 2.469416 -3.459265 -1.432916 |
|                  | 31| 1| 0               | 5.320089 1.150899 0.928409 |
|                  | 32| 1| 0               | 3.787143 3.059925 1.284838 |
|                  | 33| 1| 0               | 1.395772 2.869048 0.659004 |
|                  | 34| 1| 0               | -0.000810 0.423605 -1.412013 |
|                  | 35| 1| 0               | 0.101361 0.729652 2.277333 |
|                  | 36| 1| 0               | -1.176246 -0.646010 3.881745 |
|                  | 37| 1| 0               | -2.754312 -2.366982 3.059958 |
|                  | 38| 1| 0               | -1.368236 -0.788599 -2.095305 |
|                  | 39| 1| 0               | -2.925557 -2.491840 -2.842180 |
|                  | 40| 1| 0               | -4.175606 -3.885514 -1.200049 |
|                  | 41| 1| 0               | -3.831354 -3.531804 1.220112 |
|                  | 42| 1| 0               | -2.374302 1.484744 -0.911091 |
|                  | 43| 1| 0               | -1.658958 4.413337 -0.499896 |
|                  | 44| 1| 0               | -3.234701 3.836196 -1.020579 |
|                  | 45| 1| 0               | -2.351273 2.703386 -3.083951 |
|                  | 46| 1| 0               | -0.781324 3.426349 -2.676998 |
|                  | 47| 1| 0               | -0.913114 1.688285 -2.974116 |
|                  | 48| 1| 0               | -3.242480 4.292107 1.438367 |
|                  | 49| 1| 0               | -3.497544 2.567608 1.146545 |
|   |   |   |   |   |
|---|---|---|---|---|
| 50| 1 | 0 | -1.913436 | 3.146415 | 1.668048 |
| **1e (conformer 2)** | 1 | 6 | 0 | 3.968443 | -2.455672 | -1.176450 |
|   | 2 | 6 | 0 | 3.745940 | -2.567245 | 0.172590 |
|   | 3 | 6 | 0 | 2.716432 | -1.827230 | 0.813149 |
|   | 4 | 6 | 0 | 1.889704 | -0.944694 | 0.035862 |
|   | 5 | 6 | 0 | 2.158854 | -0.857267 | -1.360723 |
|   | 6 | 6 | 0 | 3.163958 | -1.587706 | -1.948078 |
|   | 7 | 6 | 0 | 2.499497 | -1.942902 | 2.208329 |
|   | 8 | 6 | 0 | 1.506995 | -1.219670 | 2.820740 |
|   | 9 | 6 | 0 | 0.688577 | -0.360512 | 2.061051 |
|   | 10| 6| 0 | 0.850637 | -0.212420 | 0.698825 |
|   | 11| 6| 0 | -0.059094 | 0.788935 | -0.029533 |
|   | 12| 6| 0 | -1.540244 | 0.574166 | 0.275616 |
|   | 13| 6| 0 | -2.241004 | -0.557814 | -0.256947 |
|   | 14| 6| 0 | -2.220130 | 1.481470 | 1.058773 |
|   | 15| 6| 0 | -3.591452 | 1.317008 | 1.359244 |
|   | 16| 6| 0 | -4.285314 | 0.243961 | 0.865061 |
|   | 17| 6| 0 | -3.634410 | -0.714266 | 0.045086 |
|   | 18| 6| 0 | -1.628317 | -1.539648 | -1.083129 |
|   | 19| 6| 0 | -2.342749 | -2.603603 | -1.581680 |
|   | 20| 6| 0 | -3.714520 | -2.751536 | -1.281611 |
|   | 21| 6| 0 | -4.411666 | -1.825234 | -0.485064 |
|   | 22| 8| 0 | 0.274554 | 2.126307 | 0.351571 |
|   | 23| 6| 0 | 1.486245 | 2.669597 | -0.204813 |
|   | 24| 6| 0 | 1.251591 | 3.211847 | -1.625717 |
|   | 25| 6| 0 | 1.974049 | 3.723655 | 0.782640 |
|   | 26| 6| 0 | 0.203132 | 4.323827 | -1.727937 |
|   | 27| 1| 0 | 4.757419 | -3.027098 | -1.651852 |
|   | 28| 1| 0 | 4.358613 | -3.227539 | 0.777605 |
|   | 29| 1| 0 | 1.568144 | -0.200031 | -1.985193 |
|   | 30| 1| 0 | 3.342386 | -1.495851 | -3.013577 |
|   | 31| 1| 0 | 3.131424 | -2.612969 | 2.781555 |
|   | 32| 1| 0 | 1.341941 | -1.308856 | 3.888519 |
|   | 33| 1| 0 | -0.097640 | 0.194505 | 2.559185 |
|   | 34| 1| 0 | 0.065810 | 0.682980 | -1.110489 |
|   | 35| 1| 0 | -1.687208 | 2.341688 | 1.439221 |
|   | 36| 1| 0 | -4.089535 | 2.052291 | 1.981459 |
|   | 37| 1| 0 | -5.338921 | 0.112645 | 1.088247 |
|   | 38| 1| 0 | -0.576435 | -1.463465 | -1.321923 |
|   | 39| 1| 0 | -1.847324 | -3.337350 | -2.207635 |
|   | 40| 1| 0 | -4.266960 | -3.595256 | -1.679535 |
|   | 41| 1| 0 | -5.394786 | -1.928704 | -0.246902 |
|   | 42| 1| 0 | 2.240192 | 1.875603 | -0.260661 |
|   | 43| 1| 0 | 2.215277 | 3.563036 | -2.012823 |
|   | 44| 1| 0 | 0.956954 | 2.379687 | -2.274828 |
|   | 45| 1| 0 | 2.874599 | 4.216092 | 0.405749 |
|   | 46| 1| 0 | 1.209140 | 4.484461 | 0.953198 |
|   | 47| 1| 0 | 2.208141 | 3.258192 | 1.741833 |
|   | 48| 1| 0 | 0.031704 | 4.596496 | -2.772517 |
|   | 49| 1| 0 | -0.748793 | 3.998282 | -1.303030 |
|   | 50| 1| 0 | 0.515502 | 5.228424 | -1.199880 |
|   |   |   | Energy (a.u.) | Z (number of electrons) | Coordinates (Å) |
|---|---|---|---------------|----------------------|-----------------|
| 1 | 6 | 0 | 3.460528      | 1.00000              | 1.012345, 0.00000, 0.00000 |
| 2 | 6 | 0 | 3.158457      | 1.00000              | 0.98752, 0.97852, 0.96752 |
| 3 | 6 | 0 | 1.601099      | 1.00000              | 0.55768, 0.44232, 0.33768 |
| 4 | 6 | 0 | 1.948041      | 1.00000              | 0.66578, 0.55678, 0.44322 |
| 5 | 6 | 0 | 2.846588      | 1.00000              | 0.45378, 0.34278, 0.23788 |
| 6 | 6 | 0 | 1.937325      | 1.00000              | 1.012345, 0.00000, 0.00000 |
| 7 | 6 | 0 | 1.042831      | 1.00000              | 0.98752, 0.97852, 0.96752 |
| 8 | 6 | 0 | 0.412437      | 1.00000              | 0.66578, 0.55678, 0.44322 |
| 9 | 6 | 0 | 0.663683      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|10 | 6 | 0 | -0.035292     | 1.00000              | 0.66578, 0.55678, 0.44322 |
|11 | 6 | 0 | 0.663683      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|12 | 6 | 0 | -1.546590     | 1.00000              | 0.66578, 0.55678, 0.44322 |
|13 | 6 | 0 | -2.386447     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|14 | 6 | 0 | -2.117942     | 1.00000              | 0.66578, 0.55678, 0.44322 |
|15 | 6 | 0 | -3.512377     | 1.00000              | 0.66578, 0.55678, 0.44322 |
|16 | 6 | 0 | -4.338051     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|17 | 6 | 0 | -3.801593     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|18 | 6 | 0 | -1.891725     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|19 | 6 | 0 | -2.736379     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|21 | 6 | 0 | -3.801593     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|22 | 6 | 0 | -0.484109     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|23 | 6 | 0 | 1.703835      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|24 | 6 | 0 | 2.386661      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|25 | 6 | 0 | 3.059807      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|26 | 6 | 0 | 4.167214      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|27 | 6 | 0 | 3.625179      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|28 | 6 | 0 | 1.503458      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|29 | 6 | 0 | 3.087620      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|30 | 6 | 0 | 2.419398      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|31 | 6 | 0 | 0.813229      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|32 | 6 | 0 | -0.297612     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|33 | 6 | 0 | 0.130594      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|34 | 6 | 0 | -1.479456     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|35 | 6 | 0 | -3.921927     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|36 | 6 | 0 | -5.409786     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|37 | 6 | 0 | -0.829660     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|38 | 6 | 0 | -2.329017     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|39 | 6 | 0 | -4.784360     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|40 | 6 | 0 | -5.712647     | 1.00000              | 0.55768, 0.44232, 0.33768 |
|41 | 6 | 0 | 2.419475      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|42 | 6 | 0 | 1.103993      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|43 | 6 | 0 | 3.399390      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|45 | 6 | 0 | 1.766402      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|46 | 6 | 0 | 2.424589      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|47 | 6 | 0 | 3.666271      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|48 | 6 | 0 | 3.635670      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|49 | 6 | 0 | 4.435931      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|50 | 6 | 0 | 4.806651      | 1.00000              | 0.55768, 0.44232, 0.33768 |
|   |   |   | 3.844052 | 0.207193 | 0.018301 |
|---|---|---|---------|---------|---------|
| 4 | 6 | 0 | 2.460110 | -0.016235 | -0.285015 |
| 5 | 6 | 0 | 2.116663 | -1.216394 | -0.965830 |
| 6 | 6 | 0 | 3.074902 | -2.133892 | -1.327960 |
| 7 | 6 | 0 | 4.230263 | 1.392975 | 0.695790 |
| 8 | 6 | 0 | 3.290056 | 2.324295 | 1.050460 |
| 9 | 6 | 0 | 1.925741 | 2.114463 | 0.746458 |
|10 | 6 | 0 | 1.498394 | 0.975067 | 0.100407 |
|11 | 6 | 0 | 0.015752 | 0.787672 | -0.215184 |
|12 | 6 | 0 | -0.643385 | -0.307402 | 0.637167 |
|13 | 6 | 0 | -1.476181 | -1.332436 | 0.079034 |
|14 | 6 | 0 | -0.468549 | -0.254432 | 2.004812 |
|15 | 6 | 0 | -1.078275 | -1.182867 | 2.871625 |
|16 | 6 | 0 | -1.870928 | -2.180632 | 2.362322 |
|17 | 6 | 0 | -2.089112 | -2.283006 | 0.966311 |
|18 | 6 | 0 | -1.735414 | -1.476930 | -1.314782 |
|19 | 6 | 0 | -2.535877 | -2.484000 | -1.798492 |
|20 | 6 | 0 | -3.132155 | -3.414688 | -0.918631 |
|21 | 6 | 0 | -2.911110 | -3.310592 | 0.431241 |
|22 | 6 | 0 | -0.639861 | 2.039664 | 0.001653 |
|23 | 6 | 0 | -1.911402 | 2.219202 | -0.648185 |
|24 | 6 | 0 | -2.676154 | 3.235060 | 0.203328 |
|25 | 6 | 0 | -1.704656 | 2.667502 | -2.095429 |
|26 | 6 | 0 | -4.113244 | 3.492712 | -0.259607 |
|27 | 1 | 0 | 5.182063 | -2.638971 | -1.317227 |
|28 | 1 | 0 | 5.849428 | -0.577297 | -0.131461 |
|29 | 1 | 0 | 1.081963 | -1.426977 | -1.198956 |
|30 | 1 | 0 | 2.782233 | -3.040817 | -1.845164 |
|31 | 1 | 0 | 5.279885 | 1.548246 | 0.922364 |
|32 | 1 | 0 | 3.585011 | 3.233041 | 1.563384 |
|33 | 1 | 0 | 1.195737 | 2.866009 | 1.012372 |
|34 | 1 | 0 | -0.057020 | 0.525368 | -1.274201 |
|35 | 1 | 0 | 0.162877 | 0.520676 | 2.423015 |
|36 | 1 | 0 | -0.911272 | -1.105977 | 3.940051 |
|37 | 1 | 0 | -2.340525 | -2.903211 | 3.019024 |
|38 | 1 | 0 | -1.301468 | -0.781094 | -2.020761 |
|39 | 1 | 0 | -2.712701 | -2.564094 | -2.865205 |
|40 | 1 | 0 | -3.761330 | -4.204633 | -1.312557 |
|41 | 1 | 0 | -3.365048 | -4.017535 | 1.117984 |
|42 | 1 | 0 | -2.461516 | 1.269953 | -0.631279 |
|43 | 1 | 0 | -2.680257 | 2.859301 | 1.230526 |
|44 | 1 | 0 | -2.108904 | 4.172784 | 0.214558 |
|45 | 1 | 0 | -2.658088 | 2.754263 | -2.622338 |
|46 | 1 | 0 | -1.201533 | 3.638045 | -2.120876 |
|47 | 1 | 0 | -1.089183 | 1.953886 | -2.649039 |
|48 | 1 | 0 | -4.625169 | 4.163024 | 0.435330 |
|49 | 1 | 0 | -4.149676 | 3.957367 | -1.248172 |
|50 | 1 | 0 | -4.689054 | 2.562920 | -0.305225 |

**1e (conformer 5)**

|   |   |   | 4.001389 | -2.617206 | -1.392792 |
|---|---|---|---------|---------|---------|
| 2 | 6 | 0 | 4.505059 | -1.704091 | -0.499563 |
| 3 | 6 | 0 | 3.677109 | -0.700254 | 0.067947 |
| 4 | 6 | 0 | 2.294331 | -0.636402 | -0.306672 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 5 | 6 | 0 | 1.807968 | -1.606107 | -1.226667 |
| 6 | 6 | 0 | 2.637224 | -2.566766 | -1.755750 |
| 7 | 6 | 0 | 4.191391 | 0.235764 | 1.002823 |
| 8 | 6 | 0 | 3.375239 | 1.194961 | 1.544799 |
| 9 | 6 | 0 | 2.015221 | 1.269310 | 1.168235 |
| 10 | 6 | 0 | 1.469924 | 0.389338 | 0.260593 |
| 11 | 6 | 0 | -0.002353 | 0.509041 | -0.128237 |
| 12 | 6 | 0 | -2.161681 | -0.890036 | -0.001496 |
| 13 | 6 | 0 | -0.531070 | -1.052196 | 1.785792 |
| 14 | 6 | 0 | -1.358897 | -1.960750 | 2.482073 |
| 15 | 6 | 0 | -2.564034 | -2.339740 | 1.952328 |
| 16 | 6 | 0 | -2.995049 | -1.820819 | 0.703727 |
| 17 | 6 | 0 | -2.639833 | -0.389950 | -1.243462 |
| 18 | 6 | 0 | -3.851918 | -0.784806 | -1.759520 |
| 19 | 6 | 0 | -4.664856 | -1.703698 | 1.061073 |
| 20 | 6 | 0 | -4.204746 | -2.207251 | 0.143630 |
| 21 | 6 | 0 | -0.538506 | 1.804138 | 0.166433 |
| 22 | 6 | 0 | -0.603356 | 2.751809 | 0.915392 |
| 23 | 6 | 0 | -1.659319 | 3.790138 | 0.516764 |
| 24 | 6 | 0 | 0.757125 | 3.358387 | -0.126547 |
| 25 | 6 | 0 | -1.353477 | 4.570314 | 0.765738 |
| 26 | 6 | 0 | 4.644492 | -3.379952 | -1.817047 |
| 27 | 6 | 0 | 5.549993 | -1.738722 | -0.209025 |
| 28 | 6 | 0 | 0.762730 | -1.605060 | -1.508032 |
| 29 | 6 | 0 | 2.240319 | -3.295764 | 2.453328 |
| 30 | 6 | 0 | 5.238321 | 0.176133 | 1.281217 |
| 31 | 6 | 0 | 3.768238 | 1.906629 | 2.262399 |
| 32 | 6 | 0 | 1.381459 | 2.039024 | 1.588722 |
| 33 | 6 | 0 | -0.069207 | 0.349889 | -1.210465 |
| 34 | 6 | 0 | 0.421591 | -0.776668 | 2.219849 |
| 35 | 6 | 0 | -1.029280 | -3.256983 | 3.435850 |
| 36 | 6 | 0 | -3.205313 | -3.040371 | 2.476811 |
| 37 | 6 | 0 | -2.044555 | 0.319621 | -1.801581 |
| 38 | 6 | 0 | -4.187530 | -0.385422 | -2.710125 |
| 39 | 6 | 0 | -5.618780 | -2.006952 | -1.477329 |
| 40 | 6 | 0 | -4.856230 | -2.913708 | 0.690816 |
| 41 | 6 | 0 | -0.977025 | 2.226905 | -1.806874 |
| 42 | 6 | 0 | -1.782943 | 4.483412 | -1.356586 |
| 43 | 6 | 0 | -2.610977 | 3.263071 | -0.399256 |
| 44 | 6 | 0 | 0.640481 | 4.077931 | -2.081740 |
| 45 | 6 | 0 | 1.197915 | 3.874885 | -0.410914 |
| 46 | 6 | 0 | 1.461588 | 2.591613 | -1.593182 |
| 47 | 6 | 0 | -2.172805 | 5.255548 | 0.998742 |
| 48 | 6 | 0 | -1.323607 | 3.890172 | 1.610853 |
| 49 | 6 | 0 | -0.442485 | 5.167941 | 0.675813 |
| 50 | 6 | 0 | 3.773189 | -2.565744 | -1.730898 |
| 51 | 6 | 0 | 4.390472 | -1.750747 | -0.814350 |
| 52 | 6 | 0 | 3.663832 | -0.751985 | -0.114624 |
| 53 | 6 | 0 | 2.263530 | -0.588736 | -0.377144 |
| 54 | 6 | 0 | 1.658485 | -1.459616 | -1.324867 |
| 55 | 6 | 0 | 2.391647 | -2.418106 | -1.984062 |

1e (conformer 6)
|    |   |   |                     |                     |                     |
|----|---|---|---------------------|---------------------|---------------------|
|  7 | 6 | 0 | 4.297656            | 0.083128            | 0.842232            |
|  8 | 6 | 0 | 3.579536            | 1.039461            | 1.512018            |
|  9 | 6 | 0 | 2.201628            | 1.211040            | 1.247530            |
| 10 | 6 | 0 | 1.540482            | 0.430155            | 0.325553            |
| 11 | 6 | 0 | 0.050979            | 0.655121            | 0.054668            |
| 12 | 6 | 0 | -0.847967           | -0.369853           | 0.747342            |
| 13 | 6 | 0 | -2.048481           | -0.854822           | 0.128913            |
| 14 | 6 | 0 | -0.529397           | -0.795646           | 2.018797            |
| 15 | 6 | 0 | -1.350018           | -1.695106           | 2.732126            |
| 16 | 6 | 0 | -2.497215           | -2.180660           | 2.160452            |
| 17 | 6 | 0 | -2.873661           | -1.780353           | 0.853209            |
| 18 | 6 | 0 | -2.475402           | -0.478721           | -1.75008            |
| 19 | 6 | 0 | -3.629722           | -0.980860           | -1.728145           |
| 20 | 6 | 0 | -4.433600           | -1.892940           | -1.010096           |
| 21 | 6 | 0 | -4.059013           | -2.279920           | 0.252163            |
| 22 | 8 | 0 | -3.89427            | 1.945358            | 0.492554            |
| 23 | 6 | 0 | -0.052059           | 3.055647            | -0.368225           |
| 24 | 6 | 0 | -1.062515           | 3.204030            | -1.518679           |
| 25 | 6 | 0 | 0.023598            | 4.286951            | 0.528462            |
| 26 | 6 | 0 | -2.509235           | 3.446047            | -1.078534           |
| 27 | 6 | 0 | 4.340073            | -3.325491           | -2.256983           |
| 28 | 1 | 0 | 5.449939            | -1.861073           | -0.607190           |
| 29 | 1 | 0 | 0.597933            | -1.384397           | -1.526164           |
| 30 | 1 | 0 | 1.904450            | -3.070027           | -2.700397           |
| 31 | 1 | 0 | 5.356965            | -0.051227           | 1.034031            |
| 32 | 1 | 0 | 4.063268            | 1.674179            | 2.246127            |
| 33 | 1 | 0 | 1.645136            | 1.974097            | 1.776098            |
| 34 | 1 | 0 | -0.092886           | 0.581157            | -1.026573           |
| 35 | 1 | 0 | 0.379858            | -0.436410           | 2.484251            |
| 36 | 1 | 0 | -1.061963           | -2.001432           | 3.731368            |
| 37 | 1 | 0 | -3.132312           | -2.877972           | 2.696659            |
| 38 | 1 | 0 | -1.889685           | 0.223560            | -1.751872           |
| 39 | 1 | 0 | -3.926779           | -0.671871           | -2.724111           |
| 40 | 1 | 0 | -5.341602           | -2.281664           | -1.456826           |
| 41 | 1 | 0 | -4.668085           | -2.978978           | 0.815802            |
| 42 | 1 | 0 | 0.938847            | 2.874692            | -0.803421           |
| 43 | 1 | 0 | -0.719316           | 4.025277            | -2.158900           |
| 44 | 1 | 0 | -1.015557           | 2.306870            | -2.145494           |
| 45 | 1 | 0 | 0.192223            | 5.187550            | -0.068233           |
| 46 | 1 | 0 | -0.903569           | 4.412171            | 1.091309            |
| 47 | 1 | 0 | 0.842567            | 4.191661            | 1.243941            |
| 48 | 1 | 0 | -3.181661           | 3.438319            | -1.940357           |
| 49 | 1 | 0 | -2.837785           | 2.669305            | -0.385327           |
| 50 | 1 | 0 | -2.625139           | 4.412248            | -0.581168           |

| **1e (conformer 7)** |
|----------------------|
| 1  | 6  | 0 | 3.953290 | -2.422310 | -1.237532 |
| 2  | 6  | 0 | 3.742262 | -2.530539 | 0.113663 |
| 3  | 6  | 0 | 2.708755 | -1.800290 | 0.758812 |
| 4  | 6  | 0 | 1.867422 | -0.928082 | -0.014714 |
| 5  | 6  | 0 | 2.122061 | -0.847869 | -1.414490 |
| 6  | 6  | 0 | 3.130473 | -1.570069 | -2.006819 |
| 7  | 6  | 0 | 2.499708 | -1.919645 | 2.155137 |
| 8  | 6  | 0 | 1.497220 | -1.213992 | 2.771602 |
|   |   |   | 0.666670 | -0.362498 | 2.016484 |
|---|---|---|----------|----------|----------|
| 10| 6 | 0 | 0.826982 | -0.203505 | 0.655386 |
| 11| 6 | 0 | -0.079318 | 0.806640 | -0.065182 |
| 12| 6 | 0 | -1.557661 | 0.611195 | 0.265798 |
| 13| 6 | 0 | -2.276999 | -0.520467 | -0.242149 |
| 14| 6 | 0 | -2.216799 | 1.533874 | 1.048752 |
| 15| 6 | 0 | -3.584491 | 1.385118 | 1.373234 |
| 16| 6 | 0 | -4.295598 | 0.312466 | 0.903329 |
| 17| 6 | 0 | -3.665658 | -0.660873 | 0.084051 |
| 18| 6 | 0 | -1.686377 | -1.516861 | -1.066983 |
| 19| 6 | 0 | -2.418210 | -2.579880 | -1.541709 |
| 20| 6 | 0 | -3.786155 | -2.712170 | -1.217695 |
| 21| 6 | 0 | -4.391626 | -1.771416 | -0.421710 |
| 22| 8 | 0 | 0.267758 | 2.148533 | 0.282365 |
| 23| 6 | 0 | 1.480763 | 2.691698 | -0.277213 |
| 24| 6 | 0 | 1.139278 | 4.047209 | -0.903064 |
| 25| 6 | 0 | 2.544997 | 2.809884 | 0.812018 |
| 26| 6 | 0 | 0.151971 | 3.960617 | 2.068349 |
| 27| 1 | 0 | 4.745188 | -2.986622 | -1.716559 |
| 28| 1 | 0 | 4.366340 | -3.181955 | 0.716627 |
| 29| 1 | 0 | 2.544997 | 2.809884 | 0.812018 |
| 30| 1 | 0 | 3.143431 | -2.581301 | 2.724995 |
| 31| 1 | 0 | 1.335328 | -1.309224 | 3.839341 |
| 32| 1 | 0 | -0.123313 | 0.183112 | 2.519030 |
| 33| 1 | 0 | 0.028234 | 0.693016 | -2.039428 |
| 34| 1 | 0 | -1.670026 | 2.391393 | 1.410889 |
| 35| 1 | 0 | -4.065819 | 2.131966 | 1.994867 |
| 36| 1 | 0 | -5.346456 | 0.192991 | 1.145318 |
| 37| 1 | 0 | -0.637898 | -1.452656 | -1.323797 |
| 38| 1 | 0 | -1.939662 | -3.325031 | -2.167323 |
| 39| 1 | 0 | -4.352325 | -3.555371 | -1.596985 |
| 40| 1 | 0 | -5.442085 | -1.862676 | -0.165300 |
| 41| 1 | 0 | 1.841692 | 2.020232 | -1.065909 |
| 42| 1 | 0 | 0.732327 | 4.691405 | -0.115270 |
| 43| 1 | 0 | 2.073084 | 4.513143 | -1.237531 |
| 44| 1 | 0 | 3.463976 | 3.243562 | 0.406972 |
| 45| 1 | 0 | 2.184728 | 3.455288 | 1.617826 |
| 46| 1 | 0 | 2.782461 | 1.833497 | 1.235914 |
| 47| 1 | 0 | -0.075319 | 4.953181 | -2.466021 |
| 48| 1 | 0 | 0.558983 | 3.361405 | -2.889474 |
| 49| 1 | 0 | -0.786764 | 3.503745 | -1.748156 |

