Supplementary Materials for

Michael Acceptors Tuned by the Pivotal Aromaticity of Histidine to Block COVID19 Activity

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Materials and Methods
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Computational details: All DFT static calculations were performed with the Gaussian 16 rev.a1 set of programs, using the B3LYP functional of Becke–Lee, Parr, and Yang, together with the Grimme D3 correction term to the electronic energy. The electronic configuration of the molecular systems for main-group atoms was described with the small split-valence basis set 3-21G(d) due to the size of the target species. The geometry optimizations were performed without symmetry constraints, and analytical frequency calculations were carried out for the characterization of the located stationary points. These frequencies were used to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects at 298.15 K. The pressure of 1354 atm was considered in our calculations based on the work of Martin et al., who determined that this pressure simulates the experimental density of liquid water for the ideal water gas including the deformations performed by the surrounding water solvent in aqueous media.

Energies were obtained by single-point calculations on the optimized geometries with the B3LYP-D3 functional and the 6-31G(d,p) basis set, and estimating solvent effects with the universal solvation model SMD of Cramer and Truhlar, using H2O as solvent. The reported free energies in this work include energies obtained at the B3LYP-D3/6-31G(d,p) level of theory corrected with zero-point energies, thermal corrections, and entropy effects evaluated at 298.15 K, achieved at the B3LYP-D3/3-21G(d) level. Tests with other functionals, and larger basis sets were carried out (see SI), with almost undistinguishable geometrical parameters.

Aromaticity was evaluated by means of the nucleus-independent chemical shift (NICS), proposed by Schleyer and coworkers, as a magnetic descriptor of aromaticity. NICS is defined as the negative value of the absolute magnetic shielding computed at a ring center or at any other interesting point of the system. Rings with large negative NICS values are considered as aromatic. NICS values were computed using the gauge-including atomic orbital method (GIAO). The magnetic shielding tensor was calculated for ghost atoms located at the center of the rings determined by the non-weighted mean of the heavy atoms coordinates. In this case, values close to 1 are indicative of aromatic structures, while values close to 0 indicate non-aromaticity.

Models preparation: The part of the X-Ray structures (space groups (C2 and P212121)) that is evaluated by DFT includes the whole inhibitor (82 atoms), and all the surrounding aminoacids (roughly 500 atoms in a range of 7-12 Å). The reliability and feasibility of the computational scheme used here is based on recent results, where systems of 500 atoms could generate kinetic and thermodynamic results with low quantitative errors for the Diels-Alder reaction.
to 162 is quite rigid. On the other hand, there would be His41, which is part of a helix, which is in a flexible region.

All in all, the analysis of the real systems was performed at 3 different levels, the first model including all the amino acid chains included in the 10 Å sphere. Unfortunately, this was unaffordable, not only because of the thermal corrections, but also because of the optimization of the geometry that entails the flexibility of the different parts between the chosen part of the M\textsuperscript{pro} and the inhibitor 13b. The second still included the entire inhibitor, but removes the fragments around histidine His41, further from the active site where C-S bond formation takes place. The third model is the same as the second model, but including His41, for its active role in the C-S bond formation. In fact, this third model can use the same energy reference as the second, simply by considering the group containing histidine His41.

Benchmark

Actually, the study on COVID started by a benchmark based on a further simplified fourth model, where the SH group was just linked to a methyl, and the keto of the amide group of the inhibitor 13b just surrounded by the CONH(CH\textsubscript{3}) moiety on one side and CH(CH\textsubscript{3})NHCO(CH\textsubscript{3}) on the other side. For the sake of consistency the most widely used functional ever was used, namely B3LYP of Becke and Perdew, and including the dispersion correction D3 by Grimme. The discrepancy between the most accurate basis sets, as well as taking into account the enormous size of the systems under study, had to be taken into account and given the corresponding weight. Solvent effects were also tested, including explicit and/or implicit models. Because water is the solvent, the use of explicit molecules that help proton transfers was mandatory.

The small models of the active center of M\textsuperscript{pro} with the inhibitor 13b, simplified or not, allowed to obtain the right image for this reference point of benchmark.

It is necessary to make the initial incision that all the energies discussed are made from the fragments separately as an energy reference, although the adducts or intermediates have also been calculated, but it has been used as a reference since in all cases they are energetically disadvantaged. However, in the case of where the activity is, it could be controversial which value would be the most real. But here it is mandatory the honesty, even if it was against the results presented, to take the values of the worst possible scenario. Therefore, one might think that the values for the energy barriers of the transition states, as well as the deprotonations, could be overestimated. However, free energies in solvent are calculated at P = 1354 atm to correct this overestimation, following the advice of Martin and coworkers.\textsuperscript{6}

Going to the 3 models, thus to the results that validate the conclusions of the manuscript, the addition of Michael, where the SH group interacted with the keto of the amide of inhibitor 13b was tested and with and without implicit solvent, and it was concluded that the results varied very slightly. And this then allowed the study of systems up to 500 atoms, which would not have been possible otherwise. In Table S1 it can be seen that the formation of the C-S bond requires only 1.7 kcal/mol less at P = 1 atm and even 1.1 kcal/mol more at P = 1354 atm, validating the convergence of values including implicit solvent effects in the geometry optimizations or not. Interestingly, explicit water molecules assistance did not affect much in geometry optimizations, and only in the transition state was the addition of one explicit water molecule favorable. In the other intermediates studied, the presence of water molecules did not imply additional stabilization, from a thermodynamic point of view.

The size of the calculation basis set was a major concern for this work, and although it started with the dual-polarization Def2SVP, it had to be switched to 3-21G(d) as the systems would not
have allowed to take into account all the agents discussed in the study, such as the histidine His41 of Mpro. The barrier of C-S bond formation through the addition of Michael meant a reduction of the barrier, specifically 1.7 kcal/mol. Therefore, although the chosen base, 3-21G(d) gives values close to larger entities. But also, emphasizing that the barriers arranged in the study may be slightly overestimated.

Characterization of the role of His41

The addition of the histidine His41 in the formation of the C-S bond, thanks to its potential role in deprotonating the thiol group was also relevant. Thermodynamically deprotonation of the thiol moiety in unfavorable by 42.1 and 43.3 kcal/mol by the model without or with the inhibitor 13b, respectively. However, these values decrease to 18.5 and 19.8 kcal/mol when the proton is caught by the nitrogen of the histidine. Bearing the negatively charged species once deprotonated the thiol group, here implicit solvent effects were also included in the geometry optimizations. And with just 8.1 kcal/mol it was possible to deprotonate the thiol group, whereas this was not feasible without those implicit solvent effects. Thus, this is a hint that the incapacity of using implicit solvent effects in the geometry optimizations underestimates the proton abstraction power of the histidine.

Focusing the study on the 5-membered ring of histidine His41, the 2 tautomers were studied, that is, with either of the two protonated nitrogen atoms, which turned out to be almost isoenergetic, as well as the possible proton migration between the two nitrogen atoms. With the help of a range of one to five water molecules it was found that this step was kinetically not that facile, with barriers of 46.1, 27.6, 19.7, 17.0 and 17.7 kcal/mol, respectively, in agreement with the work of Mo and coworkers, even requiring less kinetic effort. Even though this energy input is feasible, it is not easy for a chain of four water molecules to be placed between the histidine,17 the thiol moiety, and with the inhibitor in the area around.

But given the flexibility of rotation of the 5-membered ring of any histidine, with an energy barrier of 1.9 kcal/mol, it could be reoriented in the best way if there is enough space around it, which is the case given the maps stereos obtained with Cavallo's SambVca2.1 package.14 Following this argument, this change in the protonated nitrogen could be done by deprotonating the thiol group of the Mpro more feasibly. Without the role of the thiol group, the protonation of the two nitrogen atoms was found to be unfavorable and could not occur spontaneously. The required energy cost of the additional proton was 285.7 kcal/mol. This is not affordable taking into account any parametrized value for biological systems (262.2 kcal/mol).18,19 On the other hand, past calculations have a wide range from 250 to 273 kcal/mol. The latter values could be attainable.20 Moreover, a NICS analysis (see computational details) was performed (see Table S2).

The third model, with the C2 group space, with the thiol group in close proximity to the inhibitor, describes two possible intermediates, displayed in Fig. S1c and S1d. If the thiol group does not lose the proton, we have a possible intermediate, but if it establishes a H-bond with histidine, we have the most stable structure (see Fig. S1c). If then the proton of histidine would be in the other nitrogen with respect to the typical expected one we have an alternative intermediate just 0.5 kcal/mol higher in energy (see Fig. S1d). In both cases it is unexpected that histidine can capture the proton of the thiol group, kinetically requiring only 3.7 and 5.7 kcal/mol, respectively (see Fig. S1c and S1d). And what is more hopeful is that thermodynamically the resulting species is almost isoenergetic. Interestingly, the biprotonated structure with an H-bond with the anionic sulfur is 2.8 kcal/mol with the nitrogen atom farthest from the aminoacids chain of Mpro to which this 5-membered ring belongs. To point out that the reactant complex with both moieties, i.e.
inhibitor and the simplified Mpro is placed 3.3 kcal/mol above in energy (see Fig. S1a), therefore both species are interested in finding each other to get a H-bond.

In addition, Fig. S1e shows the expected structure after the C-S bond formation, with a H-bond between the oxygen atom of the hydroxyl and the NH moiety of the close His41, while Fig. S2f displays a more stable conformation by 7.7 kcal/mol, where there is a H-bond between the hydroxyl and the nitrogen without a proton of His41. Geometrically, by comparison with the corresponding X-Ray data (see Table S3), it is an evidence that the computed values in schemes e and f of Fig. S1 are feasible.

The analysis of the absolute and relative errors in Table S3 could lead to the conclusion that the protonation of the hydroxyl group goes along with the protonation of the NH group of His41 closer to it. However, the N···O distance is too short for systems where the NH fragment is the other, compared to X-ray structures. Therefore, in this study it is confirmed that the short piece of His41 it is not enough, specially for the latter protonation scheme of His41. Probably the most real scenario is that the 5-membered ring of the His41 rotates freely and this would explain why the C-N distances are almost identical for both nitrogen atoms, when only one is protonated.

The direct formation of the C-S bond, without deprotonation of the thiol group, using model 2, is displayed in Fig. S2. The reactant complex and the product are placed 19.2 and 24.0 kcal/mol below than the separated reactants, with a transition state that links them with an energy barrier of 36.1 kcal/mol. The latter energy barrier decreases by 9.0 kcal/mol when assisted with an explicit water molecule. Explicit water molecules can help in the kinetics here only, because thermodynamically they represent a destabilization of at least 6.1 kcal/mol for the intermediate and product.

In order to validate the results, calculations were also performed starting from the X-Ray with space group P2₁₂₁₂₁, for both protomers, A and B. For protomer A, with model 1, the reactant complex is 15.2 kcal/mol more stable than the two moieties separately. If it is checked the direct formation of the C-S bond between them, it is localized a transition state with an energy barrier of 32.5 kcal/mol, that decreases 7.1 kcal/mol assisted by an explicit water molecule. This means to proceed via a 6-membered transition state instead of a constrained 4-membered one. And the final product is placed 28.2 kcal/mol. Interestingly the latter product is 2.3 kcal/mol more stable again when the closest nitrogen of H41 assists with a H-bond with the hydroxyl group. For the sake of consistency, when freezing all heteroatoms, thus except for hydrogens, from the X-Ray geometry, this difference following the same trend is 1.3 kcal/mol. Switching to the more simplified model 2, the reactant complex is just 7.9 kcal/mol more stable, and the product 10.2 kcal/mol. And including the imidazole in model 3, from the reactant complex bearing the free pair of electrons of the N of the histidine closer to the thiol is favored by 3.0 kcal/mol. And for the corresponding product this difference is nearly identical, 2.2 kcal/mol (and freezing all atoms except for the hydrogens 2.8 kcal/mol). For the protomer B, neither significant trend nor energy difference were observed. And it was checked again for model 2 that the direct C-S bond formation assisted with a water molecule displays an energy barrier of 27.8 kcal/mol, which is not feasible at room temperature, and highly disfavored with respect to the deprotonation of the thiol by the imidazole group of His41.

Steric maps

To characterize the occupation around Cys145, using the sulfur as a center, steric maps were performed. The orientation for the steric map in Fig. 1g is plotted in Fig. S3 (the steric map is performed in the xy plane). Next, in Tables S4-S6 the steric maps together with the %V_{bur} values
are included (total and by quadrants). The analyses reveal that the reactive pocket must describe what is around the thiol group in a radius of at least 7 Å, and more detailed using 10 Å.

NCIplots
To highlight the role of stabilization between inhibitor 13b and Mpro, non-covalent interactions (NCI) are traced in Fig. S4, calculated using the NCIplot program developed by Contreras-Garcia and coworkers,\textsuperscript{21} on the optimized structure of the largest model of the X-ray structures, as well as the transition state leading to the formation of the C-S bond and the previous intermediate as well. The differences are very small, and there are basically favorable interactions where there are hydrogen bonds between the inhibitor 13b and Mpro. Fig. S4 shows the NCI plot for the structure corresponding to what the product would be for model 3 from the X-Ray with space group C2. Since it is difficult to distinguish which are the main interactions we can summarize basically from 13b with a quite long list of aminoacids from Mpro: Cys145, Asn142, Gly143, Phe140, His163, Glu166, Thr26, Gln189, His164, and Phe140. Of course for the calculated intermediates including His41 the favorable interactions with the thiol are particularly remarkable in the NCI plots.

Energy data and xyz coordinates
All xyz coordinates and absolute energy data of the computed geometry optimizations, and single point energy calculations in solvent, are included in Table S7.
Figure S1. Optimized structures mimicking the center of the X-Ray structures with space group C2 (main distances in Å; free energies referred to the separated species in kcal/mol; the structures are simplified for the sake of clarity) of (a) the interaction of the SH and imidazole of H41 of Mpro; (b) deprotonated thiol moiety; (c) and (d) deprotonation of the thiol by any of both N atoms of the imidazole; (e) product with a H-bond of the imidazole with the hydroxyl group; and (f) product with a H-bond of the hydroxyl with the free nitrogen atom of the imidazole.
**Figure S2.** Reaction profile of the direct C-S bond formation between inhibitor 13b and the thiol moiety for model 2 of X-Ray with space group C2 (free energies in kcal/mol; the structures are simplified for the sake of clarity).
Figure S3. Orientation of the x, y, z axes of the steric map of the active site in the crystallographic structure (space group C2) of the protease Mpro. On the z axis there is the sulfur atom of the glycine that bonds to 13b, the carbon atom of the carbonyl at the origin, while its oxygen atom is on the xz plane (in Å).
Figure S4. NCIplot of the model 3 from the X-Ray with space group C2 (left), detailed snapshot of the C-S bond (right). The isosurface represents a value of 0.4 with a color scale for the reduced density gradient from −0.05 (red) to 0.05 (blue).
**Table S1.** Interaction of the model system of the thiol moiety (CH$_3$-SH) of Mpro together with the inhibitor 13b, and the 5-membered ring of the histidine His41 (free energies in kcal/mol).

| Basis set | Geometry optimization | Single point energy calculation | Single point energy calculation |
|-----------|-----------------------|---------------------------------|---------------------------------|
|           | 3-21G(d)              | 6-31G(d,p)                       | Def2TZVP                        |
| Energy type | $E_{\text{gas}}$ | $G_{\text{gas}}$ | $E_{\text{solv}}$ | $G_{\text{solv}}$ | $E_{\text{solv}}$ | $G_{\text{solv}}$ |
| Separate reactants | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Reactant complex | -9.8 | -1.4 | -4.8 | 6.3 | 2.1 | -3.3 | 7.9 | 3.6 |
| Reactant complex + H$_2$O | -36.8 | -11.5 | -10.7 | 14.6 | 6.0 | -3.8 | 21.4 | 12.9 |
| Reactant complex + 2H$_2$O | -69.9 | -23.2 | -18.5 | 19.2 | 6.4 | -7.2 | 30.4 | 17.6 |
| TS | 29.2 | 40.1 | 34.7 | 45.6 | 41.4 | 37.1 | 48.0 | 43.8 |
| TS + H$_2$O | -20.7 | 3.6 | 8.7 | 33.1 | 24.6 | 17.4 | 41.8 | 33.2 |
| TS + 2H$_2$O | -58.3 | -20.3 | -2.8 | 35.2 | 22.4 | 11.5 | 49.5 | 36.7 |
| Product | -14.6 | 1.0 | -7.5 | 8.0 | 3.7 | -4.8 | 10.8 | 6.5 |
| Product + H$_2$O | -36.4 | -8.0 | -13.7 | 14.7 | 6.2 | -5.7 | 22.7 | 14.1 |
| Product + 2H$_2$O | -67.8 | -26.0 | -20.4 | 21.3 | 8.5 | -7.1 | 34.6 | 21.8 |
| Separate reactants$^a$ | 111.1 | 105.0 | 48.2 | 42.1 | 42.1 |
| Separate reactants$^b$ | 123.4 | 126.2 | 15.7 | 18.5 | 18.5 |
| Reactant complex$^a$ | 77.8 | 84.8 | 40.5 | 47.6 | 43.3 |
| Reactant complex$^b$ | 90.0 | 106.1 | 8.0 | 24.0 | 19.8 |

| Basis set | SVP | 6-31G(d,p) | Def2TZVP |
|-----------|-----|-----------|----------|
| Energy type | $E_{\text{gas}}$ | $G_{\text{gas}}$ | $E_{\text{solv}}$ | $G_{\text{solv}}$ | $E_{\text{solv}}$ | $G_{\text{solv}}$ |
| Separate reactants | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Reactant complex | -7.9 | 3.6 | -5.5 | 6.0 | 1.7 | -4.2 | 7.3 | 3.0 |
| Reactant complex + H$_2$O | -23.2 | 0.5 | -14.3 | 9.4 | 0.9 | -8.6 | 15.1 | 6.6 |
| TS | 30.7 | 41.8 | 35.8 | 46.9 | 42.6 | 39.5 | 50.6 | 46.3 |
| TS + H$_2$O | -0.7 | 23.3 | 7.5 | 31.5 | 22.9 | 16.6 | 40.6 | 32.0 |
| Product | -10.2 | 6.1 | -8.4 | 7.9 | 3.6 | -5.3 | 11.0 | 6.7 |
| Product + H$_2$O | -22.8 | 5.7 | -16.1 | 12.4 | 3.9 | -8.7 | 19.8 | 11.3 |

| Basis set | 3-21G(d) | 6-31G(d,p) | Def2TZVP |
|-----------|---------|-----------|----------|
| Energy type | $E_{\text{gas}}$ | $G_{\text{gas}}$ | $E_{\text{solv}}$ | $G_{\text{solv}}$ | $E_{\text{solv}}$ | $G_{\text{solv}}$ |
| Separate reactants | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Reactant complex | -9.4 | 2.1 | 5.9 | 5.9 | 1.6 | -4.1 | 7.5 | 3.2 |
| Reactant complex + H$_2$O | -31.6 | -7.3 | 12.2 | 12.2 | 9.2 | -5.2 | 19.0 | 16.0 |
| TS | 28.3 | 38.8 | 44.7 | 44.7 | 40.4 | 35.8 | 46.3 | 42.0 |
| TS + H$_2$O | -17.8 | 7.0 | 31.4 | 31.4 | 28.4 | 15.4 | 40.2 | 37.2 |
| Product | -15.3 | -0.6 | 5.7 | 5.7 | 1.5 | -6.4 | 8.3 | 4.0 |
| Product + H$_2$O | -34.3 | -6.8 | 13.3 | 13.3 | 10.3 | -6.2 | 21.3 | 18.3 |
| Separate reactants$^a$ | 49.6 | 43.8 | 42.4 | 42.4 | 42.4 |
| Separate reactants$^b$ | 12.2 | 15.0 | 18.3 | 18.3 | 18.3 |
| Reactant complex$^a$ | 31.4 | 38.1 | 42.8 | 42.8 | 38.5 |

(a) The thiol group is deprotonated; (b) using imidazole as proton acceptor
Table S2. NICS(0, 1 and -1)$_{iso}$ aromaticity results (in ppm) of the studied 5-membered ring of histidine His41. B3LYP-D3 was used for all calculations.

| Computational method | NICS(0) | NICS(1) | NICS(-1) |
|----------------------|---------|---------|----------|
| ![Diagram](image1.png) | -12.65  | -11.53  | -11.53   |
| ![Diagram](image2.png) | -13.08  | -10.98  | -10.98   |
| ![Diagram](image3.png) | -11.53  | -9.73   | -9.74    |
| ![Diagram](image4.png) | -13.08  | -10.98  | -10.98   |
| ![Diagram](image5.png) | -11.77  | -9.83   | -9.83    |
| ![Diagram](image6.png) | -13.15  | -10.86  | -10.86   |
| ![Diagram](image7.png) | -14.22  | -10.34  | -10.34   |
| ![Diagram](image8.png) | -13.17  | -9.47   | -9.47    |
| ![Diagram](image9.png) | -11.75  | -9.84   | -9.84    |

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Table S3. Comparison of the imidazole for the computed models and X-Ray data (in Å).

| Computational model | Protonation product scheme | Model 2 | Model 1 | X-Ray |
|---------------------|---------------------------|---------|---------|-------|
|                     |                           | C2      | C2      | prot A | prot A | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prote | peptide | section | and | its | consequences. | 

| Computational model | Protonation product scheme | Model 2 | Model 1 | X-Ray |
|---------------------|---------------------------|---------|---------|-------|
|                     |                           | C2      | C2      | prot A | prot A | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prot A | prot A | prot B | prot B | prote | peptide | section | and | its | consequences.
Table S4. Steric maps of the active site in the crystallographic structure (space group C2) of the protease M<sub>pro</sub>.

| C2     | Total | Quadrant | V<sub>f</sub> | V<sub>b</sub> | V<sub>t</sub> | %V<sub>f</sub> | %V<sub>b</sub> |
|--------|-------|----------|--------------|--------------|--------------|---------------|---------------|
| 3.5 Å  | 33.4% | SW       | 30.6         | 14.3         | 44.9         | 68.1          | 31.9          |
|        |       | NW       | 34.9         | 9.9          | 44.9         | 77.8          | 22.2          |
|        |       | NE       | 26.9         | 17.9         | 44.9         | 60.1          | 39.9          |
|        |       | SE       | 27.1         | 17.8         | 44.9         | 60.4          | 39.6          |
| 5.0 Å  | 38.7% | SW       | 64.4         | 66.4         | 130.8        | 49.3          | 50.7          |
|        |       | NW       | 100.6        | 30.2         | 130.8        | 76.9          | 23.1          |
|        |       | NE       | 78.7         | 52.1         | 130.8        | 60.2          | 39.8          |
|        |       | SE       | 76.8         | 54.0         | 130.8        | 58.7          | 41.3          |
| 7.0 Å  | 47.8% | SW       | 127.3        | 231.7        | 359.1        | 35.5          | 64.5          |
|        |       | NW       | 216.7        | 142.4        | 359.1        | 60.4          | 39.6          |
|        |       | NE       | 226.6        | 132.4        | 359.1        | 63.1          | 36.9          |
|        |       | SE       | 179.2        | 179.8        | 359.1        | 49.9          | 50.1          |
| 10.0 Å | 53.6% | SW       | 454.3        | 592.7        | 1046.9       | 43.4          | 56.6          |
|        |       | NW       | 525.1        | 521.9        | 1046.9       | 50.2          | 49.8          |
|        |       | NE       | 559.1        | 487.8        | 1046.9       | 53.4          | 46.6          |
|        |       | SE       | 403.6        | 643.4        | 1046.9       | 38.5          | 61.5          |
Table S5. Steric map of the active site in the crystallographic structure (protomer A, space group P2₁₂₁) of the protease M_pro.

| P2₁₂₁₂₁ (Å) | Total   | Quadrant | V_f | V_b | V_t | %V_f | %V_b |
|--------------|---------|----------|-----|-----|-----|-------|-------|
| 3.5 Å        | 31.6%   | SW       | 31.8| 13.1| 44.9| 70.8  | 29.2  |
|              |         | NW       | 34.2| 10.7| 44.9| 76.2  | 23.8  |
|              |         | NE       | 27.4| 17.5| 44.9| 61.0  | 39.0  |
|              |         | SE       | 29.4| 15.5| 44.9| 65.4  | 34.6  |
| 5.0 Å        | 36.9%   | SW       | 66.7| 64.2| 130.8| 51.0 | 49.0  |
|              |         | NW       | 98.6| 32.2| 130.8| 75.4 | 24.6  |
|              |         | NE       | 80.0| 50.8| 130.8| 61.2 | 38.8  |
|              |         | SE       | 84.9| 45.9| 130.8| 64.9 | 35.1  |
| 7.0 Å        | 46.6%   | SW       | 117.2| 241.9| 359.1| 32.6 | 67.4  |
|              |         | NW       | 223.0| 136.0| 359.1| 62.1 | 37.9  |
|              |         | NE       | 227.7| 131.3| 359.1| 63.4 | 36.6  |
|              |         | SE       | 199.4| 159.7| 359.1| 55.5 | 44.5  |
| 10.0 Å       | 52.4%   | SW       | 413.9| 633.1| 1046.9| 39.5 | 60.5  |
|              |         | NW       | 553.6| 493.4| 1046.9| 52.9 | 47.1  |
|              |         | NE       | 571.4| 475.6| 1046.9| 54.6 | 45.4  |
|              |         | SE       | 453.6| 593.4| 1046.9| 43.3 | 56.7  |
**Table S6.** Steric map of the active site in the crystallographic structure (protomer B, space group P2\(_1\)2\(_1\)2\(_1\)) of the protease M\(^{\text{pro}}\).

| Quadrant | Vf  | Vb  | Vt  | %Vf | %Vb |
|----------|-----|-----|-----|-----|-----|
| SW       | 31.3| 13.5| 44.9| 69.8| 30.2|
| NW       | 35.2| 9.7 | 44.9| 78.5| 21.5|
| NE       | 27.7| 17.2| 44.9| 61.6| 38.4|
| SE       | 28.3| 16.5| 44.9| 63.2| 36.8|
| NW       | 35.2| 9.7 | 44.9| 78.5| 21.5|
| NE       | 27.7| 17.2| 44.9| 61.6| 38.4|
| SE       | 28.3| 16.5| 44.9| 63.2| 36.8|

**3.5 Å**

| Quadrant | Vf  | Vb  | Vt  | %Vf | %Vb |
|----------|-----|-----|-----|-----|-----|
| SW       | 69.9| 60.9| 130.8| 53.5| 46.5|
| NW       | 103.3| 27.5| 130.8| 78.9| 21.1|
| NE       | 78.9| 51.9| 130.8| 60.3| 39.7|
| SE       | 79.9| 50.9| 130.8| 61.1| 38.9|

**5.0 Å**

| Quadrant | Vf  | Vb  | Vt  | %Vf | %Vb |
|----------|-----|-----|-----|-----|-----|
| SW       | 131.9| 227.1| 359.1| 36.7| 63.3|
| NW       | 228.6| 130.4| 359.1| 63.7| 36.3|
| NE       | 220.4| 138.7| 359.1| 61.4| 38.6|
| SE       | 180.7| 178.3| 359.1| 50.3| 49.7|

**7.0 Å**

| Quadrant | Vf  | Vb  | Vt  | %Vf | %Vb |
|----------|-----|-----|-----|-----|-----|
| SW       | 451.5| 595.5| 1046.9| 43.1| 56.9|
| NW       | 552.7| 494.3| 1046.9| 52.8| 47.2|
| NE       | 573.0| 473.9| 1046.9| 54.7| 45.3|
| SE       | 394.6| 652.4| 1046.9| 37.7| 62.3|

**10.0 Å**
Table S7. Cartesian coordinates and energy data of DFT-optimized structures (selected distances in Å), absolute gas and solvent phase energy values (in a.u.).

| Structure | Zero-point correction | Thermal correction to Energy | Thermal correction to Enthalpy | Thermal correction to Gibbs Free Energy | Sum of electronic and zero-point Energies | Sum of electronic and thermal Energies | Sum of electronic and thermal Enthalpies | Sum of electronic and thermal Free Energies | SOLVENT |
|---|---|---|---|---|---|---|---|---|---|
| CH$_3$SH | 0.046594 (Hartree/Particle) | 0.050189 | 0.051133 | 0.022349 | -436.584103 | -436.580508 | -436.579564 | -436.608348 | -438.7084419 |
| 13b (simplified) | 0.197873 (Hartree/Particle) | 0.211235 | 0.212179 | 0.157376 | -605.654794 | -605.641432 | -605.640488 | -605.695291 | -609.2334273 |
| CH$_3$SH + 13b(simplified) reactant complex | 0.246368 (Hartree/Particle) | 0.264825 | 0.265769 | 0.197504 | -1042.252588 | -1042.243131 | -1042.233187 | -1042.301453 | -1047.9495377 |
| H | 0.022383 | -1.424798 | 1.311740 |
| H | -0.658244 | -1.870302 | -0.279675 |
| H | 1.802812 | 2.066580 | -1.149690 |
| H | 3.412467 | 1.721284 | 1.362109 |
| H | 4.211724 | 1.645308 | -0.232321 |
| H | 2.699337 | -0.468403 | -1.264644 |
| H | 2.790465 | -2.940820 | 0.943143 |
| H | -1.718890 | -1.818656 | 1.171108 |
| H | -5.745212 | -0.153876 | -0.306857 |
| H | -4.874453 | 1.154955 | -1.156618 |
| H | 3.532928 | 3.190614 | 0.352488 |

**CH$_3$SH + 13b(simplified) + H$_2$O reactant complex**

| Energy correction | 0.271581 (Hartree/Particle) |
| Thermal correction to Energy | 0.291965 |
| Thermal correction to Enthalpy | 0.292910 |
| Thermal correction to Gibbs Free Energy | 0.221910 |
| Sum of electronic and zero-point Energies | -1118.244365 |
| Sum of electronic and thermal Energies | -1118.223981 |
| Sum of electronic and thermal Enthalpies | -1118.223037 |
| Sum of electronic and thermal Free Energies | -1118.294037 |
| SOLVENT: -1124.3894646 |

| CH$_3$SH + 13b(simplified) transition state |
| Energy correction | 0.242846 (Hartree/Particle) |
| Thermal correction to Energy | 0.260069 |
| Thermal correction to Enthalpy | 0.261013 |
| Thermal correction to Gibbs Free Energy | 0.197108 |
| Sum of electronic and zero-point Energies | -1042.194059 |
| Sum of electronic and thermal Energies | -1042.176836 |
| Sum of electronic and thermal Enthalpies | -1042.175892 |
| Sum of electronic and thermal Free Energies | -1042.239798 |
| SOLVENT: -1047.8865328 |
### CH$_3$SH + 13b(simplified) + H$_2$O transition state

| H      | 0.428364 | 1.636612 | 2.080829 |
|--------|----------|----------|----------|
| H      | -1.522980| -1.454668| -1.504629|
| H      | -3.816337| -1.705282| 0.425227 |
| H      | -4.121880| -1.461992| -1.319122|
| H      | -2.941410| 2.958003 | -0.497686|
| H      | 1.343486 | 0.471126 | 3.080829 |
| H      | 4.859926 | -0.509036| -1.308500|
| H      | 3.657886 | 0.683940 |-1.864926 |
| H      | -3.440037| -3.006892| -0.739191|
| H      | -0.287974| 0.758408 | -1.580045|

Zero-point correction= 0.268274 (Hartree/Particle)
Thermal correction to Energy= 0.287230
Thermal correction to Enthalpy= 0.288175
Thermal correction to Gibbs Free Energy= 0.220558
Sum of electronic and zero-point Energies= -1118.222132
Sum of electronic and thermal Energies= -1118.203176
Sum of electronic and thermal Enthalpies= -1118.202231
Sum of electronic and thermal Free Energies= -1118.269848

SOLVENT: -1124.3585618

### CH$_3$SH + 13b(simplified) product

| H      | 0.428364 | 1.636612 | 2.080928 |
|--------|----------|----------|----------|
| H      | -1.522980| -1.454668| -1.504629|
| H      | -3.816337| -1.705282| 0.425227 |
| H      | -4.121880| -1.461992| -1.319122|
| H      | -2.941410| 2.958003 | -0.497686|
| H      | 1.343486 | 0.471126 | 3.080829 |
| H      | 4.859926 | -0.509036| -1.308500|
| H      | 3.657886 | 0.683940 |-1.864926 |
| H      | -3.440037| -3.006892| -0.739191|
| H      | -0.287974| 0.758408 | -1.580045|

Zero-point correction= 0.249779 (Hartree/Particle)
Thermal correction to Energy= 0.266737
Thermal correction to Enthalpy= 0.267682
Thermal correction to Gibbs Free Energy= 0.204496
Sum of electronic and zero-point Energies= -1118.256820
Sum of electronic and thermal Energies= -1118.239862
Sum of electronic and thermal Enthalpies= -1118.238917
Sum of electronic and thermal Free Energies= -1118.302103

SOLVENT: -1047.9538974
### CH₃SH + 13b(simplified) + H₂O product

Zero-point correction = 0.274486 (Hartree/Particle)
Thermal correction to Energy = 0.293828
Thermal correction to Enthalpy = 0.294772
Thermal correction to Gibbs Free Energy = 0.227018

Sum of electronic and zero-point Energies = -1118.240934
Sum of electronic and thermal Energies = -1118.221592
Sum of electronic and thermal Enthalpies = -1118.220647
Sum of electronic and thermal Free Energies = -1118.288401

SOLVENT: -1124.3943345

13SimpliPROD+H₂Og SCF Done: -1118.51541945 A.U.