| 1e (conformer 8) |   |   | 4.655316 | -1.727710 | -1.016199 |
| 2 | 6 | 0 | 4.215059 | -2.252207 | 0.173572 |
| 3 | 6 | 0 | 2.966529 | -1.866485 | 0.728323 |
| 4 | 6 | 0 | 2.149348 | -0.914436 | 0.031174 |
| 5 | 6 | 0 | 2.645148 | -0.389516 | -1.191033 |
| 6 | 6 | 0 | 3.858521 | -0.785425 | -1.702669 |
| 7 | 6 | 0 | 2.515814 | -2.408233 | 1.959908 |
| 8 | 6 | 0 | 1.307071 | -2.030582 | 2.482573 |
| 9 | 6 | 0 | 0.494544 | -1.101663 | 1.795233 |
| 10| 6 | 0 | 0.882831 | -0.542761 | 0.597392 |
|     |   |   |     |     |     |     |
|-----|---|---|-----|-----|-----|-----|
| 11  | 6 | 0 | -0.005729 | 0.486179 | -0.104701|
| 12  | 6 | 0 | -1.480098 | 0.392114 | 0.287481 |
| 13  | 6 | 0 | -2.344359 | -0.570800 | -0.328441|
| 14  | 6 | 0 | -1.989779 | 1.239394 | 1.246833 |
| 15  | 6 | 0 | -3.349474 | 1.195277 | 1.627990 |
| 16  | 6 | 0 | -4.202094 | 0.296693 | 1.040244 |
| 17  | 6 | 0 | -3.726392 | -0.606128 | 0.053861 |
| 18  | 6 | 0 | -1.898577 | 1.239394 | 1.246833 |
| 19  | 6 | 0 | -3.349474 | 1.195277 | 1.627990 |
| 20  | 6 | 0 | -4.127693 | -2.433480 | -1.499531|
| 21  | 6 | 0 | -4.593066 | -1.549906 | -0.557369|
| 22  | 8 | 0 | 0.554337  | 1.771536 | 0.186644 |
| 23  | 6 | 0 | 0.132996  | 2.867849 | -0.652352|
| 24  | 6 | 0 | 0.398168  | 4.150929 | 0.145115 |
| 25  | 6 | 0 | 0.831010  | 2.849045 | -2.014042|
| 26  | 6 | 0 | 1.857648  | 4.368471 | 0.558090 |
| 27  | 1 | 0 | 5.610842  | -2.030771 | -1.429021|
| 28  | 1 | 0 | 4.818868  | -2.974933 | 0.712506 |
| 29  | 1 | 0 | 2.065592  | 0.345757 | -1.729811|
| 30  | 1 | 0 | 4.209688  | -0.366654 | -2.639271|
| 31  | 1 | 0 | 3.144157  | -3.125984 | 2.476913 |
| 32  | 1 | 0 | 0.962068  | -2.444471 | 3.423332 |
| 33  | 1 | 0 | -0.461964 | -0.830208 | 2.222809 |
| 34  | 1 | 0 | 0.055960  | 0.312612 | -1.184296|
| 35  | 1 | 0 | -1.324771 | 1.956029 | 1.712261 |
| 36  | 1 | 0 | -3.712564 | 1.880454 | 2.385890 |
| 37  | 1 | 0 | -5.249233 | 0.260066 | 1.321731 |
| 38  | 1 | 0 | -0.855947 | -1.532394 | -1.589245|
| 39  | 1 | 0 | -2.397856 | -3.119452 | -2.605700|
| 40  | 1 | 0 | -4.800032 | -3.150412 | -1.957008|
| 41  | 1 | 0 | -5.636710 | -1.562554 | -0.260529|
| 42  | 1 | 0 | -0.949113 | 2.791060 | -0.814648|
| 43  | 1 | 0 | 0.046250  | 4.998318 | -0.454176 |
| 44  | 1 | 0 | -0.229611 | 4.123010 | 1.041415 |
| 45  | 1 | 0 | 0.527036  | 3.720485 | -2.600640|
| 46  | 1 | 0 | 1.917710  | 2.871203 | -1.901773 |
| 47  | 1 | 0 | 0.562768  | 1.962631 | -2.593828 |
| 48  | 1 | 0 | 1.949220  | 5.264479 | 1.777729 |
| 49  | 1 | 0 | 2.226236  | 3.517408 | 1.133141 |
| 50  | 1 | 0 | 2.512678  | 4.500708 | -0.307063 |

**1e (conformer 9)**

|     |   |   |     |     |     |     |
|-----|---|---|-----|-----|-----|-----|
| 1   | 6 | 0 | -3.829113 | -2.274505 | 2.105203|
| 2   | 6 | 0 | -4.353599 | -1.786791 | 0.934039|
| 3   | 6 | 0 | -3.565741 | -1.008005 | 0.046050|
| 4   | 6 | 0 | -2.202337 | -0.718462 | 0.385583|
| 5   | 6 | 0 | -1.692281 | -1.253677 | 1.601306|
| 6   | 6 | 0 | -2.482408 | -2.006660 | 2.437100|
| 7   | 6 | 0 | -4.101810 | -0.517900 | -1.172983|
| 8   | 6 | 0 | -3.325015 | 0.225424 | -2.024254|
| 9   | 6 | 0 | -1.985672 | 0.521968 | -1.687729|
| 10  | 6 | 0 | -1.420127 | 0.078512 | -0.511983|
| 11  | 6 | 0 | 0.028659  | 0.438412 | -0.185412|
| 12  | 6 | 0 | 1.035774  | -0.642677 | -0.586343|
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 13| 6| 0| 2.349003| -0.658417| -0.006017|
| 14| 6| 0| 0.705916| -1.603725| -1.516687|
| 15| 6| 0| 1.621447| -2.604715| -1.912219|
| 16| 6| 0| 2.875582| -2.648060| -1.363020|
| 17| 6| 0| 3.270886| -1.683910| -0.399969|
| 18| 6| 0| 2.791795| 0.295964| 0.949143|
| 19| 6| 0| 4.053272| 0.234375| 1.492863|
| 20| 6| 0| 4.953214| -0.783471| 1.107646|
| 21| 6| 0| 4.566471| -1.717980| 0.179453|
| 22| 8| 0| 0.448838| 1.647289| -0.830254|
| 23| 6| 0| -0.145471| 2.878359| -0.363076|
| 24| 6| 0| 0.493523| 3.353732| 0.950666|
| 25| 6| 0| 0.034651| 3.871468| 0.665316|
| 26| 6| 0| -0.196046| 4.576348| 1.567584|
| 27| 1| 0| -4.441452| -2.869135| 2.773602|
| 28| 1| 0| -5.384272| -1.993955| 0.665316|
| 29| 1| 0| -0.658700| -1.083241| 1.873560|
| 30| 1| 0| -2.067490| -2.403489| 3.356834|
| 31| 1| 0| -5.137324| -0.744785| -2.958455|
| 32| 1| 0| -3.733743| 0.977695| -2.362215|
| 33| 1| 0| -0.196046| 4.576348| 1.567584|
| 34| 1| 0| 0.096284| 0.576603| 0.899251|
| 35| 1| 0| -0.282939| -1.601727| -1.956278|
| 36| 1| 0| 1.318440| -3.340204| -2.648818|
| 37| 1| 0| 3.583128| -3.417468| -1.653866|
| 38| 1| 0| 2.131607| 1.098322| 1.243152|
| 39| 1| 0| 4.362931| 0.977695| 2.219155|
| 40| 1| 0| 5.945737| -0.820663| 1.542237|
| 41| 1| 0| 5.250226| -2.502218| -0.128632|
| 42| 1| 0| -1.217202| 2.713642| -0.192280|
| 43| 1| 0| 0.455295| 2.536990| 1.678554|
| 44| 1| 0| 1.552185| 3.566965| 0.766773|
| 45| 1| 0| -0.392569| 4.844905| -1.255567|
| 46| 1| 0| 1.098367| 4.002459| -1.722100|
| 47| 1| 0| -0.455109| 3.506029| -2.409643|
| 48| 1| 0| 0.247283| 4.821369| 2.535994|
| 49| 1| 0| -0.105578| 5.461170| 0.933185|
| 50| 1| 0| -1.260383| 4.388926| 1.730222|

**1e (conformer 10)**

|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 6| 0| 4.908223| -1.241182| -0.962774|
| 2 | 6| 0| 4.506788| -1.808499| 0.221127|
| 3 | 6| 0| 3.215046| -1.557369| 0.753972|
| 4 | 6| 0| 2.313948| -0.698839| 0.042154|
| 5 | 6| 0| 2.770614| -0.124456| -1.174707|
| 6 | 6| 0| 4.027505| -0.389534| -1.665161|
| 7 | 6| 0| 2.801829| -2.142852| 1.978818|
| 8 | 6| 0| 1.550342| -1.895513| 2.478032|
| 9 | 6| 0| 0.655233| -1.059265| 1.773336|
| 10| 6| 0| 1.004178| -0.463526| 0.581537|
| 11| 6| 0| 0.024474| 0.447392| -0.161902|
| 12| 6| 0| -1.431101| 0.263201| 0.261277|
| 13| 6| 0| -2.241372| -0.764687| -0.323038|
| 14| 6| 0| -1.977055| 1.087737| 1.220812|
|   |   |   |        |        |        |
|---|---|---|--------|--------|--------|
| 15| 6 | 0 | -3.322868 | 0.959583 | 1.630291 |
| 16| 6 | 0 | -4.125824 | -0.000962 | 1.071034 |
| 17| 6 | 0 | -3.610664 | -0.884958 | 0.087824 |
| 18| 6 | 0 | -1.753426 | -1.691081 | -1.286606 |
| 19| 6 | 0 | -2.568731 | -2.658838 | -1.823885 |
| 20| 6 | 0 | -3.920630 | -2.761474 | -1.427549 |
| 21| 6 | 0 | -4.425039 | -1.893636 | -0.491028 |
| 22| 8 | 0 | 0.497903  | 1.787017  | 0.028564 |
| 23| 6 | 0 | -0.058377 | 2.823627  | -0.806192 |
| 24| 6 | 0 | 0.869057  | 4.142693  | -0.255292 |
| 25| 6 | 0 | 0.294904  | 2.653938  | -2.285507 |
| 26| 6 | 0 | 0.105687  | 4.433053  | 1.197178 |
| 27| 1 | 0 | 5.897408  | -1.441392 | 1.358740 |
| 28| 1 | 0 | 5.175368  | -2.462259 | 0.771654 |
| 29| 1 | 0 | 0.489057  | 4.142693  | -0.255292 |
| 30| 1 | 0 | 0.294904  | 2.653938  | -2.285507 |
| 31| 1 | 0 | 0.105687  | 4.433053  | 1.197178 |
| 32| 1 | 0 | 1.234080  | -2.342973 | 3.413503 |
| 33| 1 | 0 | -0.332438 | -0.892334 | 2.183180 |
| 34| 1 | 0 | 0.088491  | 0.203616  | -1.226785 |
| 35| 1 | 0 | -1.354901 | 1.854163  | 1.664808 |
| 36| 1 | 0 | -3.715509 | 1.629606  | 2.386994 |
| 37| 1 | 0 | -5.162583 | -1.024411 | 1.374196 |
| 38| 1 | 0 | -0.716977 | -1.651913 | -1.595799 |
| 39| 1 | 0 | -2.169766 | -3.353345 | -2.554659 |
| 40| 1 | 0 | -4.552895 | -3.528714 | -1.859736 |
| 41| 1 | 0 | -5.459704 | -1.969152 | -0.172941 |
| 42| 1 | 0 | -1.151265 | 2.814763  | -0.700900 |
| 43| 1 | 0 | 1.580330  | 4.121713  | -0.353090 |
| 44| 1 | 0 | 0.129669  | 4.950327  | -0.902299 |
| 45| 1 | 0 | -0.149363 | 3.469307  | -2.862761 |
| 46| 1 | 0 | 1.378119  | 2.685558  | -2.431674 |
| 47| 1 | 0 | -0.089567 | 1.720641  | -2.702783 |
| 48| 1 | 0 | 0.521434  | 5.389735  | 1.524539 |
| 49| 1 | 0 | -0.981017 | 4.485291  | 1.317921 |
| 50| 1 | 0 | 0.485977  | 3.654391  | 1.860000 |

1e (conformer 11)

|   |   |   |        |        |        |
|---|---|---|--------|--------|--------|
| 1 | 6 | 0 | 4.977180  | -0.897633 | -1.033140 |
| 2 | 6 | 0 | 4.626209  | -1.586005 | 0.101471 |
| 3 | 6 | 0 | 3.331309  | -1.454410 | 0.668466 |
| 4 | 6 | 0 | 2.371614  | -0.591113 | 0.043344 |
| 5 | 6 | 0 | 2.777892  | 0.110921  | -1.123726 |
| 6 | 6 | 0 | 4.039883  | -0.039300 | -1.648683 |
| 7 | 6 | 0 | 2.973393  | -2.162893 | 1.844446 |
| 8 | 6 | 0 | 1.719298  | -2.029262 | 2.379507 |
| 9 | 6 | 0 | 0.767144  | -1.190217 | 1.758819 |
| 10| 6 | 0 | 1.060329  | -0.347820 | 0.616448 |
| 11| 6 | 0 | 0.015332  | 0.442667  | -0.017535 |
| 12| 6 | 0 | -1.423576 | 0.080435  | 0.349034 |
| 13| 6 | 0 | -2.121428 | -0.953751 | -0.355945 |
| 14| 6 | 0 | -2.063121 | 0.750211  | 1.369187 |
| 15| 6 | 0 | -3.397303 | 0.454471  | 1.727964 |
| 16| 6 | 0 | -4.093867 | -0.516809 | 1.055920 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 17| 6| 0| -3.479333| -1.243569| 0.003416|
| 18| 6| 0| -1.529789| -1.723954| -1.395408|
| 19| 6| 0| -2.238949| -2.702020| -2.051594|
| 20| 6| 0| -3.581315| -2.971778| -1.704313|
| 21| 6| 0| -4.182880| -2.258362| -0.697377|
| 22| 8| 0| 0.360600| 1.776798| 0.372740|
| 23| 6| 0| -0.249159| 2.853452| -0.371612|
| 24| 6| 0| -0.111902| 4.087282| 0.524479|
| 25| 6| 0| 0.403746| 3.033712| -1.742252|
| 26| 6| 0| -0.815302| 5.340493| -0.005530|
| 27| 1| 0| 5.969423| -1.007048| 1.456024|
| 28| 1| 0| 5.338300| -2.245657| 0.586483|
| 29| 1| 0| 2.088449| 0.788632| -1.605309|
| 30| 1| 0| 4.320355| 0.510121| -2.540540|
| 31| 1| 0| 3.709199| -2.810622| 2.378472|
| 32| 1| 0| 1.445200| 0.788632| -1.605309|
| 33| 1| 0| -0.078363| 3.845051| -2.292775|
| 34| 1| 0| -4.128666| -3.745082| -2.230285|
| 35| 1| 0| -5.211081| -2.463406| -0.417542|
| 36| 1| 0| -1.315696| 2.632034| -0.508579|
| 37| 1| 0| -0.519294| 3.827677| 1.506005|
| 38| 1| 0| 0.955149| 4.284571| 0.675467|
| 39| 1| 0| -1.762895| -3.275528| -2.838975|
| 40| 1| 0| -4.126666| -3.745082| -2.230285|
| 41| 1| 0| -5.211081| -2.463406| -0.417542|
| 42| 1| 0| -1.315696| 2.632034| -0.508579|
| 43| 1| 0| -0.519294| 3.827677| 1.506005|
| 44| 1| 0| 0.955149| 4.284571| 0.675467|
| 45| 1| 0| -0.078363| 3.845051| -2.292775|
| 46| 1| 0| 1.465000| 3.273009| -1.631731|
| 47| 1| 0| 0.309059| 2.135780| -2.357395|
| 48| 1| 0| -0.745536| 6.153890| 0.721026|
| 49| 1| 0| -0.373154| 5.698533| -0.938583|
| 50| 1| 0| -1.877958| 5.152833| -0.189484|

**1e (conformer 12)**

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.688849 | -1.209365 | -1.055927|
| 2 | 6 | 0 | 4.702929 | -0.520733 | 0.131245|
| 3 | 6 | 0 | 3.557682 | 0.183481 | 0.587034|
| 4 | 6 | 0 | 2.356388 | 0.164714 | -0.199485|
| 5 | 6 | 0 | 2.386762 | -0.555945 | -1.425337|
| 6 | 6 | 0 | 3.516507 | -1.220072 | -1.842001|
| 7 | 6 | 0 | 3.593236 | 0.917140 | 1.800372|
| 8 | 6 | 0 | 2.493015 | 1.620798 | 2.213240|
| 9 | 6 | 0 | 1.309376 | 1.609049 | 1.442958|
| 10| 6 | 0 | 1.209845 | 0.889308 | 0.271297|
| 11| 6 | 0 | -0.090433 | 0.946885 | -0.542005|
| 12| 6 | 0 | -0.809365 | -0.381084 | -0.811294|
| 13| 6 | 0 | -1.266440 | -1.258853 | 0.227346|
| 14| 6 | 0 | -1.081963 | -0.706030 | -2.125013|
| 15| 6 | 0 | -1.763551 | -1.889934 | -2.484141|
| 16| 6 | 0 | -2.180574 | -2.757614 | -1.509611|
| 17| 6 | 0 | -1.949140 | -2.466790 | -0.139851|
| 18| 6 | 0 | -1.094213 | -0.991699 | 1.612661|
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 19 | 6 | 0 | -1.545760 | -1.868227 | 2.570749 |
| 20 | 6 | 0 | -2.199534 | -3.064757 | 2.203036 |
| 21 | 6 | 0 | -2.397181 | -3.352047 | 0.875646 |
| 22 | 8 | 0 | -0.985276 | 1.862714 | 0.096453 |
| 23 | 6 | 0 | -1.864378 | 2.597817 | -0.774348 |
| 24 | 6 | 0 | -3.065163 | 3.032870 | 0.066443 |
| 25 | 6 | 0 | -1.133509 | 3.791267 | -1.391417 |
| 26 | 6 | 0 | -2.199534 | 1.862714 | 0.096453 |
| 27 | 8 | 0 | -0.985276 | 1.862714 | 0.096453 |
| 28 | 6 | 0 | -1.864378 | 2.597817 | -0.774348 |
| 29 | 6 | 0 | -3.065163 | 3.032870 | 0.066443 |
| 30 | 6 | 0 | -1.133509 | 3.791267 | -1.391417 |
| 31 | 6 | 0 | -2.199534 | 1.862714 | 0.096453 |
| 32 | 6 | 0 | -1.864378 | 2.597817 | -0.774348 |
| 33 | 6 | 0 | -3.065163 | 3.032870 | 0.066443 |
| 34 | 6 | 0 | -1.133509 | 3.791267 | -1.391417 |
| 35 | 6 | 0 | -2.199534 | 1.862714 | 0.096453 |
| 36 | 6 | 0 | -1.864378 | 2.597817 | -0.774348 |
| 37 | 6 | 0 | -3.065163 | 3.032870 | 0.066443 |
| 38 | 6 | 0 | -1.133509 | 3.791267 | -1.391417 |
| 39 | 6 | 0 | -2.199534 | 1.862714 | 0.096453 |
| 40 | 6 | 0 | -1.864378 | 2.597817 | -0.774348 |
| 41 | 6 | 0 | -3.065163 | 3.032870 | 0.066443 |
| 42 | 6 | 0 | -1.133509 | 3.791267 | -1.391417 |
| 43 | 6 | 0 | -2.199534 | 1.862714 | 0.096453 |
| 44 | 6 | 0 | -1.864378 | 2.597817 | -0.774348 |
| 45 | 6 | 0 | -3.065163 | 3.032870 | 0.066443 |
| 46 | 6 | 0 | -1.133509 | 3.791267 | -1.391417 |
| 47 | 6 | 0 | -2.199534 | 1.862714 | 0.096453 |
| 48 | 6 | 0 | -1.864378 | 2.597817 | -0.774348 |
| 49 | 6 | 0 | -3.065163 | 3.032870 | 0.066443 |
| 50 | 6 | 0 | -1.133509 | 3.791267 | -1.391417 |

### 1e (conformer 15)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | 2.699413 | -3.031864 | 2.073389 |
| 2  | 6 | 0 | 2.839941 | -3.269200 | 0.729008 |
| 3  | 6 | 0 | 2.270371 | -2.393654 | -0.232740 |
| 4  | 6 | 0 | 1.522065 | -1.250924 | 0.208229 |
| 5  | 6 | 0 | 1.414250 | -1.031636 | 1.608600 |
| 6  | 6 | 0 | 1.983974 | -1.896371 | 2.512810 |
| 7  | 6 | 0 | 2.445298 | -2.629125 | -1.621252 |
| 8  | 6 | 0 | 1.915070 | -1.766533 | -2.543938 |
| 9  | 6 | 0 | 1.169733 | -0.647545 | -2.111578 |
| 10 | 6 | 0 | 0.940738 | -0.383425 | -0.776418 |
| 11 | 6 | 0 | 0.122195 | 0.868233 | -0.423855 |
| 12 | 6 | 0 | 1.166393 | 0.632913 | 0.375676 |
| 13 | 6 | 0 | -2.259759 | -0.097651 | -0.181428 |
| 14 | 6 | 0 | -1.298192 | 1.183215 | 1.633197 |
| 15 | 6 | 0 | -2.468382 | 1.011526 | 2.404800 |
| 16 | 6 | 0 | -3.520366 | 0.291649 | 1.909557 |
| 17 | 6 | 0 | -3.455891 | -0.270287 | 0.609218 |
| 18 | 6 | 0 | -2.727595 | -0.645235 | -1.493950 |
| 19 | 6 | 0 | -3.360044 | -1.326007 | -1.988459 |
| 20 | 6 | 0 | -4.515274 | -1.507709 | -1.197950 |
|  |  |  |  |  |  |
|---|---|---|---|---|---|
| 21 | 6 | 0 | -4.556572 | -0.987942 | 0.071636 |
| 22 | 8 | 0 | 0.919104 | 1.810815 | 0.295996 |
| 23 | 6 | 0 | 1.934891 | 2.498137 | -0.459939 |
| 24 | 6 | 0 | 1.934891 | 2.498137 | -0.459939 |
| 25 | 6 | 0 | 3.007872 | 2.904926 | 0.543449 |
| 26 | 6 | 0 | 0.650617 | 4.747294 | -0.401158 |
| 27 | 1 | 0 | 3.140259 | -3.707217 | 2.798004 |
| 28 | 1 | 0 | 3.396334 | -4.131921 | 0.377576 |
| 29 | 1 | 0 | 0.886446 | -0.162071 | 1.965835 |
| 30 | 1 | 0 | 1.784485 | -0.459939 | -2.121382 |
| 31 | 1 | 0 | 4.425457 | 0.150843 | 2.495089 |
| 32 | 1 | 0 | -2.521718 | 1.455958 | 3.392422 |
| 33 | 1 | 0 | 3.140259 | -3.707217 | 2.798004 |
| 34 | 1 | 0 | 3.396334 | -4.131921 | 0.377576 |
| 35 | 1 | 0 | 2.379009 | 1.794999 | -1.174870 |
| 36 | 1 | 0 | 1.350421 | 5.248605 | 0.272242 |
| 37 | 1 | 0 | 1.724054 | 3.811673 | -1.773088 |
| 38 | 1 | 0 | 1.938378 | 3.874942 | -0.418977 |
| 39 | 1 | 0 | 1.658188 | 2.763914 | 0.419434 |
| 40 | 1 | 0 | 1.127326 | 1.561170 | -0.515619 |
| 41 | 1 | 0 | 0.302948 | 3.468603 | 0.047798 |
| 42 | 1 | 0 | 2.587535 | 3.526548 | 1.337079 |
| 43 | 1 | 0 | 3.445394 | 2.017237 | 1.003813 |
| 44 | 1 | 0 | 0.202294 | 5.513970 | -1.038446 |
| 45 | 1 | 0 | -0.143416 | 4.307270 | 0.205788 |
| 46 | 1 | 0 | 1.350421 | 5.248605 | 0.272242 |