### CH₃SH + 13b(simplified) + 2H₂O product

Zero-point correction = 0.296114 (Hartree/Particle)
Thermal correction to Energy = 0.318658
Thermal correction to Enthalpy = 0.319602

Thermal correction to Gibbs Free Energy = 0.243698

Sum of electronic and zero-point Energies = -1194.232270
Sum of electronic and thermal Energies = -1194.209727
Sum of electronic and thermal Enthalpies = -1194.208783
Sum of electronic and thermal Free Energies = -1194.284687

SOLVENT: -1200.8325127
### CH$_3$SH + 13b(simplified) + 2H$_2$O transition state

| Atom | x   | y   | z   |
|------|-----|-----|-----|
| H    | -1.261314 | -1.835741 | 0.555971 |
| H    | -2.419163 | -0.244425 | 2.823168 |
| H    | -3.458381 | -0.914505 | 1.543040 |
| H    | -0.270483 | -2.088695 | -0.999988 |
| H    | -2.820343 | 3.216694  | -0.320044 |
| H    | 1.854698  | 3.209279  | 0.079085  |
| H    | 5.350553  | -1.444668 | -0.365899 |
| H    | 4.443575  | -0.957979 | -1.822485 |
| H    | -2.600790 | -2.018880 | 2.658996  |
| O    | -1.043077 | -2.764965 | -0.904108 |
| H    | -0.700521 | -3.691945 | -0.930561 |
| H    | -2.445153 | -2.101008 | -1.314157 |
| H    | -2.584304 | 0.050965  | -1.372586 |
| O    | -3.257727 | -1.483174 | -1.372586 |
| O    | -3.792861 | -1.638957 | -0.552209 |

Zero-point correction: 0.293424 (Hartree/Particle)
Thermal correction to Energy: 0.314123
Thermal correction to Enthalpy: 0.315068
Thermal correction to Gibbs Free Energy: 0.244264
Sum of electronic and zero-point Energies: -1194.230801
Sum of electronic and thermal Energies: -1194.210102
Sum of electronic and thermal Enthalpies: -1194.209157
Sum of electronic and thermal Free Energies: -1194.279961

SOLVENT: -1200.807527

### CH$_3$SH + 13b(simplified) + 2H$_2$O product

| Atom | x   | y   | z   |
|------|-----|-----|-----|
| C    | -1.709904 | 2.441517 | -1.214311 |
| S    | -0.600536 | 1.048494 | -1.671230 |
| H    | -2.639941 | 2.389507 | -1.787880 |
| H    | -1.921188 | 2.380717 | -0.140964 |
| C    | 4.237040  | -0.897627 | -0.967151 |
| C    | 3.339514  | -0.879627 | -0.967151 |
| O    | 3.396649  | -0.970033 | 1.327431 |
| N    | 2.459257  | 0.521742  | -0.118889 |
| C    | 1.355515  | 0.840769  | 0.784676 |
| C    | 1.138321  | 2.565111  | 0.855493 |
| O    | 0.482645  | -1.233791 | -0.026428 |
| C    | -1.679565 | 0.193252  | 1.119277 |
| O    | -1.450324 | 1.302587  | 1.630973 |
| N    | -2.020066 | -0.872145 | 1.168778 |
| C    | -3.289476 | -0.760708 | 1.984503 |
| H    | 5.005858  | -1.574418 | -0.594002 |
| H    | 2.346525  | 0.822043  | -1.083393 |
| H    | 1.680607  | 0.455659  | 1.762560 |
| H    | 0.297227  | 2.584452  | 1.505050 |
| H    | 0.930149  | 2.748134  | -0.144420 |
| H    | -1.766375 | -1.776024 | 0.761688 |
| H    | -3.303904 | -1.438795 | 2.764447 |
| H    | -3.364760 | 0.279396  | 2.251869 |
| H    | -0.394556 | -2.154531 | -0.428466 |
| H    | -1.206715 | 3.871934  | -1.429916 |
| H    | 2.057104  | 2.816498  | 1.230015 |
| H    | 3.633758  | -1.413429 | -1.723835 |
| H    | 4.703316  | -0.220001 | -1.431152 |
| H    | -4.143105 | -0.995119 | 1.256539 |
| O    | -1.291522 | -2.768420 | -0.688409 |
| O    | -1.098200 | -3.705111 | -0.929398 |
| C    | -2.505143 | -1.952665 | -1.420531 |
| H    | -1.777896 | -0.153759 | -1.832411 |
| H    | -2.583587 | -1.045794 | -1.812914 |
| H    | -3.271743 | -0.786870 | -1.146565 |

Zero-point correction: 0.299430 (Hartree/Particle)
Thermal correction to Energy: 0.314123
Thermal correction to Enthalpy: 0.315068
Thermal correction to Gibbs Free Energy: 0.250200
Sum of electronic and zero-point Energies: -1194.239885
Sum of electronic and thermal Energies: -1194.218743
Sum of electronic and thermal Enthalpies: -1194.217799
Sum of electronic and thermal Free Energies: -1194.289115

SOLVENT: -1200.835619
### CH$_3$S$^-$

| Atom | x  | y  | z  |
|------|----|----|----|
| C    | -1.17633 | 0.228777 | 1.021522 |
| O    | -1.477957 | 1.300233 | 1.603772 |
| N    | -1.918851 | -0.904831 | 1.148593 |
| C    | -3.029948 | -0.949241 | 2.117504 |
| H    | 4.669674 | -0.271840 | -1.331643 |
| H    | 2.481881 | 0.829080 | -1.005253 |
| H    | 1.454098 | 0.260734 | 1.693499 |
| H    | 0.337289 | 2.561798 | 1.547478 |
| H    | 1.230102 | 2.843072 | 0.030009 |
| H    | -1.664691 | -1.767335 | 0.649871 |
| H    | -3.199418 | 0.073304 | 2.458641 |
| H    | -3.935896 | -1.344290 | 1.645609 |
| H    | -0.305868 | -1.752747 | -0.668731 |
| H    | -0.639759 | 3.468526 | -1.231928 |
| H    | 2.129387 | 2.618975 | 1.540941 |
| H    | 4.797618 | -1.874877 | -0.545186 |
| H    | 3.475670 | -1.541776 | -1.697469 |
| H    | -2.772382 | -1.579638 | 2.975403 |
| O    | -1.517117 | -2.617869 | -0.908604 |
| H    | -1.438886 | -3.517358 | -1.306593 |
| H    | -2.215450 | -1.986683 | -1.396945 |
| H    | -2.216206 | -0.113223 | -1.921040 |
| H    | -0.969182 | -0.771884 | -1.726476 |
| H    | -3.311267 | -0.494444 | -0.833065 |

#### CH$_3$S$^-$ + 13b(simplified) reactant complex

| Atom | x  | y  | z  |
|------|----|----|----|
| C    | 2.149400 | -2.390652 | -0.151500 |
| S    | 1.330069 | -1.298177 | -1.381971 |
| H    | 3.116109 | -2.748491 | -0.530899 |
| C    | 2.323510 | -1.807507 | 0.763786 |
| C    | 4.391999 | 0.563536 | -0.982912 |
| C    | 3.398918 | 0.180913 | 0.132151 |
| O    | 3.776537 | -0.293454 | 1.225500 |
| N    | -2.112162 | 0.394216 | -0.212521 |
| C    | -0.956017 | 0.118060 | 0.651855 |
| O    | -0.870125 | -1.349756 | 1.085876 |
| C    | 0.246736 | 0.691681 | -0.138808 |

### H$_2$O

| Atom | x  | y  | z  |
|------|----|----|----|
| H    | 0.000000 | 0.784895 | -0.491722 |
| O    | 0.000000 | 0.000000 | 0.122931 |
| H    | 0.000000 | -0.784895 | -0.491722 |

#### H$_2$O + 13b(simplified) reactant complex

| Atom | x  | y  | z  |
|------|----|----|----|
| C    | 2.149400 | -2.390652 | -0.151500 |
| S    | 1.330069 | -1.298177 | -1.381971 |
| H    | 3.116109 | -2.748491 | -0.530899 |
| C    | 2.323510 | -1.807507 | 0.763786 |
| C    | 4.391999 | 0.563536 | -0.982912 |
| C    | 3.398918 | 0.180913 | 0.132151 |
| O    | 3.776537 | -0.293454 | 1.225500 |
| N    | -2.112162 | 0.394216 | -0.212521 |
| C    | -0.956017 | 0.118060 | 0.651855 |
| O    | -0.870125 | -1.349756 | 1.085876 |
| C    | 0.246736 | 0.691681 | -0.138808 |
### CH$_3$S$^-$ + 13b(simplified) + H$_2$O reactant complex

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| O    | 0.024869 | 1.497840 | -1.098105|
| C    | 1.567733 | 0.706963 | 0.584871 |
| O    | 1.811689 | 0.080497 | 1.648772 |
| N    | 2.453191 | 1.563163 | -0.019801|
| C    | 3.876840 | 1.459945 | 0.272725 |
| H    | -4.281699| -0.125463| -1.828069|
| H    | -1.818908| 0.889057 | 1.562481 |
| H    | -1.033150| 0.737122 | 1.562481 |
| H    | 0.016666 | -1.463594| 1.709492 |
| H    | -0.768849| -1.969046| 0.193415 |
| H    | 2.119831 | 1.910378 | -0.917962|
| H    | 3.950473 | 0.959575 | 1.242666 |
| H    | 4.400648 | 0.848290 | -0.476643|
| H    | 1.527839 | -3.256992| 0.104263 |
| H    | -1.782338| -1.593464| 1.636757 |
| H    | -5.403810| 0.491106 | -0.581339|

Zero-point correction= 0.260561 (Hartree/Particle)  
Thermal correction to Energy= 0.279901  
Thermal correction to Enthalpy= 0.280846  
Thermal correction to Gibbs Free Energy= 0.212577

Sum of electronic and zero-point Energies= -1117.712834  
Sum of electronic and thermal Energies= -1117.693493  
Sum of electronic and thermal Enthalpies= -1117.692549  
Sum of electronic and thermal Free Energies= -1117.760818

SOLVENT: -1123.909065

### CH$_3$S$^-$ + 13b(simplified) reactant complex (isomer)

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| O    | 1.895654 | -1.678150| 1.791576 |
| S    | -0.591860| -2.660265| 0.394238 |
| H    | 0.571907 | -2.336033| 2.551190 |
| C    | -3.925361| -0.638070| -0.244070|
| C    | -3.034400| 0.608091 | -0.203135|
| O    | -3.476426| 1.778430 | -0.131592|
| N    | -1.712318| 0.316877 | -0.272290|
| C    | -0.724055| 1.404187 | -0.208813|
| C    | -0.612040| 1.960030 | 1.227448 |
| O    | 0.131437 | -1.678150| 1.791576 |
| C    | 3.876840 | 1.459945 | 0.272725 |
| H    | -4.281699| -0.125463| -1.828069|
| H    | -1.818908| 0.889057 | 1.562481 |
| H    | -1.033150| 0.737122 | 1.562481 |
| H    | 0.016666 | -1.463594| 1.709492 |
| H    | -0.768849| -1.969046| 0.193415 |
| H    | 2.119831 | 1.910378 | -0.917962|
| H    | 3.950473 | 0.959575 | 1.242666 |
| H    | 4.400648 | 0.848290 | -0.476643|
| H    | 1.527839 | -3.256992| 0.104263 |
| H    | -1.782338| -1.593464| 1.636757 |
| H    | -5.403810| 0.491106 | -0.581339|

Zero-point correction= 0.236400 (Hartree/Particle)  
Thermal correction to Energy= 0.253289  
Thermal correction to Enthalpy= 0.254233  
Thermal correction to Gibbs Free Energy= 0.191202

Sum of electronic and zero-point Energies= -1117.712834  
Sum of electronic and thermal Energies= -1117.712834  
Sum of electronic and thermal Enthalpies= -1117.712834  
Sum of electronic and thermal Free Energies= -1117.712834

SOLVENT: -1123.909065

### CH$_3$S$^-$ + 13b(simplified) proct reactant complex

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | -0.114950| 2.694809 | 0.040518 |
| S    | -0.519454| 1.540712 | 1.394917 |
| H    | 0.768763 | 3.305003 | 0.269544 |
| O    | 0.103438 | 2.062998 | -0.841925|
| C    | 0.597679 | 0.866977 | -0.683090|
| C    | 1.808927 | -0.436768| -0.512920|
| O    | -2.504331| -0.775166| -0.519813|
| C    | 0.180564 | 1.223673 | -0.155223|
| C    | 2.105962 | 2.777246 | 0.291652 |
| C    | -0.563222| 0.845115 | -0.816012|
| O    | 0.051191 | 0.218783 | -1.344696|
| C    | -0.008694| -0.208694| -1.225655|
| H    | 2.241267 | -2.465772| -0.654773|

Zero-point correction= 0.260561 (Hartree/Particle)  
Thermal correction to Energy= 0.292201  
Thermal correction to Enthalpy= 0.283246  
Thermal correction to Gibbs Free Energy= 0.214281

Sum of electronic and zero-point Energies= -1117.712834  
Sum of electronic and thermal Energies= -1117.712834  
Sum of electronic and thermal Enthalpies= -1117.712834  
Sum of electronic and thermal Free Energies= -1117.712834

SOLVENT: -1123.909065
### CH$_3$SH + H$_4$Imidazole

Zero-point correction= 0.147938 (Hartree/Particle)
Thermal correction to Energy= 0.158322
Thermal correction to Enthalpy= 0.159266
Thermal correction to Gibbs Free Energy= 0.109274
Sum of electronic and zero-point Energies= -700.570915
Sum of electronic and thermal Energies= -700.560531
Sum of electronic and thermal Enthalpies= -700.559587
Sum of electronic and thermal Free Energies= -700.609579

SOLVENT: -704.276925

### CH$_3$SH + 13b(simplified) + H$_4$Imidazole reactant complex

Zero-point correction= 0.347767 (Hartree/Particle)
Thermal correction to Energy= 0.373048
Thermal correction to Enthalpy= 0.373948
Thermal correction to Gibbs Free Energy= 0.288762
Sum of electronic and zero-point Energies= -1306.258223
Sum of electronic and thermal Energies= -1306.232986
Sum of electronic and thermal Enthalpies= -1306.232042
Sum of electronic and thermal Free Energies= -1306.317228

SOLVENT: -1313.528189
### CH₃SH + 13b(simplified) + H₄₁imidazole product

| Bond          | Energy (hartree) | Atomic Number | X  | Y  | Z  |
|---------------|------------------|---------------|----|----|----|
| C-C           | 0.351636         | 3             | 0.803334 | 2.712450 | -1.602667 |
| S-S           | 0.376005         | 3             | 0.657135 | 0.877626 | -1.717961 |
| H-H           |                  | 3             | 0.214910 | 3.130732 | -2.425101 |
| C-C           | -1306.261988     | 3             | 4.692598 | -2.385382 | -0.808806 |
| O-H           |                  | 3             | 4.945231 | 0.643596 | 0.880598 |
| N-C           |                  | 3             | 2.905221 | 1.401569 | 0.237628 |
| C-O           |                  | 3             | -0.150029 | 0.944392 | 1.039877 |
| O-H           |                  | 3             | -0.248580 | 2.187093 | 1.136903 |
| N-C           |                  | 3             | -0.285695 | 0.062424 | 1.871076 |
| C-C           | -1306.238563     | 3             | 4.575460 | -2.139700 | -1.869843 |
| O-H           |                  | 3             | 2.284689 | -1.515683 | -0.674055 |
| N-C           |                  | 3             | 2.048879 | -0.232900 | 1.645967 |
| C-C           | -1306.237619     | 3             | 2.253462 | 2.292799 | 1.108534 |
| O-H           |                  | 3             | 3.114494 | 1.782504 | -0.392707 |
| N-C           |                  | 3             | -0.599740 | -0.916977 | 1.648394 |
| C-C           | -1306.317051     | 3             | -1.677837 | 1.587353 | 2.907411 |
| O-H           |                  | 3             | -2.704214 | 0.137802 | 2.695422 |
| N-C           |                  | 3             | -0.667900 | -1.184400 | -0.480042 |
| C-C           | -1313.528152     | 3             | 1.842507 | 3.032061 | 1.694456 |
| O-H           |                  | 3             | 3.853840 | 1.364646 | 1.168941 |
| N-C           |                  | 3             | 5.743520 | -2.570023 | -0.585247 |
| C-C           | -1306.61362425   | 3             | 4.108368 | -3.288547 | -0.596404 |
| O-H           |                  | 3             | -1.379103 | 0.129771 | 3.896313 |
| N-C           |                  | 3             | -5.858100 | -1.133231 | 0.129765 |
| C-C           | -1306.737094     | 3             | -4.470877 | -0.881696 | -0.284584 |
| O-H           |                  | 3             | -0.646855 | 0.254691 | -0.991955 |
| N-C           |                  | 3             | -2.712277 | 0.171531 | -1.215026 |
| C-C           | -76.337094       | 3             | -2.238024 | -0.955522 | -0.689701 |
| O-H           |                  | 3             | -3.225398 | -1.619190 | -1.08538 |
| N-C           |                  | 3             | -5.943976 | -2.079397 | 0.673939 |
| C-C           | -76.334258       | 3             | -6.256971 | -0.337879 | 0.787612 |
| O-H           |                  | 3             | -2.131390 | 0.913163 | -1.712187 |
| N-C           |                  | 3             | -3.21738 | -2.567812 | 0.387680 |
| C-C           | -76.333314       | 3             | -4.669897 | 1.013405 | -1.282101 |
| O-H           |                  | 3             | -6.551248 | -1.198988 | -0.739457 |

### H₂O (geometry optimization with SVP basis set)

| Bond          | Energy (hartree) | Atomic Number | X  | Y  | Z  |
|---------------|------------------|---------------|----|----|----|
| C-H           | 0.021229         | 3             | 0.000000 | 0.756663 | -0.481374 |
| O-H           |                  | 3             | 0.000000 | 0.000000 | 0.120343 |
| H-H           |                  | 3             | 0.000000 | -0.756663 | -0.481374 |

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**SOLVENT:** -1313.5281525

**SOLVENT:** -76.4322049
### 13b(simplified) (geometry optimization with SVP basis set)

| Property                                      | Value                          |
|-----------------------------------------------|--------------------------------|
| Zero-point correction                         | 0.195226 (Hartree/Particle)    |
| Thermal correction to Energy                  | 0.209202                       |
| Thermal correction to Enthalpy                | 0.210146                       |
| Thermal correction to Gibbs Free Energy       | 0.152701                       |
| Sum of electronic and zero-point Energies     | -608.561691                    |
| Sum of electronic and thermal Energies        | -608.547715                    |
| Sum of electronic and thermal Enthalpies      | -608.546771                    |
| Sum of electronic and thermal Free Energies   | -608.604217                    |
| SOLVENT:                                     | -609.2353353                   |

### CH$_3$SH (geometry optimization with SVP basis set)

| Property                                      | Value                          |
|-----------------------------------------------|--------------------------------|
| Zero-point correction                         | 0.045666 (Hartree/Particle)    |
| Thermal correction to Energy                  | 0.049262                       |
| Thermal correction to Enthalpy                | 0.050206                       |
| Thermal correction to Gibbs Free Energy       | 0.021446                       |
| Sum of electronic and zero-point Energies     | -438.517374                    |
| Sum of electronic and thermal Energies        | -438.513779                    |
| Sum of electronic and thermal Enthalpies      | -438.512834                    |
| Sum of electronic and thermal Free Energies   | -438.541594                    |
| SOLVENT:                                     | -438.7082799                   |

### CH$_3$SH + 13b(simplified) reactant complex (geometry optimization with SVP basis set)

| Property                                      | Value                          |
|-----------------------------------------------|--------------------------------|
| Zero-point correction                         | 0.246368 (Hartree/Particle)    |
| Thermal correction to Energy                  | 0.264825                       |
| Thermal correction to Enthalpy                | 0.265769                       |
| Thermal correction to Gibbs Free Energy       | 0.197504                       |
| Sum of electronic and zero-point Energies     | -1042.252588                   |
| Sum of electronic and thermal Energies        | -1042.234131                   |
| Sum of electronic and thermal Enthalpies      | -1042.233187                   |
| Sum of electronic and thermal Free Energies   | -1042.301453                   |
| SOLVENT:                                     | -1047.9495377                  |

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S26
### CH$_3$SH + 13b(simplified) + H$_2$O reactant complex (geometry optimization with SVP basis set)

| Atom | x   | y   | z   |
|------|-----|-----|-----|
| H    | 1.802812 | 2.066580 | -1.149690 |
| H    | 3.412467 | 1.721284 | 1.362109 |
| H    | 4.211724 | 1.645308 | -0.232321 |
| H    | 2.699937 | -0.468403 | -1.264644 |
| H    | 2.790465 | -2.940820 | 0.943143 |
| H    | -1.718890 | -1.816856 | 1.711080 |
| H    | -5.745212 | -0.153876 | -0.306857 |
| H    | -4.874453 | 1.154955 | 1.156618 |
| H    | 3.532928 | 3.190614 | 0.352488 |

Zero-point correction = 0.267983 (Hartree/Particle)
Thermal correction to Energy = 0.289774
Thermal correction to Enthalpy = 0.290718
Thermal correction to Gibbs Free Energy = 0.215460

Sum of electronic and zero-point Energies = -1123.447208
Sum of electronic and thermal Energies = -1123.425417
Sum of electronic and thermal Enthalpies = -1123.424472
Sum of electronic and thermal Free Energies = -1123.499731

SOLVENT: -1124.3985353

### CH$_3$SH + 13b(simplified) transition state (geometry optimization with SVP basis set)

| Atom | x   | y   | z   |
|------|-----|-----|-----|
| C    | -2.549656 | 2.023897 | -0.479133 |
| S    | 0.276302 | 2.095986 | -0.379721 |
| H    | -2.719515 | 1.283248 | -1.229798 |
| C    | -1.519245 | 1.721340 | 0.509856 |
| C    | 1.212808 | -1.665394 | 0.301878 |
| C    | -0.995663 | -1.900992 | 2.754715 |
| H    | -0.574247 | -0.381389 | 1.330014 |
| C    | 0.392341 | 2.219746 | 0.557674 |
| H    | 0.923443 | 1.774169 | -1.094336 |
| C    | -2.874195 | 3.093309 | -0.589940 |
| C    | 2.128833 | 2.312501 | 0.130026 |
| H    | 5.668552 | -1.130868 | -0.123816 |
| H    | 4.488010 | -1.382419 | -1.398602 |
| C    | -3.923263 | -1.816745 | 2.288434 |
| O    | -2.285505 | -2.388905 | -1.423856 |
| H    | -2.402782 | -3.332831 | -1.592330 |
| H    | -2.532559 | -0.068282 | -1.594116 |

Zero-point correction = 0.239462 (Hartree/Particle)
Thermal correction to Energy = 0.257295
Thermal correction to Enthalpy = 0.258240
Thermal correction to Gibbs Free Energy = 0.191763

Sum of electronic and zero-point Energies = -1047.031496
Sum of electronic and thermal Energies = -1047.013662
Sum of electronic and thermal Enthalpies = -1047.012718
Sum of electronic and thermal Free Energies = -1047.079195

SOLVENT: -1047.8865328

S27
CH$_3$SH + 13b(simplified) + H$_2$O transition state (geometry optimization with SVP basis set)

Zero-point correction= 0.265082 (Hartree/Particle)
Thermal correction to Energy= 0.284560
Thermal correction to Enthalpy= 0.285504
Thermal correction to Gibbs Free Energy= 0.215909
Sum of electronic and zero-point Energies= -1123.414264
Sum of electronic and thermal Energies= -1123.394786
Sum of electronic and thermal Enthalpies= -1123.393842
Sum of electronic and thermal Free Energies= -1123.463437
SOLVENT: -1124.363896

CH$_3$SH + 13b(simplified) product (geometry optimization with SVP basis set)

Zero-point correction= 0.247174 (Hartree/Particle)
Thermal correction to Energy= 0.264692
Thermal correction to Enthalpy= 0.265636
Thermal correction to Gibbs Free Energy= 0.200137
Sum of electronic and zero-point Energies= -1047.089032
Sum of electronic and thermal Energies= -1047.071514
Sum of electronic and thermal Enthalpies= -1047.070570
Sum of electronic and thermal Free Energies= -1047.136069
SOLVENT: -1047.9570237
### CH$_3$SH + 13b(simplified) + H$_2$O product (geometry optimization with SVP basis set)

| Atom  | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-------|--------------|--------------|--------------|
| C     | -1.743385    | 2.642167     | 0.604949     |
| S     | -0.554994    | 1.866755     | -0.548598    |
| H     | -1.828153    | 3.682245     | 0.253837     |
| C     | 4.162429     | 0.015552     | -0.885810    |
| C     | 3.063747     | -0.572836    | -0.014165    |
| O     | 3.001276     | -1.760334    | 0.247568     |
| N     | 2.153362     | 0.346321     | 0.445893     |
| C     | 0.891592     | -0.045432    | 1.035755     |
| C     | 0.638708     | 0.707186     | 2.340739     |
| O     | -0.248768    | 0.063653     | -0.025201    |
| C     | 0.021551     | 0.562093     | -1.177940    |
| C     | -1.537553    | -0.601479    | 0.523383     |
| O     | -2.239586    | -0.074030    | 1.376437     |
| N     | -1.755009    | -1.853992    | 0.030999     |
| C     | -2.862347    | -2.675629    | 0.413342     |
| H     | 4.512444     | 0.992494     | -0.516506    |
| H     | 2.202845     | 1.296096     | 0.091955     |
| H     | 0.986447     | -1.124191    | 1.237189     |
| H     | -0.350751    | 0.475199     | 2.755211     |
| H     | 0.701947     | 1.794721     | 2.176968     |
| H     | -1.079774    | -2.174387    | -0.663488    |
| H     | -3.450254    | -2.130214    | 1.164807     |
| H     | -3.512248    | -2.913585    | -0.445344    |
| H     | -0.430008    | -0.446478    | -1.899653    |
| H     | -1.369584    | 2.630110     | 1.635033     |
| H     | 1.414394     | 0.332022     | 3.070438     |
| H     | 5.001443     | -0.690135    | -0.926472    |
| H     | 3.769332     | 0.156397     | -1.906480    |
| H     | -2.506099    | -3.620814    | 0.856092     |
| O     | -1.760306    | 0.091780     | -2.911242    |
| H     | -1.431698    | 0.400703     | -3.767944    |
| H     | -1.777546    | 0.908858     | -2.358974    |

### H$_2$O (geometry optimization with SVP basis set)

| Atom  | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-------|--------------|--------------|--------------|
| H     | 0.000000     | 0.780472     | -0.493724    |
| O     | 0.000000     | 0.000000     | 0.123431     |
| H     | 0.000000     | -0.780472    | -0.493724    |

### 13b(simplified) (geometry optimization with SMD)

| Atom  | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-------|--------------|--------------|--------------|
| C     | -4.077205    | -1.011582    | -0.218668    |
| C     | -2.954794    | 0.011962     | -0.253629    |
| O     | -3.130327    | 1.262984     | -0.537123    |

Zero-point correction: 0.197425 (Hartree/Particle)
Thermal correction to Energy: 0.023565
Thermal correction to Enthalpy: 0.023565
Thermal correction to Gibbs Free Energy: 0.158237

Sum of electronic and zero-point Energies: -605.673522

SOLVENT: -6.4308305
| Sum of electronic and thermal Energies | -605.660995 |
|---------------------------------------|-------------|
| Sum of electronic and thermal Enthalpies | -605.660050 |
| Sum of electronic and thermal Free Energies | -605.712710 |

**SOLVENT:** -609.2341999

### CH₃SH (geometry optimization with SMD)

| Zero-point correction | 0.046530 (Hartree/Particle) |
|-----------------------|-----------------------------|
| Thermal correction to Energy | 0.050115 |
| Thermal correction to Enthalpy | 0.051059 |
| Thermal correction to Gibbs Free Energy | 0.042304 |
| Sum of electronic and zero-point Energies | -436.585591 |
| Sum of electronic and thermal Energies | -436.582006 |
| Sum of electronic and thermal Enthalpies | -436.581062 |
| Sum of electronic and thermal Free Energies | -436.609817 |

**SOLVENT:** -438.7084606

### CH₃SH + 13b(simplified) reactant complex (geometry optimization with SMD)

| Zero-point correction | 0.246232 (Hartree/Particle) |
|-----------------------|-----------------------------|
| Thermal correction to Energy | 0.264355 |
| Thermal correction to Enthalpy | 0.265300 |
| Thermal correction to Gibbs Free Energy | 0.198986 |
| Sum of electronic and zero-point Energies | -1042.271891 |
| Sum of electronic and thermal Energies | -1042.253768 |
| Sum of electronic and thermal Enthalpies | -1042.252824 |
| Sum of electronic and thermal Free Energies | -1042.319137 |

**SOLVENT:** -1047.9516763
CH₃SH + 13b(simplified) + H₂O reactant complex (geometry optimization with SMD)

Zero-point correction= 0.270935 (Hartree/Particle)
Thermal correction to Energy= 0.29112
Thermal correction to Enthalpy= 0.292066
Thermal correction to Gibbs Free Energy= 0.221255

Sum of electronic and zero-point Energies= -1118.270778
Sum of electronic and thermal Energies= -1118.250591
Sum of electronic and thermal Enthalpies= -1118.249647
Sum of electronic and thermal Free Energies= -1118.320458

SOLVENT: -1124.3926965

CH₃SH + 13b(simplified) transition state (geometry optimization with SMD)

Zero-point correction= 0.242443 (Hartree/Particle)
Thermal correction to Energy= 0.259553
Thermal correction to Enthalpy= 0.260497
Thermal correction to Gibbs Free Energy= 0.197241

Sum of electronic and zero-point Energies= -1042.215556
Sum of electronic and thermal Energies= -1042.198446
Sum of electronic and thermal Enthalpies= -1042.197502
Sum of electronic and thermal Free Energies= -1042.260759

SOLVENT: -1047.8881197
### CH$_3$SH + 13b(simplified) + H$_2$O transition state (geometry optimization with SMD)

| Property                               | Value                      |
|----------------------------------------|----------------------------|
| Zero-point correction                  | 0.268849 (Hartree/Particle) |
| Thermal correction to Energy           | 0.287515                   |
| Thermal correction to Enthalpy         | 0.288459                   |
| Thermal correction to Gibbs Free Energy| 0.222046                   |
| Sum of electronic and zero-point Energies| -1118.250856             |
| Sum of electronic and thermal Energies | -1118.232189               |
| Sum of electronic and thermal Enthalpies| -1118.232145              |
| Sum of electronic and thermal Free Energies| -1118.297658            |

**SOLVENT:** -1124.3629941

### CH$_3$SH + 13b(simplified) + H$_2$O transition state (geometry optimization with SMD)

| Property                               | Value                      |
|----------------------------------------|----------------------------|
| Zero-point correction                  | 0.248940 (Hartree/Particle) |
| Thermal correction to Energy           | 0.265935                   |
| Thermal correction to Enthalpy         | 0.266879                   |
| Thermal correction to Gibbs Free Energy| 0.204004                   |
| Sum of electronic and zero-point Energies| -1042.278479              |
| Sum of electronic and thermal Energies | -1042.261484               |
| Sum of electronic and thermal Enthalpies| -1042.260540              |
| Sum of electronic and thermal Free Energies| -1042.323414            |

**SOLVENT:** -1047.9570028
### Zero-point correction=  0.273850 (Hartree/Particle)
Thermal correction to Energy=  0.293181
Thermal correction to Enthalpy=  0.294126
Thermal correction to Gibbs Free Energy=  0.226419

Sum of electronic and zero-point Energies=  -1118.272159
Sum of electronic and thermal Energies=  -1118.252827
Sum of electronic and thermal Enthalpies=  -1118.251883
Sum of electronic and thermal Free Energies=  -1118.319589

SOLVENT: -1124.396146

### CH₃SH

| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | 1.140472 | -2.518421 | 0.052534 |
| S    | 1.242336  | -1.533876  | -1.274927 |
| H    | 2.994261  | -2.983594  | -0.323515 |
| C    | 3.805736  | 1.822785  | 0.314473 |

### CH₃S⁻ + 13b(simplified) reactant complex (geometry optimization with SMD)

| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | 2.074844  | -2.518421  | 0.052534 |
| S    | 1.242336  | -1.533876  | -1.274927 |
| H    | 2.994261  | -2.983594  | -0.323515 |
| C    | 3.805736  | 1.822785  | 0.314473 |

### SOLVENT: -1047.462602
### CH₃S⁻ + 13b(simplified) product (geometry optimization with SMD)

#### Zero-point correction
0.235984 (Hartree/Particle)

#### Thermal correction to Energy
0.252897

#### Thermal correction to Enthalpy
0.253841

#### Thermal correction to Gibbs Free Energy
0.191113

#### Sum of electronic and zero-point Energies
-1041.799146

#### Sum of electronic and thermal Energies
-1041.782234

#### Sum of electronic and thermal Enthalpies
-1041.781290

#### Sum of electronic and thermal Free Energies
-1041.844018

#### SOLVENT: -1047.4671892

### CH₃S⁻ + 13b(simplified) + H₂O reactant complex (geometry optimization with SMD)

#### Zero-point correction
0.260237 (Hartree/Particle)

#### Thermal correction to Energy
0.279683

#### Thermal correction to Enthalpy
0.280627

#### Thermal correction to Gibbs Free Energy
0.211614

#### Sum of electronic and zero-point Energies
-1117.797127

#### Sum of electronic and thermal Energies
-1117.777682

#### Sum of electronic and thermal Enthalpies
-1117.776738

#### Sum of electronic and thermal Free Energies
-1117.845750

#### SOLVENT: -1123.9125663
H41imidazole Tautomer

Zero-point correction= 0.099388 (Hartree/Particle)
Thermal correction to Energy= 0.104678
Thermal correction to Enthalpy= 0.105622
Thermal correction to Gibbs Free Energy= 0.070777
Sum of electronic and zero-point Energies= -263.972628
Sum of electronic and thermal Energies= -263.967338
Sum of electronic and thermal Enthalpies= -263.966394
Sum of electronic and thermal Free Energies= -264.001238
SOLVENT: -265.5641215

H41imidazole

Zero-point correction= 0.0999113 (Hartree/Particle)
Thermal correction to Energy= 0.104503
Thermal correction to Enthalpy= 0.105447
Thermal correction to Gibbs Free Energy= 0.070147
Sum of electronic and zero-point Energies= -263.972589
Sum of electronic and thermal Energies= -263.967199
Sum of electronic and thermal Enthalpies= -263.966255
Sum of electronic and thermal Free Energies= -264.001555
SOLVENT: -265.5629172

H41imidazole TS Stautomerization

Zero-point correction= 0.098987 (Hartree/Particle)
Thermal correction to Energy= 0.103574
Thermal correction to Enthalpy= 0.104518
Thermal correction to Gibbs Free Energy= 0.071150
Sum of electronic and zero-point Energies= -263.972105
Sum of electronic and thermal Energies= -263.967519
Sum of electronic and thermal Enthalpies= -263.966574
Sum of electronic and thermal Free Energies= -263.999942
SOLVENT: -265.5615167

H41imidazole TS Stautomerization+1H2O

Zero-point correction= 0.119253 (Hartree/Particle)
Thermal correction to Energy= 0.125925
Thermal correction to Enthalpy= 0.126869
Thermal correction to Gibbs Free Energy= 0.088631

PENTIL SCF Done: -264.072015796 A.U.
C     -2.144670    -0.028765     0.000041
C     -0.651751     0.061765    -0.000104
N      0.187627    -1.054404    -0.000083
C      1.496667    -0.595973     0.000081
N      1.536262     0.730122     0.000054
C      0.197010     1.145228    -0.000019
H     -2.570370     0.978416    -0.000610
H     -2.517434    -0.555252    -0.888164
H      2.343963    -1.259375    -0.000237
H     -0.072739     2.186957    -0.000073
H     -0.116867    -2.020255     0.000279
H     -2.517319    -0.554046     0.889019

PENTIL histidine SCF Done: -264.071702123 A.U.
C     -2.164735    -0.017075    -0.000098
C     -0.667751     0.022478    -0.000159
N      0.097954    -1.160565    -0.000071
C      1.367315    -0.771057    -0.000039
N      1.466780    0.607929    -0.000007
C      0.164896    1.113411     0.000007
H     -2.578913    0.995826    -0.000030
H     -2.534981    -0.548542    -0.884287
H      2.229013    -1.415874    -0.000007
H     -0.049103    2.167016    -0.000067
H      2.316969    1.156745    -0.000007
H     -2.535011    -0.548511     0.884267

PENTIL histidine TS SCF Done: -264.071092404 A.U.
PentilPENTIL histidineTS SCF Done: -264.071092404 A.U.
C     -2.328372    -0.355346     0.000898
C     -0.668269     0.022478    -0.000159
N      0.094942    -1.157633    -0.000071
C      1.366751    -0.771057    -0.000039
N      1.466780    0.607929    -0.000007
C      0.166956    1.115336    -0.000079
H     -2.484929    -1.063161     0.001097
H     -2.538973    0.474030     0.887886
H      2.226139    -1.420690     0.000143
H     -0.037759    2.170367    -0.000076
H      2.320602    1.151432    -0.000238
H     -2.584288    0.472314    -0.884942

PENTIL-TSH1 SCF Done: -340.001598389 A.U.
C     -2.328372    -0.355346     0.002744
C     -0.926093     0.171452     0.012110
N      0.114069    0.138259    1.805375
C      1.041222    0.776219    0.785459
| Energy Component                                      | Value                      |
|------------------------------------------------------|----------------------------|
| Sum of electronic and zero-point Energies            | -339.882345                |
| Sum of electronic and thermal Energies               | -339.875674                |
| Sum of electronic and thermal Enthalpies             | -339.874729                |
| Sum of electronic and thermal Free Energies          | -339.912968                |
| SOLVENT:                                             | -341.930387                |

| H41imidazoleTStautomerization+2H2O                  |
|------------------------------------------------------|
| Zero-point correction                                | 0.143780                   |
| Thermal correction to Energy                         | 0.152381                   |
| Thermal correction to Enthalpy                       | 0.153325                   |
| Thermal correction to Gibbs Free Energy              | 0.110502                   |
| Sum of electronic and zero-point Energies            | -415.925297                |
| Sum of electronic and thermal Energies               | -415.916696                |
| Sum of electronic and thermal Enthalpies             | -415.915752                |
| Sum of electronic and thermal Free Energies          | -415.958575                |
| SOLVENT:                                             | -418.403513                |

| H41imidazoleTStautomerization+3H2O                  |
|------------------------------------------------------|
| Zero-point correction                                | 0.168649                   |
| Thermal correction to Energy                         | 0.179137                   |
| Thermal correction to Enthalpy                       | 0.180081                   |
| Thermal correction to Gibbs Free Energy              | 0.132831                   |
| Sum of electronic and zero-point Energies            | -491.947471                |
| Sum of electronic and thermal Energies               | -491.934243                |
| Sum of electronic and thermal Enthalpies             | -491.933299                |
| Sum of electronic and thermal Free Energies          | -491.980549                |
| SOLVENT:                                             | -494.8602745               |

| H41imidazoleTStautomerization+4H2O                  |
|------------------------------------------------------|
| Zero-point correction                                | 0.190618                   |
| Thermal correction to Energy                         | 0.203506                   |
| Thermal correction to Enthalpy                       | 0.204450                   |
| Thermal correction to Gibbs Free Energy              | 0.151554                   |
| Sum of electronic and zero-point Energies            | -567.953622                |
| Sum of electronic and thermal Energies               | -567.940734                |
| Sum of electronic and thermal Enthalpies             | -567.939790                |
| Sum of electronic and thermal Free Energies          | -567.992686                |

| PENTIL-TSH2 SCF Done: -416.09076988 A.U.            |
|------------------------------------------------------|
| C                                                   | 2.43172                    |
| N                                                   | 0.632322                   |
| O                                                   | 0.344326                   |
| H                                                   | -0.432432                  |
| C                                                   | 0.650486                   |
| N                                                   | 2.796272                   |
| O                                                   | 2.143345                   |
| H                                                   | -1.067008                  |
| C                                                   | 0.865535                   |
| N                                                   | -0.273889                  |
| O                                                   | -1.619835                  |
| H                                                   | 1.863377                   |
| C                                                   | -0.236431                  |
| N                                                   | -1.955336                  |
| O                                                   | 2.630077                   |
| N                                                   | 1.338124                   |
| O                                                   | 0.955252                   |
| H                                                   | -0.656880                  |
| C                                                   | 0.315355                   |
| N                                                   | 2.720423                   |
| O                                                   | 3.484769                   |
| H                                                   | -0.853247                  |
| C                                                   | 0.288729                   |
| N                                                   | 0.853986                   |
| O                                                   | -2.029749                  |
| H                                                   | 2.688795                   |
| C                                                   | 0.402589                   |
| N                                                   | -0.000303                  |
| O                                                   | -2.768897                  |
| H                                                   | 3.331097                   |
| C                                                   | -0.460594                  |
| N                                                   | 1.027430                   |
| O                                                   | -1.951523                  |
| H                                                   | -0.361252                  |

| PENTIL-TSH3 SCF Done: -492.11337936 A.U.            |
|------------------------------------------------------|
| C                                                   | 2.43172                    |
| N                                                   | 0.632322                   |
| O                                                   | 0.344326                   |
| H                                                   | -0.432432                  |
| C                                                   | 0.650486                   |
| N                                                   | 2.796272                   |
| O                                                   | 2.143345                   |
| H                                                   | -1.067008                  |
| C                                                   | 0.865535                   |
| N                                                   | -0.273889                  |
| O                                                   | -1.619835                  |
| H                                                   | 1.863377                   |
| C                                                   | -0.236431                  |
| N                                                   | -1.955336                  |
| O                                                   | 2.630077                   |
| N                                                   | 1.338124                   |
| O                                                   | 0.955252                   |
| H                                                   | -0.656880                  |
| C                                                   | 0.315355                   |
| N                                                   | 2.720423                   |
| O                                                   | 3.484769                   |
| H                                                   | -0.853247                  |
| C                                                   | 0.288729                   |
| N                                                   | 0.853986                   |
| O                                                   | -2.029749                  |
| H                                                   | 2.688795                   |
| C                                                   | 0.402589                   |
| N                                                   | -0.000303                  |
| O                                                   | -2.768897                  |
| H                                                   | 3.331097                   |
| C                                                   | -0.460594                  |
| N                                                   | 1.027430                   |
| O                                                   | -1.951523                  |
| H                                                   | -0.361252                  |

| PENTIL-TSH4 SCF Done: -568.144239804 A.U.           |
|------------------------------------------------------|
| C                                                   | 2.793144                   |
| N                                                   | 1.413614                   |
| O                                                   | 1.059422                   |
| H                                                   | -0.259831                  |
| C                                                   | -0.771253                  |
| N                                                   | 0.285915                   |
| O                                                   | 3.517993                   |

| PENTIL-TSH4 SCF Done: -568.144239804 A.U.           |
|------------------------------------------------------|
| C                                                   | 2.793144                   |
| N                                                   | 1.413614                   |
| O                                                   | 1.059422                   |
| H                                                   | -0.259831                  |
| C                                                   | -0.771253                  |
| N                                                   | 0.285915                   |
| O                                                   | 3.517993                   |

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### H41imidazole Tautomer (geometry optimization with SMD)

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -2.141744  | -0.028300  | 0.000005   |
| C    | -0.651150  | 0.063301   | -0.000022  |
| N    | 0.186903   | -1.050598  | -0.000026  |
| C    | 1.490332   | -0.602179  | 0.000025   |
| N    | 1.540651   | 0.731174   | 0.000012   |
| C    | 0.196075   | 1.148137   | 0.000008   |
| H    | -2.572478  | 0.976832   | -0.000027  |
| H    | -2.507323  | -0.561505  | -0.886346  |
| H    | 2.331094   | -1.273488  | -0.000091  |
| H    | 0.062462   | 2.198288   | -0.000011  |
| H    | -0.120244  | -2.019495  | 0.000114   |
| H    | -2.507294  | -0.561421  | 0.886426   |

SOLVENT: -265.5641553

### H41imidazole (geometry optimization with SMD)

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 2.166927   | 0.007902   | -0.000032  |
| C    | 0.670130   | 0.009006   | 0.000057   |
| N    | -0.107161  | -1.169009  | 0.000001   |
| C    | -1.38436   | -0.758972  | 0.000001   |
| N    | -1.468784  | 0.630007   | -0.000013  |
| C    | -0.157790  | 1.107643   | 0.000008   |
| H    | 2.568635   | 0.995957   | 0.000018   |
| H    | 2.550687   | -0.542003  | 0.884326   |
| H    | -2.250575  | -1.391240  | 0.000000   |
| H    | 0.062462   | 2.160188   | 0.000013   |
| H    | -2.311274  | 1.168585   | -0.000022  |
| H    | 2.550689   | -0.542007  | -0.884337  |

SOLVENT: -265.5629706

### H41imidazole H+

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -2.185499  | 0.007902   | -0.000032  |
| C    | -0.694596  | 0.072241   | 0.000057   |
| N    | 0.129025   | -1.066317  | 0.000019   |
| C    | 1.428920   | -0.71748  | -0.000027  |
| N    | 1.462286   | 0.631597   | -0.000017  |
| C    | 0.159284   | 1.141788   | 0.000034   |
| H    | 2.598673   | 1.018902   | 0.000101   |
| H    | 2.554427   | -0.51324  | -0.890761  |
| H    | 2.274961   | -1.375066  | 0.000068   |
| H    | -0.053782  | 2.194508   | 0.000056   |
| H    | -0.211425  | -0.025359  | 0.000007   |
| H    | 2.310079   | 1.193898   | -0.000146  |
| H    | 2.554560   | -0.513509  | 0.890470   |

SOLVENT: -266.0337766
### H41imidazoleH⁺ (geometry optimization with SMD)

| Term                                      | Value                      | Source          |
|-------------------------------------------|----------------------------|-----------------|
| Zero-point correction=                   | 0.113280 (Hartree/Particle) |                 |
| Thermal correction to Energy=             | 0.118580                   |                 |
| Thermal correction to Enthalpy=           | 0.119525                   |                 |
| Thermal correction to Gibbs Free Energy=  | 0.084689                   |                 |
| Sum of electronic and zero-point Energies=| -264.450962                |                 |
| Sum of electronic and thermal Energies=   | -264.446561                |                 |
| Sum of electronic and thermal Enthalpies= | -264.444717                |                 |
| Sum of electronic and thermal Free Energies=| -264.479553                |                 |
| SOLVENT:                                  | -266.0340663               |                 |

### space group C2, model 1, product (heteroatoms frozen, free hydrogens)

| Term                                      | Value                      | Source          |
|-------------------------------------------|----------------------------|-----------------|
| Zero-point correction=                   | 2.538013 (Hartree/Particle) |                 |
| Thermal correction to Energy=             | 2.656405                   |                 |
| Thermal correction to Enthalpy=           | 2.657349                   |                 |
| Thermal correction to Gibbs Free Energy=  | 2.383710                   |                 |
| Sum of electronic and zero-point Energies=| -8195.579091               |                 |
| Sum of electronic and thermal Energies=   | -8195.460699               |                 |
| Sum of electronic and thermal Enthalpies= | -8195.459755               |                 |
| Sum of electronic and thermal Free Energies=| -8195.73394                |                 |
| SOLVENT:                                  | -8243.0804481              |                 |
| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| C    | -8.279302 | -3.038457 | -4.567420 |
| O    | -7.325927 | -3.752241 | -4.175634 |
| N    | -5.017317 | -4.998422 | -3.102558 |
| C    | -5.014449 | -6.326515 | -3.173587 |
| O    | -4.023696 | -7.038656 | -2.953634 |
| N    | -5.017317 | -4.998422 | -3.102558 |
| C    | -3.788781 | -4.225780 | -2.816688 |
| C    | -3.942344 | -2.810247 | -3.364142 |
| C    | -2.664890 | -2.066543 | -3.195562 |
| N    | -1.483931 | -2.524449 | -2.697980 |
| O    | -0.519138 | -1.713055 | -3.42657 |
| N    | -1.046754 | -0.747221 | -2.616167 |
| C    | -2.379979 | -0.950956 | -1.315115 |
| O    | -4.299813 | -4.039862 | -0.512225 |
| N    | -2.126977 | -4.453171 | -0.977062 |
| C    | -1.588869 | -4.693934 | 0.408894  |
| C    | -1.140919 | -5.888832 | 0.850057  |
| C    | -2.707167 | -6.859664 | 0.967815  |
| N    | -2.627887 | -7.450679 | 2.167875  |
| C    | -3.621204 | -8.288254 | 1.938282  |
| C    | -3.904669 | -8.27203 | 0.661866  |
| C    | -3.101549 | -7.363524 | 0.041454  |
| C    | -0.436182 | -3.489021 | 0.621085  |
| N    | 0.490421  | -3.274036 | -0.312373 |
| C    | 1.715425  | -2.527484 | 0.071357  |
| C    | 2.653521  | -3.438641 | 0.879331  |
| S    | 3.689958  | -6.030493 | 1.319427  |
| C    | 5.247856  | -5.967915 | 0.467446  |
| C    | 4.929776  | -1.994924 | -1.127384 |
| C    | 2.257881  | -2.440789 | -2.277977 |
| N    | 3.424229  | -1.110858 | -0.811805 |
| C    | 4.378199  | -0.521753 | -1.769394 |
| C    | 4.227440  | 0.991525  | -1.816621 |
| C    | 5.000813  | 1.628406  | -2.906868 |
| S    | 4.847559  | 3.108077  | -3.178109 |
| C    | 5.846109  | 3.844040  | -3.105984 |
| C    | 3.691023  | 3.519652  | -3.474434 |
| C    | 5.759430  | 1.000714  | -1.135707 |
| C    | 6.035557  | -0.975343 | -0.130783 |
| N    | 6.549805  | -1.492319 | -2.284568 |
| C    | 7.940239  | -1.945486 | -2.069429 |
| C    | 8.213587  | -1.644526 | -2.984739 |
| C    | 7.352113  | -4.378635 | -2.691202 |
| C    | 7.444511  | -5.348759 | -3.822047 |
| C    | 7.743894  | -5.051398 | -1.375775 |
| C    | 8.690164  | -0.784798 | -2.325042 |
| C    | 8.527150  | 0.197475  | -2.980318 |
| N    | 10.143693 | -0.871233 | -1.826375 |
| C    | 11.084492 | 0.246388 | -1.888815 |
| C    | 12.441497 | -0.355959 | -1.477459 |
| C    | 12.183562 | -1.826330 | -1.183492 |
| C    | 10.687969 | -1.950955 | -1.505317 |
| C    | 11.194320 | 0.931838  | -3.256819 |
| C    | 11.139817 | 2.145905  | -3.275437 |
| C    | 11.128050 | 0.183150  | -4.359402 |
| C    | 7.993333  | 1.357527  | 3.433657  |
| C    | 7.104733  | 1.163235  | 2.444804  |
| C    | 7.540681  | 1.647606  | 1.148216  |
| C    | 8.571999  | 2.625990  | 0.921208  |
| C    | 9.892190  | 2.060702  | 1.473544  |
| C    | 8.673776  | 2.897911  | -0.587269 |
| C    | 8.227526  | 3.954117  | 1.608752  |
| C    | 5.939495  | 0.507796  | 2.427384  |
| C    | 5.234082  | 0.058172  | 3.491790  |
| C    | 3.887276  | -0.453804 | 3.188058  |
| C    | 3.440814  | -0.460350 | 2.001304  |
| C    | 5.664422  | 0.083697  | 4.832656  |
| C    | 4.892345  | -0.727671 | 5.832073  |
| C    | 3.571133  | -0.877302 | 5.520050  |
| C    | 3.098742  | -0.935693 | 4.251811  |
| C    | 1.757964  | -1.415425 | 3.914443  |
| C    | 1.099444  | -2.273074 | 5.025940  |
| C    | 1.893805  | 3.503695  | 5.330428  |
| C    | 1.181629  | -0.707759 | 5.939550  |
| C    | 1.513516  | -0.707167 | 4.452672  |
| C    | 0.959847  | -0.816699 | 3.587732  |
| O    | 1.209721  | 0.883477  | 4.152375  |
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N  -0.020324  -0.314632  2.677669  
C   -0.903421  0.754414  2.327067  
C   -0.900132  1.100219  0.803852  
C    0.397876  1.776777  0.480030  
C    0.720719  2.004491 -0.980723  
O     0.487838  1.171727 -1.852006  
N    1.324632  3.196408 -1.122985  
C    1.535386  3.889367  0.152864  
C    0.530025  3.190447  1.059979  
C   -2.193854  0.260031  2.972107  
O   -2.052867 -0.278005  4.340775  
C   -3.113436  1.396462  3.168686  
O   -3.452119  2.006207  2.171265  
N   -3.348752  1.550722  4.472608  
C   -4.416042  2.561230  4.974445  
C   -3.678303  3.825380  5.398088  
C   -2.247090  3.888250  5.409103  
C   -1.633945  4.055671  5.815555  
C   -2.374429  6.175784  6.214324  
C   -3.769069  6.122692  6.206943  
C   -4.412805  4.950076  5.799694  
H   -2.510606 -4.746564  8.481690  
H   -2.985132 -6.170287  7.544221  
H   -2.480905 -3.803131  3.187675  
H   -3.096677 -2.364007  7.096062  
H   -2.163483 -5.758423  4.821684  
H   -2.571769  3.854131 -5.052552  
H   -1.445753  2.145296 -3.545866  
H   -0.077634  2.134609 -4.650116  
H   -3.816054  1.739554 -4.612630  
H   -5.002758 -0.014099 -5.866818  
H   -3.742551 -1.549444 -7.322184  
H   -0.143165  4.778884 -6.327800  
H   -1.317877 -1.285137 -7.563557  
H   -2.373897  5.123855 -3.214975  
H   -0.247333  6.127521 -1.982055  
H   -1.547284  8.219114 -1.370017  
H   -2.967580  7.526864 -2.127037  
H   -1.706241  7.856964 -4.340393  
H   -0.608038  7.665395 -3.491431  
H   -1.582077  9.239231 -4.514332  
H   -0.154600  9.422388 -2.747997  
H   -3.818129  9.242761 -3.729453  
H   -2.273385 10.233296 -2.907300  
H   -2.192709 10.008937 -4.665792  
H   -0.672953  6.796632  0.407855  
H   -1.646859  4.974253  2.173204  
H   -2.213874  6.867888  3.693595  
H   -1.935889  7.898651  2.356748  
H   -1.253801  7.892005  4.220483  
H   -0.326560  8.620920  4.355577  
H   -3.642751  3.804944  2.158839  
H   -5.595220  4.055062  2.928293  
H   -6.067501  5.492173  1.876822  
H   -4.322717  3.628815 -0.063718  
H   -6.678475  2.777468 -1.587018  
H   -4.789980  3.735417 -2.778184  
H   -4.997564  2.030236 -3.234745  
H   -2.951706  3.170708 -1.604101  
H   -4.464626  1.187156  0.739539  
H   -4.658907 -1.483205 -0.135835  
H   -4.906452 -2.123351  2.280320  
H   -5.093169 -0.406860  2.668295  
H   -6.036540 -3.175249 -0.273302  
H   -8.885736 -2.813475  0.441641  
H   -8.115825 -4.286906 -2.019811  
H   -7.381493 -1.348788 -2.065215  
H   -9.629322 -1.519560 -3.853903  
H   -8.287712 -0.431277 -5.505856  
H   -6.785546 -0.891664 -4.680033  
H   -7.962098  0.539090 -2.956443  
H   -8.995469 -4.270177 -6.014052  
H   -9.963400 -2.847625 -5.730701  
H   -5.865231 -4.471333 -3.358752  
H   -2.973944 -4.605402 -3.381306  
H   -7.605797 -2.293842 -2.841665  
H   -4.210989 -2.891203 -4.423352  
H   -0.531989 -1.631058 -3.526157  
H   -0.068487 -0.232319 -2.027409  
H   -0.525099  0.049586 -2.224211  

| H     | -1.475054 | -4.585641 | -1.746836 |
|-------|-----------|-----------|-----------|
| H     | -2.412871 | -4.122870 | 2.079002  |
| H     | -3.175974 | -1.646586 | -1.015932 |
| H     | -2.117949 | -3.143688 | 3.033144  |
| H     | 0.396066  | -4.859046 | -1.307234 |
| H     | 1.438324  | -1.681834 | 0.705752  |
| H     | 2.201735  | -3.759422 | 1.867334  |
| H     | 3.604496  | -2.932282 | 1.036529  |
| H     | 3.366676  | -2.426545 | -0.700749 |
| H     | 1.848157  | -2.14638 | 0.031381  |
| H     | 5.968520  | -6.612937 | 0.981185  |
| H     | 1.438324  | -1.681834 | 0.705752  |
| H     | 4.048416  | -0.952099 | -2.742441 |
| H     | 3.167590  | 1.197640  | -2.002544 |
| H     | 4.492646  | 1.401027  | -0.832809 |
| H     | 4.851465  | 1.197640  | -2.002544 |
| H     | 6.149280  | 1.531107  | -2.716155 |
| H     | 6.302884  | -1.327417 | -3.257045 |
| H     | 7.992786  | -2.228153 | -1.013273 |
| H     | 8.030850  | 2.812791  | -4.81179  |
| H     | 9.271414  | -3.425975 | -2.935878 |
| H     | 6.310288  | -4.037931 | -2.690382 |
| H     | 8.806323  | -5.333802 | -1.404592 |
| H     | 7.587962  | -3.960658 | -0.514234 |
| H     | 7.138050  | -4.944507 | -4.778756 |
| H     | 8.474870  | -5.749884 | -3.936343 |
| H     | 6.800225  | -6.249455 | -3.627674 |
| H     | 10.777290 | 1.044072  | -1.234199 |
| H     | 13.177589 | -0.232297 | -2.275304 |
| H     | 12.816501 | 0.166584  | -0.593197 |
| H     | 12.539994 | -2.434084 | -2.024693 |
| H     | 12.709184 | -2.171656 | -0.288348 |
| H     | 10.373089 | -1.908777 | -0.000288 |
| H     | 10.346141 | -2.957705 | -1.428232 |
| H     | 10.881256 | -0.797679 | -4.323876 |
| H     | 6.645204  | 0.483736  | 5.037661  |
| H     | 5.131731  | -0.350408 | 6.895364  |
| H     | 2.908210  | -1.205128 | 6.302913  |
| H     | 1.847485  | -2.045786 | 3.032377  |
| H     | 0.944010  | -1.607994 | 5.912501  |
| H     | 0.088061  | -2.493161 | 4.662784  |
| H     | 2.943213  | -3.377501 | 5.562109  |
| H     | 0.144972  | -5.626423 | 6.219457  |
| H     | 1.756268  | -5.358158 | 6.588180  |
| H     | 2.305668  | -5.354076 | 4.093468  |
| H     | 0.708949  | -4.524096 | 3.743795  |
| H     | -0.172930 | -1.241833 | 2.257180  |
| H     | -0.561324 | 1.618566  | 2.895739  |
| H     | -1.758660 | 1.737802  | 0.593344  |
| H     | -1.003470 | 0.181777  | 0.217463  |
| H     | 1.223294  | 1.504038  | 0.886640  |
| H     | 1.591757  | 3.551679  | -2.041271 |
| H     | 2.564757  | 3.750264  | 0.596179  |
| H     | 1.327772  | 4.959482  | 0.082582  |
| H     | -0.439059 | 3.689933  | 0.962275  |
| H     | 0.835360  | 3.215315  | 2.107038  |
| H     | -2.990155 | 0.839303  | 5.040769  |
| H     | -5.129402 | 2.799092  | 4.180220  |
| H     | -4.963947 | 2.137352  | 5.821991  |
| H     | -1.704336 | 3.066850  | 5.102502  |
| H     | -0.550612 | 5.993367  | 5.811214  |
| H     | -1.861366 | 7.077852  | 6.529847  |
| H     | -4.354052 | 6.892643  | 6.511215  |
| H     | -5.497858 | 4.910987  | 5.786562  |
| H     | -2.436687 | -1.243740 | 4.432009  |
| H     | 8.152167  | 3.804935  | 2.690616  |
| H     | 7.268354  | 4.322982  | 1.230478  |
| H     | 9.003832  | 4.694733  | 1.397113  |
| H     | 8.009991  | 1.971716  | 1.155529  |
| H     | 9.532999  | 3.548578  | -0.779723 |
| H     | 7.765100  | 3.777092  | -0.971960 |
| H     | 10.997462 | 1.103237  | 0.979305  |
| H     | 10.718536 | 2.749219  | 1.268532  |
| H     | 9.797110  | 1.809059  | 2.544986  |
| Atom | X   | Y   | Z     |
|------|-----|-----|-------|
| H    |  5.596107 |  0.215724 |  1.499956 |
| H    |  11.128300 |  0.653704 | -5.256860 |
| H    |   3.666354 |  4.494112 | -3.681388 |
| H    | -1.291912 | -5.627595 |  7.544728 |
| H    | -5.994514 | -6.733140 | -3.473751 |

**Space group C2, model 1, reactantM**

Zero-point correction= 1.846347 (Hartree/Particle)
Thermal correction to Energy= 1.960646
Thermal correction to Enthalpy= 1.961590
Thermal correction to Gibbs Free Energy= 1.684815

Sum of electronic and zero-point Energies= -6202.125820
Sum of electronic and thermal Energies= -6202.011521
Sum of electronic and thermal Enthalpies= -6202.010577
Sum of electronic and thermal Free Energies= -6202.287351

SOLVENT: -6237.7092688

| Atom | X   | Y   | Z     |
|------|-----|-----|-------|
| C    | -3.626232 | -5.893409 |  5.529409 |
| C    | -3.615754 | -4.486651 |  5.020612 |
| N    | -2.455819 | -3.822744 |  4.626706 |
| C    | -2.810393 | -2.564408 |  4.210445 |
| N    | -4.127625 | -2.382161 |  4.324843 |
| C    | -4.644541 | -3.584074 |  4.829600 |
| C    |  0.718053 |  3.480901 | -2.199375 |
| C    |  0.702885 |  2.008438 | -1.695246 |
| C    |  0.879137 |  0.939196 | -2.758254 |
| C    |  0.262955 |  1.033734 | -4.014777 |
| C    |  0.280840 | -0.046958 | -4.899600 |
| C    |  0.921964 | -1.238321 | -4.199996 |
| C    | -1.526271 | -0.256014 | -2.415797 |
| C    |  1.555591 | -1.333281 | -3.305963 |
| C    |  0.413441 |  4.360524 |  0.946738 |
| C    | -2.289026 |  3.743753 |  0.131428 |
| C    | -1.607714 |  7.526792 | -0.769964 |
| C    | -2.602889 |  8.577693 | -1.034800 |
| C    | -0.303104 |  7.962874 | -0.138473 |
| C    | -2.162909 |  4.302933 |  1.402078 |
| C    | -2.997149 |  3.440538 |  0.938103 |
| C    | -2.140785 |  4.549557 |  2.703805 |
| C    | -3.245677 |  4.053207 |  3.555979 |
| C    | -3.117458 |  4.729347 |  4.944829 |
| C    | -1.695681 |  4.720071 |  5.500316 |
| O    | -0.732545 |  5.159167 |  4.826882 |
| N    | -1.543854 |  4.247295 |  6.758605 |
| C    | -0.450849 |  4.605015 |  2.923279 |
| O    | -6.433883 |  5.818184 |  2.660984 |
| N    | -5.548562 |  3.708866 |  2.713367 |
| C    | -7.875800 |  4.190636 |  2.061999 |
| N    | -8.656491 |  3.813744 |  0.556014 |
| N    | -7.933219 |  3.863043 | -0.067832 |
| N    | -5.662657 |  3.452614 |  0.004347 |
| C    | -5.585783 |  2.937151 | -1.362484 |
| C    | -4.846362 |  3.614534 | -2.203880 |
| C    | -3.154252 |  3.299881 | -1.670403 |
| C    | -5.301655 |  4.423781 | -1.333220 |
| O    | -4.927667 |  0.811504 | -2.373702 |
| N    | -5.410419 |  0.812126 | -0.154131 |
| O    | -5.057600 | -0.598535 |  0.017831 |
| N    | -5.372142 | -1.031651 |  1.449398 |
| O    | -4.671217 |  0.157249 |  2.710739 |
| C    | -5.890373 | -1.426299 | -1.007698 |
| O    | -7.080023 | -1.173091 | -1.253651 |
| N    | -5.134528 | -2.382655 | -1.597883 |
| C    | -5.590239 | -3.156993 | -2.745971 |
| C    | -4.920142 | -2.691843 | -4.055705 |
| C    | -4.312120 | -3.407773 | -5.068620 |
| N    | -4.456188 | -1.401648 | -4.033333 |
| C    | -3.918389 | -0.815819 | -5.252539 |
| O    | -3.458308 |  0.652484 | -4.996044 |
| O    | -4.870301 |  1.546461 | -4.839607 |
| O    | -2.720348 | -1.626484 | -5.780218 |
| O    | -1.973780 | -2.344447 | -5.106098 |
| N    | -2.452601 | -1.358503 | -7.093324 |
| C    | -1.256224 | -5.141062 | -2.851552 |
| O    | -0.685061 | -5.039987 | -1.887772 |
| N    | -1.593810 | -3.814183 | -2.890540 |
| C    | -1.207981 | -2.905401 | -1.799000 |
| O    | -1.605770 | -1.467519 | -2.148159 |
| N    | -1.453211 | -0.596049 | -0.947305 |
| N    | -0.722644 | -0.976854 |  0.192261 |
|   |   |   |   |
|---|---|---|---|
| H  | -6.828365  | 5.237676  | 2.167734  |
| H  | -4.809632  | 3.468107  | 0.565794  |
| H  | -6.568348  | 3.105187  | -1.817972 |
| H  | -4.672825  | 4.694856  | -2.209301 |
| H  | -6.568348  | 3.105187  | -1.817972 |
| H  | -4.672825  | 4.694856  | -2.209301 |
| H  | -6.568348  | 3.105187  | -1.817972 |
| H  | -4.672825  | 4.694856  | -2.209301 |
| H  | -6.568348  | 3.105187  | -1.817972 |
| H  | -4.672825  | 4.694856  | -2.209301 |
| H  | -6.568348  | 3.105187  | -1.817972 |
| H  | -4.672825  | 4.694856  | -2.209301 |
| H  | -6.568348  | 3.105187  | -1.817972 |
| H  | -4.672825  | 4.694856  | -2.209301 |
| H  | -6.568348  | 3.105187  | -1.817972 |
| H  | -4.672825  | 4.694856  | -2.209301 |

**space group C2, model 2, reactant13b (heteroatoms frozen, free hydrogens)**
Zero-point correction= 0.687576 (Hartree/Particle)
Thermal correction to Energy= 0.726710
Thermal correction to Enthalpy= 0.727655
Thermal correction to Gibbs Free Energy= 0.615262

Sum of electronic and zero-point Energies= -1993.602522
Sum of electronic and thermal Energies= -1993.563388
Sum of electronic and thermal Enthalpies= -1993.562444
Sum of electronic and thermal Free Energies= -1993.674837

SOLVENT: -2005.3734451

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SCF Done: -1994.29009845 A.U.

O     -3.679237     0.974483     2.117668
C     -3.651450     1.075902     0.871109
O     -4.616451     0.670413     0.015388
C     -5.954408     0.159438     0.543372
C     -6.688565     1.371915     1.211112
C     -7.602744     -0.363778    -0.741626
C     -5.767520    -0.954934     1.582195
N     -2.588971     1.587463     0.168031
C     -1.367379     1.978083     0.715828
C     -0.328742     2.088579    -0.292999
O     -0.543896     1.845720    -1.520139
C     -1.092780     2.193723     2.043797
C     -0.228078     2.527887     2.443619
C     -0.221177     2.609549     1.511726
N     -0.947337     2.415963     0.173343
C     -2.048779     2.550715    -0.853428
C     -3.269421     3.204338    -0.506125
C     -2.923437     -0.363778    -1.625362
C     -1.596682    -1.333322    -1.625362
C     -0.628114    -1.987031    -2.635610
C     -0.785423    -1.376943    -2.575628
C     -1.379211    -2.278855    -3.397447
O     -1.441616    -2.822916    -4.473373
N     -2.903895    -2.866568    -2.709866
C     -2.955625    -1.573245    -1.484021
C     -1.445472    -1.343304    -1.853452
C     -3.067099    -1.893839    -1.836858
O     -3.784944    -1.554972    -2.720242
C     -3.286863    -2.494934    -0.757440
O     -3.063372    -4.179362    -0.895349
N     -3.678819    -2.319802     0.361457
C     -3.979406    -2.968161     1.677623
C     -2.709563    -2.515328    -2.652256
C     -2.164086    -1.225077    -2.599502
C     -1.268243    -0.792200     3.583307
C     -0.897602    -1.656930     4.624697
C     -1.416238    -2.955475     4.662459
C     -2.313036    -3.381231     3.680736
C     -1.885546     2.081100     2.766020
H     -0.453536     2.716348     3.484079
H     -2.244352     2.831452     1.766579
C     -1.597451     2.683351    -1.786694
C     -3.762609     2.801983     0.384565
C     -3.981117     3.070279    -1.331148
H     -4.917570     5.340097    -1.144951
C     -4.016595     6.626240    -0.207988
C     -1.970480     6.248530    -1.665258
H     -2.877712     4.962810    -2.597553
H     -0.815689     6.060739    -2.165031
C     -1.278455    -1.600407    -0.609884
C     -0.575971    -3.054732    -2.390397
H     -1.025792    -1.910533    -3.650316
H     -0.803308    -3.710195    -3.015596
C     -3.629169    -3.054565    -3.018680
H     -3.853088    -0.630194    -1.644642
C     -3.431132    -2.107616    -0.664077
H     -1.093467    -2.193717    -0.604314
C     -1.259872    -0.421192    -0.643522
H     -3.742221    -1.290434     0.299448
H     -3.747303    -4.046946     1.526003
H     -4.779020    -2.723938     2.099448
H     -2.448458    -0.535455     1.813818
C     -0.881356     0.213980     3.537752
C     -0.210989    -1.322438     1.594010
C     -1.116253    -3.637951     5.448776
C     -2.701006    -4.393143     3.707810
C     -5.472952    -0.530085     2.543799
C     -4.998204    -1.664928    -1.270461
H     -6.721210    -1.482073     1.691304
H     -6.638782    -0.431662    -1.490902
H     -7.615770    -0.708396    -0.525689
H     -6.014082    -1.197526    -1.137995
H     -6.786725     2.152262     0.359343
space group C2, model 2 (simplified), reactantM (heteroatoms frozen, free hydrogens)

Zero-point correction=  0.850960 (Hartree/Particle)
Thermal correction to Energy=  0.901970
Thermal correction to Enthalpy=  0.902915
Thermal correction to Gibbs Free Energy=  0.765211
Sum of electronic and zero-point Energies=  -2950.856095
Sum of electronic and thermal Energies=  -2950.805084
Sum of electronic and thermal Enthalpies=  -2950.804140
Sum of electronic and thermal Free Energies=  -2950.941843

SOLVENT:  -2967.7976381

| H     | -7.685523 | 1.068865 | 1.454474 |
|-------|-----------|---------|----------|
| H     | -6.129405 | 1.763186 | 1.976065 |
| H     | -2.608109 | 1.566222 | -0.852785|
| H     | 2.277468  | 4.932490 | 0.457382 |

| C     | -1.133776 | 4.604998 | 0.752564 |
|-------|-----------|---------|----------|
| C     | -0.304201 | 4.450017 | 2.081744 |
| C     | 0.858986  | 3.502944 | 1.865069 |
| C     | 0.605664  | 2.133643 | 1.754364 |
| C     | 1.627468  | 1.256255 | 1.416207 |
| C     | 2.934588  | 1.708488 | 1.247456 |
| C     | 2.169269  | 3.967329 | 1.669102 |
| C     | 3.205287  | 3.075238 | 1.380394 |
| C     | -2.373236 | 3.677181 | 0.707399 |
| O     | -3.494364 | 4.045892 | 1.187507 |
| H     | -0.477384 | 4.443921 | -1.06234 |
| C     | -0.958919 | 4.055892 | 2.863170 |
| C     | 0.063160  | 5.438096 | 2.377955 |
| C     | -0.388549 | 1.769010 | 1.945541 |
| C     | 1.359459  | 2.255959 | 1.261518 |
| C     | 3.752210  | 1.044874 | 0.996035 |
| C     | 2.374536  | 5.031002 | 1.746409 |
| H     | -2.719930 | 2.370061 | 0.101343 |
| C     | -3.355293 | 1.654376 | -0.199271|
| C     | -3.490630 | 1.487362 | -1.74952 |
| C     | -3.654770 | 2.834562 | -2.479418|
| C     | -3.812898 | 2.561579 | -3.991132|
| C     | -4.858971 | 3.639220 | -1.931415|
| C     | -3.335570 | 0.236437 | 0.354175 |
| O     | -2.285739 | -0.464565 | 0.529515 |
| O     | -1.824040 | 2.142608 | -0.296094|
| O     | -4.216759 | 2.182000 | 0.208151 |
| O     | -4.37728 | 0.824063 | -1.957999|
| O     | -2.575655 | 0.991474 | -2.087456|
| N     | -2.741235 | 3.419196 | -2.316919|
| O     | -4.680866 | 3.967972 | -0.908137|
| C     | -5.023617 | 4.529080 | -2.556635|
| C     | -5.768345 | 3.024911 | -1.975258|
| C     | -2.961344 | 1.986643 | -4.376663|
| C     | -4.728713 | 1.986161 | -4.174624|
| C     | -3.878168 | 3.503271 | -4.547327|
| N     | -4.555373 | -0.303694 | 0.482654|
| C     | -4.762079 | -1.755048 | 0.621423|
| C     | -6.285465 | -2.027338 | 0.632108 |
| O     | -7.096218 | -1.075843 | 1.499075 |
| O     | -7.086774 | 0.164905 | 1.241944 |
| O     | -7.809456 | -1.633177 | 2.491147 |
| O     | -4.230626 | -2.439200 | -0.659922 |
| O     | -4.728714 | -2.162551 | -1.764561|
| N     | -5.421234 | 0.255910 | 0.480488 |
| C     | -4.268848 | -2.135147 | 1.518629 |
| C     | -6.453099 | -3.071062 | 0.882551 |
| O     | -6.605174 | -1.858884 | -0.403337 |
| O     | -8.440659 | -1.079877 | 3.078709 |
| N     | -7.739508 | -2.631511 | 2.661712 |
| C     | -3.255711 | -3.364653 | -0.459657 |
| C     | 2.623883 | -0.001532 | -1.614032|
| C     | -1.254412 | -3.405306 | -1.964887|
| O     | -0.534299 | -3.921819 | -2.832266|
| C     | -2.720384 | -3.400095 | 0.417615 |
| C     | -2.488267 | -5.074338 | -1.451902 |
| O     | -3.823229 | -3.847022 | -2.472938|
| N     | -0.930437 | -2.268615 | -2.179066|
| C     | -2.93967 | -1.565412 | -2.60549 |
| C     | 0.094974 | -0.078100 | -1.975374 |
| O     | -0.296356 | 0.700721 | -0.789036|
| C     | 1.369303 | -1.620705 | -0.552492 |
| O     | 2.490522 | -1.104843 | -0.825434 |
| C     | -1.570817 | -1.844001 | -0.600965 |
| O     | 0.698887 | -2.080735 | -2.498535|
| H     | -0.737262 | -0.043357 | -2.740581|
| H     | 0.976459 | 0.338836 | -2.377684|
| H     | -0.943629 | 0.168829 | -0.240235|
space group C2, model 2 (simplified), 13b