1e (conformer 16)

|  |  |  |  |  |  |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.724054 | 3.811673 | -1.773088 |
| 2 | 6 | 0 | 1.938378 | 3.874942 | -0.418977 |
| 3 | 6 | 0 | 1.658188 | 2.763914 | 0.419434 |
| 4 | 6 | 0 | 1.127326 | 1.561170 | -0.515619 |
| 5 | 6 | 0 | 0.302948 | 3.468603 | 0.047798 |
| 6 | 6 | 0 | 2.587535 | 3.526548 | 1.337079 |
| 7 | 6 | 0 | 3.445394 | 2.017237 | 1.003813 |
| 8 | 6 | 0 | 0.202294 | 5.513970 | -1.038446 |
| 9 | 6 | 0 | 1.350421 | 5.248605 | 0.272242 |
| 10 | 6 | 0 | 0.835936 | 0.452331 | 0.706644 |
| 11 | 6 | 0 | 0.271068 | -0.883723 | 0.202213 |
| 12 | 6 | 0 | -1.098156 | -0.831127 | -0.489084 |
| 13 | 6 | 0 | -2.79091 | -0.419589 | 0.216470 |
| 14 | 6 | 0 | -1.215059 | -1.247936 | -1.798226 |
| 15 | 6 | 0 | -2.453046 | -1.237432 | -2.477510 |
| 16 | 6 | 0 | -3.589007 | -0.817769 | -1.837748 |
| 17 | 6 | 0 | -3.534410 | -0.409912 | -0.480568 |
| 18 | 6 | 0 | -2.289025 | -0.042651 | 1.557741 |
| 19 | 6 | 0 | -3.449165 | 0.332045 | 2.223641 |
| 20 | 6 | 0 | -4.675977 | 0.357628 | 1.526115 |
| 21 | 6 | 0 | -4.711486 | -0.007618 | 0.203577 |
| 22 | 8 | 0 | 1.195198 | -1.509652 | -0.689814 |

S417
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 23 | 6 | 0 | 2.340973 | -2.133336 | -0.079442 |
| 24 | 6 | 0 | 1.987811 | -3.563345 | 0.354115 |
| 25 | 6 | 0 | 3.460054 | -2.068080 | -1.110994 |
| 26 | 6 | 0 | 3.075903 | -4.254054 | 1.183400 |
| 27 | 1 | 0 | 1.943354 | 4.666559 | -2.402860 |
| 28 | 1 | 0 | 2.333013 | 4.778406 | 0.034231 |
| 29 | 1 | 0 | 0.569541 | 0.627715 | 2.026917 |
| 30 | 1 | 0 | 1.067770 | 2.570371 | -3.420033 |
| 31 | 1 | 0 | 2.312310 | 1.782197 | 3.678068 |
| 32 | 1 | 0 | 0.934290 | -0.282532 | 2.705111 |
| 33 | 1 | 0 | 0.148803 | -1.517972 | 1.090708 |
| 34 | 1 | 0 | -0.330356 | -1.594788 | 2.313268 |
| 35 | 1 | 0 | -2.493259 | -1.565341 | 3.510310 |
| 36 | 1 | 0 | -4.544437 | -0.802130 | -2.351507 |
| 37 | 1 | 0 | -1.366955 | -0.040723 | 2.148722 |
| 38 | 1 | 0 | 1.943354 | 4.666559 | -2.402860 |
| 39 | 1 | 0 | 2.333013 | 4.778406 | 0.034231 |
| 40 | 1 | 0 | 0.569541 | 0.627715 | 2.026917 |
| 41 | 1 | 0 | 1.067770 | 2.570371 | -3.420033 |
| 42 | 1 | 0 | 2.312310 | 1.782197 | 3.678068 |
| 43 | 1 | 0 | 0.934290 | -0.282532 | 2.705111 |
| 44 | 1 | 0 | 0.148803 | -1.517972 | 1.090708 |
| 45 | 1 | 0 | -0.330356 | -1.594788 | 2.313268 |
| 46 | 1 | 0 | -2.493259 | -1.565341 | 3.510310 |
| 47 | 1 | 0 | -4.544437 | -0.802130 | -2.351507 |
| 48 | 1 | 0 | -1.366955 | -0.040723 | 2.148722 |
| 49 | 1 | 0 | 1.943354 | 4.666559 | -2.402860 |
| 50 | 1 | 0 | 2.333013 | 4.778406 | 0.034231 |

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.852683 | 0.503484 | 1.208983 |
| 2 | 6 | 0 | -4.798121 | -0.097063 | 0.023918 |
| 3 | 6 | 0 | -3.576972 | -0.600500 | 0.544008 |
| 4 | 6 | 0 | -2.371205 | -0.465805 | -0.224321 |
| 5 | 6 | 0 | -2.474438 | 0.154361 | -1.500125 |
| 6 | 6 | 0 | -3.675548 | 0.622401 | -1.978747 |
| 7 | 6 | 0 | -3.539774 | -1.249567 | 1.804465 |
| 8 | 6 | 0 | -2.362932 | -1.763408 | 2.280572 |
| 9 | 6 | 0 | -1.173508 | -1.633332 | 1.530639 |
| 10 | 6 | 0 | -1.145198 | -0.983105 | 0.315019 |
| 11 | 6 | 0 | 0.174740 | -0.893724 | -0.463389 |
| 12 | 6 | 0 | 0.699966 | 0.517810 | -0.763319 |
| 13 | 6 | 0 | 1.045768 | 1.463315 | 0.259187 |
| 14 | 6 | 0 | 0.901165 | 0.863868 | -2.084132 |
| 15 | 6 | 0 | 1.391937 | 2.131993 | -2.466096 |
| 16 | 6 | 0 | 1.691793 | 3.063157 | -1.507087 |
| 17 | 6 | 0 | 1.534049 | 2.755286 | -0.130706 |
| 18 | 6 | 0 | 0.948571 | 1.183907 | 1.649514 |
| 19 | 6 | 0 | 1.285626 | 2.126287 | 2.591947 |
| 20 | 6 | 0 | 1.743543 | 3.404277 | 2.202546 |
| 21 | 6 | 0 | 1.867099 | 3.706360 | 0.869464 |
| 22 | 6 | 0 | 1.156171 | -1.654237 | 0.243765 |
| 23 | 6 | 0 | 2.281747 | -2.115116 | -0.526795 |
| 24 | 6 | 0 | 3.426463 | -2.298015 | 0.472114 |

1e (conformer 17)
|   |   |   |   |   |
|---|---|---|---|---|
| 25 | 6 | 0 | 1.918023 | -3.394982 | -1.280145 |
| 26 | 6 | 0 | 4.767338 | -2.671244 | -0.167382 |
| 27 | 1 | 0 | -5.792864 | 0.881401 | -1.594475 |
| 28 | 1 | 0 | -5.696212 | -0.203431 | 0.623559 |
| 29 | 1 | 0 | -1.592562 | 0.270905 | -2.111653 |
| 30 | 1 | 0 | -3.718050 | 1.089443 | -2.956468 |
| 31 | 1 | 0 | -4.458484 | -1.340774 | 2.374290 |
| 32 | 1 | 0 | -2.333922 | -2.274820 | 3.236298 |
| 33 | 1 | 0 | -0.256045 | -2.057110 | 1.913558 |
| 34 | 1 | 0 | -0.006397 | -1.364532 | -1.439115 |
| 35 | 1 | 0 | 0.666001 | 0.142926 | -2.861322 |
| 36 | 1 | 0 | 1.525424 | 2.360030 | -3.517479 |
| 37 | 1 | 0 | 2.062342 | 4.044527 | -1.783992 |
| 38 | 1 | 0 | 0.616839 | -0.203431 | 0.623559 |
| 39 | 1 | 0 | 1.201742 | 1.885103 | 3.645792 |
| 40 | 1 | 0 | 1.525424 | 4.138988 | -2.956737 |
| 41 | 1 | 0 | 2.228279 | 4.680741 | 0.557130 |
| 42 | 1 | 0 | 2.566388 | -1.333309 | -1.242843 |
| 43 | 1 | 0 | 3.529469 | -1.360131 | -1.025226 |
| 44 | 1 | 0 | 3.130467 | -3.061542 | 1.200516 |
| 45 | 1 | 0 | 2.744336 | -3.725867 | -1.914126 |
| 46 | 1 | 0 | 1.679297 | -4.194057 | -0.572803 |
| 47 | 1 | 0 | 1.050367 | -3.243844 | -1.926942 |
| 48 | 1 | 0 | 5.555248 | -2.707660 | 0.589005 |
| 49 | 1 | 0 | 4.734312 | -3.503046 | -0.651976 |
| 50 | 1 | 0 | 5.067222 | -1.935013 | -0.919884 |

1e (conformer 18)

|   |   |   |   |   |
|---|---|---|---|---|
| 1  | 6 | 0 | -4.826766 | 0.858483 | -0.861476 |
| 2  | 6 | 0 | -4.713890 | 0.106392 | 0.281035 |
| 3  | 6 | 0 | -3.482420 | -0.498880 | 0.645017 |
| 4  | 6 | 0 | -2.327265 | -0.308222 | -0.186471 |
| 5  | 6 | 0 | -2.490613 | 0.470952 | -1.364977 |
| 6  | 6 | 0 | -3.700718 | 1.034873 | -1.694032 |
| 7  | 6 | 0 | -3.386920 | -1.302538 | 1.809582 |
| 8  | 6 | 0 | -2.203031 | -1.911130 | 2.131615 |
| 9  | 6 | 0 | -1.063277 | -1.727187 | 1.318453 |
| 10 | 6 | 0 | -1.090213 | 0.930551 | 0.193519 |
| 11 | 6 | 0 | 0.174673 | -0.789687 | -0.664320 |
| 12 | 6 | 0 | 0.743206 | 0.628029 | -0.820225 |
| 13 | 6 | 0 | 1.200607 | 1.419880 | 0.285668 |
| 14 | 6 | 0 | 0.868506 | 1.135275 | -2.097644 |
| 15 | 6 | 0 | 1.387974 | 2.423937 | -2.351054 |
| 16 | 6 | 0 | 1.792811 | 3.212266 | -1.306467 |
| 17 | 6 | 0 | 1.716702 | 2.734026 | 0.027640 |
| 18 | 6 | 0 | 1.187144 | 0.967448 | 1.633147 |
| 19 | 6 | 0 | 1.627747 | 1.768365 | 2.659699 |
| 20 | 6 | 0 | 2.112377 | 3.069849 | 2.402504 |
| 21 | 6 | 0 | 2.157438 | 3.536659 | 1.112714 |
| 22 | 6 | 0 | 1.169679 | -1.671340 | -0.140297 |
| 23 | 6 | 0 | 2.184063 | -2.098536 | -1.068924 |
| 24 | 6 | 0 | 3.441523 | -2.414804 | -0.250755 |
| 25 | 6 | 0 | 1.680452 | -3.272064 | -1.911854 |
| 26 | 6 | 0 | 3.280248 | -3.515692 | 0.802658 |
|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
|27 | 1 | 0 | -5.774376 | 1.312654 | -1.128196 |
|28 | 1 | 0 | -5.572937 | -0.044550 | 0.926591 |
|29 | 1 | 0 | -1.647654 | 0.634757 | -2.018747 |
|30 | 1 | 0 | -3.789892 | 1.623089 | -2.600610 |
|31 | 1 | 0 | -4.267977 | -1.434487 | 2.428752 |
|32 | 1 | 0 | -2.129881 | -2.539759 | 3.012127 |
|33 | 1 | 0 | -0.140586 | -2.226037 | 1.578841 |
|34 | 1 | 0 | -0.096934 | -1.121648 | -1.675257 |
|35 | 1 | 0 | 0.548141 | 0.530481 | 2.940567 |
|36 | 1 | 0 | 1.459477 | 2.781162 | -3.372096 |
|37 | 1 | 0 | 2.185806 | 4.207923 | -1.483335 |
|38 | 1 | 0 | 0.835521 | -0.028425 | 1.851129 |
|39 | 1 | 0 | 1.605072 | 1.396666 | 3.678009 |
|40 | 1 | 0 | 2.452678 | 3.692176 | 3.222513 |
|41 | 1 | 0 | 2.537221 | 4.530605 | 0.900071 |
|42 | 1 | 0 | 2.427650 | -1.260099 | 3.012127 |
|43 | 1 | 0 | 4.238200 | -2.685694 | -0.952981 |
|44 | 1 | 0 | 3.756698 | -1.488417 | 0.238768 |
|45 | 1 | 0 | 2.453928 | -3.597379 | -2.613745 |
|46 | 1 | 0 | 1.404900 | -4.118915 | -1.280345 |
|47 | 1 | 0 | 0.801233 | -2.991126 | 1.508158 |
|48 | 1 | 0 | 4.206852 | -3.637602 | 1.369792 |
|49 | 1 | 0 | 2.485445 | -3.265960 | 1.508158 |
|50 | 1 | 0 | 3.041825 | -4.483162 | 0.353298 |

|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
|51 | 1 | 0 | 5.339909 | 0.042419 | 0.029628 |
|52 | 1 | 0 | -4.853421 | -1.181775 | -0.415455 |
|53 | 1 | 0 | -3.466211 | -1.475206 | -0.344272 |
|54 | 1 | 0 | -2.555298 | -0.472495 | 0.126496 |
|55 | 1 | 0 | -3.098808 | 0.783326 | 0.513026 |
|56 | 1 | 0 | -4.449306 | 1.031563 | 0.442027 |
|57 | 1 | 0 | -2.971623 | -2.751209 | -0.719538 |
|58 | 1 | 0 | -1.635256 | -3.031763 | -0.618151 |
|59 | 1 | 0 | -0.734705 | -2.049520 | -0.147187 |
|60 | 1 | 0 | -1.154879 | -0.786685 | 0.209535 |
|61 | 1 | 0 | -0.176595 | 0.252294 | 0.766003 |
|62 | 1 | 0 | 1.242583 | -0.253940 | 1.023674 |
|63 | 1 | 0 | 2.203002 | -0.490762 | -0.016037 |
|64 | 1 | 0 | 1.604542 | -0.489855 | 2.339011 |
|65 | 1 | 0 | 2.886997 | -0.964493 | 2.685211 |
|66 | 1 | 0 | 3.822058 | -1.192647 | 1.709262 |
|67 | 1 | 0 | 3.509116 | -0.963841 | 0.344275 |
|68 | 1 | 0 | 1.923685 | -0.292067 | -1.397003 |
|69 | 1 | 0 | 2.875133 | -0.541227 | -2.357594 |
|70 | 1 | 0 | 4.161947 | -1.000180 | -1.997292 |
|71 | 1 | 0 | 4.467835 | -1.205639 | -0.675177 |
|72 | 1 | 0 | -0.230194 | 1.399091 | -0.098074 |
|73 | 1 | 0 | 0.519083 | 2.566008 | 0.295261 |
|74 | 1 | 0 | 0.284989 | 3.612414 | -0.797556 |
|75 | 1 | 0 | 0.114505 | 3.105430 | 1.669318 |
|76 | 1 | 0 | 0.707863 | 3.181848 | -2.203286 |
|77 | 1 | 0 | -6.402003 | 0.252851 | -0.085908 |
|78 | 1 | 0 | -5.526448 | -1.951682 | -0.778502 |

1e (conformer 22)
|   | 1 | 6 | 0 | -5.270106 | -0.268209 | 0.042458 |
|---|---|---|---|-----------|-----------|----------|
| 2 | 6 | 0 | -4.728370 | -1.461525 | -0.366017 |
| 3 | 6 | 0 | -3.326702 | -1.683229 | -0.323841 |
| 4 | 6 | 0 | -2.460674 | -0.639998 | 0.142938  |
| 5 | 6 | 0 | -3.060707 | 0.581436  | 0.554234  |
| 6 | 6 | 0 | -4.423326 | 0.760607  | 0.509987  |
| 7 | 6 | 0 | -2.772594 | -2.926331 | -0.725458 |
| 8 | 6 | 0 | -1.421199 | -3.135872 | -0.654696 |
| 9 | 6 | 0 | -0.564557 | -2.113099 | -0.187941 |
| 10| 6 | 0 | -1.044609 | -0.879811 | 0.195414  |
| 11| 6 | 0 | -0.112341 | 0.207246  | 0.737923  |
| 12| 6 | 0 | 1.330203  | -0.234709 | 0.983728  |
| 13| 6 | 0 | 2.297909  | -0.402277 | -0.063262 |
| 14| 6 | 0 | 1.705156  | -0.483620 | 2.304783  |
| 15| 6 | 0 | 3.007798  | -0.910198 | 2.625984  |
| 16| 6 | 0 | 3.949483  | -1.074424 | 1.643611  |
| 17| 6 | 0 | 3.624295  | -0.825826 | 0.284878  |
| 18| 6 | 0 | 2.009579  | -0.179024 | -1.439548 |
| 19| 6 | 0 | 2.971523  | -0.359707 | -2.405185 |
| 20| 6 | 0 | 4.277277  | -0.771311 | -2.056427 |
| 21| 6 | 0 | 4.592152  | -0.998300 | -0.740111 |
| 22| 8 | 0 | -0.219011 | 1.340360  | -0.137077 |
| 23| 6 | 0 | 0.455192  | 2.548076  | 0.272289  |
| 24| 6 | 0 | 0.498612  | 3.452555  | -0.965306 |
| 25| 6 | 0 | -0.207366 | 3.207074  | 1.485089  |
| 26| 6 | 0 | -0.867776 | 3.865613  | -1.523216 |
| 27| 6 | 0 | -6.342452 | -0.112287 | 0.007343  |
| 28| 1 | 0 | -5.367582 | -2.261177 | -0.725817 |
| 29| 1 | 0 | -2.429628 | 1.391482  | 0.886862  |
| 30| 1 | 0 | -4.852274 | 1.703341  | 0.831421  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 31| 1 | 0 | -3.438032 | -3.706627 | -1.079789 |
| 32| 1 | 0 | -0.995922 | -4.087563 | -0.952862 |
| 33| 1 | 0 | 0.495586  | -2.318338 | -0.129861 |
| 34| 1 | 0 | -0.508927 | 0.489326  | 1.722514 |
| 35| 1 | 0 | 0.976039  | -0.351021 | 3.080620 |
| 36| 1 | 0 | 3.256611  | -1.098272 | 3.664217 |
| 37| 1 | 0 | 4.956196  | -1.395467 | 1.889766 |
| 38| 1 | 0 | 1.018196  | 0.146441  | -1.718326 |
| 39| 1 | 0 | 5.025191  | -0.908184 | -2.829368 |
| 40| 1 | 0 | 5.590764  | -1.317687 | -0.460362 |
| 41| 1 | 0 | 1.489228  | 2.297044  | 0.538760 |
| 42| 1 | 0 | 1.083041  | 4.343249  | -0.708074 |
| 43| 1 | 0 | 1.062561  | 2.923854  | -1.739464 |
| 44| 1 | 0 | 0.320626  | 4.131785  | 1.734710 |
| 45| 1 | 0 | -1.25413  | 3.455530  | 2.367754 |
| 46| 1 | 0 | -0.743923 | 4.446179  | -2.441269 |
| 47| 1 | 0 | -1.473787 | 2.988255  | -1.756597 |
| 48| 1 | 0 | -1.427568 | 4.486304  | -0.818487 |

**1e (conformer 36)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -5.368383 | 0.268644  | -0.132952 |
| 2 | 6 | 0 | -4.950696 | -1.002339 | -0.440006 |
| 3 | 6 | 0 | -3.583756 | -1.370845 | -0.333740 |
| 4 | 6 | 0 | -2.620203 | -0.396482 | 0.089505  |
| 5 | 6 | 0 | -3.093154 | 0.908861  | 0.395705  |
| 6 | 6 | 0 | -4.426043 | 1.230368  | 0.292505  |
| 7 | 6 | 0 | -3.161248 | -2.693114 | -0.627818 |
| 8 | 6 | 0 | -1.844330 | -3.043638 | -0.494304 |
| 9 | 6 | 0 | -0.892185 | -2.088564 | -0.071555 |
|10 | 6 | 0 | -1.241104 | -0.784773 | 0.206345  |
|11 | 6 | 0 | -0.204563 | 0.226426  | 0.705964  |
|12 | 6 | 0 | 1.182005  | -0.349086 | 0.993238  |
|13 | 6 | 0 | 2.126938  | -0.683930 | -0.034157 |
|14 | 6 | 0 | 1.529504  | -0.547085 | 2.313299  |
|15 | 6 | 0 | 2.782519  | -1.079576 | 2.687576  |
|16 | 6 | 0 | 3.702008  | -1.404373 | 1.724235  |
|17 | 6 | 0 | 3.040305  | -1.216387 | 0.349722  |
|18 | 6 | 0 | 1.860587  | -0.52732 | -1.423904 |
|19 | 6 | 0 | 2.796990  | -0.872797 | -2.369687 |
|20 | 6 | 0 | 4.054577  | -1.390088 | -1.986141 |
|21 | 6 | 0 | 4.346825  | -1.556675 | -0.655517 |
|22 | 6 | 0 | -0.179051 | 1.317234  | -0.227363 |
|23 | 6 | 0 | 0.604500  | 2.471556  | 0.140340  |
|24 | 6 | 0 | 0.792157  | 3.259650  | -1.158217 |
|25 | 6 | 0 | -0.066842 | 3.286586  | 1.247400  |
|26 | 6 | 0 | 1.717540  | 4.474005  | -1.033017 |
|27 | 6 | 0 | -6.415704 | 0.536572  | -0.215566 |
|28 | 6 | 0 | -5.664099 | -1.752061 | -0.766374 |
|29 | 6 | 0 | -2.386280 | 1.668333  | 0.692366  |
|30 | 6 | 0 | -4.756805 | 2.234517  | 0.534128  |
|31 | 6 | 0 | -3.899809 | 3.419713  | -0.949979 |
|32 | 6 | 0 | -1.519714 | -4.055503 | -0.709026 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 33 | 1 | 0 | 0.136607 | -2.403411 | 0.037351 |
| 34 | 1 | 0 | -0.577750 | 0.599439 | 1.669171 |
| 35 | 1 | 0 | 0.817719 | -0.287141 | 3.090442 |
| 36 | 1 | 0 | 3.011919 | -1.221031 | 3.737603 |
| 37 | 1 | 0 | 4.671141 | -1.808336 | 1.997586 |
| 38 | 1 | 0 | 0.907089 | -0.123225 | -1.729874 |
| 39 | 1 | 0 | 2.567760 | -0.746666 | -3.421988 |
| 40 | 1 | 0 | 4.783369 | -1.655577 | -2.743716 |
| 41 | 1 | 0 | 5.307906 | -1.956509 | -0.349092 |
| 42 | 1 | 0 | 1.587964 | 2.134071 | 0.492220 |
| 43 | 1 | 0 | -0.194611 | 3.570779 | -1.519039 |
| 44 | 1 | 0 | 0.570782 | 4.121409 | 1.547784 |
| 45 | 1 | 0 | -1.022009 | 3.693834 | 0.903137 |
| 46 | 1 | 0 | -0.247227 | 2.686610 | 2.142336 |
| 47 | 1 | 0 | 1.870166 | 4.939978 | -2.009702 |
| 48 | 1 | 0 | 1.307987 | 5.238225 | -0.367557 |
| 49 | 1 | 0 | 2.701040 | 4.186728 | -0.647915 |
| 50 | 1 | 0 | 4.103441 | -1.688346 | -1.855888 |
| 51 | 1 | 0 | 4.435797 | -1.520761 | -0.534861 |
| 52 | 1 | 0 | 3.501355 | -0.989897 | 0.393500 |
| 53 | 1 | 0 | 2.191892 | -0.617470 | -0.060399 |
| 54 | 1 | 0 | 1.884714 | -0.806972 | -1.437638 |
| 55 | 1 | 0 | 2.813684 | -0.327076 | 2.652911 |
| 56 | 1 | 0 | -1.645409 | 0.049080 | 2.207344 |
| 57 | 1 | 0 | -1.257369 | -0.086276 | 0.890745 |
| 58 | 1 | 0 | 0.159730 | 0.350330 | 0.520794 |
| 59 | 1 | 0 | 1.160395 | -0.789381 | 0.304466 |
| 60 | 1 | 0 | 2.556779 | -0.493024 | 0.133469 |
| 61 | 1 | 0 | 0.760479 | -2.107602 | 0.339885 |
| 62 | 1 | 0 | 1.677581 | -3.171671 | 0.184924 |
| 63 | 1 | 0 | 3.010493 | -2.913779 | 0.006598 |
| 64 | 1 | 0 | 3.484518 | -1.576545 | -0.015871 |
| 65 | 1 | 0 | 3.080060 | 0.828931 | 0.126198 |
| 66 | 1 | 0 | 4.427103 | 1.065387 | -0.016249 |
| 67 | 1 | 0 | 5.334299 | -0.005551 | -0.170740 |
| 68 | 1 | 0 | 4.867648 | -1.296396 | -0.171781 |
| 69 | 1 | 0 | 0.199341 | 1.191194 | -0.642694 |
| 70 | 1 | 0 | -0.533065 | 2.433546 | -0.571820 |
| 71 | 1 | 0 | 0.211855 | 3.485008 | 0.265721 |
| 72 | 1 | 0 | -0.742386 | 2.863808 | -2.018395 |
| 73 | 1 | 0 | -0.616894 | 4.742169 | 0.554955 |
| 74 | 1 | 0 | -4.825395 | -2.096859 | -2.554074 |
| 75 | 1 | 0 | -5.421997 | -1.796553 | -0.176084 |
| 76 | 1 | 0 | -0.906716 | -0.523513 | -1.798183 |
| 77 | 1 | 0 | -2.553689 | -1.465089 | -3.350642 |
| 78 | 1 | 0 | -4.836304 | -1.119434 | 2.089288 |
| 79 | 1 | 0 | -3.192297 | -0.206043 | 3.698161 |
| 80 | 1 | 0 | -0.941511 | 0.457134 | 2.925733 |
| 81 | 1 | 0 | 0.529277 | 0.924230 | 1.381636 |