Zero-point correction=                           0.689702 (Hartree/Particle)
Thermal correction to Energy=                    0.729732
Thermal correction to Enthalpy=                  0.730676
Thermal correction to Gibbs Free Energy=         0.616237
Sum of electronic and zero-point Energies=          -1993.624508
Sum of electronic and thermal Energies=             -1993.584478
Sum of electronic and thermal Enthalpies=           -1993.583534
Sum of electronic and thermal Free Energies=        -1993.697972

SOLVENT: -2005.3851379

| N | 1.139577 | -2.160075 | 0.654115 |
| C | 2.265907 | -2.125922 | 1.607265 |
| C | 3.419163 | -3.092505 | 0.321363 |
| H | 0.247798 | -2.395100 | 0.903917 |
| H | 2.712322 | -1.316453 | 3.048629 |
| C | 3.486640 | -2.865903 | 1.004874 |
| O | 3.419163 | -3.892505 | 0.321363 |
| H | 2.575025 | -1.084181 | 1.693862 |
| H | 2.712322 | -3.164653 | 3.454629 |
| H | 1.033261 | -3.319578 | 2.955679 |
| N | 4.649864 | -2.193233 | 1.287840 |
| C | 5.876506 | -2.432352 | 0.521850 |
| C | 6.224698 | -1.222685 | -0.377693 |
| O | 7.394273 | -0.933302 | -0.683674 |
| H | 4.609103 | -1.326265 | 1.816759 |
| H | 5.677403 | -3.310262 | -0.099799 |
| H | 6.739878 | -2.624799 | 1.161814 |
| C | 7.394273 | -0.933302 | -0.683674 |
| C | 6.224698 | -1.222685 | -0.377693 |
| O | 7.394273 | -0.933302 | -0.683674 |
| H | 4.609103 | -1.326265 | 1.816759 |
| H | 5.677403 | -3.310262 | -0.099799 |
| H | 6.739878 | -2.624799 | 1.161814 |
| C | 7.394273 | -0.933302 | -0.683674 |
| C | 6.224698 | -1.222685 | -0.377693 |
| O | 7.394273 | -0.933302 | -0.683674 |
| H | 4.609103 | -1.326265 | 1.816759 |
| H | 5.677403 | -3.310262 | -0.099799 |
| H | 6.739878 | -2.624799 | 1.161814 |
| C | 7.394273 | -0.933302 | -0.683674 |
| C | 6.224698 | -1.222685 | -0.377693 |
| O | 7.394273 | -0.933302 | -0.683674 |
| H | 4.609103 | -1.326265 | 1.816759 |
| H | 5.677403 | -3.310262 | -0.099799 |
| H | 6.739878 | -2.624799 | 1.161814 |
| C | 7.394273 | -0.933302 | -0.683674 |
| C | 6.224698 | -1.222685 | -0.377693 |
| O | 7.394273 | -0.933302 | -0.683674 |
| H | 4.609103 | -1.326265 | 1.816759 |
| H | 5.677403 | -3.310262 | -0.099799 |
| H | 6.739878 | -2.624799 | 1.161814 |

S47
| Atom | x    | y    | z    |
|------|------|------|------|
| C    | 2.110189 | -3.004618 | 2.912013 |
| C    | 2.614461  | -3.938796  | 2.002968 |
| C    | 3.660476  | -3.589169  | 1.144468 |
| H    | -6.609651 | -0.021377  | 1.399065 |
| H    | -7.367939 | 0.823391   | 0.023105 |
| H    | -7.933507 | -0.802475  | 0.483035 |
| H    | -7.428656 | -1.566505  | -1.992262 |
| H    | -6.859917 | 0.091597   | -2.332552 |
| H    | -5.777988 | -1.294084  | -2.618147 |
| H    | -5.113245 | -2.003653  | 0.980335 |
| H    | -6.333769 | -2.853764  | -0.008870 |
| H    | -4.718947 | -2.492697  | -0.696560 |
| H    | -2.746230 | 1.584236   | 2.571698 |
| H    | -0.595280 | 2.384445   | 3.630908 |
| H    | 1.336758  | 2.932947   | 2.168223 |
| H    | 1.064671  | 3.119686   | -1.451010 |
| H    | 3.282350  | 3.873025   | -0.691786 |
| H    | 2.950100  | 3.409856   | 0.957083 |
| H    | 1.078060  | 5.201417   | 1.026124 |
| H    | 3.748369  | 6.250978   | -0.186645 |
| H    | 2.522044  | 7.244217   | 0.738076 |

**Zero-point correction= 0.852584 (Hartree/Particle)**
**Thermal correction to Energy= 0.905329**
**Thermal correction to Enthalpy= 0.906273**
**Thermal correction to Gibbs Free Energy= 0.765818**

**Sum of electronic and zero-point Energies= -2950.903797**
**Sum of electronic and thermal Energies= -2950.851052**
**Sum of electronic and thermal Enthalpies= -2950.851008**
**Sum of electronic and thermal Free Energies= -2950.990563**

**SOLVENT: -2967.8038553**
|   |    X     |    Y     |    Z    |
|---|---------|---------|--------|
|H | 4.552394 | 4.366793 | -0.269925 |
|H | 5.029365 | 5.486240 | 1.021077 |
|H | 5.855788 | 3.921810 | 0.866703 |
|H | 3.527221 | 3.599702 | 3.892386 |
|H | 5.240880 | 3.630251 | 3.412482 |
|H | 4.289393 | 5.131755 | 3.406753 |
|N | 4.413740 | -0.254053 | -0.305405 |
|C | 4.468103 | -1.721018 | -0.243686 |
|C | 5.909331 | -2.128592 | 0.164129 |
|C | 6.991171 | -1.764464 | 1.193728 |
|O | 6.958759 | 1.887547 | -1.647282 |
|N | 8.006795 | -3.270829 | 0.835347 |
|C | 1.934327 | -3.843051 | 1.687528 |
|C | 0.618721 | -3.085381 | 1.923015 |
|O | -0.495973 | -3.621778 | 1.858277 |
|H | 2.478265 | -4.155549 | -0.364103 |
|H | 1.681837 | -4.870762 | 1.430732 |
|H | 2.546010 | -3.807444 | 2.593527 |
|N | 0.778318 | -1.742022 | 1.858277 |
|C | -0.177164 | 0.540777 | 2.581843 |
|C | 0.564765 | 1.254243 | 1.528577 |
|C | -1.186718 | -0.998831 | 0.872856 |
|O | -2.242110 | -0.779610 | 0.846030 |
|H | 1.710296 | -1.356670 | 2.308221 |
|H | -1.140871 | -1.346791 | 2.943408 |
|H | 0.359674 | 0.579281 | 3.524562 |
|H | -1.159279 | 1.009715 | 2.688145 |
|N | 1.134518 | 0.612455 | 0.979971 |
|N | -0.464470 | -1.235610 | -0.230430 |
|C | -1.080283 | -1.359984 | -1.566828 |
|C | -0.264943 | -2.356680 | -2.413462 |
|C | 1.528674 | -1.988851 | -2.592118 |
|C | -2.482457 | -2.025677 | -1.443721 |
|O | -2.530131 | -3.220110 | -1.125065 |
|H | 0.553312 | -1.261077 | -0.147617 |
|H | -1.154732 | -0.379567 | -2.037966 |
|H | -0.704439 | -2.395327 | -3.413191 |
|H | -0.369784 | -3.30742 | -1.932237 |
|N | -3.539240 | -1.243883 | -1.809981 |
|C | -4.889901 | -1.794918 | -1.699237 |
|C | -5.696101 | -1.687684 | -0.458034 |
|O | -6.843417 | -1.848666 | -0.285591 |
|H | -3.419667 | -2.503535 | -2.000389 |
|H | -4.790201 | -2.882036 | -1.661732 |
|H | -5.490242 | -1.523205 | -2.573073 |
|N | -5.113744 | -0.451237 | 0.344470 |
|C | -5.830039 | 0.909715 | 1.526729 |
|C | -4.930979 | 0.990770 | 2.411036 |
|O | -3.631211 | 0.475500 | 2.805311 |
|C | -6.980160 | 0.999845 | 0.994282 |
|O | -6.828951 | 2.228944 | 0.831975 |
|H | -4.115997 | -0.273908 | 0.232870 |
|H | -6.248044 | -0.747056 | 2.091681 |
|H | -5.493619 | 1.193209 | 3.328532 |
|H | -8.408330 | 1.941297 | 1.879418 |
|H | -3.245256 | -0.122785 | 2.092876 |
|N | -8.133840 | 0.319772 | 0.699434 |
|H | -8.875737 | 0.840771 | 0.274113 |
|H | -8.020795 | -0.689530 | 0.522714 |
|H | 1.734165 | -2.692614 | -3.662188 |
|H | 0.733932 | 4.010515 | -2.965116 |

**space group C2, model 2 (simplified), reactant complex**

| 1 | 1.547764 (Hartree/Particle) |
|---|-----------------------------|
| 2 | 1.640944 |
| 3 | 1.641888 |

**Zero-point correction=**

**Thermal correction to Energy=**

**Thermal correction to Enthalpy=**

**S49**
Thermal correction to Gibbs Free Energy= 1.417189
Sum of electronic and zero-point Energies= -4944.624252
Sum of electronic and thermal Energies= -4944.531072
Sum of electronic and thermal Enthalpies= -4944.530128
Sum of electronic and thermal Free Energies= -4944.754827

SOLVENT: -4973.2479718
|     | O     | -9.74343 | -2.755105 | -0.653625 |
|-----|-------|----------|-----------|-----------|
| H   | -6.074659 | -3.130022 | -1.447469 |
| H   | -7.582620 | -4.151965 | 0.884475  |
| H   | -8.015466 | 1.038289  | -0.686137 |
| N   | -7.915400 | -1.444100 | -0.174978 |
| C   | -8.682540 | -0.217029 | -0.347086 |
| C   | -7.810329 | 1.022577  | -0.001764 |
| O   | -7.400454 | 1.044316  | 1.393436  |
| C   | -9.106819 | -0.087341 | -1.818814 |
| O   | -8.390482 | -0.460364 | -2.762596 |
| H   | -6.938131 | -0.235294 | 0.303643  |
| H   | -8.415677 | 1.916057  | -0.775754 |
| H   | -6.954666 | 1.038289  | -0.686137 |
| N   | -10.287584 | 0.571970 | -1.989389 |
| H   | -10.621705 | 0.730162 | -2.933783 |
| H   | -10.917389 | 0.742914 | -2.154757 |
| O   | 7.098367 | 2.241378  | -0.131981 |
| C   | 6.453102 | 2.129888  | -1.197894 |
| O   | 5.924381 | 3.142715  | -1.921203 |
| C   | 6.214930 | 4.594028  | -1.547498 |
| C   | 6.787300 | 4.846204  | -1.885889 |
| C   | 5.259644 | 5.338059  | -2.482819 |
| C   | 5.901895 | 4.748733  | -0.071333 |
| N   | 6.140965 | 0.927154  | -1.781741 |
| C   | 6.408055 | -0.330033 | -1.240580 |
| C   | 5.619602 | -1.373382 | -0.817126 |
| O   | 4.789988 | -1.130832 | -2.800899 |
| C   | 7.255187 | -0.613723 | -0.199922 |
| C   | 7.369262 | -1.947708 | 0.237220  |
| C   | 6.615284 | -2.935137 | -0.290053 |
| N   | 5.776354 | -2.660748 | -1.350543 |
| C   | 4.824316 | -3.697733 | -1.899037 |
| C   | 5.332756 | -5.133830 | -1.753497 |
| C   | 6.634791 | -5.353633 | -2.495405 |
| C   | 6.901218 | -6.720033 | -3.112546 |
| C   | 6.573974 | -5.521154 | -4.009905 |
| C   | 3.546210 | -3.461900 | -1.070787 |
| O   | 3.368652 | -4.065652 | 0.022787  |
| C   | 2.739194 | -2.501906 | -1.555712 |
| C   | 1.679724 | -1.939005 | -0.709745 |
| C   | 0.872844 | -0.836564 | -1.430682 |
| C   | 1.777291 | 0.250187  | -2.042923 |
| C   | 0.884680 | 1.438486  | -2.475288 |
| O   | -0.236116 | 1.323117  | -3.009983 |
| N   | 1.526132 | 2.585311  | -2.140615 |
| C   | 2.869078 | 2.378231  | -1.574577 |
| C   | 2.788100 | 0.903567  | -1.083346 |
| C   | 0.725732 | -3.046381 | -2.470616 |
| C   | 0.259828 | -3.926605 | -0.958548 |
| C   | 0.459765 | -2.874421 | 1.250839  |
| O   | -0.504189 | -2.213674 | 1.727269  |
| N   | 1.471695 | -3.427139 | 1.936864  |
| C   | 1.694215 | -3.245545 | 3.379013  |
| C   | 2.910215 | -2.367223 | 3.676104  |
| C   | 4.025991 | -2.342781 | 2.827857  |
| C   | 4.173945 | -1.632477 | 3.194244  |
| C   | 5.215925 | -0.929002 | 4.402212  |
| C   | 4.092796 | -0.926542 | 5.236000  |
| C   | 2.947774 | -1.637991 | 4.872600  |
| H   | 7.811187 | 0.191309  | 0.257112  |
| H   | 8.047044 | -2.186792 | 1.081406  |
| H   | 6.641463 | -3.958662 | 0.051226  |
| H   | 4.671907 | -3.438702 | -2.936353 |
| H   | 5.394717 | -5.407458 | -6.695319 |
| H   | 4.552888 | -5.775949 | -2.187270 |
| H   | 6.138890 | -7.489049 | -2.989272 |
| H   | 7.920359 | -7.087098 | -3.112035 |
| H   | 7.374991 | -5.104936 | -4.664179 |
| H   | 5.594749 | -5.304568 | -4.476289 |
| H   | 3.082123 | -1.956355 | -2.352325 |
| H   | 2.147575 | -1.305446 | 0.182925  |
| H   | 0.208409 | -0.381123 | -0.686352 |
| H   | 0.236471 | -1.272880 | -2.204125 |
| H   | 2.302667 | -0.124013 | -2.931606 |
| H   | 1.041786 | 3.494380  | -2.221388 |
| H   | 3.650713 | 2.512827  | -2.327212 |
| H   | 3.064084 | 3.049480  | -0.746992 |
| H   | 2.368472 | 0.915409  | -0.079234 |
space group C2, model 2 (simplified), reactant complex+H₂O

Zero-point correction= 1.573617 (Hartree/Particle)
Thermal correction to Energy= 1.668392
Thermal correction to Enthalpy= 1.669336
Thermal correction to Gibbs Free Energy= 1.442009

Sum of electronic and zero-point Energies= -5020.636784
Sum of electronic and thermal Energies= -5020.542009
Sum of electronic and thermal Enthalpies= -5020.541065
Sum of electronic and thermal Free Energies= -5020.768392

SOLVENT: -5049.684828

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13SCUTGREATACTANT+H2O SCF Done: -5022.21040097 A.U.

C     -3.211050     3.143907    -1.246686
C     -2.922221     3.661172    -2.675985
C     -3.975910     3.161102    -3.642531
C     -3.882761     1.864241    -4.172258
C     -4.877575     1.374315    -5.021350
C     -5.971610     2.176957    -5.368262
C     -5.080914     3.952636    -3.983929
C     -6.068225     3.471332    -4.848395
C     -2.052052     3.481067    -0.312991
O     -1.167758     4.331165    -0.620820
H     -3.350992     2.056173    -1.258862
H     -1.933746     3.297519    -2.968238
C     -2.888089     4.754994    -2.662444
C     -3.032300     2.137089    -3.928686
C     -4.812465     3.588545    -5.394476
H     -6.743954     1.791398    -6.023889
H     -5.161210     4.954915    -3.575411
H     -6.912745     4.099210    -5.109822
N     -2.036852     2.783622     0.846747
C     -0.902152     2.836242     1.764785
C     -1.292670     3.460951     3.137969
C     -1.882741     4.882348     3.009468
C     -2.249731     5.397594     4.418517
C     -0.897251     5.848862     2.313880
C     -0.361050     4.426169     2.037409
O     -1.030522     0.362634     1.866651
H     -2.821045     2.146294     1.095246
H     -0.162886     3.436488     1.285765
H     -0.403014     3.486177     3.773536
H     -2.028903     2.799104     3.606988
H     -2.795533     4.816450     2.405000
H     -0.760261     5.575810     1.263660
H     -1.286623     6.872818     2.352711
H     0.077265     5.833922     2.829942
H     -2.949226     4.171741     4.918327
H     -1.346450     5.481229     5.035839
H     -2.715363     6.387251     4.356478
N     0.882120     1.386364     2.540373
N     0.543425     0.108886     2.883743
C     2.975642     0.418336     3.367556
C     3.745232     1.419294     2.519591
O     2.377219     2.568798     2.294471
O     9.437355     0.990962     2.065691
C     0.827525     -0.553623     4.088395
O     0.935598     -0.070301     5.229610
H     1.508772     2.205411     2.566075
H     1.533058     -0.552297     2.013158
H     3.510333     -0.318970     3.487671
H     2.844550     0.862831     4.362291
H     5.574093     1.018215     1.556196
space group C2, model 2 (simplified), transition state Mpro (deformation of the fragment)
| Atom | x    | y    | z    |
|------|------|------|------|
| C    | 3.505486 | 2.996911 | 1.783434 |
| C    | 2.107142 | 3.656833 | 1.012211 |
| O    | -0.165986 | 4.293438 | 0.281882 |
| C    | -0.741651 | 3.656833 | 3.179552 |
| C    | 0.266743 | 5.162129 | 2.891193 |
| C    | -0.819996 | 1.553306 | 2.011415 |
| C    | 1.767897 | 0.143081 | 1.216855 |
| C    | 4.119290 | 1.048261 | 1.166060 |
| O    | 2.604853 | 4.874661 | 2.342909 |
| C    | 4.516512 | 3.758959 | 1.700533 |
| C    | -2.043347 | 2.502001 | 0.298606 |
| C    | 3.892466 | 1.806025 | -0.070556 |
| C    | -3.00215 | 0.315378 | 0.286101 |
| H    | -0.269550 | -0.420188 | 0.440702 |
| C    | 1.161053 | 2.141077 | -0.112254 |
| C    | -4.090303 | 2.301135 | 0.449200 |
| C    | -4.407919 | 1.344997 | -1.871237 |
| C    | -2.648491 | 1.355156 | -2.090025 |
| C    | -2.598841 | 3.819039 | -1.920541 |
| C    | -4.878533 | 4.289292 | -0.409199 |
| C    | -4.798012 | 5.106701 | -1.948790 |
| C    | -5.645236 | 3.591705 | -1.587719 |
| C    | -2.946493 | 2.724849 | -4.162015 |
| C    | -4.702751 | 2.803839 | -3.921000 |
| C    | -3.760705 | 4.304221 | -4.087989 |
| N    | -4.531163 | -0.210216 | 0.297806 |
| C    | -4.786214 | -1.662078 | 0.390493 |
| C    | -6.315740 | -1.880173 | 0.422776 |
| C    | -7.079870 | -0.920994 | 1.319532 |
| C    | -7.019038 | 0.328887 | 1.109686 |
| O    | -7.826270 | -1.474728 | 2.288304 |
| C    | -8.493930 | -2.343646 | -0.906354 |
| O    | -8.850204 | -2.107690 | -1.933273 |
| H    | -5.385263 | 0.770784 | 0.329613 |
| H    | -4.289560 | -2.077628 | 1.270140 |
| H    | -6.515979 | -2.920340 | 0.666992 |
| H    | -6.646242 | -1.689508 | -0.605843 |
| H    | -8.434970 | -0.909033 | 2.889112 |
| H    | -7.804742 | -2.478599 | 2.432131 |
| N    | -3.265483 | -3.216663 | -0.740691 |
| C    | -2.633323 | -3.816267 | -1.912206 |
| C    | -1.70245 | -3.190692 | -2.240950 |
| O    | -0.519633 | -3.678313 | -3.098210 |
| H    | -2.750596 | -3.292614 | 0.145761 |
| H    | -2.492649 | -4.891519 | -1.787497 |
| H    | -3.300421 | -3.648030 | -2.762809 |
| H    | -0.986200 | -2.058388 | -1.523897 |
| C    | 0.256502 | -1.349100 | -1.779852 |
| C    | 0.063569 | 0.179106 | -1.907937 |
| O    | -0.157815 | 0.776742 | -0.591118 |
| C    | 1.308088 | -1.572285 | -0.704706 |
| H    | 2.454649 | -1.075715 | -0.882588 |
| H    | 1.645841 | -1.669942 | -0.849039 |
| C    | 0.665302 | -1.755732 | -2.711265 |
| H    | -0.767910 | 0.364410 | -2.601162 |
| O    | 0.985284 | 0.613933 | -2.299742 |
| H    | -0.66129 | 0.242413 | -0.880848 |
| N    | 0.997502 | -2.51916 | 0.407062 |
| C    | 2.034122 | -2.473424 | 1.433443 |
| C    | 1.546598 | -3.553312 | 2.415201 |
| S    | 0.545270 | -2.840433 | 3.776065 |
| C    | 3.349592 | -2.955860 | 0.773888 |
| O    | 3.396723 | -3.939307 | 0.025436 |
| H    | 0.059583 | -2.628302 | 0.569012 |
| H    | 2.215546 | -1.544213 | 1.976679 |
| H    | 2.411720 | -4.010154 | 2.907233 |
| H    | 1.004108 | -4.329910 | 1.871597 |
| N    | 4.433381 | -2.212468 | 1.575459 |
| C    | 5.736345 | -2.376675 | 0.503854 |
| C    | 6.142601 | -1.143389 | -0.331308 |
| O    | 7.325977 | -0.890283 | -0.609901 |
| H    | 4.299066 | -1.777897 | 1.720633 |
| H    | 5.634619 | -3.244546 | -0.154960 |
| H    | 6.536899 | -2.564333 | 1.225418 |
| N    | 5.900713 | -0.399363 | -0.750506 |
space group C2, model 2 (simplified), transition state

Zero-point correction= 1.544558 (Hartree/Particle)
Thermal correction to Energy= 1.636487
Thermal correction to Enthalpy= 1.637431
Thermal correction to Gibbs Free Energy= 1.416402

Sum of electronic and zero-point Energies= -4944.578218
Sum of electronic and thermal Energies= -4944.486289
Sum of electronic and thermal Enthalpies= -4944.485345
Sum of electronic and thermal Free Energies= -4944.706374

SOLVENT: -4973.189562

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SCUTgTS SCF Done: -4946.12277591 A.U.

S57
space group C2, model 2 (simplified), transition state+1H2O 13b (deformation of the fragment)

Zero-point correction= 0.681447 (Hartree/Particle)
Thermal correction to Energy= 0.716803
Thermal correction to Enthalpy= 0.717748
Thermal correction to Gibbs Free Energy= 0.613932
Sum of electronic and zero-point Energies= -1992.936741
Sum of electronic and thermal Energies= -1992.901385
Sum of electronic and thermal Enthalpies= -1992.900441
Sum of electronic and thermal Free Energies= -1993.004256

SOLVENT: -2004.8000119

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13SCUTgTS+1H2OF1 SCF Done: -1993.61818811
A.U.
O 1.611840 -1.904203 3.915306
C 1.980821 -2.430185 2.819751
O 3.146965 -2.849112 2.452932
C 5.712032 0.004530 -0.383437
C 5.408299 -1.057691 0.678260
C 6.903028 -3.799883 -1.264895
C 5.879178 1.404274 0.224831
N 1.020225 -2.630163 1.796429
O -0.324290 -2.244549 1.801244
C -0.908681 -2.266849 0.471098
O -0.261818 -2.817785 -0.559669
C -1.053690 -1.841613 2.891946
C -2.401320 -1.426905 2.725820
C -2.951287 -1.395706 1.477951
N -2.232774 -1.820913 0.381468
C -2.747921 -1.597535 -1.017585
C -4.269608 -1.878000 -1.135738
C -4.799844 -3.056060 -0.695746
C -6.043588 -3.590453 -1.376618
C -6.674470 -4.205416 -1.666484
C -2.226487 -0.181622 -1.329519
O -0.291359 0.809630 -0.949902
N -0.986221 -0.158634 -1.844944
C -0.116669 1.029405 -1.889871
| Element | X  | Y  | Z   |
|---------|----|----|-----|
| C       | 1.274914 | 0.590761 | -2.342091 |
| C       | 1.958493  | -0.471274 | -1.461047 |
| C       | 3.319559  | -0.730025 | -2.131203 |
| O       | 3.484720  | -0.829977 | -3.360046 |
| N       | 4.279122  | -0.741086 | -1.176904 |
| C       | 3.762872  | -0.581050 | 0.195603  |
| C       | 2.332967  | -0.000481 | -0.042706 |
| C       | -0.788769 | 2.140854  | -2.812600 |
| O       | -1.827095 | 1.789005  | -3.590494 |
| N       | -0.916969 | 3.435200  | -1.966412 |
| C       | -3.232967 | 4.387351  | -1.959174 |
| C       | -1.992533 | 3.361328  | -1.173877 |
| C       | -2.464624 | 4.342964  | -0.108275 |
| C       | -1.821610 | 3.849938  | 1.275873  |
| C       | -1.988044 | 2.510838  | 1.654145  |
| C       | -1.722714 | 2.112909  | 2.968129  |
| C       | -1.285190 | 3.045791  | 3.916082  |
| C       | -1.083160 | 4.374166  | 3.531969  |
| C       | -1.343769 | 4.770911  | 2.218654  |
| H       | -0.579210 | -1.823153 | 3.860043  |
| H       | -2.991431 | -1.225382 | 3.579880  |
| H       | -3.952831 | -1.104651 | 2.88794  |
| H       | -2.667589 | -2.356636 | -1.631283 |
| H       | -4.730560 | -0.853027 | -0.597253 |
| H       | -4.505180 | -1.529436 | -2.196420 |
| H       | -6.499880 | -2.986755 | -2.153483 |
| H       | -6.738021 | -1.614752 | -0.775438 |
| H       | -4.462645 | -5.186483 | -1.259374 |
| H       | -4.229535 | -0.002333 | -2.635197 |
| H       | -0.539013 | -1.059778 | -2.080845 |
| H       | -0.059626 | 1.451447  | -0.877320 |
| H       | 1.918645  | 1.476717  | -2.351984 |
| H       | 1.205539  | 0.191118  | -3.359172 |
| H       | 1.388224  | -1.403477 | -1.413435 |
| H       | 5.249921  | -0.615679 | -1.469872 |
| H       | 3.713165  | -1.538339 | 0.717008  |
| H       | 4.368227  | 1.08214  | 0.780563  |
| H       | 2.400661  | 1.085769  | -0.030395 |
| H       | 1.629407  | -0.316357 | 0.727003  |
| H       | -2.543729 | 2.483946  | -1.211528 |
| H       | -1.707540 | 5.257797  | -0.364031 |
| H       | -3.319588 | 4.562273  | -0.094090 |
| H       | -2.351121 | 1.783974  | 0.937899  |
| H       | -1.882711 | 1.076341  | 3.241796  |
| H       | -1.104166 | 2.739469  | 4.940772  |
| H       | -0.719346 | 5.099114  | 4.250848  |
| H       | -1.172374 | 5.790027  | 1.922970  |
| H       | 5.770844  | 2.189181  | -0.527953 |
| H       | 6.879758  | 1.468771  | 0.665816  |
| H       | 5.133039  | 1.574334  | 1.008875  |
| H       | 7.075740  | 0.392368  | -2.038704 |
| H       | 6.071740  | -1.329049 | -1.768728 |
| H       | 7.797387  | -0.481331 | -0.643041 |
| H       | 5.282424  | -2.036670 | 0.206170  |
| H       | 6.239061  | -1.106112 | 1.388342  |
| H       | 4.494873  | -0.787360 | 1.213819  |
| H       | 1.354906  | -2.995129 | 0.903455  |
| H       | -4.675868 | -3.267820 | 0.356573  |

space group C2, model 2 (simplified), transition state+1H2O Mpro (deformation of the fragment)

**Zero-point correction** = 0.851204 (Hartree/Particle)
**Thermal correction to Energy** = 0.901195
**Thermal correction to Enthalpy** = 0.902139
**Thermal correction to Gibbs Free Energy** = 0.767269

Sum of electronic and zero-point Energies = -2950.861845
Sum of electronic and thermal Energies = -2950.811854
Sum of electronic and thermal Enthalpies = -2950.810910
Sum of electronic and thermal Free Energies = -2950.945780

**SOLVENT:** -2967.7839368
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H  -1.145589   5.520704   0.862035
H  -1.177747   3.401442  -2.946344
H  -3.158699   2.919587  -3.578085
H  -5.383755   3.926790  -2.948634
H  -3.535436   5.731046   0.494673
H  -5.538954   5.347068  -0.916961
N   1.535208   2.084492   0.837711
C   2.947619   1.725562   0.745018
C   3.547995   1.326543   2.125912
C   3.383429   2.402436   3.218792
C   3.960927   1.860395   4.545295
C   4.074726   3.726113   2.822750
C   3.119982   0.507462  -0.170642
O   2.171861  -0.283344  -0.469669
H   0.857650   1.324713   1.034011
H   3.481270   2.582975   0.331022
H   4.612643   1.973111   1.992587
H   3.048212   0.404431   2.450617
H   2.310046   2.588772   3.347421
H   3.559480   4.189327   1.977387
H   4.050687   4.428761   3.663804
H   5.125874   3.539833   2.564953
H   3.475619   0.920367  -0.616260
H   5.037395   1.676678   4.439455
H   3.813686   2.587333   5.351504
N   4.360500   0.270289  -2.095632
C   4.644281  -0.896002   1.145721
C   6.100702  -0.794217  -1.983794
C   6.480245   0.578037  -2.514367
O   6.450851   1.582982  -1.745204
N   6.838858   0.627349  -3.810186
C   5.698416  -2.194594  -0.646528
O   5.336423  -2.435689   0.215200
H   5.127350   0.955642  -0.559007
H   3.925903  -0.914494  -2.309563
H   6.264058  -1.382327  -2.714787
H   6.720879  -0.998909  -1.103278
H   7.174429   1.486766  -4.254726
H   6.776061  -0.210653  -4.379315
N   3.540079  -3.023358  -0.962388
C   3.290502  -4.212688  -0.149250
C   2.057309  -4.081853   0.762106
O   1.623923  -5.039528   1.417712
H   1.783022  -2.721076  -1.593175
H   3.145663  -5.100547  -0.771761
H   4.169460  -4.361783   0.484698
N   1.909042  -2.827946   0.789971
C   0.341556  -2.567359   1.618968
C   0.341292  -1.102177   2.123456
O   0.019196  -0.182141  -1.015341
C   -0.978250  -2.706337   0.867549
O   -2.060641  -2.659492   1.520831
H   1.912076  -2.065019   0.245070
H   0.340467  -3.267579   2.457130
H   1.318098  -0.877660   2.569024
H   -0.462911  -0.954559   2.844039
H   0.695184  -0.313966   0.267782
N  -0.942434  -2.664417  -0.470859
C  -1.712726  -2.247330  -1.140444
C  -1.911796  -1.642297  -2.514002
S  -0.767875  -0.205608  -2.302284
C  -3.269885  -3.339181  -1.055226
O  -3.076506  -4.503689  -0.737003
H  -0.630268  -2.703849  -0.993747
H  -2.592280  -1.435401  -0.545742
H  -2.851316  -1.248156  -2.901949
H  -1.484042  -2.333101  -3.241691
N  -4.508302  -2.767256  -1.311882
C  -5.608271  -3.140933  -0.380099
C  -5.764605  -1.895269   0.528110
O  -6.783847  -1.190518   0.552838
H  -4.486524  -1.748669  -1.463353
H  -5.288219  -4.036681   0.159176
H  -6.553909  -3.310937  -0.893926
N  -5.872533  -1.290022   1.330568
C  -4.363687  -0.114027  1.397726
C  -2.954715  -0.137996  2.021898
O  -2.672769  -0.683613  3.188186
C  -4.345179   0.641701   0.046450
O  -4.142400   0.076769  -1.059907
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | -3.768882 | -2.146682 | 1.163647 |
| H    | -5.154860 | 0.262073 | 2.039202 |
| H    | -2.914855 | 1.180165 | 2.152678 |
| H    | -2.189391 | 0.002253 | 1.251351 |
| H    | -2.490459 | -1.602612 | 2.818344 |
| N    | -4.459009 | 1.975352 | 0.156278 |
| H    | -4.378432 | 2.561274 | -0.670507 |
| H    | -4.642986 | 2.427993 | 1.042773 |
| H    | -0.793544 | 3.353573 | 1.751144 |
| H    | -1.488316 | 0.166251 | -3.269607 |
|     |        |       |       |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |
| C    | 2.734145 | -2.217549 | -3.618291 |

**Space group C2, model 2 (simplified), transition state+1H2O**

Zero-point correction= 1.572523 (Hartree/Particle)
Thermal correction to Energy= 1.665387
Thermal correction to Gibbs Free Energy= 1.444712
Sum of electronic and zero-point Energies= -5020.619076
Sum of electronic and thermal Energies= -5020.526203
Sum of electronic and thermal Enthalpies= -5020.525259
Sum of electronic and thermal Free Energies= -5020.746878

**SOLVENT: -5049.6539818**
|  |  |  |  |
|---|---|---|---|
| C | 4.637268 | -0.412272 | 2.415336 |
| O | 5.850744 | -0.375313 | 2.059455 |
| H | 1.882423 | -1.618282 | 2.745681 |
| H | 4.677136 | -2.240046 | 3.528183 |
| H | 3.440062 | -3.489292 | 1.633710 |
| H | 5.001223 | -2.744141 | 1.122766 |
| H | 2.441087 | -1.459486 | 0.693803 |
| N | 3.812510 | 0.633483 | 2.271992 |
| C | 4.276650 | 1.713012 | 1.404609 |
| C | 3.129762 | 2.516941 | 0.807319 |
| S | 2.039525 | 1.354497 | -0.129464 |
| C | 5.404775 | 2.552031 | 2.056360 |
| O | 5.730665 | 2.473257 | 3.243553 |
| H | 2.831549 | 0.597485 | 2.563104 |
| H | 4.768504 | 1.240367 | 0.552478 |
| H | 3.540698 | 2.220995 | 0.084521 |
| H | 2.527112 | 3.059909 | 1.536520 |
| N | 6.107820 | 3.230503 | 1.080209 |
| C | 7.954572 | 3.165545 | 1.136207 |
| H | 6.864698 | 4.126269 | 0.928504 |
| N | 7.329280 | 0.969906 | 1.07173 |
| C | 6.985390 | 0.264612 | -1.118853 |
| H | 6.202214 | -1.052566 | -0.819631 |
| O | 6.856559 | -1.920406 | 0.146079 |
| C | 6.003898 | 1.136899 | -1.937435 |
| H | 5.325053 | 2.072627 | -1.432735 |
| H | 6.848726 | 0.689464 | 0.964446 |
| H | 7.886417 | 0.062879 | -1.703486 |
| H | 6.125464 | -1.615195 | -1.754183 |
| N | 5.185798 | -0.803327 | -0.499594 |
| C | 7.786533 | 1.473355 | 1.036369 |
| C | 5.853049 | 0.755357 | -3.215159 |
| H | 5.710650 | 1.218526 | -3.808054 |
| C | 6.414238 | 0.017320 | -3.624546 |
| H | 6.985856 | -1.406150 | -0.500179 |
| O | 6.329814 | -1.150528 | -1.534106 |
| C | -6.019808 | -2.038538 | -2.513842 |
| H | -6.589840 | -3.453888 | -2.464416 |
| C | -8.096152 | -3.370018 | -2.719628 |
| C | -5.853099 | -4.115849 | -3.631563 |
| C | -6.277628 | -4.141566 | -1.127588 |
| N | 5.785593 | 0.073882 | -1.817578 |
| C | -5.841410 | 1.198803 | -0.988193 |
| C | -4.890726 | 2.223570 | -1.384870 |
| O | -4.121620 | 2.100179 | -2.383529 |
| C | -6.646649 | 1.362852 | 0.111212 |
| C | -5.848487 | 2.547441 | 0.887614 |
| C | -5.628191 | 3.498780 | 0.558032 |
| N | -4.832698 | 3.351645 | -0.557710 |
| C | -3.676989 | 4.284441 | -0.814815 |
| C | -3.930139 | 5.727082 | -0.354940 |
| C | -5.135182 | 6.335956 | -1.035322 |
| C | -5.134320 | 7.833237 | -1.311796 |
| C | -4.969181 | 6.427776 | -2.464335 |
| C | -5.177669 | 5.000016 | -1.005177 |
| C | -5.404329 | 3.615188 | -0.018480 |
| O | -2.433937 | 3.682632 | 1.209816 |
| N | -1.866132 | 2.682388 | -0.711175 |
| C | -1.002703 | 1.650739 | -0.111335 |
| C | -0.604276 | 0.609262 | -1.204809 |
| C | -1.769719 | -0.045679 | -1.921329 |
| C | -1.101419 | -0.967249 | -2.957015 |
| O | -0.128129 | -0.636089 | -3.658977 |
| N | -1.920248 | -2.183680 | -2.902039 |
| C | -2.817734 | -2.262219 | -1.951996 |
| C | -2.585756 | -1.013589 | -1.043376 |
| C | 0.226047 | 3.514422 | 0.621913 |
| C | 0.400071 | 3.627911 | 0.417985 |
| C | 0.229143 | 1.865610 | 2.095602 |
| O | 0.912161 | 0.901859 | 2.544603 |
| N | -0.665657 | 2.583700 | 2.896621 |
| C | -1.037649 | 2.174158 | 4.179883 |
| C | -2.347486 | 1.387938 | 4.248217 |
| C | -3.425999 | 1.695749 | 3.407500 |
| C | -4.658254 | 1.058222 | 3.581821 |
| C | -4.826804 | 0.105372 | 4.591896 |
| C | -3.741716 | -0.230471 | 5.409239 |
| C   | -2.509735 | 0.402850 | 5.232469 |
| H   | -7.327663 | 0.372192 | 0.382381 |
| H   | -7.190581 | 2.696156 | 1.744378 |
| H   | -5.479409 | 4.394385 | -1.138143 |
| H   | -3.503524 | 4.246290 | -1.888936 |
| H   | -3.997168 | 5.751442 | 0.737086 |
| H   | -3.029941 | 6.291136 | -0.618961 |
| H   | -4.261274 | 8.397446 | -1.003853 |
| H   | -6.075115 | 8.364530 | -1.233356 |
| H   | -5.798715 | 6.719174 | -3.149680 |
| H   | -3.985496 | 6.755672 | -2.913356 |
| H   | -2.142737 | 2.540158 | -1.681775 |
| H   | -1.579249 | 1.130273 | 0.665417 |
| C   | 0.019272  | -0.113021 | -0.744469 |
| H   | -0.014128 | 1.189207 | -1.960528 |
| H   | -2.434892 | 0.658333 | -2.429648 |
| H   | -1.194315 | -2.978509 | -3.307636 |
| H   | -3.778263 | -2.197604 | -2.465753 |
| H   | -2.792365 | -3.178185 | -1.365413 |
| H   | -1.983089 | -1.320847 | -0.190699 |
| H   | -3.522349 | -0.594011 | -0.677351 |
| H   | -1.227729 | 3.264573 | 2.299342 |
| H   | -0.219558 | 1.579432 | 4.591851 |
| H   | -1.139411 | 3.087903 | 4.775437 |
| H   | -3.318027 | 4.250628 | 2.637931 |
| C   | -5.483453 | 1.331716 | 2.934354 |
| H   | -5.790099 | -0.372243 | 4.741566 |
| H   | -3.852742 | -0.986168 | 6.178195 |
| H   | -1.669112 | 0.129114 | 5.858767 |
| H   | 2.131685  | 4.122312 | -1.979001 |
| H   | -5.255796 | -3.939387 | -0.796584 |
| H   | -6.402314 | -5.221346 | -1.260662 |
| H   | -6.959630 | -3.793839 | -0.351710 |
| H   | -4.781781 | -4.164250 | -3.418861 |
| H   | -6.080703 | -3.536510 | -4.545691 |
| H   | -6.237000 | -5.130205 | -3.774998 |
| H   | -8.278456 | -2.830814 | -3.672328 |
| H   | -8.534699 | -4.339065 | -2.756178 |
| H   | -8.560859 | -2.771841 | -1.907919 |
| H   | -5.197357 | 0.184090 | -2.644891 |
| H   | 3.633460  | -2.844016 | -3.117869 |
| H   | -6.091756 | 5.885944 | -0.792166 |
| O   | 1.356981  | 3.506442 | -1.893212 |
| H   | 0.803408  | 3.778061 | -1.017412 |
| H   | 1.842641  | 2.294980 | -1.226651 |

**space group C2, model 2 (simplified), 13b (deformation fragment)**

**Zero-point correction** = 0.684973 (Hartree/Particle)
**Thermal correction to Energy** = 0.724939
**Thermal correction to Enthalpy** = 0.725883
**Thermal correction to Gibbs Free Energy** = 0.608121
**Sum of electronic and zero-point Energies** = -1993.512509
**Sum of electronic and thermal Energies** = -1993.472542
**Sum of electronic and thermal Enthalpies** = -1993.471599
**Sum of electronic and thermal Free Energies** = -1993.589361

**SOLVENT: -2005.267941**

| X2  | 13SCUTgF1 SCF Done: -1994.19748201 A.U. |
| O   | -3.600425 0.375036 2.159463 |
| C   | -3.646386 0.892828 0.949862 |
| O   | -6.371022 0.658428 0.055084 |
| C   | -5.963549 0.058765 0.501949 |
| C   | -6.657535 1.149145 1.307660 |
| C   | -6.635020 -0.229123 -0.834892 |
| C   | -3.579686 -1.222494 1.332353 |
| N   | -2.586893 1.496683 0.323478 |
| C   | -1.359024 1.802009 0.916541 |
| O   | -0.276686 2.093362 -0.067345 |
| C   | -0.530052 2.064047 -1.314678 |
| C   | 2.805300 1.793361 2.260155 |
| C   | 2.037554 2.071857 2.710911 |
| O   | 1.223413 2.327135 1.804949 |
| O   | 0.943088 2.372213 0.455340 |
| C   | 2.044524 2.460851 -0.560068 |
| C   | 3.239550 3.304610 -0.096092 |
| C   | 2.842039 4.722592 0.257435 |
| C   | 3.841023 5.846588 0.013591 |
| C   | 2.611364 5.708166 -0.883560 |
| C   | 2.422945 0.990675 -0.752257 |
| O   | 3.073402 0.411899 0.149659 |
| N   | 1.885709 0.391671 -1.844425 |
| C   | 1.741874 -0.773359 -1.901926 |
| C   | 0.616269 -1.504707 -2.846661 |
| O   | -0.760609 -0.894803 -2.562442 |
| C   | -1.709991 -1.504601 -3.627830 |
| O   | -1.391422 -1.674047 -4.820816 |

S64
space group C2, model 2 (simplified), Mpro (deformation fragment)

Zero-point correction= 0.844419 (Hartree/Particle)
Thermal correction to Energy= 0.896059
Thermal correction to Enthalpy= 0.897004
Thermal correction to Gibbs Free Energy= 0.757567
Sum of electronic and zero-point Energies= -2950.715505
Sum of electronic and thermal Energies= -2950.663864
Sum of electronic and thermal Enthalpies= -2950.662920
Sum of electronic and thermal Free Energies= -2950.802357

SOLVENT: -2967.6456143

N  -2.862054  -1.864575  -3.018934
C  -2.924193  -1.497163  -1.945435
C  -1.419821  -1.301463  -1.230199
C   3.144502  -1.776491  -2.252330
O   4.271779  -0.893920  -2.019832
C   3.290147  -2.876758  -1.181201
O   2.992376  -4.086368  -1.381655
N   3.666736  -2.368718  -0.000081
C   3.752159  -3.177445  1.223981
C   2.622897  -2.917015  2.221112
C   2.033254  -1.653459  2.353624
C   1.121201  -1.408163  3.385792
C   0.778251  -2.422556  4.285163
C   1.337159  -3.695852  4.131292
C   2.250644  -3.940659  3.104033
H   -1.868521   1.549143  2.954133
H    0.465323   2.077523  3.767586
H    2.246462   2.904286  2.091128
H    1.588623   2.897653  1.449791
H    3.743890   2.791098  0.726203
H    3.949544   3.324244  0.937715
H    4.803528   5.576631  0.406594
H    3.862232   6.667528  0.718935
H    1.819163   6.438577  0.774382
H    2.766353   5.346956  1.846747
H    1.224058   0.937071  2.395281
H    1.488714  -1.394452  0.883782
H    0.536970  -2.595964  2.773996
H    0.857501  -1.270841  3.898017
H   -0.766747   1.096206  2.653332
H   -3.544638  -2.463258  3.509937
H   -3.497719  -0.580160  1.446841
H   -3.368102  -2.286299  0.991933
H   -1.021900  -2.266303  -0.919923
H   -1.275323  -0.580136  -0.428085
H    3.808922  -1.350025  0.039957
H    3.757428  -4.227871  0.927883
H    4.707247  -2.953137  1.712970
H    2.304737  -0.849896  1.681883
H    0.704871  -0.411788  3.488335
H    0.080963  -2.228203  5.092192
H    1.057662  -4.974477  4.804873
H    2.672182  -4.930256  2.982768
H    5.451798  -0.980269  2.347844
H   -5.013839  -1.880490  0.891496
H   -6.723618  -1.753087  1.367400
H   -6.678815   0.685138  1.432866
H   -7.649698  -0.600889  -0.664540
H   -6.062123  -0.938678  -1.381320
H   -6.797235   2.058675  0.698044
H   -7.763555   0.787401  1.596828
H   -6.110026  1.382744  2.207408
H   -2.619452  1.645631  -0.686385
H    2.194048   4.825004  1.121007

13SCUTGF2 SCF Done: -2951.5599236 A.U.

SOLVENT: -2967.6456143

C   -1.051985   4.586798   0.802556
C   -0.267863   4.444423  2.159683
C    0.587561   3.623218  2.002110
C    0.593734   2.098470  1.880983
C    1.604865   1.193621  1.573985
C    1.224058  -0.937071  1.712970
C    2.284953   3.891306  1.863555
C    3.228107   2.975421  1.607949
C    2.284121   3.693327  0.745062
C    3.838949   4.084106  1.233043
C   -0.377236   4.386175  -0.033302
C    0.955474   4.089168  2.931096
C    0.119627   5.429311  2.440496
C    0.420430   1.754387  2.016013
C    1.318511   0.172321  1.392645
C    3.735572   0.940298  1.202004
C    2.434175   4.949009  1.953005
C    4.528907   3.287135  1.500894
C   -2.151745   2.891610  0.120069

Zero-point correction= 0.844419 (Hartree/Particle)
Thermal correction to Energy= 0.896059
Thermal correction to Enthalpy= 0.897004
Thermal correction to Gibbs Free Energy= 0.757567
Sum of electronic and zero-point Energies= -2950.715505
Sum of electronic and thermal Energies= -2950.663864
Sum of electronic and thermal Enthalpies= -2950.662920
Sum of electronic and thermal Free Energies= -2950.802357

SOLVENT: -2967.6456143
| Atoms | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-------|--------------|--------------|--------------|
| C     | -3.343648    | 1.706320     | -0.201271    |
| C     | -3.529907    | 1.645668     | -1.748077    |
| C     | -3.665643    | 3.037171     | -2.401626    |
| C     | -3.836612    | 2.858625     | -3.926441    |
| C     | -4.851342    | 3.831926     | -1.808545    |
| C     | -3.302538    | 0.255297     | 0.267337     |
| O     | -2.236543    | -0.419572    | 0.448628     |
| H     | -1.254811    | 2.156231     | -0.278432    |
| H     | -4.188302    | 2.209869     | 0.269198     |
| H     | -4.413575    | 1.037233     | -1.876513    |
| H     | -2.650960    | 1.132316     | -2.158299    |
| H     | -2.738722    | 3.592169     | -2.212428    |
| H     | -4.669098    | 4.094656     | -0.761981    |
| H     | -4.999505    | 4.760587     | -2.371712    |
| H     | -5.772982    | 3.239405     | -1.879767    |
| H     | -2.999103    | 2.293782     | -4.352662    |
| H     | -4.765372    | 2.315238     | -4.403836    |
| H     | -3.885570    | 3.840968     | -4.422859    |
| C     | -4.908116    | -0.324694    | 0.348190     |
| C     | -4.677248    | -1.781172    | 0.523323     |
| C     | -6.190287    | -2.082898    | 0.628573     |
| C     | -6.958649    | -1.128555    | 1.523323     |
| O     | -7.040599    | 0.095991     | 1.213543     |
| N     | -7.519613    | -1.668324    | 2.624256     |
| C     | -4.926322    | -2.488819    | -0.760128    |
| C     | -4.785940    | -2.305938    | -1.837781    |
| H     | -5.388220    | 0.211082     | 0.344440     |
| H     | -3.818894    | -3.123035    | 0.919326     |
| H     | -6.574005    | -1.945673    | -0.389053    |
| H     | -3.165934    | -3.269774    | -2.132562    |
| O     | -4.178333    | -3.761556    | -2.998508    |
| H     | -2.576539    | -3.316952    | 0.274695     |
| H     | -2.311907    | -4.990265    | 1.613922     |
| H     | -3.182215    | -3.793402    | -2.605995    |
| N     | -0.875029    | -2.115652    | -1.494200    |
| C     | 0.353588     | -1.401232    | -1.757296    |
| C     | 0.131893     | 0.109842     | -1.987095    |
| O     | -0.195406    | 0.793654     | -0.738018    |
| N     | 1.427899     | -1.555440    | -0.685125    |
| C     | 2.566673     | -1.050570    | -0.905532    |
| H     | -1.519819    | -1.725772    | -0.769792    |
| O     | 0.756003     | -1.856001    | -2.666343    |
| H     | -0.656901    | 0.220581     | -2.748350    |
| C     | 1.065026     | 0.544033     | -2.354032    |
| O     | -0.862185    | 0.251472     | -0.200283    |
| C     | 1.152601     | -2.179870    | 0.464120     |
| C     | 2.205116     | -2.246289    | 1.491714     |
| C     | 1.649605     | -2.933776    | 2.748431     |
| C     | 0.648531     | -1.750937    | 3.515549     |
| C     | 3.466553     | -2.943782    | 0.928984     |
| O     | 3.440522     | -3.984223    | 0.262993     |
| H     | 0.229097     | -2.555551    | 0.681865     |
| H     | 2.491050     | -1.223091    | 1.756247     |
| C     | 2.461404     | -3.133072    | 3.450937     |
| C     | 1.160254     | -3.874047    | 2.491655     |
| C     | 4.604008     | -2.241599    | 1.236848     |
| C     | 5.863251     | -2.459854    | 0.517007     |
| C     | 6.259022     | -1.280280    | -0.291120    |
| C     | 7.442328     | -0.902564    | -0.526576    |
| C     | 4.525757     | -1.363909    | 1.742419     |
| C     | 5.687627     | -3.083885    | -0.153162    |
| C     | 6.694635     | -2.690501    | 1.186452     |
| C     | 5.197657     | -0.482273    | -0.743833    |
| C     | 5.433348     | 0.752236     | -1.480404    |
| C     | 4.081825     | 1.387604     | -1.917114    |
| C     | 3.347605     | 0.555428     | -2.855787    |
| C     | 6.135772     | 1.760121     | -0.556363    |
| O     | 5.908741     | 1.826916     | 0.663550     |
| H     | 4.234244     | -0.789827    | -0.597052    |
| H     | 6.046589     | 0.551522     | -2.365145    |
| H     | 4.304666     | 2.330957     | -2.423191    |
| H     | 3.503177     | 1.603833     | -1.011936    |
| H     | 3.022048     | -0.221905    | -2.30368    |
| N     | 6.940476     | 2.637908     | -1.218169    |
| H     | 7.421269     | 3.360389     | -0.685274    |
space group C2, model 2 (simplified), reactant complex

Zero-point correction= 1.550781 (Hartree/Particle)
Thermal correction to Energy= 1.642667
Thermal correction to Enthalpy= 1.643611
Thermal correction to Gibbs Free Energy= 1.422993
Sum of electronic and zero-point Energies= -4944.643570
Sum of electronic and thermal Energies= -4944.551684
Sum of electronic and thermal Enthalpies= -4944.550740
Sum of electronic and thermal Free Energies= -4944.771358

SOLVENT: -4973.2613485

H  7.209815  2.489765  -2.182724
H  -0.318180  -3.357621  5.688363
H  -1.441328  5.605735  0.720878
|   | X      | Y      | Z      |
|---|--------|--------|--------|
| C | -3.84559 | -2.68895 | 0.204317 |
| C | -2.639455 | -3.531679 | -0.039316 |
| S | -1.411467 | -3.689900 | 0.702253 |
| O | -5.249499 | -3.759668 | 1.864343 |
| H | -2.506792 | -1.535739 | 1.527012 |
| H | -4.123340 | -2.129801 | -0.738854 |
| H | -2.952370 | -4.040241 | -0.616351 |
| H | -2.080930 | -3.865024 | 0.966663 |
| N | -6.019377 | -1.520108 | -0.301005 |
| C | -7.420483 | -3.847765 | -0.016324 |
| C | -8.353690 | -2.677875 | -0.409554 |
| O | -9.522992 | -2.854500 | -0.791296 |
| H | -5.834029 | -3.117565 | -1.215004 |
| H | -7.761886 | -4.734123 | -0.555181 |
| H | -7.780900 | -1.451879 | -0.290933 |
| C | -8.533103 | -0.267084 | -0.680748 |
| C | -7.694163 | 1.016378 | -0.166352 |
| O | -7.403825 | 1.231569 | 0.982927 |
| H | -5.834029 | -3.117565 | -1.215004 |
| H | -9.466921 | -0.212757 | -0.112479 |
| H | -8.275777 | 1.872264 | -0.775110 |
| H | -6.778724 | 0.946438 | -1.028714 |
| H | -6.737285 | 0.516692 | 1.217336 |
| O | -9.971613 | 0.302528 | -2.553109 |
| H | -10.217306 | 0.330028 | -3.534389 |
| H | -10.660116 | 0.588753 | -1.866352 |
| O | 7.061296 | 1.911643 | -0.176432 |
| C | 6.435622 | 1.803481 | -1.256308 |
| O | 6.026295 | 2.875225 | -2.017503 |
| C | 6.420611 | 3.401699 | -1.648898 |
| C | 7.918145 | 4.431541 | -1.943801 |
| C | 5.556988 | 5.108132 | -2.621950 |
| C | 6.089845 | 6.326461 | -1.168493 |
| N | 6.023532 | 0.651790 | -1.823210 |
| C | 6.187946 | -0.618060 | -1.264836 |
| O | 5.339888 | -1.614801 | -0.900663 |
| H | 4.543002 | -1.348007 | -2.844562 |
| H | 6.999576 | -0.942777 | -0.207084 |
| H | 7.019168 | -2.274345 | 0.286755 |
| O | 6.217274 | -3.219059 | -0.280990 |
| N | 5.425822 | -2.908536 | -1.366919 |
| C | 4.405536 | -3.881103 | -1.882973 |
| O | 5.836431 | -5.345938 | -1.765537 |
| C | 6.126834 | -5.624507 | -2.507782 |
| C | 6.327741 | -6.996006 | -3.381718 |
| O | 6.062922 | -5.778927 | 0.403865 |
| C | 3.194480 | -3.569444 | -0.991096 |
| O | 3.207987 | -9.551166 | 0.201618 |
| H | 2.256238 | -2.763277 | -1.547956 |
| C | 1.326090 | -1.992990 | -0.697373 |
| C | 0.886722 | -0.740902 | -1.407447 |
| C | 1.879375 | 0.220623 | -1.943521 |
| O | 1.096210 | 1.956010 | -2.579199 |
| O | 0.696174 | 1.252105 | -3.259384 |
| N | 1.087338 | 2.552364 | 0.204965 |
| C | 2.915210 | 2.563358 | -1.414095 |
| C | 2.757280 | 0.907871 | -0.883008 |
| C | 0.143502 | -2.930251 | -0.147866 |
| C | 0.469374 | -4.340239 | -0.245237 |
| C | 0.116333 | -2.645562 | 1.367829 |
| O | -0.690505 | -1.841218 | 1.910092 |
| N | 1.136862 | -3.729365 | 2.005629 |
| C | 1.398811 | -3.069528 | 3.432840 |
| C | 2.644118 | -2.225014 | 3.703641 |
| C | 3.752845 | -2.251037 | 2.848153 |
| C | 4.935562 | -1.997257 | 3.210276 |
| C | 5.019096 | -0.900849 | 4.419919 |
| C | 3.900435 | -0.841531 | 5.258035 |
| C | 2.720870 | -1.497095 | 4.899556 |
| C | 7.593969 | -0.168111 | 0.250404 |
| C | 7.662167 | -2.542695 | 1.113201 |
| C | 6.164289 | -2.423253 | 0.080315 |
| C | 4.236715 | -3.606768 | -2.922821 |
| C | 4.887582 | -5.628065 | -0.708858 |
| C | 4.027500 | -5.944311 | -2.205616 |
| C | 5.528872 | -7.720230 | -3.025609 |
space group C2, model 2 (simplified) + H2O product

Zero-point correction= 1.577149 (Hartree/Particle)
Thermal correction to Energy= 1.670380
Thermal correction to Enthalpy= 1.671324
Thermal correction to Gibbs Free Energy= 1.449212

Sum of electronic and zero-point Energies= -5020.644823
Sum of electronic and thermal Energies= -5020.551593
Sum of electronic and thermal Enthalpies= -5020.550648
Sum of electronic and thermal Free Energies= -5020.772761

SOLVENT: -5049.6937109

H 7.327655 -7.412603 -3.138095
H 6.85522 -5.390078 -4.611341
H 5.087765 -5.702976 -4.493056
H 2.464466 -2.373311 -2.466249
H 1.905860 -1.686647 0.180848
H 0.184171 -0.200140 -0.684275
H 0.160864 -0.998995 -2.253750
H 2.517184 -0.247022 -2.700534
H 1.210225 3.454290 -2.360908
H 3.806488 2.475392 -2.034998
H 2.976669 3.071320 -0.589692
H 2.209462 0.950984 0.056974
H 3.715111 0.418466 -0.716806
H 1.743737 -3.845286 1.426893
H 0.521786 -2.601188 3.882930
H 1.538238 -0.281277 5.547529
H 0.569820 -4.537798 -1.215455
H 6.825516 4.186333 0.482106
H 5.101476 4.267588 0.103221
H 6.111716 5.219178 -0.073017
H 5.751248 4.785248 -3.648289
H 5.939232 6.171688 -2.524758
H 4.498531 4.952215 -2.395000
H 8.212036 4.175724 -2.980888
H 8.235320 5.462252 -1.757832
H 8.477418 3.705024 -1.286149
H 5.441106 0.675690 -2.661598
H -2.952534 5.096523 -3.506841
H 7.069778 -5.136352 -2.109974

S69
| Atom | U1   | U2   | U3   | U12  | U13  | U23  |
|------|------|------|------|------|------|------|
| C    | 5.563482 | -7.657207 | -1.836931 |
| C    | 5.306796 | -6.598178 | -2.908687 |
| C    | 2.759992 | -3.714637 | -0.189028 |
| O    | 2.751249 | -3.940606 | 1.031590 |
| N    | 1.887221 | -2.880602 | -0.861123 |
| C    | 1.082325 | -1.914297 | -0.064328 |
| C    | 0.628957 | -0.729300 | -0.915602 |
| C    | 1.697483 | 0.064446 | -1.678774 |
| C    | 2.742910 | 2.273529 | -1.760375 |
| O    | -0.156713 | -1.969512 | 2.046806 |
| N    | 1.516647 | 2.432820 | -1.571800 |
| C    | 1.002820 | -2.149328 | 4.212714 |
| C    | 2.340276 | -1.406610 | 4.186550 |
| C    | 0.635512 | -1.831502 | -1.821370 |
| C    | 6.079020 | -6.376040 | -3.603974 |
| O    | 3.863432 | 0.165363 | 5.239638 |
| H    | 1.353709 | -0.394343 | 0.275982 |
| H    | 7.375504 | -2.594454 | 1.516727 |
| H    | 5.677929 | -4.365303 | 0.839027 |
| H    | 3.654866 | -5.789833 | 0.385000 |
| H    | 3.394732 | -6.303414 | -0.981331 |
| H    | 4.733967 | -8.293580 | -1.550013 |
| H    | 6.535512 | -8.135062 | 3.272060 |
| H    | 4.602720 | -1.147009 | 3.348403 |
| C    | 4.874983 | -0.203249 | 4.343789 |
| C    | 3.863432 | 0.165363 | 5.239638 |
| C    | 2.601618 | -0.426845 | 5.154453 |
| H    | 0.087703 | -0.044817 | -0.252194 |
| H    | -0.081334 | -1.066291 | -1.678441 |
| H    | 2.325357 | -0.572254 | -2.311771 |
| H    | 1.019720 | 0.307542 | -2.980756 |
| H    | 3.639821 | 2.211591 | -2.379126 |
| H    | 2.797703 | 3.174176 | -1.151756 |
| H    | 2.048894 | 1.305219 | 0.045521 |
| H    | 3.546211 | 0.583324 | -0.567900 |
| H    | 0.952955 | -3.554549 | 2.524523 |
| H    | 0.215061 | -1.483273 | 4.572222 |
| H    | 1.078677 | -2.996228 | 4.902577 |
| H    | 3.155875 | -2.508545 | 2.523037 |
| H    | 5.367430 | -1.439435 | 2.638128 |
| H    | 5.862288 | 0.238887 | 4.249998 |
| H    | 4.058675 | 0.912354 | 6.000172 |
| H    | 1.816612 | -0.124301 | 5.837852 |
| H    | 0.619802 | -4.111472 | -1.696632 |
| H    | 5.172002 | 4.154527 | -0.664803 |
| H    | 6.311315 | 5.436767 | -1.142012 |
| H    | 6.892530 | 3.989098 | -0.295988 |
| H    | 4.564743 | 4.966863 | -2.342703 |
| H    | 5.749529 | 3.388425 | -4.448898 |
| H    | 5.976270 | 5.412303 | -3.636898 |
| H    | 8.065034 | 3.132124 | -3.704646 |
| H    | 8.348298 | 4.632462 | -2.768347 |
| H    | 8.437232 | 3.038583 | -1.958179 |
| H    | 5.112752 | 0.052428 | -2.658924 |
| H    | 3.546345 | 3.539133 | -3.344664 |
| H    | 6.420329 | -5.978066 | -1.197381 |
| H    | -0.108040 | -4.786348 | -1.538859 |
| H    | -0.070927 | -4.514523 | -0.030733 |
| H    | -0.958870 | -4.334857 | -1.799213 |

**space group C2, model 2, Mpro**

Zero-point correction= 1.219169 (Hartree/Particle)
Thermal correction to Energy= 1.293863
Thermal correction to Enthalpy= 1.294808
Thermal correction to Gibbs Free Energy= 1.111087

SHg SCF Done: -4065.628757 A.U.
### Summary of Energies

- **Sum of electronic and zero-point Energies =**  4064.409589
- **Sum of electronic and thermal Energies =**  4064.334894
- **Sum of electronic and thermal Enthalpies =**  4064.333950
- **Sum of electronic and thermal Free Energies =**  4064.517670

### SOLVENT

- **Energy =**  4087.847889

### Atomic Coordinates

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -7.001159  | 2.628265   | 0.625910   |
| C       | -7.319834  | -1.694907  | -0.327482  |
| O       | -6.239254  | 2.170688   | -0.426244  |
| H       | -5.97032   | 0.64613    | 0.234648   |
| H       | -6.34472   | 0.789727   | 1.372928   |
| H       | -6.15031   | 0.406694   | -2.61016   |
| H       | -6.875005  | -0.716233  | -1.499145  |
| H       | -8.06246   | -1.460595  | -3.591830  |
| H       | -7.87844   | 2.729456   | -2.797028  |
| H       | -6.05812   | 1.412785   | -3.536935  |
| C       | -3.71684   | -0.806319  | -3.592501  |
| C       | -3.804740  | -1.764382  | -2.817263  |
| C       | -0.885514  | 0.004654   | -2.989998  |
| H       | -5.02248   | -1.728635  | -3.724535  |
| H       | -0.061432  | -0.411391  | -0.987833  |
| N       | -0.217683  | -0.969484  | 0.856292   |
| C       | -0.73007   | 1.530341   | 2.137628   |
| C       | 0.136254   | 3.396923   | 3.297358   |
| O       | 0.134215   | 3.617349   | 2.996609   |
| C       | -2.128994  | 1.355214   | 2.933454   |
| C       | -3.338342  | 1.320191   | 2.236650   |
| C       | -3.817537  | -2.477505  | 1.611589   |
| C       | -1.851938  | -3.682410  | 2.376013   |
| N       | -3.087589  | -3.667055  | 1.721359   |
| C       | 2.260386   | -1.475181  | 2.127763   |
| C       | 2.933676   | -1.355672  | 3.175534   |
| C       | 0.414151   | -2.920149  | 0.511446   |
| O       | 0.365507   | -0.516613  | 2.290095   |
| C       | 0.335729   | 1.095753   | 4.244657   |
| O       | 0.618017   | -3.380233  | 3.308176   |
| H       | -1.727369  | -0.446129  | 3.361931   |
| H       | -3.851777  | -0.737077  | 2.106671   |
| H       | 2.179748   | -2.443198  | 1.010430   |
| H       | -1.254963  | -4.589850  | 2.390293   |
| C       | -3.463496  | 1.471574   | 2.125108   |
| N       | 2.790998   | -1.521129  | 0.876584   |
| C       | 4.232410   | -1.074134  | 0.662439   |
| C       | 4.540834   | -0.004477  | -0.834356  |
| C       | 3.791283   | -4.230769  | 0.469270   |
| C       | 2.494413   | -5.479709  | -0.344787  |
| C       | 4.096659   | -4.447295  | 1.967544   |
| C       | 4.800456   | -0.572301  | -0.221475  |
| O       | 4.177854   | -0.114363  | -1.226071  |
| H       | 2.157968   | -1.50750  | 0.085987   |
| O       | 4.697617   | -1.664345  | 1.659085   |
| H       | 5.625599   | -1.620549  | -0.065607  |
| H       | 4.242130   | -2.585739  | -1.141844  |
| H       | 2.177957   | -0.470401  | 0.314307   |
| H       | 3.784734   | -3.600078  | 2.581045   |
| H       | 3.580496   | -5.340909  | 2.332065   |
| H       | 5.175088   | -5.597049  | 2.106063   |
| H       | 3.974693   | -5.340909  | -1.408319  |
| H       | 5.280751   | -5.660552  | -2.383035  |
| H       | 3.667574   | 3.636022   | 0.014574   |
| N       | 6.079700   | -0.240299  | 0.031774   |
| C       | 6.939521   | 0.537767   | -1.015223  |
| C       | 7.221660   | -0.678962  | -2.114772  |
| C       | 7.903558   | -1.913822  | -1.540475  |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| O    | 7.837972 | -2.239760 | -0.329916 |
| N    | 5.686659 | 2.464660 | -0.824091 |
| C    | -0.709061 | 1.676435 | 2.495814 |
| S    | 7.368970 | 1.635455 | -1.658876 |
| O    | 6.601667 | 1.883164 | -2.855457 |
| H    | 6.612054 | -0.856463 | 0.650148 |
| H    | 7.874914 | 0.629032 | -2.902807 |
| H    | 7.809975 | -0.204647 | -3.455773 |
| N    | 5.491522 | 2.192851 | 0.138389 |
| C    | 5.122128 | 3.716665 | -1.333276 |
| C    | 3.584697 | 3.737566 | -1.357937 |
| O    | 2.941442 | 4.797553 | -1.327861 |
| H    | 5.495097 | 3.826627 | -2.356710 |
| H    | 5.441195 | 0.758063 | 2.901752 |
| H    | 5.423313 | 0.309557 | 3.965735 |
| C    | 1.540404 | 2.408786 | -1.282636 |
| O    | 1.324813 | 2.581404 | 0.211058 |
| O    | 0.763297 | 3.696585 | 0.685373 |
| H    | 3.568328 | 1.657116 | -1.377534 |
| H    | 3.102578 | 3.723451 | -1.783617 |
| H    | 1.628882 | 1.120451 | -2.960920 |
| H    | -0.960625 | 1.070373 | -1.687801 |
| N    | 2.557330 | -0.151487 | -1.477171 |
| C    | 1.718310 | 1.736131 | 2.455451 |
| C    | 2.879315 | 2.657627 | 2.850865 |
| S    | 5.407845 | 1.887885 | 2.448047 |
| O    | 0.392031 | 3.095387 | 3.965735 |
| C    | 1.893486 | 0.691359 | 0.533269 |
| H    | 1.900745 | 0.758063 | 2.901752 |
| H    | 2.808732 | 2.882983 | 3.910529 |
| H    | 2.802378 | 3.993239 | 2.290532 |
| H    | -0.709061 | 1.676435 | 2.495814 |
| C    | -2.050772 | 2.163855 | 2.827372 |
| C    | -2.815101 | 2.490410 | 1.533096 |
| C    | -3.981326 | 2.041489 | 3.350504 |
| H    | -0.649053 | 1.063093 | 1.688396 |
| H    | -1.922336 | 3.076854 | 3.418877 |
| H    | -2.633646 | 1.441605 | 3.401969 |
| H    | -2.108515 | 3.175235 | 0.636057 |
| C    | -2.691677 | 3.613215 | -0.630385 |
| C    | -1.564507 | 4.226381 | -1.511101 |
| O    | 0.812711 | 2.521055 | -0.840593 |
| C    | -2.676877 | 2.417927 | -1.403138 |
| O    | -2.498318 | 1.517307 | -1.846744 |
| H    | -1.164594 | 3.495864 | 0.854385 |
| H    | -3.466056 | 4.362835 | -0.445713 |
| H    | -2.035825 | 4.762415 | -2.391656 |
| H    | -0.955784 | 3.380509 | -1.849905 |
| H    | 0.057426 | 4.819926 | -0.332058 |
| N    | -4.576655 | 2.463839 | -1.688229 |
| C    | -5.060764 | 1.685140 | -2.136706 |
| H    | -5.160025 | 1.333515 | -1.174347 |
| H    | 4.235248 | 0.667916 | 2.966290 |
| H    | -6.965111 | -2.620064 | 2.084378 |