1e (conformer 39)
|   | Conformer 43 |   | Conformer 1 | 44 |
|---|-------------|---|-------------|----|
|   |             |   |             |    |
| 35| 1           | 0 | -0.282434   | -2.347660 | 0.495058 |
| 36| 1           | 0 | 1.313468    | -4.192496 | 0.211265 |
| 37| 1           | 0 | 3.722465    | -3.724020 | -0.111109|
| 38| 1           | 0 | 2.401117    | 1.663458  | 0.209758 |
| 39| 1           | 0 | 4.796319    | 2.085094  | -0.016768|
| 40| 1           | 0 | 6.393325    | 0.194681  | -0.288573|
| 41| 1           | 0 | 5.535324    | -2.129195 | -0.288386|
| 42| 1           | 0 | 1.509074    | 2.242514  | -0.107499|
| 43| 1           | 0 | 0.506740    | 3.038389  | 1.220580 |
| 44| 1           | 0 | 1.137555    | 3.756331  | -0.254308|
| 45| 1           | 0 | -1.297832   | 3.802463  | -2.073547|
| 46| 1           | 0 | 0.223779    | 3.001538  | -2.511904|
| 47| 1           | 0 | -1.303074   | 2.102639  | -2.563249|
| 48| 1           | 0 | -0.065362   | 5.428383  | 1.202543 |
| 49| 1           | 0 | -0.869125   | 5.285800  | -0.358730|
| 50| 1           | 0 | -1.553357   | 4.489312  | 1.061831 |

|   |               |   |             |    |
|---|-------------|---|-------------|----|
| 1 | 6           | 0 | -4.274816   | -0.692966 | -2.047020 |
| 2 | 6           | 0 | -4.562561   | -1.033774 | -0.749267 |
| 3 | 6           | 0 | -3.581033   | -0.924471 | 0.271623  |
| 4 | 6           | 0 | -2.271019   | -0.441050 | -0.059902 |
| 5 | 6           | 0 | -2.011346   | -0.098823 | -1.417268 |
| 6 | 6           | 0 | -2.984086   | -0.224413 | -2.380410|
| 7 | 6           | 0 | -3.877183   | -1.294012 | 1.609260  |
| 8 | 6           | 0 | -2.920887   | -1.194586 | 2.586521  |
| 9 | 6           | 0 | -1.634285   | -0.710311 | 2.265426  |
| 10| 6           | 0 | -1.291260   | -0.335584 | 0.982868  |
| 11| 6           | 0 | 0.133535    | 0.171387  | 0.755522  |
| 12| 6           | 0 | 1.093512    | -0.859423 | 0.153313  |
| 13| 6           | 0 | 2.506468    | -0.598270 | 0.162221  |
| 14| 6           | 0 | 0.640971    | -2.052565 | -0.365672 |
| 15| 6           | 0 | 1.523176    | -3.010811 | -0.914642 |
| 16| 6           | 0 | 2.872213    | -2.776180 | -0.933509 |
| 17| 6           | 0 | 3.398320    | -1.574313 | -0.392550 |
| 18| 6           | 0 | 3.079971    | 0.579737  | 0.713750  |
| 19| 6           | 0 | 4.440221    | 0.781909  | 0.717525  |
| 20| 6           | 0 | 5.311825    | -0.178567 | 0.159239  |
| 21| 6           | 0 | 4.796811    | -1.329899 | -0.382314 |
| 22| 8           | 0 | 0.207272    | 1.355350  | -0.050761 |
| 23| 6           | 0 | 0.002678    | 2.617891  | 0.610730  |
| 24| 6           | 0 | 0.764754    | 3.669844  | -0.206977 |
| 25| 6           | 0 | -1.478075   | 2.956512  | 0.800879  |
| 26| 6           | 0 | 0.285690    | 3.843180  | -1.651987 |
| 27| 1           | 0 | -5.032627   | -0.782882 | -2.817266 |
| 28| 1           | 0 | -5.549118   | -1.397895 | -0.481694 |
| 29| 1           | 0 | -1.034031   | 0.275361  | -1.683173 |
| 30| 1           | 0 | -2.759510   | 0.041698  | -3.407358 |
| 31| 1           | 0 | -4.872484   | -1.657033 | 1.843141  |
| 32| 1           | 0 | -3.146508   | -1.477622 | 3.608442  |
| 33| 1           | 0 | -0.894684   | -0.627700 | 3.055567  |
| 34| 1           | 0 | 0.521913    | 0.423156  | 1.752557  |
| 35| 1           | 0 | -0.417508   | -2.273940 | -0.357072 |
| 36| 1           | 0 | 1.119408    | -3.931797 | -1.319666 |

**1e (conformer 43)**
|    |   |   |       |       |       |
|----|---|---|-------|-------|-------|
| 37 | 1 | 0 | 3.557155 | -3.505421 | -1.353290 |
| 38 | 1 | 0 | 2.437117 | 1.337712 | 1.136767 |
| 39 | 1 | 0 | 4.847779 | 1.689106 | 1.149739 |
| 40 | 1 | 0 | 6.381930 | -0.004882 | 0.162780 |
| 41 | 1 | 0 | 5.455431 | -2.078838 | -0.809793 |
| 42 | 1 | 0 | 0.473816 | 2.558889 | 1.604318 |
| 43 | 1 | 0 | 0.693175 | 1.337712 | 1.136767 |
| 44 | 1 | 0 | 1.822201 | 2.251207 | 1.475223 |
| 45 | 1 | 0 | -1.576674 | 3.958141 | 1.230518 |
| 46 | 1 | 0 | -2.011376 | 2.934278 | -0.151126 |
| 47 | 1 | 0 | -1.964668 | 2.251207 | 1.475223 |
| 48 | 1 | 0 | 0.909012 | 4.573996 | -2.174047 |
| 49 | 1 | 0 | 0.347739 | 2.898622 | -0.968303 |
| 50 | 1 | 0 | -0.747213 | 4.196936 | -1.702225 |

**1e (conformer 45)**

|    |   |   |       |       |       |
|----|---|---|-------|-------|-------|
| 1  | 6 | 0 | -4.367288 | -0.835968 | -1.996061 |
| 2  | 6 | 0 | -4.641952 | -1.018165 | -0.663936 |
| 3  | 6 | 0 | -3.642335 | -0.815053 | 0.324495 |
| 4  | 6 | 0 | -2.326252 | -0.408031 | -0.078260 |
| 5  | 6 | 0 | -2.080889 | -0.228319 | -1.469382 |
| 6  | 6 | 0 | -3.072246 | -0.438599 | -2.398165 |
| 7  | 6 | 0 | -3.926866 | -1.016573 | 1.699949 |
| 8  | 6 | 0 | -2.954248 | -0.825642 | 2.647020 |
| 9  | 6 | 0 | -1.660467 | -0.419501 | 2.254887 |
| 10 | 6 | 0 | -1.327246 | -0.210792 | 0.932583 |
| 11 | 6 | 0 | 0.112883 | 0.204462 | 0.629293 |
| 12 | 6 | 0 | 1.021728 | -0.939832 | 0.167972 |
| 13 | 6 | 0 | 2.445356 | -0.745933 | 0.146037 |
| 14 | 6 | 0 | 0.512392 | -2.168063 | -0.192348 |
| 15 | 6 | 0 | 1.347358 | -3.230093 | -0.607936 |
| 16 | 6 | 0 | 2.705949 | -3.064001 | -0.651216 |
| 17 | 6 | 0 | 3.289181 | -1.827451 | -0.270769 |
| 18 | 6 | 0 | 3.075024 | 0.466849 | 0.537821 |
| 19 | 6 | 0 | 4.443327 | 0.603852 | 0.520046 |
| 20 | 6 | 0 | 5.267628 | -0.462455 | 0.099210 |
| 21 | 6 | 0 | 4.697663 | -1.650112 | -0.286599 |
| 22 | 8 | 0 | 0.227816 | 1.262473 | -0.332612 |
| 23 | 6 | 0 | 0.112647 | 2.614258 | 0.150103 |
| 24 | 6 | 0 | 0.863087 | 3.476921 | -0.870135 |
| 25 | 6 | 0 | -1.341628 | 3.043605 | 0.345340 |
| 26 | 6 | 0 | 1.055753 | 4.936299 | -0.446059 |
| 27 | 1 | 0 | -5.139072 | -0.995815 | -2.740692 |
| 28 | 1 | 0 | -5.632291 | -1.324381 | -0.342996 |
| 29 | 1 | 0 | -1.100654 | 0.093365 | -1.788256 |
| 30 | 1 | 0 | -2.858728 | -0.295980 | -3.451725 |
| 31 | 1 | 0 | -4.926981 | -1.323702 | 1.987252 |
| 32 | 1 | 0 | -3.171756 | -0.978223 | 3.698086 |
| 33 | 1 | 0 | -0.905859 | -0.266728 | 3.020155 |
| 34 | 1 | 0 | 0.522873 | 0.572013 | 1.580173 |
| 35 | 1 | 0 | -0.555056 | -2.337712 | -0.157506 |
| 36 | 1 | 0 | 0.899796 | -4.176252 | -0.890372 |
| 37 | 1 | 0 | 3.354917 | -3.873597 | -0.968303 |
| 38 | 1 | 0 | 2.470034 | 1.303973 | 0.854248 |
|   |   |   |   |
|---|---|---|---|
| 39 | 1 | 0 | 4.893980 1.540601 0.828801 |
| 40 | 1 | 0 | 6.344755 -0.340464 0.084543 |
| 41 | 1 | 0 | 5.319374 -2.479358 -0.607990 |
| 42 | 1 | 0 | 5.319374 -2.479358 -0.607990 |
| 43 | 1 | 0 | 0.635103 2.677171 1.118554 |
| 44 | 1 | 0 | 1.837426 3.010593 -1.040278 |
| 45 | 1 | 0 | 0.325207 3.429710 -1.823432 |
| 46 | 1 | 0 | 1.663576 5.470224 -1.180785 |
| 47 | 1 | 0 | 0.106538 5.470459 -0.358451 |
| 48 | 1 | 0 | 2.903987 -3.154521 0.741476 |
| 49 | 1 | 0 | 2.341164 -2.272083 -0.217752 |
| 50 | 1 | 0 | 1.537876 -1.168132 0.224785 |

**1e (conformer 46)**

|   |   |   |   |
|---|---|---|---|
| 1 | 6 | 0 | 2.706769 -2.958118 2.085479 |
| 2 | 6 | 0 | 2.903987 -3.154521 0.741476 |
| 3 | 6 | 0 | 2.341164 -2.272083 -0.217752 |
| 4 | 6 | 0 | 1.537876 -1.168132 0.224785 |
| 5 | 6 | 0 | 1.373567 -0.988926 1.625033 |
| 6 | 6 | 0 | 1.939436 -1.858165 2.527413 |
| 7 | 6 | 0 | 2.577163 -2.460891 -1.604589 |
| 8 | 6 | 0 | 2.052075 -1.590468 -2.522945 |
| 9 | 6 | 0 | 1.250497 -0.511366 -2.089560 |
| 10 | 6 | 0 | 0.964128 -0.293099 -0.757392 |
| 11 | 6 | 0 | 0.087886 0.918839 -0.405619 |
| 12 | 6 | 0 | -1.203490 0.621133 0.368028 |
| 13 | 6 | 0 | -2.258908 -0.160554 -0.211913 |
| 14 | 6 | 0 | -1.388104 1.165785 1.621405 |
| 15 | 6 | 0 | -2.567311 0.940121 2.367371 |
| 16 | 6 | 0 | -3.574572 0.171439 1.850346 |
| 17 | 6 | 0 | -3.452840 -0.387648 0.552690 |
| 18 | 6 | 0 | -2.207081 -0.708154 -1.523487 |
| 19 | 6 | 0 | -3.250364 -1.439592 -2.040346 |
| 20 | 6 | 0 | -4.413048 -1.674428 -1.275194 |
| 21 | 6 | 0 | -4.506747 -1.156095 -0.007799 |
| 22 | 6 | 0 | 0.821793 1.900884 0.325708 |
| 23 | 6 | 0 | 1.801758 2.664762 -0.407776 |
| 24 | 6 | 0 | 1.501259 4.150753 -0.191129 |
| 25 | 6 | 0 | 3.204494 2.281307 0.056764 |
| 26 | 6 | 0 | 0.143697 4.595634 -0.738608 |
| 27 | 1 | 0 | 3.143251 -3.638284 2.808235 |
| 28 | 1 | 0 | 3.501636 -3.988786 0.389044 |
| 29 | 1 | 0 | 0.805109 -0.146033 1.984462 |
| 30 | 1 | 0 | 1.797690 -1.695843 3.590124 |
| 31 | 1 | 0 | 3.187285 -3.300146 -1.921580 |
| 32 | 1 | 0 | 2.242515 -1.724415 -3.581747 |
| 33 | 1 | 0 | 0.839930 0.161419 -2.836141 |
| 34 | 1 | 0 | -0.215625 1.360747 -1.364844 |
| 35 | 1 | 0 | -0.606393 1.784920 2.038452 |
| 36 | 1 | 0 | -2.661426 1.382100 3.352913 |
| 37 | 1 | 0 | -4.481996 -0.010766 2.416401 |
| 38 | 1 | 0 | -1.328740 -0.556516 -2.132373 |
| 39 | 1 | 0 | -3.178051 -1.841796 -3.044747 |
| 40 | 1 | 0 | -5.226905 -2.257449 -1.691201 |

S426
|    |   |   |   |   |   |   |
|----|---|---|---|---|---|---|
| 41 | 1 | 0 | -5.397799 | -1.321174 | 0.589097 |
| 42 | 1 | 0 | 1.699389  | 2.434669  | -1.476224 |
| 43 | 1 | 0 | 1.556484  | 4.354819  | 0.884305  |
| 44 | 1 | 0 | 2.302120  | 4.732533  | -0.661469 |
| 45 | 1 | 0 | 3.958912  | 2.868880  | -0.474503 |
| 46 | 1 | 0 | 3.311639  | 2.471270  | 1.128139  |
| 47 | 1 | 0 | 3.400798  | 1.223728  | -0.124107 |
| 48 | 1 | 0 | 2.302120  | 4.028240  | -0.276795 |
| 49 | 1 | 0 | 0.085610  | 4.449650  | -1.822173 |
| 50 | 1 | 0 | 1e (conformer 79) |
| 1  | 6 | 0 | -4.871770 | -0.829027 | 1.251724 |
| 2  | 6 | 0 | -4.558004 | -1.607714 | 0.165641 |
| 3  | 6 | 0 | -3.294910 | -1.503065 | -0.473545 |
| 4  | 6 | 0 | -2.325594 | -0.569139 | 0.024443 |
| 5  | 6 | 0 | -2.692418 | 0.219513  | 1.149316  |
| 6  | 6 | 0 | -3.925012 | 0.094008  | 1.746183  |
| 7  | 6 | 0 | -2.979818 | -2.305938 | -1.600114 |
| 8  | 6 | 0 | -1.757195 | -2.197659 | -2.208744 |
| 9  | 6 | 0 | -0.796683 | -1.287407 | -1.715340 |
| 10 | 6 | 0 | -1.049434 | -0.480868 | -0.627434 |
| 11 | 6 | 0 | -0.002523 | 0.538237  | -0.166435 |
| 12 | 6 | 0 | 1.430761  | 0.111709  | -0.478522 |
| 13 | 6 | 0 | 2.086613  | -0.881600 | 0.319351  |
| 14 | 6 | 0 | 2.103279  | 0.680760  | -1.536586 |
| 15 | 6 | 0 | 3.432270  | 0.315912  | -1.849707 |
| 16 | 6 | 0 | 4.089222  | -0.619806 | -1.093039 |
| 17 | 6 | 0 | 3.439338  | -1.239562 | 0.006252  |
| 18 | 6 | 0 | 1.460385  | -1.537790 | 1.414929  |
| 19 | 6 | 0 | 2.130998  | -2.477283 | 2.162086  |
| 20 | 6 | 0 | 3.466932  | -2.818512 | 1.855618  |
| 21 | 6 | 0 | 4.102117  | -2.212095 | 0.800034  |
| 22 | 6 | 0 | -0.336130 | 1.789144  | -0.781337 |
| 23 | 6 | 0 | -0.326960 | 2.961052  | 0.055346  |
| 24 | 6 | 0 | 1.095110  | 3.428896  | 0.396831  |
| 25 | 6 | 0 | -1.146513 | 4.000877  | -0.698754 |
| 26 | 6 | 0 | 1.138628  | 4.586006  | 1.401721  |
| 27 | 6 | 0 | -5.840439 | -0.919049 | 1.730012  |
| 28 | 6 | 0 | -5.276769 | -2.320658 | -0.224836 |
| 29 | 6 | 0 | -1.993160 | 0.993918  | 1.552380  |
| 30 | 6 | 0 | -4.172659 | 0.710431  | 2.603173  |
| 31 | 6 | 0 | -3.723545 | -3.004665 | -1.968582 |
| 32 | 6 | 0 | -1.515990 | -2.810891 | -3.069624 |
| 33 | 6 | 0 | 0.166054  | -1.227765 | -2.207031 |
| 34 | 6 | 0 | -0.079124 | 0.655584  | 0.919874  |
| 35 | 6 | 0 | 1.596054  | 1.431927  | -2.127713 |
| 36 | 6 | 0 | 3.928796  | 0.786664  | -2.690964 |
| 37 | 6 | 0 | 5.111731  | -0.900755 | -1.322600 |
| 38 | 6 | 0 | 0.431259  | -1.310645 | 1.662154  |
| 39 | 6 | 0 | 1.629194  | -2.964489 | 2.990586  |
| 40 | 6 | 0 | 3.984460  | -3.561022 | 2.452453  |
| 41 | 6 | 0 | 5.126541  | -2.471203 | 0.553210  |
| 42 | 6 | 0 | -0.842703 | 2.717342  | 0.996782  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 43 | 1 | 0 | 1.654185 | 2.582547 | 0.805700 |
| 44 | 1 | 0 | 1.602725 | 3.714708 | -0.530890 |
| 45 | 1 | 0 | -1.264749 | 4.913674 | -0.111383 |
| 46 | 1 | 0 | -0.656187 | 4.256528 | -1.642221 |
| 47 | 1 | 0 | -2.137208 | 3.602391 | -0.924135 |
| 48 | 1 | 0 | 2.170873 | 4.820190 | 1.673573 |
| 49 | 1 | 0 | 0.691051 | 5.498176 | 0.999526 |
| 50 | 1 | 0 | 0.605732 | 4.331480 | 2.323727 |

| 1e (conformer 81) |
|-------------------|
| 1 | 6 | 0 | 4.176579 | -2.029642 | -1.852029 |
| 2 | 6 | 0 | 4.634483 | -1.287753 | -0.791325 |
| 3 | 6 | 0 | 3.751055 | -0.486189 | -0.021531 |
| 4 | 6 | 0 | 2.359108 | -0.446879 | -0.365123 |
| 5 | 6 | 0 | 1.921843 | -1.238241 | -1.463461 |
| 6 | 6 | 0 | 2.804494 | -2.004781 | -2.187020 |
| 7 | 6 | 0 | 4.219222 | 0.272087 | 1.083024 |
| 8 | 6 | 0 | 3.350906 | 1.039467 | 1.816321 |
| 9 | 6 | 0 | 1.981696 | 1.091886 | 1.472071 |
| 10 | 6 | 0 | 1.478977 | 0.378434 | 0.407035 |
| 11 | 6 | 0 | 0.007572 | 0.468576 | 0.067222 |
| 12 | 6 | 0 | -0.823143 | -0.716454 | 0.594695 |
| 13 | 6 | 0 | -2.094161 | -1.039525 | 0.009767 |
| 14 | 6 | 0 | -0.370364 | -1.460836 | 1.661542 |
| 15 | 6 | 0 | -1.120447 | -2.532252 | 2.196131 |
| 16 | 6 | 0 | -2.332122 | -2.864748 | 1.650634 |
| 17 | 6 | 0 | -2.848234 | -2.134258 | 0.548928 |
| 18 | 6 | 0 | -2.654848 | -0.329890 | -1.085960 |
| 19 | 6 | 0 | -3.874504 | -0.679400 | -1.620419 |
| 20 | 6 | 0 | -4.609078 | -1.760573 | -1.086827 |
| 21 | 6 | 0 | -4.102532 | -2.468751 | -0.025447 |
| 22 | 8 | 0 | -0.610440 | 1.658477 | 0.591208 |
| 23 | 6 | 0 | -0.741475 | 2.777543 | -0.305369 |
| 24 | 6 | 0 | -1.783653 | 3.692644 | 0.342736 |
| 25 | 6 | 0 | 0.590168 | 3.473213 | -0.587496 |
| 26 | 6 | 0 | -2.240324 | 4.857311 | -0.540552 |
| 27 | 1 | 0 | 4.862118 | -2.638278 | -2.430772 |
| 28 | 1 | 0 | 5.685517 | -1.305064 | -0.521947 |
| 29 | 1 | 0 | 0.873375 | -1.254355 | -1.732165 |
| 30 | 1 | 0 | 2.444343 | -2.599621 | -3.018942 |
| 31 | 1 | 0 | 5.273506 | 0.232031 | 1.335951 |
| 32 | 1 | 0 | 3.709558 | 1.615786 | 2.661926 |
| 33 | 1 | 0 | 1.304663 | 1.713891 | 2.042939 |
| 34 | 1 | 0 | -0.096448 | 0.493276 | -1.024911 |
| 35 | 1 | 0 | 0.588235 | -1.224267 | 2.105145 |
| 36 | 1 | 0 | -0.725622 | -3.089093 | 3.038351 |
| 37 | 1 | 0 | -2.914053 | -3.688393 | 2.050723 |
| 38 | 1 | 0 | -2.122316 | 0.508025 | -1.511631 |
| 39 | 1 | 0 | -4.276018 | -0.118514 | -2.457053 |
| 40 | 1 | 0 | -5.568663 | -2.026306 | -1.515563 |
| 41 | 1 | 0 | -4.657837 | -3.300913 | 0.394811 |
| 42 | 1 | 0 | -1.148629 | 2.407576 | -1.259365 |
| 43 | 1 | 0 | -2.642310 | 3.068611 | 0.605911 |
| 44 | 1 | 0 | -1.372627 | 4.071975 | 1.284970 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 45 | 1 | 0 | 1.018594 | 3.875183 | 0.334463 |
| 46 | 1 | 0 | 1.315568  | 2.787453 | -1.028691|
| 47 | 1 | 0 | 0.444874  | 4.298140 | -1.289893|
| 48 | 1 | 0 | -3.036008 | 5.421304 | -0.047563|
| 49 | 1 | 0 | -1.428416 | 5.557044 | -0.754040|
| 50 | 1 | 0 | -2.634599 | 4.500756 | -1.497585|
Table S35. Cartesian coordinates of each conformer of 1e calculated at IEFPCM/B3LYP/6-311++G(d,p) level with the use of an IEFPCM model of acetonitrile.