**space group C2, model 2, product**

**Zero-point correction** = 1.914106 (Hartree/Particle)

**Thermal correction to Energy** = 2.028897

**Thermal correction to Enthalpy** = 2.029841

**Thermal correction to Gibbs Free Energy** = 1.764594

**Sum of electronic and zero-point Energies** = -6058.101819

**Sum of electronic and thermal Energies** = -6057.987027

**Sum of electronic and thermal Enthalpies** = -6057.986083

**Sum of electronic and thermal Free Energies** = -6058.251330

**SOLVENT**: -6093.2726855

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**Zero-point correction** = 1.914106 (Hartree/Particle)

**Thermal correction to Energy** = 2.028897

**Thermal correction to Enthalpy** = 2.029841

**Thermal correction to Gibbs Free Energy** = 1.764594

**Sum of electronic and zero-point Energies** = -6058.101819

**Sum of electronic and thermal Energies** = -6057.987027

**Sum of electronic and thermal Enthalpies** = -6057.986083

**Sum of electronic and thermal Free Energies** = -6058.251330

**SOLVENT**: -6093.2726855
### Space Group C2, Model 1, Mpro (H of the thiol on imidazole)

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | 3.893654 | 2.950464 | -1.327140 |
| C    | 4.136784 | 1.461269 | -0.921353 |
| C    | 2.866416 | -2.354389 | 2.020800 |
| N    | 3.742094 | -3.538673 | 1.436733 |
| C    | 4.361023 | -3.544690 | 2.770516 |
| C    | 5.555625 | -2.598673 | 2.901877 |
| C    | 6.420949 | -2.340431 | 1.826675 |
| C    | 7.586020 | -1.599334 | 2.023692 |
| H    | 9.201943 | 0.676554 | -1.226348 |
| H    | 9.768399 | -1.752758 | -0.819008 |
| H    | 8.248583 | -3.496558 | -1.736088 |
| H    | 5.553444 | -2.799706 | -0.445663 |
| H    | 6.957667 | -4.946912 | -2.390595 |
| H    | 5.774225 | -5.193448 | -3.660868 |
| H    | 8.574982 | -3.992170 | -4.179956 |
| H    | 7.183568 | -6.629660 | -5.087452 |
| H    | 8.445191 | -6.060266 | -5.592912 |
| H    | 7.817958 | -3.957378 | -6.584090 |
| H    | 6.159364 | -4.531562 | -6.084541 |
| H    | 3.919438 | -1.760491 | -2.950743 |
| H    | 3.979123 | -1.382644 | -0.158755 |
| H    | 1.995118 | -0.157947 | -0.349538 |
| H    | 1.626527 | -0.729069 | -1.943461 |
| H    | 3.827314 | 0.354519 | -2.760959 |
| H    | 1.846336 | 3.692481 | -1.903588 |
| H    | 4.648246 | 3.292487 | -2.037701 |
| H    | 3.923098 | 3.949369 | -0.448220 |
| H    | 3.773851 | 1.324946 | 0.094917 |
| H    | 5.192472 | 1.193631 | -0.954960 |
| H    | 4.254143 | -3.912431 | 0.462434 |
| H    | 3.588121 | -3.274591 | 3.492410 |
| H    | 4.606237 | -4.565476 | 2.985773 |
| H    | 6.211249 | -2.762463 | 0.850183 |
| H    | 8.252958 | -1.442625 | 1.183052 |
| H    | 8.812529 | -0.528766 | 3.444460 |
| H    | 7.235746 | -0.898387 | 5.333122 |
| H    | 5.169701 | -2.206654 | 4.985715 |
| H    | 2.469381 | -4.226140 | -1.771117 |
| H    | 8.604345 | 4.604378 | -1.001212 |
| H    | 6.304599 | 4.671531 | -0.083473 |
| H    | 7.067156 | 6.275624 | -0.227924 |
| H    | 6.011196 | 5.801570 | -3.753917 |
| H    | 6.213480 | 7.028661 | 2.473756 |
| H    | 5.073434 | 5.676897 | 2.465518 |
| H    | 8.500601 | 5.399595 | -3.725511 |
| H    | 8.798346 | 6.505283 | -2.357758 |
| H    | 9.282852 | 4.795211 | -2.228316 |
| H    | -7.318795 | 0.173984 | -5.283038 |
| H    | 6.209600 | 1.574396 | -3.709822 |

Zero-point correction= 2.635206 (Hartree/Particle)
Thermal correction to Energy= 2.796306
Thermal correction to Enthalpy= 2.797250
Thermal correction to Gibbs Free Energy= 2.432042
Sum of electronic and zero-point Energies= -9041.702501
Sum of electronic and thermal Energies= -9041.541401
Sum of electronic and thermal Enthalpies= -9041.540547
Sum of electronic and thermal Free Energies= -9041.905665

SOLVENT: -9093.0185485
| Element | x         | y         | z         |
|---------|-----------|-----------|-----------|
| C       | -0.51055  | 1.198776  | -2.393216 |
| C       | -7.372563 | 0.054660  | -1.802555 |
| C       | -7.99800  | -0.777302 | -3.990129 |
| C       | -6.589324 | 0.359803  | -4.580925 |
| C       | -6.368323 | 3.917936  | 0.271956  |
| O       | -6.135140 | 5.134151  | -0.002310 |
| N       | -5.768173 | 3.285182  | 1.299989  |
| C       | -4.545367 | 3.812863  | 1.921221  |
| C       | -4.728537 | 3.985203  | 3.453453  |
| C       | -5.837262 | 5.011026  | 3.800288  |
| C       | -5.908545 | 5.165799  | 5.335345  |
| C       | -5.589493 | 6.375843  | 3.119384  |
| C       | -3.44298  | 2.781480  | 1.789901  |
| O       | -3.730739 | 1.535039  | 1.953429  |
| N       | -2.164973 | 3.144171  | 1.737959  |
| C       | -1.164973 | 2.171167  | 2.276925  |
| C       | 0.263344  | 2.723361  | 2.205294  |
| O       | 0.637458  | 3.145868  | 0.812052  |
| N       | 0.127588  | 4.187738  | 0.307663  |
| C       | 1.554400  | 2.006767  | 3.771248  |
| O       | -1.748792 | 3.020225  | 4.490445  |
| N       | -5.339726 | -0.910708 | 3.640741  |
| C       | -6.550822 | -0.151769 | 2.960266  |
| O       | -6.140473 | 0.484603  | 1.687930  |
| N       | -4.848951 | -1.955345 | 2.652843  |
| C       | -3.337371 | -2.015991 | 2.467230  |
| C       | -2.936225 | -2.976461 | 1.534603  |
| O       | -4.030866 | -2.992334 | 1.679762  |
| N       | -0.581591 | -1.323631 | 1.769680  |
| C       | -3.499431 | -4.795140 | 1.880476  |
| O       | -3.689620 | -4.756328 | 3.047611  |
| N       | -3.805171 | -5.108383 | 0.765996  |
| C       | -4.581486 | -6.322379 | 0.841958  |
| O       | -6.050896 | -6.028111 | 0.292383  |
| N       | -6.720822 | -7.022721 | -0.136813 |
| C       | -4.627740 | -4.802831 | 0.357261  |
| O       | -7.776799 | -4.478317 | -0.067543 |
| N       | -8.119360 | -3.040121 | 0.334101  |
| C       | -8.229816 | -2.857243 | 1.767007  |
| C       | -7.918969 | -4.675110 | -1.590156 |
| O       | -6.985195 | -4.903850 | -2.377005 |
| N       | -9.204798 | -4.537303 | -2.028705 |
| C       | -3.985151 | -5.637169 | -4.652113 |
| O       | -2.923972 | -5.359927 | -5.276090 |
| N       | -4.487894 | -4.923311 | -3.628022 |
| C       | -3.851879 | -4.657617 | -3.193317 |
| O       | -4.804547 | -2.924923 | -2.245296 |
| N       | -4.167672 | -1.721536 | -1.642009 |
| C       | -2.974603 | -1.157251 | -2.132194 |
| C       | -2.651389 | -0.161715 | -1.280025 |
| O       | -3.624114 | -0.059277 | -0.297423 |
| C       | -4.572719 | -1.052189 | -0.513641 |
| C       | -2.505754 | -3.952601 | -2.504683 |
| O       | -2.339261 | -4.035120 | -1.265920 |
| N       | -1.474011 | -4.120699 | -3.368891 |
| C       | -0.146166 | -4.381516 | -2.831268 |
| C       | 0.788463  | -5.028719 | -3.909756 |
| C       | 0.602972  | -6.509045 | -3.914248 |
| O       | 1.400167  | -7.349840 | -3.133401 |
| N       | 0.898183  | -8.629454 | -3.286768 |
| O       | -0.159776 | -8.648505 | -4.096613 |
| C       | -0.253358 | -7.316929 | -4.488985 |
| C       | 0.521892  | -3.125109 | -2.274805 |
| C       | 1.526111  | -3.264713 | -1.512349 |
| N       | 0.043714  | -1.943324 | -2.666899 |
| C       | 0.503613  | -0.679285 | -2.069384 |
| O       | 2.055451  | -0.462210 | -2.136349 |
| N       | 2.522018  | 0.222226  | -3.440322 |
| C       | 4.292851  | -0.053418 | -3.835291 |
| O       | 5.167306  | 0.981994  | -2.588987 |
| N       | -0.138502 | 0.436345  | -2.888316 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| O    | -0.500048 | 0.295610 | -4.046547 |
| N    | -0.118662 | 1.621503 | -2.217967 |
| C    | -0.490282 | 2.874612 | -1.482569 |
| C    | -1.638254 | 3.498931 | -0.270788 |
| C    | -2.325186 | 4.784980 | -0.525968 |
| C    | -3.360228 | 5.121557 | -0.703626 |
| O    | -3.080642 | 5.151059 | -0.270788 |
| C    | 0.757025  | 3.763664 | -2.917881 |
| O    | 1.836169  | 3.473397 | -2.318555 |
| N    | 0.653320  | 4.871265 | -3.661218 |
| C    | 2.307311  | 6.067743 | -5.052968 |
| C    | 2.925255  | 4.751188 | -5.610362 |
| C    | 3.490957  | 5.091957 | -7.021447 |
| O    | 4.022988  | 4.725533 | -6.873732 |
| C    | 0.106760  | 7.201385 | -3.202080 |
| O    | -0.220855 | 3.732391 | -3.406881 |
| N    | 1.786826  | 8.123525 | -2.599671 |
| C    | 1.182863  | 9.355118 | -1.996884 |
| C    | 2.244566  | 9.798558 | -0.938210 |
| C    | 3.670767  | 9.404125 | -1.688309 |
| C    | 3.247535  | 8.039955 | -2.310763 |
| N    | 0.994424  | 10.462497| -3.102489 |
| O    | 1.694063  | 11.452797| -3.147922 |
| N    | 0.018455  | 10.097293| -3.935686 |
| C    | 9.839096  | 2.327646 | -3.218621 |
| O    | 8.817143  | 3.298553 | -3.165177 |
| N    | 9.204259  | 4.630550 | -2.098206 |
| C    | 10.512088 | 5.061514 | -2.539237 |
| O    | 9.368253  | 3.725654 | -0.717185 |
| N    | 7.453756  | 2.710371 | -2.788375 |
| O    | 6.397668  | 3.565608 | -2.874064 |
| C    | 5.103262  | 2.818754 | -2.289534 |
| O    | 4.128236  | 3.463500 | -3.349585 |
| C    | 4.502723  | 5.620471 | -1.554741 |
| O    | 5.711489  | 5.710556 | -0.985204 |
| C    | 3.661273  | 6.539843 | -1.438564 |
| O    | 5.382930  | 7.271896 | -0.853947 |
| C    | 6.116078  | 3.484848 | -0.946626 |
| O    | 4.883750  | 1.574460 | -0.420888 |
| C    | 5.328869  | 1.045727 | 0.874910  |
| O    | 6.767410  | 0.460548 | 0.750515  |
| N    | 4.451960  | 0.107912 | 1.340382  |
| O    | 3.841078  | 0.877727 | 0.536201  |
| N    | 4.556081  | 0.291067 | 2.664909  |
| O    | 4.438022  | 1.066144 | 3.314718  |
| C    | 3.725848  | 1.488185 | 4.679435  |
| C    | 3.106625  | 2.813169 | 5.176799  |
| C    | 1.572183  | 2.609289 | 5.130887  |
| O    | 1.000865  | 1.613960 | 4.840508  |
| C    | 0.864449  | 3.821988 | 5.360544  |
| O    | 5.885472  | 2.994674 | 3.544846  |
| C    | 6.782552  | 1.276109 | 3.884667  |
| O    | 6.092962  | 3.408529 | 4.300003  |
| S    | 2.981976  | 4.073796 | 1.721743  |
| O    | 3.999311  | 5.034516 | 2.835422  |
| C    | 2.288638  | 6.266658 | 1.085697  |
| C    | 3.916349  | 4.252299 | 0.217136  |
| H    | 5.503955  | 5.343215 | 1.278680  |
| C    | 5.679466  | 4.281442 | 2.525210  |
| H    | 0.797117  | 4.379341 | 0.278495  |
| C    | 3.470291  | 2.608253 | 2.915854  |
| C    | 2.963113  | 5.939670 | 0.352723  |
| C    | 4.244509  | 1.892501 | 7.447493  |
| C    | 6.228055  | 3.661379 | 6.165034  |
| C    | 4.335199  | 4.110247 | 4.511726  |
| H    | 4.264065  | 4.941497 | 6.069162  |
| C    | 2.481089  | 3.544124 | 6.884022  |
| C    | 2.043705  | 4.054457 | 5.230319  |
| H    | 0.254551  | 1.998433 | 4.578575  |
| C    | 0.343476  | 1.845486 | 6.375829  |
| C    | 0.565645  | 0.473496 | 5.312040  |
| C    | 6.309215  | 0.870535 | 6.631323  |
| H    | 7.733456  | 2.265246 | -0.021896 |
| C    | 5.422925  | 1.738832 | -0.865656 |
| C    | 5.608564  | 2.985170 | -2.117218 |
| C    | 7.513885  | -0.057737 | -0.723728 |
| H    | -8.398342 | -1.813218 | -2.152766 |
| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| H    | -8.452465    | -1.546405    | -4.605977    |
| H    | -6.421901    | 2.225762     | -4.240460    |
| H    | -7.458737    | -0.397618    | 3.887874     |
| H    | -6.595189    | 2.324732     | 1.524493     |
| H    | -5.274477    | 5.704462     | 3.356349     |
| H    | -3.270415    | 3.047184     | 3.789118     |
| H    | -1.197827    | 4.054878     | 3.334372     |
| H    | 0.314267     | 3.603537     | 2.849672     |
| H    | 1.795990     | 2.606828     | -0.795506    |
| H    | 2.101871     | 1.650232     | 0.585782     |
| H    | -1.398818    | -0.029382    | 3.558378     |
| H    | -1.683473    | -0.191749    | 6.081508     |
| H    | -2.493649    | 1.393215     | 5.974299     |
| H    | -3.910554    | 0.607090     | 3.455519     |
| H    | -5.775384    | -1.450828    | 4.513590     |
| H    | -6.936190    | 0.594986     | 3.663062     |
| H    | -7.332223    | -0.862877    | 2.684643     |
| H    | -5.188652    | 0.811243     | 1.788463     |
| H    | -2.909361    | -1.365509    | 2.927242     |
| H    | -3.199793    | -2.692791    | 0.518267     |
| H    | -1.052671    | -3.520657    | 0.788767     |
| H    | -1.149478    | -3.567363    | 2.577757     |
| H    | -4.462715    | -6.585662    | 1.903800     |
| H    | -4.138002    | -7.155177    | 0.291049     |
| H    | -5.871219    | -4.087147    | 0.831103     |
| H    | -8.497365    | -5.145875    | 0.421504     |
| H    | -9.088815    | -2.749920    | -0.092304    |
| H    | -7.357166    | -2.359676    | -0.109245    |
| H    | -7.276533    | -2.880629    | 2.106009     |
| H    | -9.39708    | -4.678226    | -3.014728    |
| H    | -9.984671    | -4.455713    | -1.387577    |
| H    | -5.388629    | -5.152367    | -3.181002    |
| H    | -3.633829    | -3.039534    | -0.468886    |
| H    | -5.113684    | -3.611442    | -1.453406    |
| H    | -5.708701    | -2.654346    | -2.805018    |
| H    | -1.841756    | 0.491585     | -1.338799    |
| H    | -5.397461    | -2.010132    | 0.151521     |
| H    | -3.542678    | 0.511111     | 0.546971     |
| H    | -1.739320    | -4.404493    | -4.329864    |
| H    | -0.215339    | -5.065395    | -1.979281    |
| H    | 1.802464     | -4.773213    | -3.671604    |
| H    | 0.529897     | -4.597334    | -4.887098    |
| H    | 1.338035     | -9.483629    | -2.801680    |
| H    | -1.175362    | -7.001141    | -5.110205    |
| H    | 2.191113     | -7.066499    | -2.540539    |
| H    | -0.848864    | -1.894014    | -3.167975    |
| H    | 0.186384     | -0.653901    | -1.017393    |
| H    | 2.501021     | -1.445883    | -2.018049    |
| H    | 2.346880     | 0.144302     | -1.275133    |
| H    | 2.335729     | 1.297826     | -3.380846    |
| H    | 1.964509     | -0.181197    | -4.291904    |
| H    | 6.119826     | 0.472008     | -2.414843    |
| H    | 5.325787     | 1.990587     | -2.977995    |
| H    | 4.618888     | 1.042665     | -1.644533    |
| H    | 0.269354     | 1.662077     | -1.274902    |
| H    | -0.812135    | 2.613927     | -3.870106    |
| H    | -2.397943    | 2.714067     | -1.947872    |
| H    | -1.243297    | 3.721136     | -1.048886    |
| H    | -2.832683    | 4.643516     | -3.499801    |
| H    | -1.622498    | 5.622871     | -2.613585    |
| H    | -0.227917    | 5.153843     | -4.087345    |
| H    | 2.446236     | 5.388163     | -2.926776    |
| H    | 1.553546     | 6.439629     | -5.733342    |
| H    | 3.110313     | 6.827964     | -5.003625    |
| H    | 2.111246     | 4.019572     | -5.683151    |
| H    | 4.823911     | 4.910229     | -4.544774    |
| H    | 4.457412     | 3.274012     | -5.141492    |
| H    | 3.699303     | 3.885205     | -3.717797    |
| H    | 2.718715     | 5.040520     | -7.697363    |
space group C2, model 1, Mpro (heteroatoms frozen, free hydrogens)

| Zero-point correction | 2.608569 (Hartree/Particle) |
|-----------------------|-------------------------------|
| Thermal correction to Energy | 2.729684 |
| Thermal correction to Enthalpy | 2.730628 |
| Thermal correction to Gibbs Free Energy | 2.444241 |
| Sum of electronic and zero-point Energies | -9041.065673 |
| Sum of electronic and thermal Energies | -9040.944559 |
| Sum of electronic and thermal Enthalpies | -9040.943614 |
| Sum of electronic and thermal Free Energies | -9041.230001 |

SOLVENT: -9092.8098439

A.U.
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -8.03970   | 1.232557   | -2.161778  |
| C       | -8.42278   | 0.435090   | -3.229057  |
| C       | -7.98748   | 0.731005   | -4.499418  |
| C       | -6.833854  | 2.621451   | -3.655919  |
| C       | -7.213584  | 1.822679   | -4.714068  |
| C       | -7.297112  | 4.527880   | 0.803988   |
| O       | -6.391095  | 5.39924    | 0.723180   |
| N       | -5.96238   | 3.83234    | 5.097968   |
| C       | -5.59110   | 2.38278    | 6.03667    |
| C       | -6.85043   | 1.239330   | 6.108960   |
| O       | -7.70506   | 1.53969    | 6.536650   |
| C       | -8.27380   | 0.008471   | 5.683547   |
| C       | -7.188347  | -1.143777  | 5.842211   |
| C       | -7.769182  | -1.597380  | 5.498860   |
| C       | -8.465235  | -2.608039  | 5.472090   |
| N       | -7.530913  | -0.849295  | 3.411347   |
| C       | -8.105127  | -1.143799  | 2.074440   |
| O       | -8.167234  | 0.107679   | 2.198797   |
| C       | -6.892011  | 0.710410   | 1.086547   |
| C       | -7.295916  | 2.226214   | 1.359094   |
| C       | -8.785336  | 3.817432   | 0.388814   |
| O       | -6.057334  | -2.492727  | 1.799867   |
| C       | -5.50285   | -5.557734  | 1.183371   |
| C       | -3.929864  | -3.779397  | 1.963457   |
| S       | -2.383847  | -2.382712  | 1.692696   |
| C       | -6.004922  | -4.845646  | 1.018360   |
| O       | -5.853326  | -6.514631  | 1.854646   |
| C       | -5.823764  | -5.502056  | 0.121392   |
| C       | -6.076665  | -6.679594  | -0.508550  |
| C       | -7.901309  | -6.360019  | -1.216978  |
| O       | -8.505234  | -7.323419  | -1.674839  |
| N       | -8.387844  | -5.104645  | -1.242761  |
| C       | -9.544559  | -6.735923  | -2.111482  |
| O       | -9.963255  | -3.297855  | -1.977228  |
| C       | -10.190829 | -2.935700  | -0.616645  |
| C       | -9.146406  | -5.051136  | -3.550547  |
| O       | -7.940282  | -4.949182  | -3.870751  |
| N       | -10.108071 | -5.496303  | -4.362405  |
| S       | -4.593721  | -5.212066  | -5.828060  |
| C       | -4.549004  | -5.014474  | -5.640538  |
| C       | -5.176623  | -4.451304  | -4.260452  |
| C       | -4.535875  | -3.225413  | -3.736361  |
| C       | -5.082393  | -2.287187  | -1.391604  |
| C       | -4.985935  | -0.999743  | -2.780950  |
| N       | -4.242973  | -0.244132  | -3.637596  |
| C       | -3.762345  | 0.792529   | -2.955408  |
| N       | -4.169678  | 0.718299   | -1.743304  |
| C       | -4.935900  | -0.386031  | -1.597723  |
| C       | -3.423771  | -3.545812  | -2.708718  |
| O       | -3.366316  | -4.342275  | -1.829246  |
| C       | -2.269663  | -2.864368  | -2.794545  |
| C       | -1.112970  | -3.015828  | -1.854043  |
| C       | 0.103673   | -3.707217  | -2.526235  |
| C       | -0.151027  | -5.131788  | -2.869799  |
| N       | 0.549987   | -6.187722  | -2.339139  |
| C       | 0.143421   | -7.313617  | -2.886122  |
| N       | -0.708038  | -7.022183  | -3.794270  |
| C       | -1.002741  | -5.675248  | -3.781360  |
| N       | -0.662426  | -1.602651  | -1.236477  |
| O       | -0.238933  | -1.747191  | -0.075036  |
| N       | -0.649418  | -0.555600  | -1.933017  |
| C       | 0.056254   | 0.615248   | -1.352400  |
| C       | 1.576181   | 0.437147   | -1.497649  |
| C       | 1.981741   | -0.068645  | -2.873872  |
| S       | 3.743251   | -0.531199  | -3.029740  |
| C       | 4.306347   | 0.931395   | -3.863835  |
| C       | 3.329077   | 1.942355   | -2.013171  |
| O       | -0.911872  | 1.946241   | -3.122190  |
|   |   |   |
|---|---|---|
| N | 0.077255 | 3.004063 -1.347645 |
| C | -0.081258 | 4.388838 -1.824639 |
| C | -0.920288 | 5.202637 -1.377554 |
| C | -1.242200 | 6.596497 -1.366345 |
| C | -2.244408 | 7.413207 -0.562833 |
| O | -1.863513 | 8.533931 -0.184854 |
| O | -3.34952 | 6.949624 -0.331410 |
| C | 1.329287 | 4.926288 -2.963386 |
| O | 2.179508 | 4.685870 -1.164920 |
| N | 1.571016 | 5.551569 -3.177554 |
| C | 2.855949 | 6.189851 -3.532989 |
| C | 3.092512 | 6.014059 -5.037253 |
| C | 3.426264 | 4.537381 -5.492467 |
| C | 3.144740 | 4.448787 -7.001519 |
| C | 4.506615 | 3.941040 -5.021291 |
| C | 2.822080 | 7.651570 -3.112124 |
| O | 1.748378 | 8.223556 -2.897617 |
| N | 4.000188 | 8.304367 -2.963386 |
| C | 4.088010 | 9.661532 -2.459300 |
| C | 5.529361 | 10.113719 -2.761835 |
| C | 6.204975 | 9.846649 -3.465754 |
| N | 5.331705 | 7.731773 -3.242502 |
| C | 7.006762 | 10.660384 -3.040573 |
| O | 5.287597 | 11.478844 -2.280014 |
| C | 7.639097 | 10.581320 -4.335755 |
| N | 4.906992 | 2.399095 -3.749105 |
| C | 6.677439 | 2.399095 -3.749105 |
| C | 7.623113 | 4.420703 -2.602625 |
| C | 5.892063 | 4.407488 -1.367563 |
| C | 4.923586 | 5.957963 -1.340371 |
| C | 5.535313 | -6.76499 -1.437187 |
| O | 6.700314 | -6.76499 -1.437187 |
| C | 4.821214 | -7.931582 -1.145486 |
| C | 6.842799 | -2.89270 -0.178081 |
| O | 6.840907 | -5.184814 0.679314 |
| N | 7.641776 | -3.232299 -0.193155 |
| C | 8.611010 | -2.781216 0.843614 |
| C | 10.077868 | -2.943160 0.420884 |
| O | 8.495296 | -1.261033 0.907877 |
| C | 8.175379 | -0.678003 -0.149360 |
| N | 8.491814 | -0.648013 2.035265 |
| C | 9.056720 | 0.820500 2.152977 |
| C | 8.971351 | 1.249519 3.624102 |
| O | 8.704982 | 2.741154 3.818352 |
| C | 7.776396 | 3.048615 4.974434 |
| O | 7.441961 | 2.194067 5.801839 |
| N | 7.338094 | 4.293479 5.041275 |
| C | 10.408753 | 1.156025 1.511843 |
| O | 11.434750 | 0.698635 2.010206 |
| N | 10.405376 | 1.871057 0.391017 |
| S | 6.216699 | 2.758381 0.039286 |
| O | 7.571910 | 2.596963 -0.631648 |
| C | 5.342290 | 1.720289 -1.088785 |
| C | 5.342490 | 1.221167 -0.116059 |
| H | 3.262472 | 1.636383 2.640798 |
| H | 2.882824 | -6.878473 4.082541 |
| O | -0.482627 | -4.314519 0.765691 |
| C | 0.601555 | -5.352498 4.709503 |
| H | 1.560639 | -5.865041 0.665355 |
| H | 9.378806 | 2.282079 8.551162 |
| H | 10.88925 | 4.582884 6.976921 |
| H | 2.858369 | 4.373502 5.713391 |
| H | 8.003576 | 4.730342 7.411080 |
| H | 7.977383 | 1.862446 7.001389 |
| H | 6.754241 | 2.876940 7.773088 |
| H | 4.886533 | -0.645663 5.128588 |
| H | 5.136078 | -0.934012 6.858046 |
| H | 6.391153 | -0.099382 5.895779 |
| H | 11.975470 | -2.254575 7.124207 |
| H | 8.724549 | 3.282065 -0.301226 |
| H | -6.331813 | 2.497690 -0.469554 |
| H | -5.997929 | 3.895459 -1.519261 |
| H | -8.348218 | 0.978455 -1.160401 |
| H | -9.039502 | -0.438664 -3.048325 |
| H | -8.271589 | 0.090058 -5.327438 |
| X         | Y         | Z         |
|-----------|-----------|-----------|
| -6.200431 | 3.485060  | -3.832966 |
| -6.869416 | 2.602360  | -5.714142 |
| -8.417554 | 3.242533  | -4.332925 |
| -9.081828 | 4.093522  | -3.332950 |
| -9.547433 | 5.853628  | 2.534877  |
| -7.548149 | 7.347171  | 2.982619  |
| -9.700255 | 8.227421  | 3.193858  |
| -8.172191 | 7.672764  | 4.622052  |
| -11.122029| 5.338237  | 4.335982  |
| -10.302878| 6.486112  | 5.415419  |
| -11.123892| 7.072700  | 3.957111  |
| -5.702655 | 4.336191  | 5.345076  |
| -4.573822 | 1.912177  | 5.632743  |
| -5.030178 | 2.060250  | 8.106007  |
| -6.840999 | 3.429532  | 5.778259  |
| -2.815659 | 4.934571  | 8.066210  |
| -4.159910 | 4.191646  | 9.432142  |
| -5.355050 | -0.170146 | 5.288181  |
| -6.686458 | -1.994463 | 6.279537  |
| -8.015492 | -0.810703 | 6.446867  |
| -7.098672 | 0.697635  | 3.532254  |
| -9.103263 | -1.574224 | 2.205136  |
| -8.921019 | 0.785249  | 1.653823  |
| -8.522277 | -0.209687 | 0.237022  |
| -6.745736 | 1.324487  | 1.868616  |
| -5.703571 | -1.970456 | 2.590869  |
| -4.918385 | -3.214323 | 0.178796  |
| -3.456503 | -4.687401 | 1.577673  |
| -4.164223 | -3.945035 | 3.020235  |
| -5.136175 | -5.159936 | -0.807847 |
| -6.870322 | -7.231467 | 0.398127  |
| -6.019651 | -7.314547 | -1.701688 |
| -7.916205 | -4.350595 | -0.742023 |
| -10.382932| -5.378963 | -1.816903 |
| -10.894367| -3.157356 | -2.537825 |
| -9.188041 | -2.673335 | -2.464326 |
| -9.308530 | -2.871757 | -0.137180 |
| -9.867621 | -5.760759 | -5.312761 |
| -11.037527| -5.709477 | -4.020668 |
| -6.144759 | -4.649129 | -3.968298 |
| -4.072312 | -2.717822 | -4.591652 |
| -6.118697 | -2.757565 | -2.340064 |
| -6.347170 | -2.123927 | -3.983711 |
| -3.081671 | 1.529590  | -3.375485 |
| -5.420450 | -0.586635 | -0.657094 |
| -3.998671 | 1.386412  | -1.001734 |
| -2.161513 | -2.232006 | -3.570101 |
| -1.883338 | -3.624466 | -1.031373 |
| -0.937812 | -3.631751 | -1.815331 |
| 0.380610  | -3.121269 | -3.412700 |
| 0.531478  | -8.289474 | -2.655665 |
| -1.734432 | -5.213062 | -4.423485 |
| 1.298939  | -6.077987 | -1.664935 |
| -1.143143 | -0.392038 | -2.807764 |
| -0.186564 | 0.639715  | -0.284831 |
| 1.866587  | -0.334682 | -0.774800 |
| 2.995520  | 1.361967  | -1.219717 |
| 1.776363  | 0.768223  | -3.622054 |
| 1.378196  | -0.874929 | -3.151687 |
| 3.590504  | 0.873811  | -3.973125 |
| 3.858019  | 1.018176  | -4.858542 |
| 4.068461  | 1.830377  | -3.289314 |
| 0.650699  | 2.918984  | -0.514568 |
| -0.609585 | 4.299533  | -2.780318 |
| 1.853334  | 4.657532  | -0.661374 |
| -0.375045 | 5.268785  | 0.108228  |
| -1.674275 | 6.473653  | -2.374385 |
| -0.349730 | 7.218193  | -1.468391 |
| 0.781696  | 5.825402  | -3.744464 |
| 3.617674  | 5.661705  | -2.951919 |
| 2.235729  | 6.470889  | -5.556135 |
| 3.976812  | 6.797285  | -5.350278 |
| 2.414614  | 3.980022  | -5.045346 |
| 5.404764  | 4.533644  | -5.401529 |
| 4.671293  | 2.925672  | -5.403942 |
| 6.454384  | 3.909513  | -3.951884 |
| 2.192585  | 4.845977  | -7.373930 |
| 3.958144  | 5.008976  | -7.482073 |
space group C2, model 1, 13b (heteroatoms frozen, free hydrogens)

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 3.223076   | 3.403513   | -7.320882  |
| H    | 3.874387   | 9.667958   | -1.387942  |
| H    | 5.527902   | 11.007688  | -3.390070  |
| H    | 6.038488   | 10.365614  | -1.827742  |
| H    | 6.260577   | 9.151670   | -4.541343  |
| H    | 7.225986   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| H    | 7.342350   | 8.778141   | -3.113578  |
| H    | 5.663716   | 7.158294   | -2.363497  |
| H    | 5.336652   | 7.059372   | -4.099538  |
| H    | 3.079779   | 9.812678   | -4.915331  |
| Atoms | X        | Y        | Z        |
|-------|----------|----------|----------|
| C     | 0.286105 | 5.901782 | 1.357228 |
| C     | -0.678047| 1.466432 | 0.317240 |
| O     | -0.695331| 0.761192 | -0.692035|
| N     | -1.397308| 1.187630 | 1.417171 |
| C     | -2.298355| 0.079842 | 1.494303 |
| C     | -1.985670| -0.906521| 2.664297 |
| C     | -0.739812| -1.664722| 2.317334 |
| C     | -0.118572| -2.519384| 3.400457 |
| O     | -0.041405| -2.158615| 4.571416 |
| N     | 0.352886 | 0.817269 | 1.48205 |
| O     | -3.776724| 2.028580 | 1.671492 |
| C     | -4.703970| -0.108011| 1.066988 |
| O     | -4.874844| 1.094966 | 1.758385 |
| N     | -5.382238| 0.335151 | -0.031018|
| C     | -6.519642| -0.345330| -0.65457 |
| C     | -7.167161| 0.930347 | -1.53129 |
| C     | -8.30091 | 2.220638 | 1.373351 |
| C     | -9.527740| -0.342517| -3.801362|
| C     | -6.61024 | 2.989423 | 3.411654 |
| C     | -8.799423| 3.111530| 2.390351 |
| H     | 4.395055 | 1.480676| -2.706922|
| H     | 2.613732 | 3.048428| 1.5391052|
| H     | 0.703805 | 3.787244| -2.165556|
| H     | 0.554725 | 2.864389| 1.365839 |
| H     | -1.049273| 3.776760| -1.085135|
| H     | -1.488604| 4.032272| 0.598359 |
| H     | 1.167916 | 5.190347| -0.545934|
| H     | -1.541200| 6.590019| 1.252205 |
| H     | 0.030305 | 7.428436| -0.275934|
| H     | 1.126844 | 6.335089| 1.729205 |
| H     | -0.436653| 5.496376| 2.115852 |
| H     | -1.363509| 1.806128| 2.221218 |
| H     | -2.225998| 0.448883| 0.537654 |
| H     | -2.948185| -1.364311| 2.785411|
| H     | -1.836292| -0.345227| 3.594344 |
| H     | 0.044797 | -0.939379| 2.032034 |
| H     | 0.903712 | -3.415458| 3.391551 |
| H     | 1.103210 | -3.425415| 0.881274 |
| H     | -0.116700| -4.710075| 1.070747 |
| H     | -1.900521| -3.150383| 1.277055 |
| H     | -0.844975| -2.212918| 0.182214 |
| H     | -5.122431| 1.255652| -0.374400|
| H     | -7.032899| -0.912338| 0.128116 |
| H     | -7.205273| 0.412739| -1.052870|
| H     | -3.987046| -0.723523| 1.667159 |
| H     | -3.289509| -2.258069| 3.474213 |
| H     | -4.691089| -3.716959| 4.596318 |
| H     | -7.348935| -3.622489| 3.890191 |
| H     | -8.037126| 2.076666| 2.081735 |
| H     | 5.975552 | 2.542345| 2.472725 |
| H     | 5.418940| 3.671635| 1.212208 |
| H     | 7.008907 | -3.911940| 1.985869 |
| H     | 7.829544| -2.610679| 1.403904 |
| H     | 8.073143 | 3.953754| 0.233704 |
| H     | 6.482179 | 3.704300| 1.015060 |
| H     | 8.595279 | 0.899193| -0.360435|
| H     | 8.922471| -2.251105| -1.474471 |
| H     | 7.840343 | 0.912638| -1.969423 |
| H     | 4.047573 | -0.001996| 0.672244 |