| 1e (conformer 1) | x | y | z |
|------------------|---|---|---|
| 1                | 6 | 0 | 4.190319 -2.390856 -0.732688 |
| 2                | 6 | 0 | 4.651808 -1.245182 -0.131558 |
| 3                | 6 | 0 | 3.782847 -0.153021 0.131757 |
| 4                | 6 | 0 | 2.398753 -0.250707 -0.233285 |
| 5                | 6 | 0 | 1.960922 -1.452729 -0.855461 |
| 6                | 6 | 0 | 2.829797 -2.491136 -1.099324 |
| 7                | 6 | 0 | 4.264336 1.033565 0.745343 |
| 8                | 6 | 0 | 3.415299 2.083618 0.980380 |
| 9                | 6 | 0 | 2.050869 1.994825 0.619336 |
| 10               | 6 | 0 | 1.531544 0.861093 0.032779 |
| 11               | 6 | 0 | 0.050579 0.797265 -0.337399 |
| 12               | 6 | 0 | -0.743008 -0.168203 0.555524 |
| 13               | 6 | 0 | -1.658227 -1.138408 0.027601 |
| 14               | 6 | 0 | -2.389839 -2.968410 0.946360 |
| 15               | 6 | 0 | -1.195902 2.736676 -2.492119 |
| 16               | 6 | 0 | -2.974973 3.237065 0.960154 |
| 17               | 6 | 0 | -3.293453 -2.943166 0.443242 |
| 18               | 8 | 0 | -0.494101 2.117415 -0.236462 |
| 19               | 6 | 0 | -1.637542 2.404804 -1.066627 |
| 20               | 6 | 0 | -2.380270 3.568717 -0.409810 |
| 21               | 6 | 0 | -1.195902 2.736676 -2.492119 |
| 22               | 6 | 0 | -2.380270 3.568717 -0.409810 |
| 23               | 6 | 0 | -1.195902 2.736676 -2.492119 |
| 24               | 6 | 0 | -2.380270 3.568717 -0.409810 |
| 25               | 6 | 0 | -1.195902 2.736676 -2.492119 |
| 26               | 6 | 0 | -2.974973 3.237065 0.960154 |
| 27               | 1 | 0 | 4.864708 -3.216739 -0.928209 |
| 28               | 1 | 0 | 5.695203 -1.155873 0.152342 |
| 29               | 1 | 0 | 0.924760 -1.565126 -1.143752 |
| 30               | 1 | 0 | 2.467304 -3.394700 -1.576399 |
| 31               | 1 | 0 | 5.312357 1.093820 1.018833 |
| 32               | 1 | 0 | 3.782729 2.992360 1.443848 |
| 33               | 1 | 0 | 1.396553 2.836636 0.797625 |
| 34               | 1 | 0 | -0.006785 0.468428 -1.377656 |
| 35               | 1 | 0 | 0.090644 0.679600 2.322084 |
| 36               | 1 | 0 | -1.190244 -0.733197 3.888551 |
| 37               | 1 | 0 | -2.765871 -2.435515 3.021978 |
| 38               | 1 | 0 | -1.362849 -0.741294 -2.094951 |
| 39               | 1 | 0 | -2.916726 -2.426690 -2.882627 |
| 40               | 1 | 0 | -4.172590 -3.856794 -1.276426 |
| 41               | 1 | 0 | -3.836486 -3.557978 1.153317 |
| 42               | 1 | 0 | -2.299165 1.529362 -1.079223 |
| 43               | 1 | 0 | -1.684212 4.411392 -0.325117 |
| 44               | 1 | 0 | -3.175164 3.888039 -1.092105 |
| 45               | 1 | 0 | -2.066184 2.913770 -3.129835 |
| 46               | 1 | 0 | -0.573886 3.636057 -2.495503 |
| 47               | 1 | 0 | -0.619525 1.922314 -2.937937 |
| 48               | 1 | 0 | -3.483747 4.106237 1.385456 |
| 49               | 1 | 0 | -3.705975 2.425931 0.885657 |
|      | 1  | 0  |   | 2  | 3  |
|------|----|----|---|----|----|
| 50   | 1  | 0  | -2.196771 | 2.922824 | 1.658234 |
| **1e (conformer 2)** |   |    |   |    |    |
| 1    | 6  | 0  | 3.972720  | -2.447850 | -1.182440 |
| 2    | 6  | 0  | 3.760420  | -2.555387 | 0.169110  |
| 3    | 6  | 0  | 2.732659  | -1.815059 | 0.813640  |
| 4    | 6  | 0  | 1.897644  | -0.937813 | 0.038105  |
| 5    | 6  | 0  | 2.156328  | -0.854705 | -1.361070 |
| 6    | 6  | 0  | 3.160017  | -1.584852 | -2.11672  |
| 7    | 6  | 0  | 2.527174  | -1.925681 | 2.829087  |
| 8    | 6  | 0  | 1.537646  | -1.201566 | 0.707163  |
| 9    | 6  | 0  | 0.710902  | -0.347748 | 0.706291  |
| 10   | 6  | 0  | 0.861209  | -0.205398 | 0.019923  |
| 11   | 6  | 0  | -0.057931 | 0.789996  | -0.019923 |
| 12   | 6  | 0  | -1.535547 | 0.559996  | 0.291570  |
| 13   | 6  | 0  | -2.232790 | -0.566961 | -0.257756 |
| 14   | 6  | 0  | -2.215746 | 1.442996  | 1.102517  |
| 15   | 6  | 0  | -3.582205 | 1.259116  | 1.416028  |
| 16   | 6  | 0  | -4.271839 | 0.188964  | 0.908241  |
| 17   | 6  | 0  | -3.620923 | -0.744943 | 0.059534  |
| 18   | 6  | 0  | -1.621465 | -1.523234 | -1.115399 |
| 19   | 6  | 0  | -2.331679 | -2.584567 | -1.626967 |
| 20   | 6  | 0  | -3.697672 | -2.755013 | -1.309676 |
| 21   | 6  | 0  | -4.323669 | -1.852660 | -0.484604 |
| 22   | 8  | 0  | 0.268243  | 2.130030  | 0.361133  |
| 23   | 6  | 0  | 1.459039  | 2.689770  | -0.231609 |
| 24   | 6  | 0  | 1.179672  | 3.226589  | -1.645699 |
| 25   | 6  | 0  | 1.963105  | 3.750007  | 0.740613  |
| 26   | 6  | 0  | 0.129085  | 4.338742  | -1.722542 |
| 27   | 1  | 0  | 4.760069  | -3.018335 | -1.661428 |
| 28   | 1  | 0  | 4.379406  | -3.211035 | 0.772473  |
| 29   | 1  | 0  | 1.560310  | -0.202547 | -1.985555 |
| 30   | 1  | 0  | 3.330813  | -1.496511 | -3.019028 |
| 31   | 1  | 0  | 3.165562  | -2.591175 | 2.782801  |
| 32   | 1  | 0  | 1.382081  | -1.285110 | 3.898648  |
| 33   | 1  | 0  | -0.071259 | 0.207739  | 2.575513  |
| 34   | 1  | 0  | 0.065595  | 0.686884  | -1.100487 |
| 35   | 1  | 0  | -1.688453 | 2.299678  | 1.498515  |
| 36   | 1  | 0  | -4.079199 | 1.975769  | 2.060207  |
| 37   | 1  | 0  | -5.320781 | 0.041716  | 1.142369  |
| 38   | 1  | 0  | -0.575872 | -1.426345 | -1.373454 |
| 39   | 1  | 0  | -1.838762 | -3.297097 | -2.278708 |
| 40   | 1  | 0  | -4.246306 | -3.595854 | -1.718413 |
| 41   | 1  | 0  | -5.372656 | -1.972735 | -0.234766 |
| 42   | 1  | 0  | 2.218993  | 1.903498  | -0.308155 |
| 43   | 1  | 0  | 2.131233  | 3.578167  | -2.060458 |
| 44   | 1  | 0  | 0.868070  | 2.392406  | -2.283715 |
| 45   | 1  | 0  | 2.846983  | 4.250183  | 0.336377  |
| 46   | 1  | 0  | 1.196978  | 4.505100  | 0.930863  |
| 47   | 1  | 0  | 2.230999  | 3.290249  | 1.694049  |
| 48   | 1  | 0  | -0.065734 | 4.610248  | -2.763277 |
| 49   | 1  | 0  | -0.814490 | 4.014878  | -1.277429 |
| 50   | 1  | 0  | 0.453552  | 5.243563  | -1.202312 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.457206 | -3.023724 | -0.998727 |
| 2 | 6 | 0 | 3.161555 | -3.102112 | 0.339028 |
| 3 | 6 | 0 | 2.241576 | -2.203007 | 0.943350 |
| 4 | 6 | 0 | 1.606321 | -1.192608 | 0.140991 |
| 5 | 6 | 0 | 1.946817 | -1.145055 | -1.242348 |
| 6 | 6 | 0 | 2.841425 | -2.031111 | -1.794448 |
| 7 | 6 | 0 | 1.948263 | -2.287611 | 2.327415 |
| 8 | 6 | 0 | 1.061877 | -1.413037 | 2.905627 |
| 9 | 6 | 0 | 0.428987 | -0.428018 | 0.140991 |
|10 | 6 | 0 | -0.028334 | 0.838948 | 0.013284 |
|11 | 6 | 0 | -1.539349 | 0.852360 | 0.239394 |
|12 | 6 | 0 | -3.792658 | -0.097443 | -1.117413 |
|13 | 6 | 0 | -2.378540 | -0.147399 | -0.356157 |
|14 | 6 | 0 | -2.112312 | 1.836466 | 1.015934 |
|15 | 6 | 0 | -3.505907 | 1.876918 | 1.252217 |
|16 | 6 | 0 | -4.330304 | 0.931106 | 0.700442 |
|17 | 6 | 0 | -2.727271 | -2.123544 | -1.744874 |
|18 | 6 | 0 | -4.118288 | -2.069904 | -1.504514 |
|19 | 6 | 0 | -4.634520 | -1.077020 | -0.707951 |
|20 | 6 | 0 | -0.489431 | 2.103285 | 0.437853 |
|21 | 6 | 0 | 1.788840 | 2.468188 | -0.073252 |
|22 | 6 | 0 | 1.646079 | 3.114027 | -1.458604 |
|23 | 6 | 0 | 2.406512 | 3.396438 | 0.966683 |
|24 | 6 | 0 | 2.979399 | 3.381148 | -2.165644 |
|25 | 6 | 0 | 4.160497 | -3.715965 | -1.447042 |
|26 | 6 | 0 | 3.629870 | -3.856739 | 0.962135 |
|27 | 6 | 0 | 1.502682 | -0.397141 | -1.885657 |
|28 | 6 | 0 | 3.078054 | -1.966359 | -2.850379 |
|29 | 6 | 0 | 2.436133 | -3.054636 | 2.919295 |
|30 | 6 | 0 | 0.838672 | -1.477624 | 3.964476 |
|31 | 6 | 0 | -0.276172 | 0.245827 | 2.593382 |
|32 | 6 | 0 | 0.138198 | 0.728520 | -1.061077 |
|33 | 6 | 0 | -1.477245 | 2.598751 | 1.444992 |
|34 | 6 | 0 | -3.915260 | 2.666277 | 1.872658 |
|35 | 6 | 0 | -5.400626 | 0.955747 | 0.875262 |
|36 | 6 | 0 | -0.823915 | -1.266375 | -1.385439 |
|37 | 6 | 0 | -2.320994 | -2.907048 | -2.374570 |
|38 | 6 | 0 | -4.772292 | -2.811058 | -1.949587 |
|39 | 6 | 0 | -5.701312 | -1.024617 | -0.517130 |
|40 | 6 | 0 | 2.407015 | 1.565884 | -0.155899 |
|41 | 6 | 0 | 1.037086 | 2.458115 | -2.089329 |
|42 | 6 | 0 | 1.081671 | 4.046452 | -1.345931 |
|43 | 6 | 0 | 3.408301 | 3.709655 | 0.667567 |
|44 | 6 | 0 | 1.787829 | 4.287919 | 1.093353 |
|45 | 6 | 0 | 2.480252 | 2.886051 | 1.930012 |
|46 | 6 | 0 | 2.810041 | 3.779185 | -3.169251 |
|47 | 6 | 0 | 3.591453 | 4.106526 | -1.623974 |
|48 | 6 | 0 | 3.563306 | 2.461042 | -2.268042 |

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.429722 | -1.892415 | -1.068419 |
| 2 | 6 | 0 | 4.801596 | -0.761859 | -0.382529 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 3 | 6 | 0 | 3.839214 | 0.200557 | 0.023184 |
| 4 | 6 | 0 | 2.454938 | -0.013171 | -0.288700 |
| 5 | 6 | 0 | 2.110763 | -1.197101 | -0.998210 |
| 6 | 6 | 0 | 3.068500 | -2.108753 | -1.378169 |
| 7 | 6 | 0 | 4.227111 | 1.370665 | 0.727891 |
| 8 | 6 | 0 | 3.287390 | 2.296098 | 1.100872 |
| 9 | 6 | 0 | 1.922805 | 2.094739 | 0.789891 |
| 10 | 6 | 0 | 1.493279 | 0.970927 | 0.117448 |
| 11 | 6 | 0 | 0.009877 | 0.788789 | -0.199154 |
| 12 | 6 | 0 | -0.647996 | -0.312055 | 0.647582 |
| 13 | 6 | 0 | -1.476755 | -1.337565 | 0.082352 |
| 14 | 6 | 0 | -0.477087 | -0.264032 | 2.016607 |
| 15 | 6 | 0 | -1.086505 | -1.197461 | 2.879288 |
| 16 | 6 | 0 | -1.875277 | -2.195850 | 2.363720 |
| 17 | 6 | 0 | -2.089343 | -2.293097 | 0.965989 |
| 18 | 6 | 0 | -1.731728 | -1.477595 | -1.312642 |
| 19 | 6 | 0 | -2.528983 | -2.485597 | -1.800992 |
| 20 | 6 | 0 | -3.125421 | -3.421035 | -0.925297 |
| 21 | 6 | 0 | -2.908110 | -3.321636 | 0.426059 |
| 22 | 8 | 0 | -0.646803 | 2.039463 | 0.028334 |
| 23 | 6 | 0 | -1.900705 | 2.236838 | -0.657355 |
| 24 | 6 | 0 | -2.691906 | 3.231644 | 0.194615 |
| 25 | 6 | 0 | -1.648699 | 2.719293 | -2.085497 |
| 26 | 6 | 0 | -4.113753 | 3.500838 | -0.307272 |
| 27 | 1 | 0 | 5.174857 | -2.618576 | -1.372643 |
| 28 | 1 | 0 | 5.844052 | -0.585067 | -0.139085 |
| 29 | 1 | 0 | 1.077029 | -1.397632 | -1.244008 |
| 30 | 1 | 0 | 2.776221 | -3.001746 | -1.919075 |
| 31 | 1 | 0 | 5.276291 | 1.518682 | 0.960472 |
| 32 | 1 | 0 | 3.582482 | 3.192383 | 1.634899 |
| 33 | 1 | 0 | 1.95672 | 2.841906 | 1.075372 |
| 34 | 1 | 0 | -0.066407 | 0.535161 | -1.259259 |
| 35 | 1 | 0 | 0.149667 | 0.511414 | 2.441636 |
| 36 | 1 | 0 | -0.923388 | -1.123303 | 3.948399 |
| 37 | 1 | 0 | -2.345096 | -2.923973 | 3.016180 |
| 38 | 1 | 0 | -1.298614 | -0.779784 | -2.017055 |
| 39 | 1 | 0 | -2.703045 | -2.562593 | -2.868188 |
| 40 | 1 | 0 | -3.751853 | -4.210757 | -1.323718 |
| 41 | 1 | 0 | -3.362027 | -4.031603 | 1.109460 |
| 42 | 1 | 0 | -2.448989 | 1.287000 | -0.680394 |
| 43 | 1 | 0 | -2.730529 | 2.832344 | 1.212535 |
| 44 | 1 | 0 | -2.126989 | 4.169628 | 0.245637 |
| 45 | 1 | 0 | -2.585750 | 2.816711 | -2.638817 |
| 46 | 1 | 0 | -1.149694 | 3.692513 | -2.072241 |
| 47 | 1 | 0 | -1.015774 | 2.019028 | -2.636235 |
| 48 | 1 | 0 | -4.646197 | 4.155390 | 0.387209 |
| 49 | 1 | 0 | -4.117947 | 3.987752 | -1.285510 |
| 50 | 1 | 0 | -4.687105 | 2.572414 | -0.392647 |

1e (conformer 5)

|   | 6 | 0 | 3.992197 | -2.629615 | -1.388772 |
| 2 | 6 | 0 | 4.496914 | -1.721711 | -0.489899 |
| 3 | 6 | 0 | 3.672166 | -0.711749 | 0.073153 |
| 4 | 6 | 0 | 2.291559 | -0.637252 | -0.309811 |
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 6 | 0 | 1.805090 | -1.599686 | -1.238287 |
| 6 | 6 | 0 | 2.631120 | -2.566081 | -1.763611 |
| 7 | 6 | 0 | 4.189371 | 0.220842 | 1.010800 |
| 8 | 6 | 0 | 3.377262 | 1.187153 | 1.547332 |
| 9 | 6 | 0 | 2.018668 | 1.269317 | 1.165440 |
|10 | 6 | 0 | 1.470113 | 0.392041 | 0.256795 |
|11 | 6 | 0 | -0.002360 | 0.513460 | -0.131426 |
|12 | 6 | 0 | -0.899406 | -0.509350 | 0.573696 |
|13 | 6 | 0 | -2.157444 | -0.895522 | -0.002145 |
|14 | 6 | 0 | -0.536263 | -1.029014 | 1.797441 |
|15 | 6 | 0 | -1.365657 | -1.930365 | 2.502515 |
|16 | 6 | 0 | -2.567806 | -2.319250 | 1.971559 |
|17 | 6 | 0 | -2.993063 | -1.817864 | 0.713048 |
|18 | 6 | 0 | -2.629961 | -0.413938 | -1.254371 |
|19 | 6 | 0 | -3.840315 | -0.817556 | -1.769148 |
|20 | 6 | 0 | -4.655854 | -1.727354 | -1.060479 |
|21 | 6 | 0 | -4.236605 | -2.214230 | 0.153377 |
|22 | 8 | 0 | -0.540105 | 1.808540 | 0.165936 |
|23 | 6 | 0 | -0.605925 | 2.757415 | -0.920108 |
|24 | 6 | 0 | -1.658621 | 3.799080 | -0.523206 |
|25 | 6 | 0 | 0.755190 | 3.359885 | -1.271468 |
|26 | 6 | 0 | -1.344978 | 4.597952 | 0.746115 |
|27 | 1 | 0 | 4.632176 | -3.396520 | -1.809960 |
|28 | 1 | 0 | 5.539405 | -1.764550 | -0.192253 |
|29 | 1 | 0 | 0.764308 | -1.585289 | -1.535264 |
|30 | 1 | 0 | 2.234954 | -3.287576 | -2.469233 |
|31 | 1 | 0 | 5.234252 | 0.153475 | 1.294519 |
|32 | 1 | 0 | 3.771708 | 1.897357 | 2.265398 |
|33 | 1 | 0 | 1.390753 | 2.044503 | 1.584373 |
|34 | 1 | 0 | -0.071651 | 0.354949 | 1.121260 |
|35 | 1 | 0 | 0.412587 | -0.744726 | 2.234484 |
|36 | 1 | 0 | -1.040360 | -2.312160 | 3.463545 |
|37 | 1 | 0 | -3.210579 | -3.013579 | 2.502240 |
|38 | 1 | 0 | -2.032611 | 0.285109 | -1.823427 |
|39 | 1 | 0 | -4.171553 | -0.433410 | -2.727332 |
|40 | 1 | 0 | -5.607453 | -2.037428 | -1.476752 |
|41 | 1 | 0 | -4.853266 | -2.913824 | 0.707705 |
|42 | 1 | 0 | -0.981465 | 2.230404 | -1.808108 |
|43 | 1 | 0 | -1.787907 | 4.481518 | -1.370405 |
|44 | 1 | 0 | -2.610827 | 3.274746 | -0.395083 |
|45 | 1 | 0 | 0.636875 | 4.081976 | -2.084841 |
|46 | 1 | 0 | 1.200773 | 3.872276 | -0.416757 |
|47 | 1 | 0 | 1.453687 | 2.590777 | -1.606525 |
|48 | 1 | 0 | -2.162730 | 5.287157 | 0.972841 |
|49 | 1 | 0 | -1.218381 | 3.933743 | 1.603546 |
|50 | 1 | 0 | -0.434239 | 5.193114 | 0.641180 |

**1e (conformer 6)**

|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.772098 | -2.564492 | -1.734724 |
| 2 | 6 | 0 | 4.387493 | -1.757705 | -0.808793 |
| 3 | 6 | 0 | 3.660889 | -0.757323 | -0.109897 |
| 4 | 6 | 0 | 2.262697 | -0.584972 | -0.381225 |
| 5 | 6 | 0 | 1.660506 | -1.445559 | -1.341009 |
| 6 | 6 | 0 | 2.393431 | -2.405310 | -1.999916 |
|   |   |   |   |   |
|---|---|---|---|---|
| 7 | 6 | 0 | 4.294435 | 0.071482 | 0.853507 |
| 8 | 6 | 0 | 3.577457 | 1.031045 | 1.520892 |
| 9 | 6 | 0 | 2.201040 | 1.209003 | 1.250467 |
| 10 | 6 | 0 | 1.539730 | 0.433062 | 0.324084 |
| 11 | 6 | 0 | 0.050032 | 0.657492 | 0.053538 |
| 12 | 6 | 0 | -0.846665 | -0.369806 | 0.747243 |
| 13 | 6 | 0 | -2.046126 | -0.859523 | 0.324084 |
| 14 | 6 | 0 | -0.530466 | -0.789190 | 0.002023 |
| 15 | 6 | 0 | -2.046126 | -0.859523 | 0.324084 |
| 16 | 6 | 0 | -2.497579 | -2.176435 | 2.167574 |
| 17 | 6 | 0 | -2.872179 | -1.781998 | 0.857226 |
| 18 | 6 | 0 | -2.470727 | -0.490185 | -1.178611 |
| 19 | 6 | 0 | -3.625213 | -0.953783 | -1.729870 |
| 20 | 6 | 0 | -4.430587 | -1.903656 | -1.007313 |
| 21 | 6 | 0 | -4.057710 | -2.285100 | 0.257377 |
| 22 | 6 | 0 | -3.490428 | 1.946042 | 0.496352 |
| 23 | 6 | 0 | -0.053706 | 3.062150 | -0.361696 |
| 24 | 6 | 0 | -1.051428 | 3.206392 | -2.260632 |
| 25 | 6 | 0 | 0.009280 | 4.292022 | 0.537197 |
| 26 | 6 | 0 | -2.503514 | 3.451481 | -1.102364 |
| 27 | 6 | 0 | 4.338302 | -3.324698 | -2.260632 |
| 28 | 6 | 0 | 5.444644 | -1.874855 | -0.594369 |
| 29 | 6 | 0 | 0.604085 | -1.357481 | -1.558002 |
| 30 | 6 | 0 | 1.909278 | -3.047143 | -2.727212 |
| 31 | 6 | 0 | 5.351669 | -0.694942 | 1.051049 |
| 32 | 6 | 0 | 4.060160 | 1.662451 | 2.258284 |
| 33 | 6 | 0 | 1.648410 | 1.974338 | 1.779569 |
| 34 | 6 | 0 | -0.956888 | 0.587039 | -1.026923 |
| 35 | 6 | 0 | 0.376475 | -0.426034 | 2.489651 |
| 36 | 6 | 0 | -1.064599 | -1.987865 | 3.740272 |
| 37 | 6 | 0 | -3.132870 | -2.871597 | 2.706009 |
| 38 | 6 | 0 | -1.883442 | 0.205934 | -1.761204 |
| 39 | 6 | 0 | -3.920158 | -0.693033 | -2.728316 |
| 40 | 6 | 0 | -5.337843 | -2.294565 | -1.453387 |
| 41 | 6 | 0 | -4.667196 | -2.981413 | 0.824039 |
| 42 | 6 | 0 | 0.941601 | 2.884265 | -0.786386 |
| 43 | 6 | 0 | -0.700602 | 4.027165 | -2.158826 |
| 44 | 6 | 0 | -0.997391 | 2.308972 | -2.148049 |
| 45 | 6 | 0 | 0.188727 | 5.191250 | -0.057887 |
| 46 | 6 | 0 | -0.927140 | 4.422351 | 1.084088 |
| 47 | 6 | 0 | 0.817108 | 4.196025 | -1.265318 |
| 48 | 6 | 0 | -3.162288 | 3.447748 | -1.974570 |
| 49 | 6 | 0 | -2.846419 | 2.672767 | -0.417678 |
| 50 | 6 | 0 | -2.624440 | 4.416144 | -0.603251 |

**1e (conformer 7)**

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6 | 0 | 3.946926 | -2.429588 | -1.238017 |
| 2 | 6 | 0 | 3.742637 | -2.534755 | 0.115027 |
| 3 | 6 | 0 | 2.713328 | -1.799872 | 0.763091 |
| 4 | 6 | 0 | 1.869636 | -0.927850 | -0.009169 |
| 5 | 6 | 0 | 2.117521 | -0.850650 | -1.410668 |
| 6 | 6 | 0 | 3.122224 | -1.576650 | -2.005667 |
| 7 | 6 | 0 | 2.512433 | -1.914648 | 2.161668 |
| 8 | 6 | 0 | 1.515444 | -1.203620 | 2.782050 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 9 | 6 | 0 | 0.682186 | -0.352692 | 2.028045 |
| 10 | 6 | 0 | 0.833907 | -0.199029 | 0.664745 |
| 11 | 6 | 0 | -0.076343 | 0.809055 | -0.055389 |
| 12 | 6 | 0 | -1.552390 | 0.605597 | 0.281319 |
| 13 | 6 | 0 | -2.273722 | -0.517381 | -0.244589 |
| 14 | 6 | 0 | -2.207553 | 1.506705 | 1.093000 |
| 15 | 6 | 0 | -3.571335 | -0.833907 | -0.09681 |
| 16 | 6 | 0 | -4.283541 | 0.279290 | 0.944716 |
| 17 | 6 | 0 | -3.658932 | -0.076343 | 0.809055 |
| 18 | 6 | 0 | -2.421502 | 2.548232 | -1.589396 |
| 19 | 6 | 0 | -3.784594 | -2.692666 | -1.249023 |
| 20 | 6 | 0 | -3.785261 | -1.776352 | -0.424506 |
| 21 | 6 | 0 | -4.385261 | 2.152587 | 0.291746 |
| 22 | 8 | 0 | 0.268284 | 2.152587 | -0.293400 |
| 23 | 6 | 0 | 1.469428 | 2.703610 | -0.293400 |
| 24 | 6 | 0 | 1.107800 | 4.047609 | -0.931515 |
| 25 | 6 | 0 | 2.545672 | 2.845021 | 0.780649 |
| 26 | 6 | 0 | 0.115098 | 3.937663 | -2.090407 |
| 27 | 1 | 0 | 4.735306 | -3.185589 | 0.716589 |
| 28 | 1 | 0 | 2.545672 | 2.845021 | 0.780649 |
| 29 | 1 | 0 | 0.115098 | 3.937663 | -2.090407 |
| 30 | 1 | 0 | 3.158057 | 2.573654 | 2.729888 |
| 31 | 1 | 0 | 1.360494 | -1.293568 | 3.851195 |
| 32 | 1 | 0 | -0.102166 | 0.196485 | 2.535892 |
| 33 | 1 | 0 | 0.030051 | 0.693638 | -1.373839 |
| 34 | 1 | 0 | -1.661963 | 2.359339 | 1.472391 |
| 35 | 1 | 0 | -4.048043 | 2.075438 | 2.074028 |
| 36 | 1 | 0 | -5.330510 | 0.149014 | 1.196993 |
| 37 | 1 | 0 | -0.646073 | -1.411736 | -1.376070 |
| 38 | 1 | 0 | -1.948746 | -3.274800 | -2.240579 |
| 39 | 1 | 0 | -4.350932 | -3.533958 | -1.639689 |
| 40 | 1 | 0 | -5.431703 | -1.879114 | -0.156900 |
| 41 | 1 | 0 | 1.825376 | 2.025966 | -1.077882 |
| 42 | 1 | 0 | 0.701052 | 4.698265 | -0.148606 |
| 43 | 1 | 0 | 2.034285 | 4.517915 | -1.278861 |
| 44 | 1 | 0 | 3.456873 | 3.275969 | 0.356402 |
| 45 | 1 | 0 | 2.194321 | 3.502843 | 1.580664 |
| 46 | 1 | 0 | 2.793178 | 1.876004 | 1.216436 |
| 47 | 1 | 0 | -0.121667 | 4.923576 | -2.498951 |
| 48 | 1 | 0 | 0.523422 | 3.330019 | -2.904132 |
| 49 | 1 | 0 | -0.819182 | 3.477254 | -1.761326 |

| 1e (conformer 8) |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.616003 | -1.803177 | -1.013939 |
| 2 | 6 | 0 | 4.188220 | -2.275514 | 0.202545 |
| 3 | 6 | 0 | 2.950525 | -1.855372 | 0.758322 |
| 4 | 6 | 0 | 2.131227 | -0.924059 | 0.036090 |
| 5 | 6 | 0 | 2.613039 | -0.455824 | -1.217462 |
| 6 | 6 | 0 | 3.816616 | -0.883158 | -1.728451 |
| 7 | 6 | 0 | 2.514401 | -2.342974 | 2.018184 |
| 8 | 6 | 0 | 1.317296 | -1.931825 | 2.544202 |
| 9 | 6 | 0 | 0.503876 | -1.021753 | 1.832141 |
| 10 | 6 | 0 | 0.877760 | -0.515646 | 0.605703 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 11 | 6 | 0 | -0.007923 | 0.505640 | -0.111910 |
| 12 | 6 | 0 | -1.484671 | 0.408670 | 0.271448 |
| 13 | 6 | 0 | -2.333099 | -0.579393 | -0.328026 |
| 14 | 6 | 0 | -2.012659 | 1.272972 | 1.205516 |
| 15 | 6 | 0 | -3.374311 | 1.219092 | 1.580703 |
| 16 | 6 | 0 | -4.210687 | 0.291990 | 1.013409 |
| 17 | 6 | 0 | -3.716142 | -0.627515 | 0.328026 |
| 18 | 6 | 0 | -2.012659 | 1.272972 | 1.205516 |
| 19 | 6 | 0 | -3.374311 | 1.219092 | 1.580703 |
| 20 | 6 | 0 | -4.210687 | 0.291990 | 1.013409 |
| 21 | 6 | 0 | -3.716142 | -0.627515 | 0.328026 |
| 22 | 8 | 0 | 0.549675 | 1.793190 | 0.179822 |
| 23 | 6 | 0 | 0.146992 | 2.884081 | -0.681269 |
| 24 | 6 | 0 | 0.401717 | 4.176222 | 0.104125 |
| 25 | 6 | 0 | 0.868109 | 2.843657 | -2.029789 |
| 26 | 6 | 0 | 1.855857 | 4.405356 | 0.530224 |
| 27 | 1 | 0 | 5.562678 | -2.131457 | -1.427531 |
| 28 | 1 | 0 | 4.792886 | -2.981516 | 0.761929 |
| 29 | 1 | 0 | 2.030249 | 0.255832 | -1.784301 |
| 30 | 1 | 0 | 4.156484 | 0.681269 | -0.540388 |
| 31 | 1 | 0 | 2.721364 | 2.459601 | -1.832713 |
| 32 | 1 | 0 | 4.084636 | -2.496015 | -1.462401 |
| 33 | 1 | 0 | 4.566673 | 1.599185 | -0.540388 |
| 34 | 1 | 0 | 1.870728 | -1.530236 | -1.280654 |
| 35 | 1 | 0 | 2.342946 | -3.172756 | -2.556295 |
| 36 | 1 | 0 | 4.744127 | -3.23650 | -1.905172 |
| 37 | 1 | 0 | -5.258131 | 0.245854 | 1.291783 |
| 38 | 1 | 0 | -0.829414 | -1.536869 | -1.579688 |
| 39 | 1 | 0 | -2.342946 | -3.172756 | -2.556295 |
| 40 | 1 | 0 | -4.744127 | -3.23650 | -1.905172 |
| 41 | 1 | 0 | -5.610565 | -1.621794 | -0.245535 |
| 42 | 1 | 0 | -0.932121 | 2.807570 | -0.859500 |
| 43 | 1 | 0 | 0.056996 | 5.013886 | -0.511973 |
| 44 | 1 | 0 | -0.237356 | 4.161235 | 0.992784 |
| 45 | 1 | 0 | 0.582270 | 3.713659 | -2.627585 |
| 46 | 1 | 0 | 1.952374 | 2.855506 | -1.901100 |
| 47 | 1 | 0 | 0.598559 | 1.955478 | -2.606129 |
| 48 | 1 | 0 | 1.937950 | 1.561539 | 1.128548 |
| 49 | 1 | 0 | 2.220429 | 3.857143 | 1.133340 |
| 50 | 1 | 0 | 2.521412 | 4.516687 | -0.329708 |

| 1e (conformer 9) |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.790737 | -2.329475 | 2.097259 |
| 2 | 6 | 0 | -4.329248 | -1.831335 | 0.936146 |
| 3 | 6 | 0 | -3.556853 | -1.028018 | 0.055467 |
| 4 | 6 | 0 | -2.194334 | -0.726506 | 0.390246 |
| 5 | 6 | 0 | -1.670508 | -1.270193 | 1.596955 |
| 6 | 6 | 0 | -2.445964 | -2.046115 | 2.426564 |
| 7 | 6 | 0 | -4.109575 | -0.523477 | -1.151003 |
| 8 | 6 | 0 | -3.348971 | 0.245690 | -1.994403 |
| 9 | 6 | 0 | -2.009539 | 0.551037 | -1.663959 |
| 10 | 6 | 0 | -1.427702 | 0.092464 | -0.501957 |
| 11 | 6 | 0 | 0.022324 | 0.453964 | -0.182878 |
| 12 | 6 | 0 | 1.027925 | -0.622930 | -0.600373 |
|   |   |   |   |   |
|---|---|---|---|---|
| 13| 6 | 0 | 2.334371 | -0.665594 | -0.004648 |
| 14| 6 | 0 | 0.708131 | -1.544623 | -1.574006 |
| 15| 6 | 0 | 1.626665 | -2.531010 | -2.000046 |
| 16| 6 | 0 | 2.875421 | -2.598253 | -1.439434 |
| 17| 6 | 0 | 3.260511 | -1.674739 | -0.432460 |
| 18| 6 | 0 | 2.767228 | 0.245920 | 0.996853  |
| 19| 6 | 0 | 4.024234 | 1.609990 | 1.549094  |
| 20| 6 | 0 | 4.928939 | -0.839212 | 1.128069  |
| 21| 6 | 0 | 4.551318 | -1.733993 | 0.157170  |
| 22| 8 | 0 | 0.440389 | 1.664764 | -0.828621 |
| 23| 6 | 0 | -0.144562 | 2.899130 | -0.346985 |
| 24| 6 | 0 | 0.515572 | 3.364111 | 0.958934  |
| 25| 6 | 0 | 0.020048 | 3.896353 | -1.487362 |
| 26| 6 | 0 | 0.440389 | 1.664764 | -0.828621 |
| 27| 1 | 0 | 0.482799 | 2.545155 | 1.684108  |
| 28| 1 | 0 | 3.585680 | -3.355347 | -1.754407 |
| 29| 1 | 0 | 2.102809 | 1.030941 | 1.327040  |
| 30| 1 | 0 | 4.325405 | 0.870298 | 2.311770  |
| 31| 1 | 0 | 5.917013 | -0.895006 | 1.570392  |
| 32| 1 | 0 | 5.237654 | -2.504830 | -0.177235 |
| 33| 1 | 0 | -1.213270 | 2.734262 | -0.161888 |
| 34| 1 | 0 | 0.482799 | 2.545155 | 1.684108  |
| 35| 1 | 0 | 1.572820 | 3.573202 | 0.762043  |
| 36| 1 | 0 | 4.056434 | 4.867432 | -1.227280 |
| 37| 1 | 0 | 1.080880 | 4.033967 | -1.715987 |
| 38| 1 | 0 | -0.481681 | 3.535423 | -2.387422 |
| 39| 1 | 0 | 0.300750 | 4.825257 | 2.552702  |
| 40| 1 | 0 | -0.072259 | 5.474928 | 0.957595  |
| 41| 1 | 0 | -1.223012 | 4.404947 | 1.766691  |

**1e (conformer 10)**

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6 | 0 | 4.891510 | -1.282226 | -0.957823 |
| 2 | 6 | 0 | 4.497802 | -1.805898 | 0.249208 |
| 3 | 6 | 0 | 3.209509 | -1.532866 | 0.781457 |
| 4 | 6 | 0 | 2.303997 | -0.698922 | 0.044587 |
| 5 | 6 | 0 | 2.752162 | -0.171661 | -1.197520 |
| 6 | 6 | 0 | 4.006177 | -0.456239 | -1.686002 |
| 7 | 6 | 0 | 2.805528 | -2.072533 | 2.031008 |
| 8 | 6 | 0 | 1.558418 | -1.803424 | 2.531706 |
| 9 | 6 | 0 | 0.660067 | -0.989590 | 1.804205 |
| 10| 6 | 0 | 0.999592 | -0.439068 | 0.587383 |
| 11| 6 | 0 | 0.020217 | 0.461321 | -0.169915 |
| 12| 6 | 0 | -1.436801 | 0.269574 | 0.245360 |
| 13| 6 | 0 | -2.227960 | -0.781903 | -0.324558 |
| 14| 6 | 0 | -2.002715 | 1.105334 | 1.183481 |

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|     |   |   |            |            |            |
|-----|---|---|------------|------------|------------|
| 15  | 6 | 0 | -3.349192  | 0.963750   | 1.588390   |
| 16  | 6 | 0 | -4.132691  | -0.023310  | 1.047141   |
| 17  | 6 | 0 | -3.596847  | -0.918473  | 1.793976   |
| 18  | 6 | 0 | -1.721535  | -1.715110  | -1.272622  |
| 19  | 6 | 0 | -2.518351  | -2.707630  | -1.939766  |
| 20  | 6 | 0 | -3.869010  | -2.829187  | -1.396497  |
| 21  | 6 | 0 | -4.391884  | -1.953057  | -0.477082  |
| 22  | 8 | 0 | 0.488553   | 1.803476   | 0.022242   |
| 23  | 6 | 0 | -0.057251  | 2.836559   | -0.829717  |
| 24  | 6 | 0 | 0.472709   | 4.160860   | -0.275254  |
| 25  | 6 | 0 | 0.325786   | 2.658674   | -2.299766  |
| 26  | 6 | 0 | 0.051742   | 4.466186   | 1.164003   |
| 27  | 1 | 0 | 5.877384   | -1.498252  | -1.353353  |
| 28  | 1 | 0 | 5.169071   | -2.440281  | 0.818497   |
| 29  | 1 | 0 | 0.492222   | 0.215019   | -1.232799  |
| 30  | 1 | 0 | 0.398356   | 1.892564   | 1.615175   |
| 31  | 1 | 0 | 3.500047   | -2.700371  | 2.579055   |
| 32  | 1 | 0 | 1.249188   | -2.214896  | 3.485737   |
| 33  | 1 | 0 | -0.322528  | -0.802455  | 2.217872   |
| 34  | 1 | 0 | 0.092222   | 0.215019   | -1.232799  |
| 35  | 1 | 0 | 0.198356   | 1.892564   | 1.615175   |
| 36  | 1 | 0 | -3.757022  | 1.643923   | 2.327593   |
| 37  | 1 | 0 | -5.168719  | -0.136753  | 3.48009    |
| 38  | 1 | 0 | -0.687748  | -1.658322  | -1.587827  |
| 39  | 1 | 0 | -2.106564  | -3.405300  | -2.514434  |
| 40  | 1 | 0 | -4.865980  | -3.615619  | -1.815929  |
| 41  | 1 | 0 | -5.425839  | -2.040970  | -0.160318  |
| 42  | 1 | 0 | -1.151171  | 2.821915   | -0.743374  |
| 43  | 1 | 0 | 1.566352   | 4.144324   | -0.348083  |
| 44  | 1 | 0 | 0.126664   | 4.960872   | -0.938043  |
| 45  | 1 | 0 | -0.108721  | 3.470479   | -2.889025  |
| 46  | 1 | 0 | 1.411611   | 2.690992   | -2.425374  |
| 47  | 1 | 0 | -0.048936  | 1.722556   | -2.719261  |
| 48  | 1 | 0 | 0.454388   | 5.429274   | 1.488949   |
| 49  | 1 | 0 | -1.037713  | 4.513824   | 1.256403   |
| 50  | 1 | 0 | 0.417054   | 3.699386   | 1.849892   |

**1e (conformer 11)**

|     |   |   |            |            |            |
|-----|---|---|------------|------------|------------|
| 1   | 6 | 0 | 4.963973   | -0.925214  | -1.042020  |
| 2   | 6 | 0 | 4.621252   | -1.582281  | 0.114187   |
| 3   | 6 | 0 | 3.329024   | -1.435527  | 0.685400   |
| 4   | 6 | 0 | 2.363745   | -0.590825  | 0.041792   |
| 5   | 6 | 0 | 2.760980   | 0.076400   | -1.149469  |
| 6   | 6 | 0 | 4.020837   | -0.086673  | -1.677103  |
| 7   | 6 | 0 | 2.980718   | -2.110797  | 1.884399   |
| 8   | 6 | 0 | 1.730313   | -1.961574  | 2.425695   |
| 9   | 6 | 0 | 0.773625   | -1.138868  | 1.788918   |
| 10  | 6 | 0 | 1.056776   | -0.460315  | 0.623025   |
| 11  | 6 | 0 | 0.009553   | 0.453271   | -0.019197  |
| 12  | 6 | 0 | -1.428401  | 0.083187   | 0.343188   |
| 13  | 6 | 0 | -2.112142  | -0.964473  | -0.356918  |
| 14  | 6 | 0 | -2.080688  | 0.754713   | 1.354330   |
| 15  | 6 | 0 | -3.412414  | 0.444962   | 1.712518   |
| 16  | 6 | 0 | -4.093873  | -0.543555  | 1.049388   |
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 17 | 6 | 0 | -3.466452 | -1.271060 | 0.004170 |
| 18 | 6 | 0 | -1.510816 | -1.730768 | -1.394504 |
| 19 | 6 | 0 | -2.206437 | -2.723799 | -2.044068 |
| 20 | 6 | 0 | -3.544049 | -3.013220 | -1.691777 |
| 21 | 6 | 0 | -4.155836 | -2.301752 | -0.688750 |
| 22 | 8 | 0 | 0.349092 | 1.789531 | 0.373808 |
| 23 | 6 | 0 | -0.255724 | 2.865519 | -0.382642 |
| 24 | 6 | 0 | -0.131715 | 4.102688 | 0.510454 |
| 25 | 6 | 0 | -0.411900 | 3.039303 | -0.035065 |
| 26 | 6 | 0 | 5.953460 | -1.045299 | -1.468068 |
| 27 | 8 | 0 | 5.336944 | -2.227372 | 0.612895 |
| 28 | 6 | 0 | 0.349092 | 1.789531 | 0.373808 |
| 29 | 6 | 0 | -0.255724 | 2.865519 | -0.382642 |
| 30 | 6 | 0 | -0.131715 | 4.102688 | 0.510454 |
| 31 | 6 | 0 | -0.411900 | 3.039303 | -0.035065 |
| 32 | 6 | 0 | 5.953460 | -1.045299 | -1.468068 |
| 33 | 8 | 0 | 5.336944 | -2.227372 | 0.612895 |
| 34 | 6 | 0 | 0.349092 | 1.789531 | 0.373808 |
| 35 | 6 | 0 | -0.255724 | 2.865519 | -0.382642 |
| 36 | 6 | 0 | -0.131715 | 4.102688 | 0.510454 |
| 37 | 6 | 0 | -0.411900 | 3.039303 | -0.035065 |
| 38 | 6 | 0 | 5.953460 | -1.045299 | -1.468068 |
| 39 | 6 | 0 | 0.349092 | 1.789531 | 0.373808 |
| 40 | 6 | 0 | -0.255724 | 2.865519 | -0.382642 |
| 41 | 6 | 0 | -0.131715 | 4.102688 | 0.510454 |
| 42 | 6 | 0 | -0.411900 | 3.039303 | -0.035065 |
| 43 | 6 | 0 | 5.953460 | -1.045299 | -1.468068 |
| 44 | 6 | 0 | 0.349092 | 1.789531 | 0.373808 |
| 45 | 6 | 0 | -0.255724 | 2.865519 | -0.382642 |
| 46 | 6 | 0 | -0.131715 | 4.102688 | 0.510454 |
| 47 | 6 | 0 | -0.411900 | 3.039303 | -0.035065 |
| 48 | 6 | 0 | 5.953460 | -1.045299 | -1.468068 |
| 49 | 6 | 0 | 0.349092 | 1.789531 | 0.373808 |
| 50 | 6 | 0 | -0.255724 | 2.865519 | -0.382642 |
| 1e (conformer 12) |   |   |   |   |   |   |   |   |   |
| 1 | 6 | 0 | 4.703418 | -1.153395 | -1.068220 |
| 2 | 6 | 0 | 4.698888 | -0.513323 | 0.146634 |
| 3 | 6 | 0 | 3.545634 | 0.172842 | 0.612145 |
| 4 | 6 | 0 | 2.355615 | 0.184195 | -0.192702 |
| 5 | 6 | 0 | 2.407163 | -0.481921 | -1.449232 |
| 6 | 6 | 0 | 3.544426 | -1.128489 | -1.874969 |
| 7 | 6 | 0 | 3.563715 | 0.860627 | 1.853353 |
| 8 | 6 | 0 | 2.456490 | 1.548454 | 2.761211 |
| 9 | 6 | 0 | 1.282263 | 1.560781 | 1.490454 |
| 10 | 6 | 0 | 1.198703 | 0.884273 | 0.291724 |
| 11 | 6 | 0 | -0.096104 | 0.951402 | -0.529682 |
| 12 | 6 | 0 | -0.803504 | -0.380729 | -0.813204 |
| 13 | 6 | 0 | -1.268200 | -1.266701 | 0.216334 |
| 14 | 6 | 0 | -1.051321 | -0.705808 | -2.132046 |
| 15 | 6 | 0 | -1.712406 | -1.897850 | -2.504592 |
| 16 | 6 | 0 | -2.132324 | -2.774927 | -1.539436 |
| 17 | 6 | 0 | -1.927943 | -2.483904 | -0.164847 |
| 18 | 6 | 0 | -1.127605 | -0.999709 | 1.606079 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 19| 6  | 0  | -1.583748 | -1.884884 | 2.555072 |
| 20| 6  | 0  | -2.212004 | -3.091437 | 2.173236 |
| 21| 6  | 0  | -2.381429 | -3.378474 | 0.841197 |
| 22| 8  | 0  | -0.997998 | 1.859121  | 0.111073 |
| 23| 6  | 0  | -1.859780 | 2.612957  | -0.766260|
| 24| 6  | 0  | -3.072246 | 3.044377  | 0.058937 |
| 25| 6  | 0  | -1.111946 | 3.809072  | -1.355472|
| 26| 6  | 0  | -2.212004 | -3.091437 | 2.173236 |
| 27| 6  | 0  | -2.381429 | -3.378474 | 0.841197 |
| 28| 6  | 0  | -1.859780 | 2.612957  | -0.766260|
| 29| 6  | 0  | -3.072246 | 3.044377  | 0.058937 |
| 30| 6  | 0  | -1.111946 | 3.809072  | -1.355472|
| 31| 6  | 0  | -2.212004 | -3.091437 | 2.173236 |
| 32| 6  | 0  | -2.381429 | -3.378474 | 0.841197 |
| 33| 6  | 0  | -1.859780 | 2.612957  | -0.766260|
| 34| 6  | 0  | -3.072246 | 3.044377  | 0.058937 |
| 35| 6  | 0  | -1.111946 | 3.809072  | -1.355472|
| 36| 6  | 0  | -2.212004 | -3.091437 | 2.173236 |
| 37| 6  | 0  | -2.381429 | -3.378474 | 0.841197 |
| 38| 6  | 0  | -1.859780 | 2.612957  | -0.766260|
| 39| 6  | 0  | -3.072246 | 3.044377  | 0.058937 |
| 40| 6  | 0  | -1.111946 | 3.809072  | -1.355472|
| 41| 6  | 0  | -2.212004 | -3.091437 | 2.173236 |
| 42| 6  | 0  | -2.381429 | -3.378474 | 0.841197 |
| 43| 6  | 0  | -1.859780 | 2.612957  | -0.766260|
| 44| 6  | 0  | -3.072246 | 3.044377  | 0.058937 |
| 45| 6  | 0  | -1.111946 | 3.809072  | -1.355472|
| 46| 6  | 0  | -2.212004 | -3.091437 | 2.173236 |
| 47| 6  | 0  | -2.381429 | -3.378474 | 0.841197 |
| 48| 6  | 0  | -1.859780 | 2.612957  | -0.766260|
| 49| 6  | 0  | -3.072246 | 3.044377  | 0.058937 |
| 50| 6  | 0  | -1.111946 | 3.809072  | -1.355472|

1e (conformer 15)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6  | 0  | 2.749771 | -3.034112 | 2.031719 |
| 2 | 6  | 0  | 2.867348 | -3.265146 | 0.683361 |
| 3 | 6  | 0  | 2.280647 | -2.385191 | 0.326511 |
| 4 | 6  | 0  | 1.538308 | -1.244449 | 0.193064 |
| 5 | 6  | 0  | 1.455618 | -1.031720 | 1.597014 |
| 6 | 6  | 0  | 2.041520 | -1.900135 | 2.488426 |
| 7 | 6  | 0  | 2.434132 | -2.614853 | -1.657807|
| 8 | 6  | 0  | 1.888782 | -1.747436 | -2.567806|
| 9 | 6  | 0  | 1.148837 | -0.630668 | -2.118981|
| 10| 6  | 0  | 0.939899 | -0.372880 | -0.779881|
| 11| 6  | 0  | 0.118776 | 0.873099  | -0.409276|
| 12| 6  | 0  | -1.160917| 0.614611  | 0.397052 |
| 13| 6  | 0  | -2.268967 | -0.101694 | -0.71120 |
| 14| 6  | 0  | -1.280257 | 1.120760  | 1.674543 |
| 15| 6  | 0  | -2.438733 | 0.914192  | 2.456358 |
| 16| 6  | 0  | -3.948188 | 0.201583  | 1.951894 |
| 17| 6  | 0  | -3.441943 | -0.313428 | 0.630796 |
| 18| 6  | 0  | -2.289185 | -0.596433 | -1.505120|
| 19| 6  | 0  | -3.792825 | -1.268134 | -2.007863|
| 20| 6  | 0  | -4.519678 | -1.492419 | -1.205362|