**space group C2, model 1, product (heteroatoms frozen, free hydrogens)**

**GAS:** -11038.2121830

**SOLVENT:** -11098.3084298

SciCUT13e SCF Done: -11038.2121830 A.U.
|      | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| S    | 5.970108  | -2.965420 | 5.118822  |
| C    | 5.362056  | -1.317365 | 5.473430  |
| C    | 9.940686  | -3.343100 | 5.852606  |
| O    | 9.293109  | -3.078770 | 4.808474  |
| N    | 11.164255 | -2.845493 | 6.094531  |
| C    | -7.614334 | 3.960868  | -1.643564 |
| C    | -6.525293 | 3.107334  | -2.277068 |
| C    | -6.984900 | 2.223347  | -4.242899 |
| C    | -7.864554 | 1.185937  | -3.159535 |
| O    | -6.957533 | 0.382148  | -4.26814 |
| N    | -7.588433 | 4.132773  | 0.794655  |
| C    | -7.094415 | 4.513459  | 2.141578  |
| C    | -8.25668  | 5.182643  | 2.921249  |
| C    | -8.94150  | 6.361352  | 2.277002  |
| C    | -10.30715 | 6.619803  | 3.006735  |
| C    | -8.15587  | 7.629178  | 2.271334  |
| C    | -6.91079  | 3.293720  | 2.900457  |
| O    | -6.79364  | 2.123515  | 2.440586  |
| N    | -5.946063 | 3.543100  | 4.043232  |
| C    | -5.588093 | 2.499028  | 5.043636  |
| C    | -5.294202 | 3.121824  | 6.407733  |
| O    | -4.193918 | 3.939022  | 6.421973  |
| O    | -3.323381 | 4.044226  | 5.415094  |
| N    | -3.707262 | 5.332295  | 7.565327  |
| C    | -6.724400 | 1.478750  | 5.118780  |
| O    | -7.840892 | 1.861910  | 5.482012  |
| N    | -6.645818 | 0.219602  | 4.758597  |
| C    | -7.447074 | -0.874875 | 4.901376  |
| C    | -8.001757 | -1.351558 | 3.576137  |
| O    | -8.751938 | -2.532653 | 3.877799  |
| N    | -7.682160 | -0.669799 | 2.476387  |
| C    | -8.221108 | -0.992313 | 1.131292  |
| C    | -8.184591 | 0.221366  | 0.222581  |
| O    | -8.676979 | 0.748506  | 0.114655  |
| C    | -7.446785 | -2.147439 | 0.495471  |
| O    | -7.997256 | -2.750574 | -0.469283 |
| N    | -6.242646 | -2.465735 | 0.996582  |
| C    | -5.426043 | -3.595978 | 0.460264  |
| C    | -4.197107 | -3.850742 | 1.299383  |
| S    | -3.015808 | -2.528301 | 1.013554  |
| C    | -6.290868 | -4.845228 | 0.313648  |
| O    | -7.186116 | -5.070406 | 1.132173  |
| N    | -6.103768 | -5.560367 | -0.784571 |
| C    | -6.936509 | -6.708533 | -1.152508 |
| C    | -8.182977 | -6.354444 | -1.924970 |
| O    | -8.821707 | -7.302456 | -2.365317 |
| N    | -5.979885 | -5.076145 | -2.023457 |
| C    | -9.69891 | -4.689425 | -2.952611 |
| O    | -10.042015 | -3.221865 | -2.896372 |
| O    | -10.300187 | -2.787727 | -1.562578 |
| C    | -9.265186 | -5.088874 | -4.359778 |
| O    | -8.043631 | -5.062403 | -4.641627 |
| N    | -10.218597 | -5.513463 | -5.189980 |
| O    | -6.700993 | -5.563834 | -5.799692 |
| O    | -3.509686 | -5.446973 | -6.220439 |
| N    | -5.244136 | -4.731400 | -4.935272 |
| C    | -4.556616 | -5.195561 | -4.438522 |
| C    | -5.595082 | -2.501738 | -3.977385 |
| C    | -4.918281 | -1.232566 | -3.597192 |
| N    | -4.102893 | -0.556888 | -4.457374 |
| C    | -3.591291 | 0.478777 | -3.838359 |
| N    | -4.047688 | 0.483680 | -2.601582 |
| C    | -4.878860 | -0.570306 | -2.440023 |
| O    | -3.503428 | -3.853124 | -3.354541 |
| C    | -3.842607 | -4.594350 | -2.455254 |
| N    | -2.308792 | -3.238646 | -3.407801 |
| C    | -1.206063 | -3.410495 | -2.431379 |
| C    | -0.000284 | -4.195516 | -3.024422 |
| C    | -0.318846 | -6.194940 | -3.340777 |
| C    | 0.301105 | -6.858605 | -2.714506 |
| C    | 0.146365 | -7.811291 | -3.229037 |
| N    | -1.017706 | -7.511413 | -4.184950 |
| C    | -1.65488 | -6.155237 | -4.238132 |
| C    | -0.709072 | -2.087236 | -1.853287 |
| O    | -0.325150 | -2.112622 | -0.674287 |
|   |   |   |   |
|---|---|---|---|
| N | -0.598791 | -0.984688 | -2.596102 |
| C | 0.148337 | 0.171272 | -2.037945 |
| C | 1.660448 | -0.094523 | -2.114596 |
| C | 2.092240 | -0.620557 | -3.453409 |
| S | 3.826476 | -1.247183 | -3.516213 |
| C | 4.500960 | 0.146389 | -4.388557 |
| C | 0.138138 | 1.478294 | -2.768994 |
| O | -0.677282 | 1.472155 | -3.899940 |
| N | 0.296779 | 2.553597 | -2.133937 |
| C | 0.238012 | 3.921999 | -2.675051 |
| C | -0.590998 | 4.822665 | -1.762453 |
| O | -1.372240 | 8.225803 | -1.285726 |
| C | 2.092240 | -0.620557 | -3.453409 |
| S | 3.826476 | -1.247183 | -3.516213 |
| C | 4.500960 | 0.146389 | -4.388557 |
| C | 0.138138 | 1.478294 | -2.768994 |
| O | -0.677282 | 1.472155 | -3.899940 |
| N | 0.296779 | 2.553597 | -2.133937 |
| C | 0.238012 | 3.921999 | -2.675051 |
| C | -0.590998 | 4.822665 | -1.762453 |
| O | -1.372240 | 8.225803 | -1.285726 |
| C | 1.682898 | 4.373215 | -2.846280 |
| O | 2.485343 | 4.126250 | -1.936364 |
| N | 2.001873 | 4.932836 | -4.009434 |
| C | 3.332729 | 5.486878 | -4.339451 |
| C | 3.615622 | 5.229665 | -5.824415 |
| C | 3.701690 | 3.748111 | -6.210516 |
| C | 3.654700 | 3.577567 | -7.716616 |
| C | 4.965131 | 3.083744 | -5.661691 |
| C | 3.364064 | 6.936415 | -3.982699 |
| O | 3.518412 | 9.343401 | -5.330769 |
| C | 7.377085 | -4.509474 | -4.792638 |
| C | 9.239673 | -4.707855 | -4.510953 |
| C | 9.994344 | -5.187359 | -5.753623 |
| C | 9.893794 | -3.471405 | -3.908883 |
| C | 6.606664 | -3.032357 | -3.253747 |
| C | 6.557341 | -5.269204 | -2.808574 |
| C | 5.693291 | -5.153390 | -1.606479 |
| C | 4.660111 | -6.285542 | -1.567638 |
| C | 5.197580 | -7.700089 | -1.581211 |
| O | 6.395599 | -7.801114 | -1.949711 |
| C | 4.421207 | -8.601479 | -1.278035 |
| C | 6.068173 | -5.033789 | -0.385834 |
| C | 6.519921 | -5.888591 | 0.507854 |
| O | 6.250900 | -4.022742 | -0.419370 |
| C | 6.339324 | -3.756529 | 0.640657 |
| C | 9.885353 | -3.387919 | 0.284187 |
| C | 8.379428 | -2.050304 | 0.635656 |
| C | 8.132107 | -1.501155 | -0.451931 |
| C | 8.724084 | -1.410325 | 1.749270 |
| C | 9.080894 | 0.048710 | 1.812741 |
| C | 8.891348 | 0.546828 | 3.259739 |
| O | 8.700926 | 2.057788 | 3.796888 |
| C | 7.747983 | 2.465391 | 4.838630 |
| C | 7.335771 | 1.668240 | 5.332506 |
| N | 7.777142 | 3.734264 | 4.479981 |
| C | 10.399803 | 0.282205 | 1.212535 |
| O | 11.379403 | -0.206973 | 1.770501 |
| N | 10.478223 | 0.945730 | 0.063133 |
| S | 6.361227 | 2.040162 | -0.493142 |
| C | 7.729810 | 1.776244 | -1.101934 |
| C | 5.484780 | 3.001818 | -1.699239 |
| C | 5.409775 | 0.546822 | -0.617991 |
| C | 4.511603 | 0.548185 | 1.971308 |
| C | 3.595558 | 5.267082 | 1.944452 |
| C | 3.032398 | 6.352047 | 0.412462 |
| C | 3.221103 | 7.765241 | 0.667444 |
| C | 4.723530 | 8.063600 | 0.548159 |
| C | 2.403774 | 8.559871 | -0.355276 |
| C | 2.71422 | 8.132121 | 2.063585 |
| N | 3.037042 | 4.076655 | 0.967568 |
| C | 3.269722 | 2.910502 | 1.633279 |
| C | 2.367525 | 1.802979 | 1.300247 |
| O | 1.442582 | 1.940404 | 0.443489 |
| C | 4.253682 | 2.733354 | 2.620587 |
| C | 4.361846 | 1.501220 | 2.352838 |
| H                  | x       | y       | z       |
|-------------------|---------|---------|---------|
| -3.741983         | -4.792997 | 0.980589 |
| -4.467809         | -3.949780 | 2.356781 |
| -5.382675         | -5.279846 | -1.463764 |
| -7.630900         | -7.205838 | -0.234115 |
| -6.360492         | -7.404045 | -1.529813 |
| -8.112508         | -6.918107 | -0.537977 |
| -9.958778         | -8.267659 | -6.119187 |
| -11.171694        | -5.656199 | -4.878192 |
| -6.236905         | -4.859936 | -6.771575 |
| -4.035186         | -3.072305 | -5.293801 |
| -6.163187         | -2.904889 | -3.127665 |
| -6.930232         | -2.338810 | -4.806272 |
| -2.863842         | 1.107347  | -2.421320 |
| -5.413978         | -0.700664 | -1.517899 |
| -3.833125         | 1.200671  | -1.894666 |
| -2.158688         | -2.615779 | -4.199483 |
| -1.640552         | -3.967271 | -1.602822 |
| 0.817915          | -1.344490 | -2.291926 |
| 0.336351          | -3.663976 | -3.924052 |
| 0.181495          | -7.895324 | -2.945645 |
| -1.848277         | -5.684168 | -4.927061 |
| 1.052256          | -6.386334 | -2.040523 |
| -1.073373         | -0.818749 | -3.484002 |
| -0.119338         | 0.297874  | -0.958936 |
| 1.198178          | -0.849161 | -1.357393 |
| 2.198445          | 0.814298  | -1.831110 |
| 1.959119          | 0.131878  | -2.439847 |
| 1.453840          | -1.466246 | -3.723672 |
| 5.588164          | 0.027124  | -4.452716 |
| 4.093696          | 0.212289  | -5.402166 |
| 4.290663          | 1.079795  | -3.860554 |
| 0.750709          | 2.451810  | -1.212270 |
| -0.260322         | 3.825898  | -3.646359 |
| -1.552729         | 4.319228  | -1.613497 |
| -0.086320         | 4.098724  | -0.790137 |
| -1.219012         | 6.062553  | -3.374207 |
| 0.113471          | 6.774412  | -2.449902 |
| 1.251501          | 5.228877  | -4.620035 |
| 4.041841          | 4.945292  | -3.704682 |
| 2.805196          | 5.707671  | -6.395872 |
| 4.540658          | 5.733115  | -6.125504 |
| 2.827263          | 3.245446  | -5.773250 |
| 5.853931          | 3.615091  | -6.036474 |
| 5.035107          | 2.048664  | -5.998482 |
| 4.994668          | 3.994069  | -4.569751 |
| 2.741971          | 4.011184  | -8.143190 |
| 4.517010          | 4.068123  | -8.188021 |
| 3.682660          | 2.516325  | -7.988078 |
| 4.467959          | 8.991830  | -2.306168 |
| 6.262453          | 10.155358 | -4.291798 |
| 6.673051          | 9.550847  | -2.684399 |
| 6.932002          | 8.211437  | -5.335737 |
| 7.820185          | 7.894449  | -3.855126 |
| 6.142175          | 6.534399  | -3.099036 |
| 5.877228          | 6.192577  | -4.841873 |
| 3.811674          | 9.025916  | -5.864015 |
| 7.430338          | 2.536061  | -5.217435 |
| 7.365833          | 5.438690  | -5.244361 |
| 9.289737          | 5.508705  | -3.752374 |
| 9.610059          | 6.153655  | -6.102963 |
| 11.062424         | 5.294552  | -5.536475 |
| 9.854690          | 4.449777  | -6.556080 |
| 9.341519          | -3.101847 | -3.036228 |
| 9.913819          | -2.669444 | -4.656207 |
| 10.923746         | -3.690383 | -3.608273 |
| 6.763191          | -6.210206 | -3.131566 |
| 5.714878          | -4.197377 | -1.726505 |
| 4.050859          | -6.171423 | -0.668438 |
| 4.012869          | -6.173071 | -2.446966 |
| 7.376248          | -3.300168 | -1.144056 |
| 8.129915          | -4.029777 | 1.594522 |
| 10.532991         | -3.367071 | 1.029029 |
| 10.087201         | -3.390305 | -0.693195 |
| 8.931856          | -1.938582 | 2.604934 |
| 8.258515          | 0.531714  | 1.177877 |
| 9.706988          | 0.213444  | 3.790207 |
### space group C2, model 3, reactant complex

|   |   |   |   |
|---|---|---|---|
| C  | 5.062212 | -5.392413 | -3.197881 |
| C  | 1.449942 | -4.06970 | -3.187919 |
| C  | 5.062212 | -5.392413 | -3.197881 |
| C  | 1.449942 | -4.06970 | -3.187919 |
| C  | 5.062212 | -5.392413 | -3.197881 |
| C  | 1.449942 | -4.06970 | -3.187919 |
| C  | 5.062212 | -5.392413 | -3.197881 |
| C  | 1.449942 | -4.06970 | -3.187919 |
| C  | 5.062212 | -5.392413 | -3.197881 |
| C  | 1.449942 | -4.06970 | -3.187919 |
| C  | 5.062212 | -5.392413 | -3.197881 |
| C  | 1.449942 | -4.06970 | -3.187919 |
| C          | -6.425266   | 1.842337   | -2.715301   |
| C          | -3.136365   | 1.429495   | -3.995933   |
| C          | 2.256450    | 1.261104   | -5.037011   |
| C          | -0.410303   | 1.973929   | -3.644957   |
| C          | -0.891429   | 1.515869   | -4.872834   |
| C          | -0.829906   | 4.224132   | 0.655170    |
| O          | 0.317193    | 4.749826   | 0.753542    |
| C          | -1.542790   | 3.820960   | 1.732640    |
| C          | 0.895202    | 3.568462   | 3.021550    |
| C          | -1.554177   | 4.372228   | 4.166551    |
| C          | 0.191448    | 1.357272   | 2.867922    |
| C          | -0.130552   | 1.621195   | 4.256488    |
| C          | 0.105359    | 0.196985   | 4.640504    |
| C          | 0.872764    | 0.049980   | 5.829066    |
| C          | 2.266869    | 0.516366   | 5.431221    |
| C          | 2.475560    | 1.665597   | 4.970363    |
| C          | -4.071908   | -1.80818   | 3.303190    |
| C          | -5.140172   | -2.320032  | 3.053361    |
| C          | -3.559078   | -0.713688  | 2.484886    |
| C          | -4.331365   | -0.266959  | 1.334997    |
| C          | -4.564458   | 1.268891   | 1.312852    |
| C          | -3.623701   | 1.929149   | 0.781799    |
| C          | -3.715554   | -0.538116  | -0.019532   |
| C          | -4.444115   | -0.658282  | -1.034174   |
| C          | -2.461014   | -1.027696  | -0.162651   |
| C          | -2.011910   | -1.274271  | -1.557278   |
| C          | -0.652332   | -1.967537  | -1.649234   |
| S          | 0.740671    | -0.944025  | -1.042292   |
| C          | -3.012955   | -2.238457  | -2.228504   |
| C          | -3.928866   | -2.394022  | -1.686912   |
| C          | -3.363778   | -1.846034  | -3.483630   |
| C          | -4.430801   | -2.528566  | -4.219110   |
| C          | -5.712788   | -1.676039  | -4.326249   |
| C          | -6.559779   | -1.851890  | -5.219254   |
| C          | -5.836017   | -0.730846  | -3.359689   |
| C          | -6.994051   | 0.156477   | -3.372895   |
| C          | -6.834405   | 1.238505   | -2.271721   |
| C          | -6.868147   | 0.689978   | -0.934478   |
| C          | -7.049213   | 0.882959   | -4.723983   |
| C          | -6.038440   | 1.391904   | -5.237759   |
| C          | -8.301880   | 1.026768   | -5.236209   |
| C          | 4.371839    | 4.458770   | -1.456993   |
| C          | 3.601355    | 3.610601   | -1.938047   |
| C          | 2.406301    | 3.858157   | -2.559444   |
| C          | 2.072214    | 5.306127   | -2.921065   |
| C          | 3.174497    | 5.831667   | -3.851658   |
| C          | 0.742995    | 5.169130   | -3.664105   |
| C          | 1.931862    | 6.140040   | -1.643651   |
| C          | 3.848499    | 2.257638   | -1.918637   |
| C          | 4.985561    | 1.659715   | -1.379867   |
| C          | 4.874664    | 0.219575   | -1.367794   |
| C          | 3.840625    | 0.365999   | -1.829401   |
| C          | 6.093424    | 2.282901   | -0.854678   |
| C          | 7.105101    | 1.502609   | -0.238288   |
| C          | 6.989696    | 0.143999   | -0.184194   |
| C          | 5.909067    | 0.489575   | -0.769496   |
| C          | 5.736051    | -1.903550  | -0.697280   |
| C          | 7.051087    | -2.760576  | -0.706375   |
| C          | 7.971776    | -2.367535  | -1.849067   |
| C          | 8.597057    | -3.461625  | -2.706601   |
| C          | 7.489299    | -2.768580  | -3.278995   |
| C          | 4.906037    | -2.280886  | 0.579035    |
| C          | 5.402084    | -2.745372  | 1.619401    |
| C          | 3.606038    | -1.937047  | 0.402493    |
| C          | 2.688483    | -1.996349  | 1.467444    |
| C          | 2.157758    | -0.897371  | 1.995872    |
| C          | 2.728887    | 0.651679   | 1.308537    |
| C          | 1.651632    | 1.752333   | 1.332717    |
| C          | 0.417616    | 1.559655   | 1.262179    |
| C          | 2.261646    | 2.952568   | 1.431191    |
| C          | 3.724926    | 2.876914   | 1.616841    |
|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| C   | 3.939655  | 1.665215  | 1.958174  |
| C   | 1.491880  | -2.93923  | 0.983430  |
| O   | 0.717147  | -3.827149 | 1.003497  |
| C   | -2.164880 | -3.96279  | 1.270756  |
| C   | -2.488945 | -5.13937  | 2.182215  |
| O   | -1.593896 | -6.194003 | 2.388119  |
| N   | -1.939021 | -7.266002 | 3.215667  |
| C   | -3.182401 | -7.29137  | 3.848584  |
| H   | 4.906173  | -6.173688 | -2.285242 |
| H   | 4.861562  | -6.246531 | -4.05506  |
| H   | 0.323293  | 2.839356  | -1.324626 |
| H   | 0.419051  | 1.273265  | -4.131800 |
| H   | 2.519182  | 3.969260  | -0.598740 |
| H   | 0.941290  | 1.183637  | -0.481734 |
| H   | 1.032393  | 1.503956  | 4.458915  |
| H   | -3.246328 | 6.212560  | 5.296814  |
| H   | -1.630179 | 6.466127  | 5.995890  |
| H   | -2.256648 | 7.660405  | 4.904775  |
| H   | 0.730000  | 2.131908  | 4.493709  |
| H   | 0.216366  | -0.402271 | 3.791948  |
| H   | 0.869470  | -0.990369 | 6.163334  |
| H   | 0.480920  | 0.681370  | 6.633718  |
| H   | -0.496491 | -0.149347 | 5.255675  |
| H   | 3.097737  | -1.334804 | 5.911881  |
| H   | -1.345047 | -1.723596 | 3.649439  |
| H   | -3.255783 | -3.003359 | 4.770468  |
| H   | -3.723714 | -1.403114 | 5.415681  |
| H   | -2.774973 | -0.125642 | 2.796848  |
| H   | 5.290570  | -0.794029 | 1.377295  |
| H   | -4.807077 | 1.608381  | 2.326410  |
| H   | -5.382768 | 1.480192  | 6.235730  |
| H   | -2.610976 | 1.630333  | 1.402010  |
| H   | -1.830719 | -1.125879 | 0.636191  |
| H   | -1.992287 | -0.319643 | -2.081862 |
| H   | -0.467911 | -2.186543 | -2.705279 |
| H   | -0.670188 | -2.913057 | -1.108158 |
| H   | 3.068434  | -0.927844 | -3.815980 |
| H   | -4.653441 | -3.442333 | -3.658112 |
| H   | -4.126419 | -2.791814 | -5.234428 |
| H   | -5.140369 | -0.632448 | -2.619048 |
| H   | -7.915122 | -0.406836 | -3.190642 |
| H   | -7.673538 | 1.934906  | -2.354325 |
| H   | -5.905265 | 1.785593  | -2.486668 |
| H   | -6.016753 | 0.144570  | -0.848896 |
| H   | -8.408458 | 1.314832  | -6.119630 |
| H   | -9.072934 | 0.460699  | -4.905290 |
| H   | 6.145338  | 3.359374  | -0.874374 |
| H   | 7.961717  | 1.983055  | 0.212669  |
| H   | 7.003566  | -0.490755 | 0.309450  |
| H   | 5.140315  | -2.246004 | -1.571336 |
| H   | 7.539370  | -2.075892 | 0.270001  |
| H   | 6.792381  | -3.814543 | -0.808125 |
| H   | 8.575697  | -1.843383 | -1.683479 |
| H   | 8.346671  | -4.487338 | -2.458282 |
| H   | 9.604543  | -3.311678 | -3.075707 |
| H   | 7.766418  | -1.834760 | -4.018425 |
| H   | 6.503739  | -3.004756 | -3.404981 |
| H   | 3.347146  | -1.540331 | -0.505408 |
| H   | 3.116289  | -2.540089 | 2.278736  |
| H   | 2.394790  | -0.550288 | 3.061401  |
| H   | 1.079053  | -0.522282 | 1.884415  |
space group C2, model 3, transition state proton transfer (H on imidazole of H41)

| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| H       | 2.921876  | 0.462003  | 0.249303  |
| H       | 1.717955  | 3.811885  | 1.265563  |
| H       | 4.241488  | 3.187050  | 0.708028  |
| H       | 4.037572  | 3.519482  | 2.444456  |
| H       | 3.855906  | 1.262506  | 3.043435  |
| H       | 4.904171  | 0.997248  | 1.605477  |
| H       | -0.211283 | -4.517024 | 0.446722  |
| H       | -2.476141 | -3.035157 | 1.751255  |
| H       | -2.685156 | -4.015923 | 0.305843  |
| H       | -0.618022 | -6.181877 | 1.917253  |
| H       | -1.234979 | -8.076717 | 3.366491  |
| H       | -3.450248 | -8.121711 | 4.491751  |
| H       | -5.039164 | -6.237239 | 4.150982  |
| H       | -4.421826 | -3.329722 | 2.714242  |
| H       | 1.643191  | -1.695108 | -1.795418 |
| H       | 2.901819  | 6.265994  | -1.174805 |
| H       | 1.263085  | 5.646398  | -0.933426 |
| H       | 1.522620  | 7.121080  | -1.909318 |
| H       | 0.858167  | 4.527717  | -4.541640 |
| H       | 0.408565  | 6.161556  | -3.982229 |
| H       | -0.012029 | 4.725488  | -3.015884 |
| H       | 3.268656  | 5.176584  | -4.724054 |
| H       | 2.901340  | 6.836233  | -4.189651 |
| H       | 4.125401  | 5.874848  | -3.319108 |
| H       | 3.147458  | 1.598548  | -2.262024 |
| H       | 6.116727  | -5.292456 | -3.237575 |
| H       | -1.283061 | 4.734351  | -1.375284 |

Zero-point correction= 1.648716 (Hartree/Particle)
Thermal correction to Energy= 1.746811
Thermal correction to Enthalpy= 1.747755
Thermal correction to Gibbs Free Energy= 1.514332
Sum of electronic and zero-point Energies= -5208.665560
Sum of electronic and thermal Energies= -5208.567465
Sum of electronic and thermal Enthalpies= -5208.566521
Sum of electronic and thermal Free Energies= -5208.799944

SOLVENT: -5238.816541
space group C2, model 3, transition state proton transfer (H on imidazole of H41) isomer (Mpro distorted)

Zero-point correction= 1.648907 (Hartree/Particle)
Thermal correction to Energy = 1.747075
Thermal correction to Enthalpy = 1.748019
Thermal correction to Gibbs Free Energy = 1.514541
Sum of electronic and zero-point Energies = -5208.688608
Sum of electronic and thermal Energies = -5208.590440
Sum of electronic and thermal Enthalpies = -5208.589496
Sum of electronic and thermal Free Energies = -5208.822973

RXsimp22REACTANT--HFqst3 SCF Done: -5210.337514 A.U.

C      4.246488     2.383540     -0.673644
C      3.107714     2.144364     -0.139363
N      2.777075     3.030716     -0.100971
C      1.859052     2.432247     -2.823513
C      1.583572     1.226225     -2.768045
C      2.346377     1.027258     -2.902743
C     -1.653680     3.449645      1.991826
C     -1.840559     2.508354      0.761076
C     -2.704933     3.053998    -0.321418
C     -4.119163     3.178795     -2.390197
C     -4.988508     3.586900    -1.102728
C     -4.483432     3.833422    -2.387115
C     -2.245199     3.231111    -1.605839
C     -3.112100     3.697056    -2.637030
C     -0.627901     2.791299      2.909441
O      0.517108     3.268595      3.123115
N     -1.050702     1.601245      3.424531
C     -0.128765     0.620256      3.948197
C     -0.491553     1.577273      6.368942
O     -0.828704     1.164440      7.818803
C     -0.846445     2.349776      6.320765
C     -0.220718     -0.703025      3.221244
O     -1.188902     -0.953340      2.449741
N      0.742202     -1.959308      3.472963
C      0.694967     -2.951284      2.889682
C      1.814544     -3.798562      3.546086
C      3.128045     -3.157955      3.124320
O      3.454626     -2.037820      3.605569
C      3.778618     -3.764088      2.110240
C     -0.657208     -3.629594      3.153951
O     -1.194671     -3.678124      4.270256
N      1.144126     -4.200682      2.014258
C     -2.244713     -4.852646      2.002419
C     -3.577371     -3.928822      1.528409
C     -4.652149     -4.381634      1.089109
N     -3.322954     -2.590903      1.665601
C     -4.417485     -1.643837      1.467894
C     -5.402416     -0.572847      2.583206
C     -3.405896     -0.855500      2.434741
C     -3.437456     -0.878217      0.157204
O     -5.365891     -2.281213    -0.215324
N     -3.216867     -0.862217    -0.543255
C     -3.132913     -0.024459    -1.758251
C     -1.754033     -0.197569    -2.421068
S     -0.450479     -0.020044    -1.141804
C     -4.225956     -0.502284      2.722687
O     -4.340380     -1.700117    -0.344633
N      5.532145      0.030569    -3.174218
C     -6.317040     -2.100045     3.808392
C     -7.511948     -0.738212     -2.984306
O     -8.638103     0.867169     -3.527098
N     -7.227146     1.045316     -1.701490
C     -8.248219     1.556549     -0.752431
C     -7.691052     1.546511      6.875856
O     -7.508791     0.210723      1.225279
C     -8.609399     0.312903     -1.134624
O     -8.156730     0.984852    -0.489096
N     -9.398046     3.115350    -2.223480
C     -4.856645     4.445832     0.898589
O     -4.402375     4.086661     0.194209
C     -3.320343     4.636574     0.855509
C     -4.246450     5.696666    -0.145758
C     -3.294046     6.917996     0.121024
C     -1.335981     5.967680     -1.863333
C     -1.868168     5.048237      1.124942
N     -4.902070     3.061369    -0.962846
C     -5.933900     2.199132    -0.602380
C     -5.986800     0.968894    -1.394875
O     -5.065376     0.825583    -2.343907
C     -6.848514     2.362097      0.409412
C     -7.730124     1.297082      0.721984
C     -7.644073     0.114901     0.046340
C     -6.754545     -0.035413    -1.006068
C     -4.668553     -1.371442    -1.630051
C     -7.654852     -3.358668    -1.583227
C     -8.864802     -1.796777    -2.315561
C     -9.705984     -2.779648    -3.011966

SOLVENT: -5238.8260043
space group C2, model 3, reaction intermediate (H on imidazole of H41) isomer distorted
Zero-point correction= 1.653110 (Hartree/Particle)
Thermal correction to Energy= 1.751358
Thermal correction to Enthalpy= 1.752302
Thermal correction to Gibbs Free Energy= 1.518640
Sum of electronic and zero-point Energies= -5208.686233
Sum of electronic and thermal Energies= -5208.587985
Sum of electronic and thermal Enthalpies= -5208.587041
Sum of electronic and thermal Free Energies= -5208.820704

SOLVENT: -5238.8286183
| Atom | x   | y   | z   |
|------|-----|-----|-----|
| H    | 2.663763 | -3.920108 | -3.622162 |
| H    | 2.025636 | -1.304900 | 3.285650  |
| H    | -0.877371 | -0.985705 | 3.917471  |
| H    | -0.277292 | 0.416951  | 5.878174  |
| H    | 1.444940  | 0.224791  | 5.522245  |
| H    | 1.300085  | -2.021366 | 5.996679  |
| H    | -0.818490 | -3.120322 | 7.082677  |
| H    | -1.654527 | -1.627019 | 6.608837  |
| H    | -0.841557 | 2.901540  | 1.793790  |
| H    | 1.662188  | 3.794927  | 4.660610  |
| H    | -4.810911 | 3.291024  | 1.535031  |
| H    | -3.428413 | 4.673726  | 1.721941  |
| H    | 0.682878  | 4.031524  | 1.091880  |
| H    | 2.467996  | 5.729826  | 1.310653  |
| H    | 2.694746  | 5.167012  | 2.966395  |
| H    | 2.448680  | 2.267664  | 2.024208  |
| H    | 5.659769  | 2.219814  | 1.439683  |
| H    | 4.509048  | 1.052771  | 3.551648  |
| H    | 5.453532  | 0.016673  | 2.427406  |
| H    | 2.548173  | 0.146552  | 2.343458  |
| H    | 2.344383  | 1.218168  | -0.135951 |
| H    | 3.229902  | -1.019898 | -1.455010 |
| H    | 1.574702  | -0.351967 | -3.12683  |
| H    | 1.079926  | 1.199276  | -2.867873 |
| H    | 4.793036  | -1.494399 | -2.856350 |
| H    | 6.334173  | 0.812828  | -3.924907 |
| H    | 6.325646  | -0.771156 | -4.824773 |
| H    | 6.297860  | -0.771464 | -1.317750 |
| H    | 9.103425  | -0.991087 | -0.848151 |
| H    | 8.365364  | -2.115748 | 1.301527  |
| H    | 6.717266  | -2.151559 | 0.674909  |
| H    | 6.764895  | 0.172351  | 0.654136  |
| H    | 9.540146  | -4.132439 | -2.597122 |
| H    | 9.433968  | -2.375980 | -2.860549 |
| H    | 9.661453  | -3.212343 | 1.026487  |
| H    | -8.449128 | -1.306609 | 1.521482  |
| H    | -8.209751 | 0.811415  | 0.253592  |
| H    | -6.121955 | 1.145166  | -2.691521 |
| H    | -7.790615 | 2.648606  | -0.606108 |
| H    | -7.210765 | 3.283028  | -2.131280 |
| H    | -9.268889 | 0.981969  | -1.949026 |
| H    | -9.419889 | 3.896053  | -3.038423 |
| H    | -10.753537| 2.647267  | -3.113282 |
| H    | -9.239481 | 1.116648  | -4.461318 |
| H    | -7.008087 | 2.368711  | -4.379752 |
| H    | -3.945938 | 0.969903  | -2.171075 |
| H    | -2.861943 | 2.926932  | -0.235938 |
| H    | -2.426012 | 1.476400  | 1.405490  |
| H    | -1.295732 | 0.683529  | 0.333650  |
| H    | -3.570016 | -0.636137 | -0.405169 |
| H    | -2.201293 | -2.606668 | 2.787548  |
| H    | -6.837473 | -2.269684 | 2.368767  |
| H    | -4.211127 | -1.175875 | 3.644252  |
| H    | -4.206312 | 0.675891  | 2.234259  |
| H    | -5.321310 | -0.240254 | 1.205826  |
| H    | 0.370949  | 2.774199  | -3.129159 |
| H    | 1.985978  | 3.394565  | -0.757339 |
| H    | 2.606018  | 3.220509  | -2.389000 |
| H    | 0.687868  | 5.504155  | -2.883543 |
| H    | 0.262067  | 7.976074  | -3.001282 |
| H    | 2.261587  | 9.095902  | -2.040133 |
| H    | 4.039608  | 7.726199  | -0.964558 |
| H    | 3.818792  | 5.278880  | -0.832791 |
| H    | -0.909987 | -0.543158 | -2.252247 |
| H    | -2.715544 | -4.869994 | 1.898692  |
| H    | -1.389994 | -4.132660 | 0.975227  |
| H    | -1.205327 | -5.771385 | 1.629289  |
| H    | -1.796281 | -6.247125 | -2.085800 |
| H    | -0.698816 | -6.701694 | -0.761541 |
| H    | -0.775330 | -5.011925 | -1.293281 |
| H    | -3.738818 | -7.275951 | -0.822717 |
| H    | -2.703865 | -7.700020 | 0.565032  |
| H    | -4.146178 | -6.677181 | 0.809106  |
| H    | -4.405724 | -2.735194 | -1.748263 |
space group C2, model 3, reaction intermediate (H on imidazole of H41) isomer2 distorted

Zero-point correction= 1.653084 (Hartree/Particle)
Thermal correction to Energy= 1.751224
Thermal correction to Enthalpy= 1.752168
Thermal correction to Gibbs Free Energy= 1.518683
Sum of electronic and zero-point Energies= -5208.662889
Sum of electronic and thermal Energies= -5208.564749
Sum of electronic and thermal Enthalpies= -5208.563805
Sum of electronic and thermal Free Energies= -5208.797290