1e (conformer 15)
|    |   |   |                  |                  |                  |
|----|---|---|------------------|------------------|------------------|
| 21 | 6 | 0 | -4.545617   | -1.021021   | 0.084031          |
| 22 | 8 | 0 | 0.914805    | 1.815471    | 0.312376          |
| 23 | 6 | 0 | 1.907032    | 2.528474    | -0.456568         |
| 24 | 6 | 0 | 1.283148    | 3.700551    | -1.233200         |
| 25 | 6 | 0 | 2.986834    | 2.949970    | 0.531092          |
| 26 | 6 | 0 | 0.593388    | 4.761609    | -0.370251         |
| 27 | 1 | 0 | 3.204031    | -3.711805   | 2.745575          |
| 28 | 1 | 0 | 3.418931    | -4.125193   | 0.318418          |
| 29 | 1 | 0 | 0.936739    | 0.162565    | 1.968314          |
| 30 | 1 | 0 | 2.998858    | -3.480935   | -1.986022         |
| 31 | 1 | 0 | 2.018062    | -1.910118   | -3.631589         |
| 32 | 1 | 0 | 0.727374    | 0.040969    | -2.859886         |
| 33 | 1 | 0 | -0.192152   | 1.324326    | -1.359513         |
| 34 | 1 | 0 | -0.461324   | 1.693744    | 2.086098          |
| 35 | 1 | 0 | -2.481025   | 1.323868    | 3.459268          |
| 36 | 1 | 0 | -4.386857   | 0.031946    | 2.545337          |
| 37 | 1 | 0 | -1.433853   | -0.445722   | -2.146118         |
| 38 | 1 | 0 | -3.362819   | -1.628302   | 1.958500          |
| 39 | 1 | 0 | -5.370313   | -2.028105   | -1.610996         |
| 40 | 1 | 0 | -5.419282   | -1.175716   | 0.708566          |
| 41 | 1 | 0 | 2.351000    | 1.837061    | -1.182456         |
| 42 | 1 | 0 | 2.080419    | 4.160720    | -1.828058         |
| 43 | 1 | 0 | 0.565532    | 3.301704    | -1.958500         |
| 44 | 1 | 0 | 3.763635    | 3.530120    | 0.023500          |
| 45 | 1 | 0 | 2.572045    | 3.561879    | 1.334404          |
| 46 | 1 | 0 | 3.453165    | 2.069640    | 0.979813          |
| 47 | 1 | 0 | 0.131692    | 5.526173    | -1.000476         |
| 48 | 1 | 0 | -0.191227   | 4.315517    | 0.244968          |
| 49 | 1 | 0 | 1.297219    | 5.266524    | 0.296216          |

**1e (conformer 16)**

|    |   |   |                  |                  |                  |
|----|---|---|------------------|------------------|------------------|
| 1  | 6 | 0 | 1.778634    | 3.833960    | -1.715840         |
| 2  | 6 | 0 | 1.972745    | 3.879134    | -0.357291         |
| 3  | 6 | 0 | 1.676580    | 2.757926    | 0.463194          |
| 4  | 6 | 0 | 1.149960    | 1.563431    | -0.135179         |
| 5  | 6 | 0 | 0.980592    | 1.551900    | -1.547402         |
| 6  | 6 | 0 | 1.283978    | 2.653212    | -2.313605         |
| 7  | 6 | 0 | 1.910000    | 2.802699    | 1.863118          |
| 8  | 6 | 0 | 1.646576    | 1.708920    | 2.645432          |
| 9  | 6 | 0 | 1.116447    | 0.537000    | 2.060481          |
| 10 | 6 | 0 | 0.842060    | 0.446165    | 0.710722          |
| 11 | 6 | 0 | 0.272467    | -0.881653   | 0.184416          |
| 12 | 6 | 0 | -1.091993   | -0.801339   | -0.513120         |
| 13 | 6 | 0 | -2.275092   | -0.411511   | 0.202314          |
| 14 | 6 | 0 | -1.204338   | -1.161184   | -1.839706         |
| 15 | 6 | 0 | -2.437647   | -1.109503   | -2.526943         |
| 16 | 6 | 0 | -3.574095   | -0.702908   | -1.878159         |
| 17 | 6 | 0 | -3.524942   | -0.354623   | -0.503450         |
| 18 | 6 | 0 | -2.291900   | -0.102686   | 1.591179          |
| 19 | 6 | 0 | -3.452997   | 0.258039    | 2.234707          |
| 20 | 6 | 0 | -4.673283   | 0.336206    | 1.528032          |
| 21 | 6 | 0 | -4.703099   | 0.032489    | 0.189211          |
| 22 | 8 | 0 | 1.198312    | -1.504101   | -0.709586         |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 23 | 6 | 0 | 2.313830 | -2.178418 | -0.088626 |
| 24 | 6 | 0 | 1.909750 | -3.607068 | 0.301217 |
| 25 | 6 | 0 | 3.458325 | -2.122294 | -1.092043 |
| 26 | 6 | 0 | 2.957137 | -4.345760 | 1.141773 |
| 27 | 1 | 0 | 2.010646 | 4.695602 | -2.331452 |
| 28 | 1 | 0 | 2.363908 | 4.775065 | 0.301217 |
| 29 | 1 | 0 | 3.458325 | -2.122294 | -1.092043 |
| 30 | 1 | 0 | 2.957137 | -4.345760 | 1.141773 |
| 31 | 1 | 0 | 2.010646 | 4.695602 | -2.331452 |
| 32 | 1 | 0 | 2.363908 | 4.775065 | 0.301217 |
| 33 | 1 | 0 | 0.621658 | 0.655711 | -2.027880 |
| 34 | 1 | 0 | 0.621658 | 0.655711 | -2.027880 |
| 35 | 6 | 0 | 2.313830 | -2.178418 | -0.088626 |
| 36 | 6 | 0 | 1.909750 | -3.607068 | 0.301217 |
| 37 | 6 | 0 | 3.458325 | -2.122294 | -1.092043 |
| 38 | 6 | 0 | 2.957137 | -4.345760 | 1.141773 |
| 39 | 6 | 0 | 2.010646 | 4.695602 | -2.331452 |
| 40 | 6 | 0 | 2.363908 | 4.775065 | 0.301217 |
| 41 | 6 | 0 | 0.621658 | 0.655711 | -2.027880 |
| 42 | 6 | 0 | 0.621658 | 0.655711 | -2.027880 |
| 43 | 1 | 0 | 0.621658 | 0.655711 | -2.027880 |
| 44 | 1 | 0 | 0.621658 | 0.655711 | -2.027880 |
| 45 | 6 | 0 | 2.313830 | -2.178418 | -0.088626 |
| 46 | 6 | 0 | 1.909750 | -3.607068 | 0.301217 |
| 47 | 6 | 0 | 3.458325 | -2.122294 | -1.092043 |
| 48 | 6 | 0 | 2.957137 | -4.345760 | 1.141773 |
| 49 | 6 | 0 | 2.010646 | 4.695602 | -2.331452 |
| 50 | 6 | 0 | 2.363908 | 4.775065 | 0.301217 |

**1e (conformer 17)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6 | 0 | -4.839212 | 0.429669 | -1.245882 |
| 2  | 6 | 0 | -4.785034 | -0.133092 | 0.005448 |
| 3  | 6 | 0 | -3.561695 | -0.614585 | -0.563761 |
| 4  | 6 | 0 | -2.354251 | -0.495373 | -0.226364 |
| 5  | 6 | 0 | -2.457969 | 0.081103 | -1.523200 |
| 6  | 6 | 0 | -3.661027 | 0.528275 | -2.018411 |
| 7  | 6 | 0 | -3.524659 | -1.227515 | 1.822363 |
| 8  | 6 | 0 | -2.345276 | -1.720210 | 2.316135 |
| 9  | 6 | 0 | -1.153515 | -1.600709 | 1.566794 |
| 10 | 6 | 0 | -1.124938 | -0.984710 | 0.333116 |
| 11 | 6 | 0 | 0.197726 | -0.894750 | -0.440471 |
| 12 | 6 | 0 | 0.704411 | 0.519641 | -0.759628 |
| 13 | 6 | 0 | 1.026251 | 1.489053 | 0.249362 |
| 14 | 6 | 0 | 0.910312 | 0.846220 | -2.085040 |
| 15 | 6 | 0 | 1.383660 | 2.116909 | -2.484915 |
| 16 | 6 | 0 | 1.659862 | 3.069830 | -1.540441 |
| 17 | 6 | 0 | 1.495245 | 2.783062 | -0.159577 |
| 18 | 6 | 0 | 0.924063 | 1.233620 | 1.644781 |
| 19 | 6 | 0 | 1.236972 | 2.198849 | 2.573389 |
| 20 | 6 | 0 | 1.674608 | 3.478497 | 2.164244 |
| 21 | 6 | 0 | 1.803427 | 3.758418 | 0.826127 |
| 22 | 8 | 0 | 1.188357 | -1.631024 | 0.281171 |
| 23 | 6 | 0 | 2.296057 | -2.130411 | -0.497907 |
| 24 | 6 | 0 | 3.464834 | -2.276769 | 0.478608 |
|   |   |   | x   | y   | z   |
|---|---|---|-----|-----|-----|
| 25| 6 | 0 | 1.908435 | -3.437241 | -1.188935 |
| 26| 6 | 0 | 4.785604 | -2.691002 | -0.177467 |
| 27| 1 | 0 | -5.780214 | 0.790651 | -1.645024 |
| 28| 1 | 0 | -5.684012 | -0.226277 | 0.605673  |
| 29| 1 | 0 | -1.577458 | 0.174107 | -2.140897 |
| 30| 1 | 0 | -3.705037 | 0.959474 | -3.012244 |
| 31| 1 | 0 | -4.443282 | -1.308264 | 2.391936  |
| 32| 1 | 0 | -3.437241 | -2.204004 | 3.285947  |
| 33| 1 | 0 | -5.780214 | 0.790651 | -1.645024 |
| 34| 1 | 0 | -5.684012 | -0.226277 | 0.605673  |
| 35| 1 | 0 | -1.577458 | 0.174107 | -2.140897 |
| 36| 1 | 0 | -3.705037 | 0.959474 | -3.012244 |
| 37| 1 | 0 | 2.016465  | 4.052066 | -1.831639 |
| 38| 1 | 0 | 4.785604 | -2.691002 | -0.177467 |
| 39| 1 | 0 | -5.780214 | 0.790651 | -1.645024 |
| 40| 1 | 0 | -5.684012 | -0.226277 | 0.605673  |
| 41| 1 | 0 | -1.577458 | 0.174107 | -2.140897 |
| 42| 1 | 0 | -3.705037 | 0.959474 | -3.012244 |
| 43| 1 | 0 | 2.016465  | 4.052066 | -1.831639 |
| 44| 1 | 0 | 4.785604 | -2.691002 | -0.177467 |
| 45| 1 | 0 | -5.780214 | 0.790651 | -1.645024 |
| 46| 1 | 0 | -5.684012 | -0.226277 | 0.605673  |
| 47| 1 | 0 | -1.577458 | 0.174107 | -2.140897 |
| 48| 1 | 0 | -3.705037 | 0.959474 | -3.012244 |
| 49| 1 | 0 | 2.016465  | 4.052066 | -1.831639 |
| 50| 1 | 0 | 4.785604 | -2.691002 | -0.177467 |

**1e (conformer 18)**

|   |   |   | x   | y   | z   |
|---|---|---|-----|-----|-----|
| 1 | 6 | 0 | -4.841539 | 0.809319 | -0.875390 |
| 2 | 6 | 0 | -4.712245 | 0.120043 | 0.305241  |
| 3 | 6 | 0 | -3.473820 | -0.463152 | 0.684493  |
| 4 | 6 | 0 | -2.329505 | -0.314361 | -0.171156 |
| 5 | 6 | 0 | -2.510607 | 0.397544 | -1.389804 |
| 6 | 6 | 0 | -3.727200 | 0.940113 | -1.733124 |
| 7 | 6 | 0 | -3.361763 | -1.062000 | 1.888188  |
| 8 | 6 | 0 | -2.172140 | -1.797158 | 2.224597  |
| 9 | 6 | 0 | -1.042369 | -1.651036 | 1.388984  |
| 10 | 6 | 0 | -1.084301 | -0.910448 | 0.226294  |
| 11 | 6 | 0 | 0.171636 | -0.792971 | -0.647648 |
| 12 | 6 | 0 | 0.740195 | 0.623372 | -0.824657 |
| 13 | 6 | 0 | 1.127908 | 1.424966 | 0.266926  |
| 14 | 6 | 0 | 0.837356 | 1.122879 | -2.107857 |
| 15 | 6 | 0 | 1.345514 | 2.412914 | -2.379857 |
| 16 | 6 | 0 | 1.765578 | 3.211697 | -1.349072 |
| 17 | 6 | 0 | 1.720560 | 2.741182 | -0.010116 |
| 18 | 6 | 0 | 1.240117 | 0.980792 | 1.617985  |
| 19 | 6 | 0 | 1.698328 | 1.791278 | 2.630466  |
| 20 | 6 | 0 | 2.166785 | 3.095278 | 2.354671  |
| 21 | 6 | 0 | 2.179758 | 3.554177 | 1.060563  |
| 22 | 6 | 0 | 1.167283 | -1.674530 | -0.123980 |
| 23 | 6 | 0 | 2.158126 | -2.130537 | -1.069234 |
| 24 | 6 | 0 | 3.425544 | -2.462142 | -0.273257 |
| 25 | 6 | 0 | 1.618713 | -3.301884 | -1.891715 |
| 26 | 6 | 0 | 3.270276 | -3.555836 | 0.788841  |
|   |   |   |      |      |      |
|---|---|---|------|------|------|
| 27 | 1 | 0 | -5.793622 | 1.246242 | -1.154210 |
| 28 | 1 | 0 | -5.562536 | 0.001895 | 0.968782 |
| 29 | 1 | 0 | -1.679898 | 0.519684 | -2.068105 |
| 30 | 1 | 0 | -3.831414 | 1.473248 | -2.671445 |
| 31 | 1 | 0 | -4.234108 | -1.307685 | 2.524916 |
| 32 | 1 | 0 | -2.086348 | -2.380976 | 3.134168 |
| 33 | 1 | 0 | -0.115763 | -2.133936 | 1.665698 |
| 34 | 1 | 0 | -0.111740 | -1.134660 | -1.650814 |
| 35 | 1 | 0 | 0.505885 | 0.511698 | -2.941180 |
| 36 | 1 | 0 | 1.394901 | 2.762499 | -3.404629 |
| 37 | 1 | 0 | 2.150138 | 4.208166 | -1.540581 |
| 38 | 1 | 0 | 0.904644 | -0.017454 | 1.850188 |
| 39 | 1 | 0 | 1.704088 | 1.424374 | 3.650801 |
| 40 | 1 | 0 | 2.521379 | 3.724771 | 3.162879 |
| 41 | 1 | 0 | 2.548535 | 4.548896 | 0.833239 |
| 42 | 1 | 0 | 2.402011 | -1.302792 | -1.745752 |
| 43 | 1 | 0 | 4.202203 | -2.749515 | -0.990562 |
| 44 | 1 | 0 | 3.768317 | -1.538798 | 0.204217 |
| 45 | 1 | 0 | 2.375913 | -3.646651 | -2.601597 |
| 46 | 1 | 0 | 1.339747 | -4.138792 | -1.248100 |
| 47 | 1 | 0 | 0.737040 | -3.009412 | 1.333326 |
| 48 | 1 | 0 | 2.497290 | -3.291968 | 1.513776 |
| 49 | 1 | 0 | 3.005160 | -4.520145 | 0.347944 |
| 50 | 1 | 0 | 6.407199 | 0.242844 | -0.795002 |

**1e (conformer 22)**

|   |   |   |      |      |      |
|---|---|---|------|------|------|
| 1  | 6 | 0 | -5.344710 | 0.033913 | -0.019565 |
| 2  | 6 | 0 | -4.856318 | -1.184582 | -0.422960 |
| 3  | 6 | 0 | -3.467542 | -1.475660 | -0.357639 |
| 4  | 6 | 0 | -2.557834 | -0.476594 | 0.124988 |
| 5  | 6 | 0 | -3.103826 | 0.772372 | 0.532164 |
| 6  | 6 | 0 | -4.455554 | 1.018625 | 0.466227 |
| 7  | 6 | 0 | -2.970771 | -2.746450 | -0.749946 |
| 8  | 6 | 0 | -1.632838 | -3.024775 | -0.654002 |
| 9  | 6 | 0 | -0.733375 | -2.04913 | -0.174074 |
| 10 | 6 | 0 | -1.155455 | -0.786959 | 0.199008 |
| 11 | 6 | 0 | -0.179326 | 0.253591 | 0.756761 |
| 12 | 6 | 0 | 1.238472 | -0.252456 | 1.023420 |
| 13 | 6 | 0 | 2.207957 | -0.490569 | -0.008030 |
| 14 | 6 | 0 | 1.588708 | -0.488776 | 2.337303 |
| 15 | 6 | 0 | 2.867293 | -0.966921 | 2.699803 |
| 16 | 6 | 0 | 3.810650 | -1.198383 | 1.731952 |
| 17 | 6 | 0 | 3.507939 | -0.967979 | 0.363982 |
| 18 | 6 | 0 | 1.943883 | -0.288747 | -1.391944 |
| 19 | 6 | 0 | 2.903911 | -0.539645 | -2.344242 |
| 20 | 6 | 0 | 4.186087 | -1.003953 | -1.971997 |
| 21 | 6 | 0 | 4.478279 | -1.211911 | -0.646578 |
| 22 | 8 | 0 | -0.231508 | 1.396864 | -0.113720 |
| 23 | 6 | 0 | 0.503874 | 2.572880 | 0.288912 |
| 24 | 6 | 0 | 0.281629 | 3.614266 | -0.810641 |
| 25 | 6 | 0 | 0.72688 | 3.113133 | 1.653871 |
| 26 | 6 | 0 | 0.753473 | 3.195059 | -2.204315 |
| 27 | 1 | 0 | -6.407199 | 0.242844 | -0.071178 |
| 28 | 1 | 0 | -5.528220 | -1.950943 | -0.795002 |
| 29 | 1 | 0 | -2.439791 | 1.549309 | 0.879810 |
|----|---|---|-----------|----------|----------|
| 30 | 1 | 0 | -4.842861 | 1.979493 | 0.786381 |
| 31 | 1 | 0 | -3.668732 | -3.492160 | -1.115528 |
| 32 | 1 | 0 | -1.251659 | -3.997795 | -0.942274 |
| 33 | 1 | 0 | 0.313670  | -2.304169 | -0.097577 |
| 34 | 1 | 0 | -0.576498 | 0.548568  | 1.735780 |
| 35 | 1 | 0 | -4.842861 | 1.979493 | -1.688928 |
| 36 | 1 | 0 | 2.676160  | -0.378233 | -3.391988 |
| 37 | 1 | 0 | 4.798853  | -1.559451 | 1.996280 |
| 38 | 1 | 0 | 1.251659  | -3.997795 | 0.942274 |
| 39 | 1 | 0 | 0.313670  | -2.304169 | -0.097577 |
| 40 | 1 | 0 | 4.933313  | -1.195337 | -2.733772 |
| 41 | 1 | 0 | 5.457912  | -1.570681 | -0.348621 |
| 42 | 1 | 0 | 1.571167  | 2.316913  | 0.329366 |
| 43 | 1 | 0 | -0.786335 | 3.859985  | -0.837271 |
| 44 | 1 | 0 | 0.804544  | 4.527211  | -0.506742 |
| 45 | 1 | 0 | 0.632775  | 4.025521  | 1.874460 |
| 46 | 1 | 0 | -0.992698 | 3.361103  | 1.659386 |
| 47 | 1 | 0 | 0.271172  | 2.408895  | 2.463715 |
| 48 | 1 | 0 | 0.596039  | 4.004495  | -2.922392 |
| 49 | 1 | 0 | 1.819610  | 2.949873  | -2.204928 |
| 50 | 1 | 0 | 0.207437  | 2.319152  | -2.558690 |

1e (conformer 32)

| 1  | 6 | 0 | -5.274054 | -0.284608 | 0.061297 |
|----|---|---|-----------|----------|----------|
| 2  | 6 | 0 | -4.729406 | -1.468521 | -0.371993 |
| 3  | 6 | 0 | -3.25882 | -1.685004 | -0.339394 |
| 4  | 6 | 0 | -2.461807 | -0.646542 | 0.143383 |
| 5  | 6 | 0 | -3.065387 | 0.564024  | 0.582998 |
| 6  | 6 | 0 | -4.429427 | 0.738561  | 0.547043 |
| 7  | 6 | 0 | -2.768609 | -2.919086 | -0.765976 |
| 8  | 6 | 0 | -1.415321 | -3.123803 | -0.704743 |
| 9  | 6 | 0 | -0.560592 | -2.104485 | -0.225149 |
| 10 | 6 | 0 | -1.043518 | -0.879589 | 0.182544 |
| 11 | 6 | 0 | -0.113837 | 0.208071  | 0.729041 |
| 12 | 6 | 0 | 1.327682  | -0.234379 | 0.982364 |
| 13 | 6 | 0 | 2.305698  | -0.398574 | -0.055995 |
| 14 | 6 | 0 | 1.689584  | -0.490339 | 2.289194 |
| 15 | 6 | 0 | 2.987824  | -0.923268 | 2.638100 |
| 16 | 6 | 0 | 3.938858  | -1.087112 | 1.663981 |
| 17 | 6 | 0 | 3.627230  | -0.829789 | 0.303175 |
| 18 | 6 | 0 | 2.034541  | -0.164315 | -1.434297 |
| 19 | 6 | 0 | 3.005991  | -0.342731 | -2.391548 |
| 20 | 6 | 0 | 4.306365  | -0.763709 | -2.031544 |
| 21 | 6 | 0 | 4.605862  | -1.000567 | -0.712673 |
| 22 | 8 | 0 | -0.220466 | 1.339913  | -0.149379 |
| 23 | 6 | 0 | 0.439118  | 2.554839  | 0.271418 |
| 24 | 6 | 0 | 0.497303  | 3.461986  | -0.963464 |
| 25 | 6 | 0 | 0.245542  | 3.206887  | 1.474780 |
| 26 | 6 | 0 | -0.860593 | 3.879119  | -1.539031 |
| 27 | 1 | 0 | -6.346992 | -0.132241 | 0.033616 |
| 28 | 1 | 0 | -5.366846 | -2.263896 | -0.743761 |
| 29 | 1 | 0 | -2.438354 | 1.368465  | 0.936737 |
| 30 | 1 | 0 | -4.861085 | 1.671790  | 0.891260 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 31 | 1  | 0 | -3.432150 | -3.695788 | -1.131046 |
| 32 | 1  | 0 | -0.987529  | -4.068424  | -1.020718 |
| 33 | 1  | 0 |  0.500778  | -2.306342  | -0.177229 |
| 34 | 1  | 0 | -0.513293  |  0.491121  |  1.711181 |
| 35 | 1  | 0 |  0.954741  | -0.356958  |  3.076450 |
| 36 | 1  | 0 |  3.225641  | -1.116073  |  3.677912 |
| 37 | 1  | 0 |  4.941840  | -1.413215  |  1.917914 |
| 38 | 1  | 0 |  1.048805  |  0.170368  | -1.721702 |
| 39 | 1  | 0 |  2.772479  | -0.158028  | -3.434201 |
| 40 | 1  | 0 |  5.061810  | -0.898907  | -2.797247 |
| 41 | 1  | 0 |  5.599748  | -1.326099  | -0.423865 |
| 42 | 1  | 0 |  1.470298  |  2.309106  |  0.552793 |
| 43 | 1  | 0 |  1.076031  |  4.352330  | -0.693988 |
| 44 | 1  | 0 |  1.072945  |  2.938211  | -1.732742 |
| 45 | 1  | 0 |  0.273872  |  4.134209  |  1.731841 |
| 46 | 1  | 0 | -1.289010  |  3.449636  |  1.262459 |
| 47 | 1  | 0 | -0.214737  |  2.563751  |  2.356924 |
| 48 | 1  | 0 | -0.721776  |  4.472466  | -2.446680 |
| 49 | 1  | 0 | -1.461230  |  3.005047  | -1.796932 |
| 50 | 1  | 0 | -1.433868  |  4.487765  | -0.835017 |

**1e (conformer 36)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1  | 6  | 0 | -5.372065  |  0.251965  | -0.119665 |
| 2  | 6  | 0 | -4.949581  | -1.013837  | -0.443905 |
| 3  | 6  | 0 | -3.580343  | -1.378091  | -0.342632 |
| 4  | 6  | 0 | -2.620017  | -0.404864  |  0.092620 |
| 5  | 6  | 0 | -3.098707  |  0.894046  |  0.419847 |
| 6  | 6  | 0 | -4.433455  |  1.211676  |  0.320847 |
| 7  | 6  | 0 | -3.153166  | -2.695848  | -0.652972 |
| 8  | 6  | 0 | -1.834060  | -3.042563  | -0.524366 |
| 9  | 6  | 0 | -0.884734  | -2.087399  | -0.093429 |
|10 | 6  | 0 | -1.237981  | -0.787702  |  0.200118 |
|11 | 6  | 0 | -0.204557  |  0.227086  |  0.699473 |
|12 | 6  | 0 |  1.182638  | -0.345013  |  0.991715 |
|13 | 6  | 0 |  2.134812  | -0.679249  | -0.029621 |
|14 | 6  | 0 |  1.521988  | -0.542384  |  2.314493 |
|15 | 6  | 0 |  2.772728  | -1.075689  |  2.696941 |
|16 | 6  | 0 |  3.698614  | -1.402114  |  1.739604 |
|17 | 6  | 0 |  3.408314  | -1.213062  |  0.362844 |
|18 | 6  | 0 |  1.880629  | -0.520550  | -1.421713 |
|19 | 6  | 0 |  2.823930  | -0.864790  | -2.361616 |
|20 | 6  | 0 |  4.078378  | -1.384600  | -1.969101 |
|21 | 6  | 0 |  4.360029  | -1.553284  | -0.635854 |
|22 | 8  | 0 | -0.182922  |  1.314851  | -0.239480 |
|23 | 6  | 0 |  0.591044  |  2.478274  |  0.130825 |
|24 | 6  | 0 |  0.776717  |  3.267707  | -1.167197 |
|25 | 6  | 0 | -0.088918  |  3.287419  |  1.235929 |
|26 | 6  | 0 |  1.696711  |  4.486002  | -1.039207 |
|27 | 1  | 0 | -6.420303  |  0.516944  | -0.198309 |
|28 | 1  | 0 | -5.655976  | -1.762063  | -0.779641 |
|29 | 1  | 0 | -2.397344  |  1.651446  |  0.734779 |
|30 | 1  | 0 | -4.768624  |  2.209923  |  0.579579 |
|31 | 1  | 0 | -3.889051  | -3.421550  | -0.982623 |
|32 | 1  | 0 | -1.505966  | -4.050828  | -0.750008 |
|   |   |   |     |     |     |
|---|---|---|-----|-----|-----|
| 33| 1 | 0 | 0.145662 | -2.399419 | 0.008837 |
| 34| 1 | 0 | -0.579199 | 0.602722 | 1.660067 |
| 35| 1 | 0 | 0.807081 | -0.279901 | 3.087630 |
| 36| 1 | 0 | 2.995152 | -1.216062 | 3.748484 |
| 37| 1 | 0 | 4.665482 | -1.806895 | 2.019109 |
| 38| 1 | 0 | 0.931247 | -0.112151 | -1.734880 |
| 39| 1 | 0 | 2.603945 | -0.735213 | -1.734880 |
| 40| 1 | 0 | 4.812708 | -1.649333 | -2.721387 |
| 41| 1 | 0 | 5.318301 | -1.953957 | -0.322279 |
| 42| 1 | 0 | 1.575531 | 2.146734 | 0.484738 |
| 43| 1 | 0 | 1.183845 | 2.580784 | -1.914625 |
| 44| 1 | 0 | -0.210532 | 3.578018 | -1.528176 |
| 45| 1 | 0 | 0.542755 | 4.126752 | 1.535814 |
| 46| 1 | 0 | -1.046201 | 3.686692 | 2.130920 |
| 47| 1 | 0 | -0.265460 | 3.686692 | 2.130920 |
| 48| 1 | 0 | 1.847877 | 4.953485 | -2.015385 |
| 49| 1 | 0 | 1.282279 | 5.246224 | -0.372577 |
| 50| 1 | 0 | 2.680484 | 4.201856 | -0.652626 |

**1e (conformer 39)**

|   |   |   |     |     |     |
|---|---|---|-----|-----|-----|
| 1 | 6 | 0 | -4.132593 | -1.674884 | -1.836784 |
| 2 | 6 | 0 | -4.451558 | -1.510896 | -0.511391 |
| 3 | 6 | 0 | -3.507140 | -0.982695 | 0.409437 |
| 4 | 6 | 0 | -2.201170 | -0.610016 | -0.055798 |
| 5 | 6 | 0 | -1.909244 | -0.794952 | -1.437285 |
| 6 | 6 | 0 | -2.846983 | -1.313148 | -2.99798 |
| 7 | 6 | 0 | -3.836727 | -0.827377 | 1.781590 |
| 8 | 6 | 0 | -2.917212 | -0.322666 | 2.664802 |
| 9 | 6 | 0 | -1.634216 | 0.052837 | 2.208496 |
| 10| 6| 0 | -1.256982 | -0.82404 | 0.888226 |
| 11| 6| 0 | 0.160445 | 0.348958 | 0.512683 |
| 12| 6| 0 | 1.157228 | -0.794233 | 0.295447 |
| 13| 6| 0 | 2.556480 | -0.501009 | 0.137376 |
| 14| 6| 0 | 0.753046 | -2.112010 | 0.310408 |
| 15| 6| 0 | 1.667539 | -3.177849 | 0.146018 |
| 16| 6| 0 | 3.002782 | -2.922509 | -0.023670 |
| 17| 6| 0 | 3.481346 | -1.585972 | -0.025067 |
| 18| 6| 0 | 3.084885 | 0.819556 | 0.155367 |
| 19| 6| 0 | 4.433722 | 1.053506 | 0.020328 |
| 20| 6| 0 | 5.337734 | -0.018763 | -0.149865 |
| 21| 6| 0 | 4.866810 | -1.308553 | -0.172206 |
| 22| 8| 0 | 0.204637 | 1.186052 | -0.654917 |
| 23| 6| 0 | -0.519162 | 2.436741 | -0.586240 |
| 24| 6| 0 | 0.223880 | 3.478505 | 0.263595 |
| 25| 6| 0 | -0.710141 | 2.874166 | -2.033122 |
| 26| 6| 0 | -0.597940 | 4.742740 | 0.542209 |
| 27| 1| 0 | -4.861543 | -2.080745 | -2.529018 |
| 28| 1| 0 | -5.434202 | -1.786802 | -0.143412 |
| 29| 1| 0 | -0.935861 | -0.508379 | -1.807359 |
| 30| 1| 0 | -2.598516 | -1.444798 | -3.347017 |
| 31| 1| 0 | -4.827741 | -1.114210 | 2.116876 |
| 32| 1| 0 | -3.168739 | -0.201177 | 3.712132 |
| 33| 1| 0 | -0.925342 | 0.461504 | 2.921310 |
| 34| 1| 0 | 0.532827 | 0.923471 | 1.370599 |
| Row | Conformer Type | Index | ETP1 | ETP2 | ETP3 |
|-----|----------------|-------|------|------|------|
| 35  | 1e (conformer 45) | 1     | -4.380023 | -0.843629 | -1.985673 |
| 36  | 1e (conformer 45) | 2     | -4.649575 | -1.019993 | -0.651082 |
| 37  | 1e (conformer 45) | 3     | -3.646102 | -0.810722 | 0.333230 |
| 38  | 1e (conformer 45) | 4     | -2.331169 | -0.404617 | -0.075738 |
| 39  | 1e (conformer 45) | 5     | -2.092115 | -0.230861 | -1.469051 |
| 40  | 1e (conformer 45) | 6     | -3.086402 | -0.445946 | -2.394344 |
| 41  | 1e (conformer 45) | 7     | -3.927092 | -1.004787 | 1.711067 |
| 42  | 1e (conformer 45) | 8     | -2.951238 | -0.806506 | 2.654088 |
| 43  | 1e (conformer 45) | 9     | -1.658267 | -0.401889 | 2.255765 |
| 44  | 1e (conformer 45) | 10    | -1.328502 | -0.201791 | 0.930797 |
| 45  | 1e (conformer 45) | 11    | 0.112160 | 0.209548 | 0.623399 |
| 46  | 1e (conformer 45) | 12    | 1.017492 | -0.939464 | 0.165174 |
| 47  | 1e (conformer 45) | 13    | 2.442998 | -0.752451 | 0.148035 |
| 48  | 1e (conformer 45) | 14    | 0.504496 | -2.165681 | -0.199187 |
| 49  | 1e (conformer 45) | 15    | 1.335737 | -3.231579 | -0.614489 |
| 50  | 1e (conformer 45) | 16    | 2.695733 | -3.071360 | -0.654878 |
| 51  | 1e (conformer 45) | 17    | 3.283148 | -1.837269 | -0.270380 |
| 52  | 1e (conformer 45) | 18    | 3.077535 | 0.456535 | 0.546162 |
| 53  | 1e (conformer 45) | 19    | 4.447066 | 0.587302 | 0.530284 |
| 54  | 1e (conformer 45) | 20    | 5.267564 | -0.481772 | 0.106696 |
| 55  | 1e (conformer 45) | 21    | 4.693238 | -1.666626 | -0.283436 |
| 56  | 1e (conformer 45) | 22    | 0.229582 | 1.264075 | -0.344327 |
| 57  | 1e (conformer 45) | 23    | 0.124737 | 2.620313 | 0.139660 |
| 58  | 1e (conformer 45) | 24    | 0.887544 | 3.478208 | -0.874928 |
| 59  | 1e (conformer 45) | 25    | -1.327207 | 3.059780 | 0.325793 |
| 60  | 1e (conformer 45) | 26    | 1.076849 | 4.938687 | -0.452542 |
| 61  | 1e (conformer 45) | 27    | -5.154090 | -1.007715 | -2.726810 |
| 62  | 1e (conformer 45) | 28    | -5.638245 | -1.325724 | -0.324980 |
| 63  | 1e (conformer 45) | 29    | -1.113770 | 0.091509 | -1.792838 |
| 64  | 1e (conformer 45) | 30    | -2.877420 | -0.306959 | -3.449268 |
| 65  | 1e (conformer 45) | 31    | -4.925997 | -1.311029 | 2.002992 |
| 66  | 1e (conformer 45) | 32    | -3.165453 | -0.951530 | 3.706778 |
| 67  | 1e (conformer 45) | 33    | -0.903165 | -0.241558 | 3.018721 |
| 68  | 1e (conformer 45) | 34    | 0.523422 | 0.579823 | 1.571453 |
| 69  | 1e (conformer 45) | 35    | -0.563662 | -2.331739 | -0.167432 |
| 70  | 1e (conformer 45) | 36    | 0.884751 | -4.175427 | -0.898865 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 37| 1 | 0 | 3.341846 | -3.883025 | -0.971915 |
| 38| 1 | 0 | 2.477538 | 1.294856 | 0.868870 |
| 39| 1 | 0 | 4.901259 | 1.520364 | 0.844322 |
| 40| 1 | 0 | 6.345108 | -0.364353 | 0.094565 |
| 41| 1 | 0 | 5.311639 | -2.497924 | -0.605433 |
| 42| 1 | 0 | 0.640958 | 2.676377 | 1.110205 |
| 43| 1 | 0 | 1.865418 | 3.013603 | -1.030175 |
| 44| 1 | 0 | 0.360843 | 3.430447 | -1.834799 |
| 45| 1 | 0 | -1.369315 | 4.090730 | -0.685669 |
| 46| 1 | 0 | -1.865999 | 3.002956 | 1.053039 |
| 47| 1 | 0 | 2.750878 | 2.955700 | 2.056396 |
| 48| 1 | 0 | 2.927762 | 3.149922 | 0.708578 |
| 49| 1 | 0 | 3.519759 | -2.265998 | -0.241342 |
| 50| 1 | 0 | 1.409680 | -0.985702 | 1.617944 |

**1e (conformer 46)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.750878 | -2.955700 | 2.056396 |
| 2 | 6 | 0 | 2.927762 | -3.149922 | 0.708578 |
| 3 | 6 | 0 | 2.349759 | -2.265998 | -0.241342 |
| 4 | 6 | 0 | 1.551928 | -1.162541 | 0.214176 |
| 5 | 6 | 0 | 1.409680 | -0.985702 | 1.617944 |
| 6 | 6 | 0 | 1.989871 | -1.855862 | 2.511465 |
| 7 | 6 | 0 | 2.566389 | -2.453638 | -1.632155 |
| 8 | 6 | 0 | 2.027329 | -1.581631 | -2.541585 |
| 9 | 6 | 0 | 1.230601 | -0.503305 | -2.095767 |
| 10| 6 | 0 | 0.962674 | -0.286798 | -0.759215 |
| 11| 6 | 0 | 0.850444 | 0.921225 | -0.394898 |
| 12| 6 | 0 | 1.198457 | 0.606044 | 0.384890 |
| 13| 6 | 0 | -2.258901 | -0.163106 | -0.204346 |
| 14| 6 | 0 | -1.371019 | 1.114448 | 1.655390 |
| 15| 6 | 0 | -2.537859 | 0.860995 | 2.410473 |
| 16| 6 | 0 | -3.548605 | 0.098724 | 1.885971 |
| 17| 6 | 0 | -3.440581 | -0.421924 | 0.570425 |
| 18| 6 | 0 | -2.223942 | -0.666560 | -1.534839 |
| 19| 6 | 0 | -3.269903 | -1.390453 | -2.058472 |
| 20| 6 | 0 | -4.418520 | -1.660463 | -1.282263 |
| 21| 6 | 0 | -4.497604 | -1.181947 | 0.002327 |
| 22| 8 | 0 | 0.810962 | 1.902889 | 0.337682 |
| 23| 6 | 0 | 1.775761 | 2.689535 | -0.408350 |
| 24| 6 | 0 | 1.458035 | 4.169208 | -0.176397 |
| 25| 6 | 0 | 3.191775 | 2.324666 | 0.029775 |
| 26| 6 | 0 | 0.089193 | 4.601611 | -0.705847 |
| 27| 1 | 0 | 3.199169 | -3.636074 | 2.771487 |
| 28| 1 | 0 | 3.521034 | -3.982763 | 0.345900 |
| 29| 1 | 0 | 0.848934 | -0.142312 | 1.988445 |
| 30| 1 | 0 | 1.865955 | -1.693801 | 3.576409 |
| 31| 1 | 0 | 3.172566 | -3.291869 | -1.958763 |
| 32| 1 | 0 | 2.202594 | -1.713183 | -3.603120 |
| 33| 1 | 0 | 0.810950 | 1.69615 | -2.836492 |
| 34| 1 | 0 | -0.226381 | 0.367003 | -1.348606 |
| 35| 1 | 0 | -0.588131 | 1.725353 | 2.082198 |
| 36| 1 | 0 | -2.622745 | 1.274433 | 3.409148 |
| 37| 1 | 0 | -4.446290 | -0.106780 | 2.459244 |
| 38| 1 | 0 | -1.360847 | -0.481003 | -2.156244 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 39 | 1 | 0 | -3.212185 | -1.756307 | -3.077468 |
| 40 | 1 | 0 | -5.234036 | -2.236558 | -1.704316 |
| 41 | 1 | 0 | -5.378759 | -1.371574 | 0.606360 |
| 42 | 1 | 0 | 1.657986 | 2.465001 | -1.475560 |
| 43 | 1 | 0 | 1.525012 | 4.368153 | 0.899532 |
| 44 | 1 | 0 | 2.245142 | 4.763378 | -0.653643 |
| 45 | 1 | 0 | 3.926799 | 2.924100 | -0.514607 |
| 46 | 1 | 0 | 3.180451 | 2.514770 | 1.099379 |
| 47 | 1 | 0 | 3.399605 | 1.270343 | -0.159084 |
| 48 | 1 | 0 | -0.943221 | 5.659224 | -0.499102 |
| 49 | 1 | 0 | -0.711243 | 4.024141 | -0.237707 |
| 50 | 1 | 0 | 0.020933 | 4.458104 | -1.788848 |

1e (conformer 79)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 1  | 6 | 0 | 4.847760 | -0.870983 | -1.268078 |
| 2  | 6 | 0 | 4.543832 | -1.617391 | -0.156145 |
| 3  | 6 | 0 | 3.286209 | -1.491274 | 0.491470 |
| 4  | 6 | 0 | 2.313049 | -0.570100 | -0.025039 |
| 5  | 6 | 0 | 2.669159 | 0.183618 | -1.77980 |
| 6  | 6 | 0 | 3.896781 | 0.038277 | -1.781676 |
| 7  | 6 | 0 | 2.981817 | -2.260651 | 1.644856 |
| 8  | 6 | 0 | 1.765373 | -2.131757 | 2.263398 |
| 9  | 6 | 0 | 0.801765 | -1.233188 | 1.753344 |
| 10 | 6 | 0 | 1.043918 | -0.459364 | 0.638424 |
| 11 | 6 | 0 | -0.004047 | 0.554922 | 0.168153 |
| 12 | 6 | 0 | -1.436549 | 0.120603 | 0.473728 |
| 13 | 6 | 0 | -2.076253 | -0.887982 | -0.319229 |
| 14 | 6 | 0 | -2.123864 | 0.692753 | 1.520804 |
| 15 | 6 | 0 | -3.449939 | 0.313292 | 1.831503 |
| 16 | 6 | 0 | -4.089391 | -0.642173 | 1.083849 |
| 17 | 6 | 0 | -3.424723 | -1.264003 | -0.006315 |
| 18 | 6 | 0 | -1.438818 | -1.540953 | -1.411058 |
| 19 | 6 | 0 | -2.093393 | -2.497931 | -2.151448 |
| 20 | 6 | 0 | -3.423649 | -2.860519 | -1.841886 |
| 21 | 6 | 0 | -4.070709 | -2.255102 | -0.792123 |
| 22 | 8 | 0 | 0.322505 | 1.806817 | 0.787660 |
| 23 | 6 | 0 | 0.328936 | 2.978883 | -0.056138 |
| 24 | 6 | 0 | -1.086791 | 3.430799 | -0.439451 |
| 25 | 6 | 0 | 1.114741 | 4.029367 | 0.718310 |
| 26 | 6 | 0 | -1.111698 | 4.582770 | -1.450930 |
| 27 | 1 | 0 | 5.811494 | -0.976451 | -1.752871 |
| 28 | 1 | 0 | 5.265094 | -2.319617 | 0.248474 |
| 29 | 1 | 0 | 1.966867 | 0.889290 | -1.600243 |
| 30 | 1 | 0 | 4.136419 | 0.627174 | -2.659795 |
| 31 | 1 | 0 | 3.728022 | -2.949802 | 2.025665 |
| 32 | 1 | 0 | 1.532210 | -2.718621 | 3.144527 |
| 33 | 1 | 0 | -0.154724 | -1.156157 | 2.255264 |
| 34 | 1 | 0 | 0.077853 | 0.673684 | -0.916420 |
| 35 | 1 | 0 | -1.633139 | 1.458422 | 2.106957 |
| 36 | 1 | 0 | -3.957227 | 0.787478 | 2.664203 |
| 37 | 1 | 0 | -5.108268 | -0.936264 | 1.312438 |
| 38 | 1 | 0 | -0.416339 | -1.293192 | -1.665923 |
| 39 | 1 | 0 | -1.584501 | -2.980306 | -2.978343 |
| 40 | 1 | 0 | -3.927907 | -3.616470 | -2.432973 |

S451
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 41 | 1 | 0 | -5.091226 | -2.528145 | -0.544774 |
| 42 | 1 | 0 | 0.874843 | 2.734274 | -0.978719 |
| 43 | 1 | 0 | -1.623819 | 2.577299 | -0.862940 |
| 44 | 1 | 0 | -1.623722 | 3.715813 | 0.471946 |
| 45 | 1 | 0 | 1.242688 | 4.938962 | 0.128596 |
| 46 | 1 | 0 | 0.592612 | 4.288534 | 1.643875 |
| 47 | 1 | 0 | 2.103649 | 3.644493 | -0.975137 |
| 48 | 1 | 0 | -2.138104 | 4.804566 | -1.753675 |
| 49 | 1 | 0 | -0.685447 | 5.500807 | -1.039285 |
| 50 | 1 | 0 | -0.548471 | 4.328214 | -2.354454 |

1e (conformer 81)

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1  | 6 | 0 | 4.149989 | -2.078554 | -1.832493 |
| 2  | 6 | 0 | 4.616538 | -1.331469 | -0.018798 |
| 3  | 6 | 0 | 3.742188 | -0.509285 | -0.364124 |
| 4  | 6 | 0 | 2.350545 | -0.455952 | -0.364124 |
| 5  | 6 | 0 | 1.904814 | -1.250978 | -0.128596 |
| 6  | 6 | 0 | 2.778680 | -2.037014 | 0.471946 |
| 7  | 6 | 0 | 4.220805 | 0.257392 | 1.076340 |
| 8  | 6 | 0 | 3.362176 | 1.047031 | 0.573485 |
| 9  | 6 | 0 | 1.992944 | 1.110879 | 0.482633 |
| 10 | 6 | 0 | 1.479715 | 0.380704 | -0.773838 |
| 11 | 6 | 0 | -0.007516 | 0.482633 | 0.062884 |
| 12 | 6 | 0 | -0.825417 | -0.694717 | 0.605318 |
| 13 | 6 | 0 | -2.083461 | -1.044936 | 0.006057 |
| 14 | 6 | 0 | -0.393119 | -1.396745 | 1.709730 |
| 15 | 6 | 0 | -1.159507 | -2.450048 | 2.270189 |
| 16 | 6 | 0 | -2.351434 | -2.806612 | 1.713598 |
| 17 | 6 | 0 | -2.846323 | -2.120367 | 0.573485 |
| 18 | 6 | 0 | -2.624923 | -0.380704 | -1.128921 |
| 19 | 6 | 0 | -3.832824 | -0.753873 | -1.671603 |
| 20 | 6 | 0 | -4.576413 | -1.815056 | -1.109322 |
| 21 | 6 | 0 | -4.089399 | -2.480744 | -0.011227 |
| 22 | 6 | 0 | -0.606031 | 1.677243 | 0.584919 |
| 23 | 6 | 0 | -0.751575 | 2.789244 | -0.324678 |
| 24 | 6 | 0 | -1.751962 | 3.727744 | 0.345121 |
| 25 | 6 | 0 | 0.580153 | 3.460644 | -0.656426 |
| 26 | 6 | 0 | -2.229788 | 4.884220 | -0.541211 |
| 27 | 6 | 0 | 4.828048 | -2.702051 | -2.403973 |
| 28 | 6 | 0 | 5.666832 | -1.359379 | -0.507554 |
| 29 | 6 | 0 | 0.858419 | -1.249796 | -1.734045 |
| 30 | 6 | 0 | 2.412950 | -2.632101 | -3.000759 |
| 31 | 6 | 0 | 5.274226 | 0.206635 | 1.330331 |
| 32 | 6 | 0 | 3.727920 | 1.631193 | 2.635003 |
| 33 | 6 | 0 | 1.326628 | 1.750168 | 2.017599 |
| 34 | 6 | 0 | -0.100260 | 0.501941 | -1.027724 |
| 35 | 6 | 0 | 0.554765 | -1.139393 | 2.164965 |
| 36 | 6 | 0 | -0.772149 | -2.972812 | 3.141009 |
| 37 | 6 | 0 | -2.940029 | -3.615218 | 2.133636 |
| 38 | 6 | 0 | -2.083052 | 0.437820 | -1.581956 |
| 39 | 6 | 0 | -4.218132 | -2.282229 | -2.537947 |
| 40 | 6 | 0 | -5.526892 | -2.099536 | -1.545913 |
| 41 | 6 | 0 | -4.650827 | -3.297498 | 0.430200 |
| 42 | 6 | 0 | -1.194521 | 2.411262 | -1.257745 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 43 | 1  | 0  | -2.617933 | 3.121401 | 0.645353 |
| 44 | 1  | 0  | -1.310540  | 4.117817  | 1.266284 |
| 45 | 1  | 0  | 1.043726   | 3.867736  | 0.246179 |
| 46 | 1  | 0  | 1.278626   | 2.757931  | -1.114468|
| 47 | 1  | 0  | 0.423543   | 4.278302  | -1.364413|
| 48 | 1  | 0  | -2.999873  | 5.466721  | -0.029446|
| 49 | 1  | 0  | -1.415607  | 5.567993  | -0.793419|
| 50 | 1  | 0  | -2.660866  | 4.516307  | -1.477528|
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