SOLVENT: -5238.82314
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 6.130157| 2.511347| -0.413860|
| C    | 7.126400| 1.427724| 0.069463 |
| C    | 7.025458| 2.311347| -0.148743|
| C    | 5.986107| -0.422311| -0.906379|
| C    | 5.802183| -1.899834| -1.122742|
| C    | 7.096400| -2.704578| -1.211896|
| C    | 7.987448| -2.437082| -2.421129|
| C    | 7.459859| -1.814939| -3.717997|
| C    | 8.464171| -1.054888| -2.854529|
| C    | 4.893775| -2.432009| 0.025780 |
| O    | 5.327366| -3.161381| 0.933125 |
| N    | 3.616573| -1.999501| -0.113986|
| C    | 2.555968| -2.273950| 0.859206 |
| C    | 2.201423| -1.046992| 1.755109 |
| C    | 2.742233| 0.331127 | 1.341730 |
| H    | 6.148991| 1.404677| 1.668149 |
| C    | 2.551699| 1.992614|
| C    | 2.875535| -0.368041| -4.631411|
| C    | 7.297543| -3.841523| -2.269900|
| C    | 4.699361| -1.940742| -5.546685|
| H    | 2.522922| 3.797701 | 0.348105 |
| H    | -0.964096| 1.836232 | 0.038089 |
| H    | 0.250262| 2.920245 | -0.624891|
| H    | -3.468537| 2.569096 | -1.227559|
| H    | -4.434840| 2.539245 | -3.527594|
| H    | -2.948890| 2.187645| -5.480337 |
| H    | 0.478819| 2.480451| -2.882498|
| H    | -0.480741| 2.108844| -5.157781|
| H    | -2.420757| 2.966836| 2.350180 |
| H    | 0.216534| 3.064708| 3.726700 |
| H    | -0.889447| 2.907648| 5.938649 |
| H    | -2.855770| 2.939921| 5.171341 |
| H    | -2.096320| 5.236729| 4.262425 |
| H    | 0.335260| 5.268328| 4.002978 |
| H    | -0.064362| 6.531904| 5.183698 |
| H    | 0.634722| 4.998438| 5.745860 |
| H    | -3.088433| 4.881867| 6.655428 |
| H    | -1.454969| 4.940227| 7.357222 |
| H    | -2.144184| 6.388204| 6.590335 |
| H    | 0.785065| 1.026972| 4.837885 |
| H    | 0.234103| -1.245224| 3.554656 |
| H    | 0.929797| -2.406174| 5.693823 |
| H    | 0.570673| -0.896659| 6.568790 |
| H    | 4.255187| -1.399888| 4.992759 |
| H    | 3.149495| -2.694985| 5.371231 |
| H    | -1.335367| -2.473311| 3.112934|
| H    | -3.240645| -3.993672| 3.929225|
| H    | -3.685348| -2.590940| 4.945034|
| H    | -2.753282| -0.736556| 2.681699 |
| H    | -5.273404| -1.070368| 1.154311|
| H    | -4.855913| 1.032782| 2.635485 |
| H    | -5.394575| 1.304790| 0.939862 |
| H    | -2.637875| 1.312272| 1.802766 |
| H    | -1.795462| -1.152234| 0.340466 |
| H    | -1.994134| 0.173575| -2.142765|
| H    | -0.486026| -1.477032| -3.157851|
| H    | -0.743178| -2.590839| -1.808861|
| H    | -3.128872| -0.072065| -3.969330|
| H    | -4.761137| -2.552894| -4.194687|
| H    | -4.309212| -1.637416| -5.653239|
| H    | -5.095118| 0.135652| -2.740805 |
| H    | 7.905854| 0.459656 | -3.241999 |
| H    | 7.672833| 2.434173| -1.673408 |
space group C2, model 3, reaction intermediate (H on imidazole of H41) isomer 3 distorted

Zero-point correction= 1.654326 (Hartree/Particle)
Thermal correction to Energy= 1.752080
Thermal correction to Enthalpy= 1.753025
Thermal correction to Gibbs Free Energy= 1.520396

Sum of electronic and zero-point Energies= -5208.665082
Sum of electronic and thermal Energies= -5208.567328
Sum of electronic and thermal Enthalpies= -5208.566383
Sum of electronic and thermal Free Energies= -5208.799012

SOLVENT: -5238.8217262

S103
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -1.599298 | 2.266661  | 4.885354  |
| C    | -2.917926 | 1.734230  | 4.313544  |
| C    | -3.208098 | 0.519005  | 5.612956  |
| C    | -3.636289 | 3.557646  | 2.334640  |
| O    | -3.208098 | 0.519005  | 4.472347  |
| N    | -3.636289 | 2.602868  | 3.575498  |
| C    | 0.888735  | 2.288244  | 4.506134  |
| O    | 1.398115  | 2.065888  | 5.612956  |
| N    | 1.383263  | 3.139029  | 3.556532  |
| C    | 2.729560  | 3.689306  | 3.653447  |
| C    | 3.694799  | 3.024678  | 2.655888  |
| O    | 4.776573  | 2.334640  | 2.334640  |
| N    | 3.263350  | 1.014151  | 1.823355  |
| C    | 4.178192  | 1.014151  | 1.373266  |
| C    | 4.542272  | 0.392914  | 2.057872  |
| O    | 3.451370  | -1.288212 | 1.862088  |
| N    | 3.709782  | 0.654152  | -0.032153 |
| C    | 3.580344  | 0.124702  | -0.788380 |
| O    | 3.451370  | 0.654152  | -1.894803 |
| N    | 3.860736  | 1.079550  | -2.437140 |
| C    | -0.649310 | 0.438543  | -1.628115 |
| C    | 3.284200  | 1.190275  | -2.756731 |
| O    | 3.542526  | 2.406429  | -2.675484 |
| N    | 3.858654  | 0.359302  | -3.674391 |
| C    | 4.995338  | 0.238519  | -4.665964 |
| O    | 7.356377  | -0.380192 | -4.762915 |
| N    | 6.344901  | -0.399129 | -2.836092 |
| C    | 7.596490  | -1.289103 | -2.655888 |
| O    | 7.077925  | -0.123568 | 0.042596  |
| N    | 7.990107  | -2.239797 | -3.007196 |
| C    | 7.797576  | -3.372567 | -2.514442 |
| O    | 8.524834  | -2.011916 | -4.229676 |
| N    | -4.330364 | -4.970536 | -0.446850 |
| C    | -3.589622 | -4.020865 | -1.094852 |
| O    | -2.324089 | -4.446777 | -1.501507 |
| C    | -2.761993 | -5.831987 | -1.297784 |
| C    | -5.753404 | -6.840162 | -2.093946 |
| C    | -0.329999 | -5.663360 | -1.896980 |
| C    | -1.667590 | -6.174504 | 0.194361  |
| O    | -3.982209 | -2.946580 | -1.517242 |
| O    | -5.154723 | -2.308877 | -1.137367 |
| C    | -5.144120 | -0.897048 | -1.471117 |
| C    | -4.198917 | -0.377380 | -2.155725 |
| C    | -6.209429 | -2.847510 | -0.449222 |
| C    | -7.241542 | -2.004525 | 0.037031  |
| C    | -7.185291 | -0.658973 | -0.182318 |
| C    | -6.672620 | -0.117480 | -0.941404 |
| C    | -6.005355 | 1.365592  | -0.094388 |
| O    | -7.308135 | 2.502027  | -0.996678 |
| C    | -8.402623 | 1.604029  | -1.933788 |
| C    | -8.827736 | 2.491745  | -3.126222 |
| C    | -8.042764 | 1.200614  | -3.350479 |
| C    | -4.984714 | 1.825465  | -0.013477 |
| C    | -5.346316 | 2.194201  | 1.126651  |
| C    | -3.714655 | 1.756113  | -0.470433 |
| C    | -2.550879 | 2.073611  | 0.368734  |
| C    | -2.090229 | 0.812174  | 1.201793  |
| C    | -2.733571 | -0.533135 | 0.925358  |
| C    | -1.713938 | -1.590489 | 1.419041  |
| O    | -0.475681 | -1.436929 | 1.371764  |
| C    | -2.715505 | -2.644804 | 1.949692  |
| C    | -3.835560 | -2.470706 | 2.017957  |
| C    | -4.000990 | -0.939234 | 1.735631  |
| C    | -1.498624 | 2.721487  | -0.525327 |
| O    | -1.815223 | 3.458667  | -1.498344 |
| C    | -0.097722 | 2.917508  | 0.041948  |
| O    | 0.337740  | 2.385345  | 1.107671  |
| C    | 0.637761  | 3.740066  | -0.799911 |
| C    | 2.027038 | 4.112186  | -0.385959 |
| C    | 2.150790 | 5.550831  | 0.100161  |
| C    | 1.150679 | 6.505815  | -0.133644 |
| C    | 1.312387 | 7.819627  | 0.316756  |
| C    | 2.464550 | 8.190647  | 1.012151  |
| C    | 3.456184 | 7.263858  | 1.258142  |
| O    | 3.304414 | 5.924795  | 0.806822  |
| C    | -5.340352 | 4.452693  | -4.367552 |
| C    | -5.71381 | 3.789427  | -6.010048 |
| O    | -3.087666 | -0.464579 | -4.631975 |
| O    | -3.064523 | 3.410406  | -2.991646 |
|   | x   | y   | z   |
|---|-----|-----|-----|
| H | -5.051283 | 0.825692 | -5.700765 |
| H | 2.868902  | -3.003932 | 1.263142  |
| H | 1.699578  | -1.793641 | 0.382618  |
| H | 0.458344  | -2.790608 | -0.345192 |
| H | 4.229014  | -2.808959 | -0.254182 |
| H | 5.632486  | -3.165562 | -2.294424 |
| H | 4.572452  | -3.159906 | -4.525871 |
| H | 0.697726  | -2.827066 | -2.669530 |
| H | 2.339021  | -2.377492 | 2.918061  |
| H | 0.451238  | -3.545729 | 4.624738  |
| H | -0.144618 | -5.469908 | 6.113156  |
| H | -1.059624 | -3.949654 | 5.304964  |
| H | 0.719681  | -3.293674 | 8.029541  |
| H | 1.652489  | -4.779996 | 7.721249  |
| H | 2.435387  | -3.184292 | 7.572858  |
| H | -1.123599 | -0.197842 | 4.566363  |
| H | -0.582846 | 1.907206  | 2.985738  |
| H | -1.534465 | 3.556712  | 4.840757  |
| H | -1.457874 | 1.935156  | 5.917034  |
| H | -3.370235 | 3.579331  | 3.525206  |
| H | 0.969927  | 3.104982  | 2.617657  |
| H | 2.749208  | 4.764208  | 3.456637  |
| H | 3.086999  | 3.494713  | 4.670767  |
| H | 2.411894  | 1.381714  | 2.530273  |
| H | 5.087328  | 1.614813  | 1.257139  |
| H | 4.745013  | -0.136894 | 3.118571  |
| H | 5.437005  | -0.712005 | 1.567260  |
| H | 2.607771  | -0.810632 | 2.181722  |
| H | 1.713069  | 1.190326  | 0.145461  |
| H | 2.224913  | -0.561274 | -2.004785 |
| H | 0.841143  | 0.823621  | -3.503267 |
| H | 0.905564  | 2.168090  | -2.356469 |
| H | 3.659640  | -0.640299 | -3.647853 |
| H | 5.034815  | 1.910363  | -4.337998 |
| H | 4.877235  | 0.594356  | -5.528216 |
| H | 5.508532  | -0.936611 | -2.251251 |
| H | 8.384919  | -0.199103 | -2.358778 |
| H | 8.319075  | -1.717251 | -0.381477 |
| H | 6.617703  | -2.063028 | -0.690100 |
| H | 6.155460  | 0.156559  | -0.256481 |
| H | 8.755337  | -2.813508 | -4.808666 |
| H | 8.343276  | -1.067671 | -4.631880 |
| H | -6.188181 | -3.900136 | -0.210097 |
| H | -8.053786 | -2.416642 | 0.618441  |
| H | -7.903834 | 0.032017  | 0.224716  |
| H | -5.546410 | 1.503343  | -2.073832 |
| H | -7.636200 | 2.165855  | 0.047480  |
| H | -7.050383 | 3.187157  | -1.244932 |
| H | -9.190741 | 1.066104  | -1.460717 |
| H | -8.306400 | 3.433167  | -3.262305 |
| H | -9.874732 | 2.520912  | -3.404251 |
| H | -8.573783 | 0.349144  | -3.758964 |
| H | -7.002889 | 1.271874  | -3.646763 |
| H | -3.567184 | 1.199643  | -1.316242 |
| H | -2.873680 | 2.815715  | 1.074402  |
| H | -2.263278 | 1.029442  | 2.246804  |
| H | -1.020387 | 0.676341  | 1.070907  |
| H | -2.871869 | -0.718518 | -0.146675 |
| H | -1.825060 | -3.462916 | 2.242777  |
| H | -4.331569 | -3.088336 | 1.273392  |
| H | -4.207809 | -2.732627 | 3.011535  |
| H | -3.973271 | -0.414138 | 2.693024  |
| H | -4.935967 | -0.723093 | 1.224660  |
| H | 0.150848  | 4.122551  | -1.529806 |
| H | 2.339948  | 3.435420  | 0.408946  |
| H | 2.656497  | 3.895171  | -1.256145 |
| H | 0.247349  | 6.226819  | -0.653996 |
| H | 0.532445  | 8.549206  | 0.128446  |
| H | 2.585526  | 9.208444  | 1.363987  |
| H | 4.348330  | 7.593171  | 1.810514  |
| H | 4.059732  | 5.184774  | 1.048390  |
| H | -1.906280 | 1.116808  | -2.984716 |
| H | -2.678252 | -6.244666 | 0.929942  |
| H | -1.102495 | -5.425707 | 0.755635  |
space group C2, model 3, reaction intermediate (H on imidazole of H41)

Zero-point correction=                           1.652572 (Hartree/Particle)
Thermal correction to Energy=                    1.751193
Thermal correction to Enthalpy=                  1.752137
Thermal correction to Gibbs Free Energy=         1.516630
Sum of electronic and zero-point Energies=          -5208.658041
Sum of electronic and thermal Energies=             -5208.559420
Sum of electronic and thermal Enthalpies=           -5208.558476
Sum of electronic and thermal Free Energies=        -5208.793983

SOLVENT: -5238.8277181

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RXsimpli22REACTANTHalN SCF Done: -5210.31061321 A.U.

S106
space group C2, model 3, product

Zero-point correction= 1.653403 (Hartree/Particle)
Thermal correction to Energy= 1.751338
Thermal correction to Enthalpy= 1.752283
Thermal correction to Gibbs Free Energy= 1.518219

Sum of electronic and zero-point Energies= -5208.691564
Sum of electronic and thermal Energies= -5208.593628
Sum of electronic and thermal Enthalpies= -5208.592684
Sum of electronic and thermal Free Energies= -5208.826747

SOLVENT: -5238.8479019
\begin{tabular}{cccc}
C & -1.219197 & -4.197249 & 6.630047 \\
C & -2.441058 & -4.059456 & 7.289959 \\
C & -3.526375 & -3.485399 & 6.620097 \\
C & -3.396826 & -3.062525 & 5.296747 \\
H & 5.200531 & -6.701168 & -2.999927 \\
H & 6.398680 & -5.432549 & -2.650005 \\
H & 2.176280 & -2.861236 & -1.995602 \\
H & 4.281786 & -5.535652 & 0.487893 \\
H & 3.900258 & -4.101311 & -3.452421 \\
H & -2.70919 & 2.844703 & -2.304422 \\
H & -0.974149 & 1.402560 & -1.167385 \\
H & 1.848956 & 1.819464 & -2.425310 \\
H & -3.61589 & 0.830601 & -2.641318 \\
H & -4.259268 & -0.888060 & -4.259422 \\
H & -2.629306 & -2.416625 & -5.334283 \\
H & 0.595986 & -0.095204 & -3.663794 \\
H & -0.186675 & -2.062324 & -4.985840 \\
H & -2.681084 & 3.678801 & -3.310814 \\
H & -0.120667 & 4.686775 & 0.623425 \\
H & -1.317538 & 6.242362 & 2.303049 \\
H & -2.878352 & 5.482620 & 1.712193 \\
H & -2.521434 & 6.751582 & -0.465356 \\
H & -0.073710 & 6.648287 & -0.715413 \\
H & -0.565551 & 8.352885 & 0.278467 \\
H & 0.151389 & 7.686320 & -1.415401 \\
H & -3.599678 & 8.044189 & 1.415401 \\
H & -1.989933 & 8.654908 & 1.894272 \\
H & -2.649922 & 9.128351 & 1.196999 \\
H & 0.307656 & 1.614368 & 0.312104 \\
H & 0.813011 & 2.091810 & -1.568136 \\
H & 0.434452 & 3.006457 & 5.402316 \\
H & 4.113662 & 2.552122 & 4.474154 \\
H & 3.070815 & 1.832160 & 5.663299 \\
H & -1.377495 & 0.296666 & 3.952268 \\
H & -3.211814 & -0.366111 & 5.630541 \\
H & -3.774347 & 1.316094 & 5.400472 \\
H & -2.911401 & 1.241274 & 2.495052 \\
H & -5.282857 & -0.231171 & 1.616818 \\
H & -5.042068 & 3.25578 & 1.196999 \\
H & -5.56467 & 1.035552 & -2.13135 \\
H & -2.802198 & 2.086557 & 0.446314 \\
H & -1.813545 & -0.623785 & 1.069362 \\
H & -2.105337 & -1.389822 & -1.641154 \\
H & -0.301756 & -2.906653 & -1.557917 \\
H & -0.442600 & -3.203245 & 0.176790 \\
H & -2.976490 & -2.990606 & -2.757813 \\
H & -4.518510 & -4.980812 & -1.164004 \\
H & -4.021690 & -5.366830 & -2.830418 \\
H & -4.900705 & -2.087260 & -2.014716 \\
H & -7.761695 & -2.306792 & -2.752888 \\
H & -7.617496 & 0.187098 & -2.989683 \\
H & -5.585650 & 0.090693 & -2.901420 \\
H & -6.080853 & -0.486744 & -0.737250 \\
H & -7.129501 & -2.974548 & -6.233505 \\
H & -7.297549 & -3.752329 & -4.644860 \\
H & 5.909159 & 2.654242 & -2.555543 \\
H & 7.840078 & 2.214091 & -0.887702 \\
H & 7.729333 & 0.189186 & 0.532462 \\
H & 5.452650 & -2.549852 & -0.101221 \\
H & 7.570150 & -1.441627 & 1.816067 \\
H & 6.953208 & -3.076878 & 1.754653 \\
H & 8.602723 & -1.818432 & -0.539191 \\
H & 9.075326 & -2.434461 & 1.364728 \\
H & 10.170194 & -3.714484 & -0.004863 \\
H & 8.267873 & -4.946464 & -1.651742 \\
H & 7.165699 & -4.533482 & -0.283019 \\
H & 4.334961 & -1.682972 & 0.191933 \\
H & 2.611454 & -1.422620 & 3.013358 \\
H & 3.061233 & 0.803000 & 2.841628 \\
H & 1.343569 & 0.751688 & 2.377479 \\
H & 2.841029 & 0.597154 & -0.072766 \\
H & 1.452423 & 3.913137 & -0.799789 \\
H & 3.970823 & 3.176732 & -1.170269 \\
H & 3.830298 & 4.361908 & 0.145674 \\
H & 3.814111 & 2.750325 & 1.847585 \\
H & 4.828814 & 1.812295 & 0.696062 \\
H & -0.188872 & -3.558044 & 2.376960 \\
H & -2.458792 & -1.731865 & 3.101322 \\
H & -2.658492 & -3.368484 & 2.497802 \\
\end{tabular}
H     -0.129360    -3.864657     4.801991
H     -0.369467    -4.632304     7.144868
H     -2.546348    -4.388092     8.317576
H     -4.475155    -3.361201     7.129852
H     -4.225489    -2.573566     4.794086
H      2.090468    -3.552808     0.751073
H      2.554424     4.690644    -4.292695
H      0.971561     4.214289    -3.656650
H      1.090975     4.925401    -5.288577
H      0.609876     1.271470    -6.047124
H      0.042357     2.909319    -6.473314
H     -0.264597     2.236958    -4.854016
H      2.946343     1.889193    -6.720058
H      2.454486     3.552027    -7.128509
H      3.766914     3.280035    -5.952872
H      3.206055     0.160626    -2.799710
H      6.003740    -6.641413    -1.420683
H     -1.460998     3.327263    -3.516021

space group C2, model 3, reaction intermediate (proton removed)

Zero-point correction=                           1.539899 (Hartree/Particle)
Thermal correction to Energy=                    1.630744
Thermal correction to Enthalpy=                  1.631688
Thermal correction to Gibbs Free Energy=         1.414321
Sum of electronic and zero-point Energies=          -4944.155581
Sum of electronic and thermal Energies=             -4944.064737
Sum of electronic and thermal Enthalpies=           -4944.063792
Sum of electronic and thermal Free Energies=        -4944.281159

SOLVENT: -4972.7615317

RXsimpli22REACTANT- SCF Done: -4945.69548025 A.U.
space group C2, model 3, reaction intermediate

Zero-point correction= 1.651408 (Hartree/Particle)
Thermal correction to Energy= 1.750329
Thermal correction to Enthalpy= 1.751274
Thermal correction to Gibbs Free Energy= 1.515116

Sum of electronic and zero-point Energies= -5208.662671
Sum of electronic and thermal Energies= -5208.563750
Sum of electronic and thermal Enthalpies= -5208.562806
Sum of electronic and thermal Free Energies= -5208.798963

SOLVENT: -5238.8272518

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RXisimpl22REACTANT180 SCF Done: -5210.31407940 A.U.

C 2.977596 0.844520 -5.021520
C -3.098462 -0.578762 -4.584933
N -1.928468 -1.167674 -3.885216
C -2.691211 -2.431939 -3.637764
N -3.507965 -2.704011 -4.160415
C -3.982226 -1.334240 -4.709571
C 1.020111 -3.062167 2.536241
C 0.346973 -2.588477 1.205546
C 0.869470 -3.316248 -0.014121
C 2.237057 -3.299014 -0.334402
C 2.713052 -4.002858 -1.448680
C 1.814812 -4.618816 -2.281138
C -0.020922 -4.000829 -0.856834
C 0.446773 -4.669774 -1.990859
C 0.436855 -2.204628 3.641638
O -0.745894 -2.367609 4.063040
N 1.232198 -1.197301 4.068021
C 0.671589 -0.010502 4.719084
C 1.317859 0.247332 6.098862
C 1.228256 -0.967294 7.048497
C 1.881887 -0.610721 8.399153
C -0.242119 -1.413411 7.259292
C 0.916070 1.205173 3.826439
|   |   |   |   |
|---|---|---|---|
| H | -2.267909 | 0.985458 | -5.846027 |
| H | -1.667450 | -3.141013 | -3.095646 |
| H | -4.940682 | -1.54746 | 1.104003 |
| H | -0.732596 | -2.745200 | 1.299016 |
| H | 0.916703 | -2.715894 | 0.281296 |
| H | 2.098114 | -2.925654 | 2.460019 |
| H | 0.511651 | -1.514746 | 1.104003 |
| H | -0.732596 | -2.745200 | 1.299016 |
| H | 2.098114 | -2.925654 | 2.460019 |
| H | 0.511651 | -1.514746 | 1.104003 |
| H | -0.732596 | -2.745200 | 1.299016 |
| H | 2.098114 | -2.925654 | 2.460019 |
| H | 0.511651 | -1.514746 | 1.104003 |
| H | -0.732596 | -2.745200 | 1.299016 |
| H | 2.098114 | -2.925654 | 2.460019 |
| H | 0.511651 | -1.514746 | 1.104003 |
| H | -0.732596 | -2.745200 | 1.299016 |
| H | 2.098114 | -2.925654 | 2.460019 |
| H | 0.511651 | -1.514746 | 1.104003 |
| H | -0.732596 | -2.745200 | 1.299016 |
| H | 2.098114 | -2.925654 | 2.460019 |
| H | 0.511651 | -1.514746 | 1.104003 |
| H | -0.732596 | -2.745200 | 1.299016 |
| H | 2.098114 | -2.925654 | 2.460019 |
| H | 0.511651 | -1.514746 | 1.104003 |
| H | -0.732596 | -2.745200 | 1.299016 |
| H | 2.098114 | -2.925654 | 2.460019 |
| H | 0.511651 | -1.514746 | 1.104003 |
### space group C2, model 3, reaction intermediate (isomer)

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | -1.464275 | -0.455562 | -2.240354 |
| H    | -3.559921 | -4.582597 | 3.829385  |
| H    | -1.849912 | -4.895774 | 2.165417  |
| H    | -2.293270 | -5.803125 | 4.136883  |
| H    | -1.390532 | -6.280888 | 0.516581  |
| H    | -1.096670 | -6.895774 | 2.165417  |
| H    | -0.528264 | -5.276796 | 1.688750  |
| H    | -3.855411 | -6.591939 | 0.739362  |
| H    | -3.642363 | -7.306106 | 2.385412  |
| H    | -4.760311 | -5.945005 | 2.105271  |
| H    | -3.315026 | -2.445401 | -0.424384 |
| H    | -3.968872 | 1.153962 | -5.396262 |
| H    | 0.775513  | -4.109755 | 2.719137  |

Zero-point correction = 1.652416 (Hartree/Particle)
Thermal correction to Energy = 1.751236
Thermal correction to Enthalpy = 1.752181
Thermal correction to Gibbs Free Energy = 1.515476

Sum of electronic and zero-point Energies = -5208.673379
Sum of electronic and thermal Energies = -5208.574558
Sum of electronic and thermal Enthalpies = -5208.573614
Sum of electronic and thermal Free Energies = -5208.810319

SOLVENT: -5238.8224391

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RXissimpl22REACTANT SCF Done: -5210.32579482 A.U.

C   -5.245349  5.354711  3.777677
C   -5.253646  3.865274  3.936910
N   -6.189115  3.217066  4.674441
C   -5.903665  1.917987  4.843270
N   -4.833396  1.689791  4.319043
C   -4.417014  2.935069  3.908635
C    2.279237  0.397503  0.169981
C    0.775513  4.109755  2.719137
C    3.043638  1.583507  2.615417
C    3.070998  2.804481  2.372378
C    3.722340  0.977679  3.630972
C    4.742289  1.736165  4.371439
C    6.187244  1.325630  4.017028
O    7.134634  1.714884  4.744560
O    6.327894  0.561975  2.914611
C    7.664510  0.167676  2.403556
C    7.558408  0.351134  0.956767
O    7.083052  0.642190  0.023827
C    8.243673  0.594926  3.295989
O    8.249770  2.144682  2.912989
N    8.673792  0.521086  4.502954
| Atom | X         | Y         | Z        |
|------|-----------|-----------|----------|
| O    | -3.798198 | -5.139011 | -1.087434|
| C    | -3.151467 | -4.244057 | -1.656203|
| O    | -1.878671 | -4.109037 | -2.158576|
| C    | -1.211551 | -5.707024 | -2.158576|
| C    | -2.039357 | -6.610893 | -3.081916|
| C    | 0.153138  | -5.377091 | -2.761724|
| C    | -1.081497 | -6.278776 | -0.743217|
| N    | -3.649615 | -2.974653 | -1.900861|
| C    | -4.868848 | -2.502281 | -1.419753|
| C    | -5.012288 | -1.069478 | -1.517159|
| O    | -4.119783 | -0.354278 | -2.113642|
| C    | -5.850448 | -3.265212 | -0.822644|
| C    | -6.952698 | -2.636389 | -0.21840|
| C    | -7.041159 | -1.271934 | -0.206792|
| N    | -6.105334 | -0.503033 | -0.867548|
| C    | -6.131078 | 1.003320  | 0.556686 |
| C    | -7.503949 | 1.586348  | -0.385942|
| C    | -8.576024 | 1.277002  | -1.411339|
| C    | -9.681571 | 2.304768  | -1.628795|
| H    | -4.487086 | 5.661346  | -3.051182|
| H    | -5.031378 | 5.845942  | -4.753086|
| H    | -6.432513 | 1.123771  | -5.19569 |
| H    | -5.802249 | 3.030123  | -2.693309|
| H    | -4.883300 | 0.793782  | -3.488959|
| H    | 3.317174  | -3.905518 | 0.708929 |
| H    | 2.501494  | 1.857419  | 0.057225 |
| H    | 0.806209  | -2.826050 | -0.845080|
| H    | 4.644538  | -2.524857 | -0.579403|
| H    | 6.153314  | -2.411611 | -2.579921|
| H    | 5.181289  | -2.242683 | -4.835318|
| H    | 1.205552  | -2.631615 | -3.161848|
| H    | 2.706257  | -2.345460 | -5.141738|
| H    | 2.666530  | -2.613494 | 2.465555 |
| H    | -0.139341 | -3.024547 | 3.408326 |
| H    | 0.531640  | -2.459437 | 5.713754 |
| H    | 2.199697  | -2.181540 | 5.208334 |
| H    | 2.447101  | -4.580992 | 4.623746 |
| H    | 0.154461  | -5.187720 | 3.940487 |
| H    | 0.621761  | -6.218427 | 5.305762 |
| H    | -0.458763 | -4.836793 | 5.583271|
| H    | 2.952165  | -3.803861 | 6.973362 |
| H    | 1.275726  | -4.173197 | 7.439847 |
| H    | 2.372583  | -5.485831 | 6.957977 |
| H    | -1.131407 | -0.987952 | 4.460855 |
| H    | -0.629550 | 1.450264  | 3.242839 |
| H    | -1.591240 | 2.443201  | 5.336688 |
| H    | -1.386082 | 0.663818  | 6.140204 |
| H    | -4.396344 | 1.465904  | 3.287475|
| H    | -3.462931 | 2.727774  | 4.042500|
| H    | 0.714099  | 2.978814  | 3.231624|
| H    | 2.562925  | 4.366666  | 4.214090|
| H    | 3.008983  | 2.904355  | 5.148363|
| H    | 2.338636  | 1.193755  | 2.670986|
| H    | 4.943807  | 1.826957  | 1.389274|
| H    | 4.835592  | -0.163093 | 3.040101 |
| H    | 5.558578  | -0.446667 | 1.423305|
space group C2, model 3, reaction intermediate (isomer1)

Zero-point correction=  1.654394 (Hartree/Particle)
Thermal correction to Energy=  1.752321
Thermal correction to Enthalpy=  1.753265
Thermal correction to Gibbs Free Energy=  1.522276

Sum of electronic and zero-point Energies=  -5208.705679
Sum of electronic and thermal Energies=  -5208.607752
Sum of electronic and thermal Enthalpies=  -5208.606808
Sum of electronic and thermal Free Energies=  -5208.837797

SOLVENT: -5238.8343406
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| O       | -0.210393 | -3.715185 | 3.186029 |
| N       | 1.414131 | -2.130574 | 3.589374 |
| C       | 0.521338 | -1.170795 | 7.977669 |
| C       | -0.198578 | -3.043276 | 6.523379 |
| C       | 0.537310 | 0.177756 | 3.514538 |
| O       | 1.447777 | 0.510080 | 2.682509 |
| N       | -0.381400 | 1.061080 | 2.898112 |
| C       | 0.306335 | 4.245689 | 2.974172 |
| O       | -0.357244 | -2.004312 | -0.118022 |
| S       | -0.228784 | 0.271596 | -0.204315 |
| C       | 1.840663 | -0.562677 | -1.364324 |
| O       | 3.603045 | 0.543631 | -1.395432 |
| S       | -3.612279 | -4.016794 | -0.322388 |
| C       | -2.321855 | 4.541282 | -0.066431 |
| O       | -5.171168 | -6.776069 | -0.942401 |
| C       | -1.747533 | -5.720932 | -0.897949 |
| O       | 2.955559 | 0.592920 | -4.488278 |
| N       | 5.730588 | 0.549881 | -2.162108 |
| C       | 7.164079 | -0.444036 | -2.859685 |
| O       | 3.827246 | 0.016747 | -2.687847 |
| N       | 3.364081 | 1.117933 | 1.856500 |
| O       | 4.268877 | 1.147958 | 1.124489 |
| N       | 3.994409 | -0.919049 | 2.329880 |
| C       | 3.603045 | 0.543631 | -0.112802 |
| C       | -3.769096 | -0.494718 | -4.659469 |
| O       | 2.356404 | 0.016747 | -2.432158 |
| N       | 3.034339 | -0.479811 | -3.442582 |
| C       | 3.760906 | -0.494718 | -4.659469 |
| O       | 2.356404 | 0.016747 | -2.432158 |
| C       | 3.034339 | -0.479811 | -3.442582 |
| O       | 3.760906 | -0.494718 | -4.659469 |
| N       | 3.034339 | -0.479811 | -3.442582 |
| C       | 3.760906 | -0.494718 | -4.659469 |
| O       | 2.356404 | 0.016747 | -2.432158 |
| N       | 3.034339 | -0.479811 | -3.442582 |
| C       | 3.760906 | -0.494718 | -4.659469 |
| O       | 2.356404 | 0.016747 | -2.432158 |
| N       | 3.034339 | -0.479811 | -3.442582 |
| C       | 3.760906 | -0.494718 | -4.659469 |
| O       | 2.356404 | 0.016747 | -2.432158 |
| N       | 3.034339 | -0.479811 | -3.442582 |
space group C2, model 3, transition state (proton of thiol removed by imidazole of H41)

Zero-point correction= 1.649159 (Hartree/Particle)
Thermal correction to Energy= 1.747205
Thermal correction to Enthalpy= 1.748149
Thermal correction to Gibbs Free Energy= 1.514061
Sum of electronic and zero-point Energies= -5208.664535
Sum of electronic and thermal Energies= -5208.566489
Sum of electronic and thermal Enthalpies= -5208.565545
Sum of electronic and thermal Free Energies= -5208.799633

SOLVENT: -5238.820385

196 RXsimpl2REACTANT--Histidine SCF Done: 5210.31369378 A.U.
| Atom | x        | y        | z        |
|------|----------|----------|----------|
| O    | 6.518804 | -3.484578| -4.119698|
| N    | 5.465171 | -3.179887| -2.171960|
| C    | 6.280999 | -4.020640| -1.261186|
| C    | 6.029809 | -3.609990| 0.203643 |
| O    | 6.494563 | -2.267600| 0.505070 |
| C    | 5.840298 | -5.490851| -1.445603|
| O    | 5.051461 | -6.037272|-0.649967 |
| N    | 6.363854 | -6.081001|-2.549857 |
| O    | -5.288759| -2.958459| 2.379893 |
| C    | -4.395622| -3.01129 | 1.520749 |
| O    | -4.318791| -3.858232| 1.515678 |
| C    | -3.520223| -4.952061| 2.582348 |
| O    | -4.491500| -5.844191| 2.438400 |
| N    | -1.979131| -5.712503| 2.201496 |
| C    | -3.143411| -4.306013| 3.966853 |
| O    | -4.565540| -2.207272| 0.405692 |
| C    | -5.297981| -1.744999| 0.054430 |
| N    | -4.933991| -0.501936| -1.097159|
| O    | -3.814641| -0.709381| -1.674971|
| C    | -6.525464| -1.027046| 0.686923 |
| O    | -7.360924| 0.019293 | 0.208204 |
| C    | -6.982188| 0.760508 | -0.869662|
| N    | -5.792347| 0.503547 | -1.517921|
| C    | -5.14951 | 1.336065 | -2.680223|
| O    | -6.444798| 1.957800 | -3.494280|
| N    | -7.386951| 0.956177 | -4.187791|
| O    | -6.858512| 0.219770 | -5.424362|
| C    | -7.131852| -0.554472| -4.139376|
| O    | -4.835674| 2.441730 | -2.106997|
| N    | -5.714313| 1.942341 | -1.764552|
| C    | -2.127776| 2.739883 | -1.130420|
| O    | -1.912781| 2.404591 | 0.963268 |
| C    | -2.693290| 1.215949 | 0.963268 |
| O    | -1.829639| 0.519684 | 2.028568 |
| N    | -0.581447| 0.425156 | 1.993671 |
| C    | -2.643656| 0.009393 | 2.972428 |
| O    | -4.064184| 0.373395 | 2.823014 |
| C    | -4.005531| 1.503871 | 1.742642 |
| O    | -0.889148| 2.651579 | -2.045134|
| N    | -1.002716| 2.657696 | -3.291642|
| C    | -0.535775| 2.897277 | -1.496297|
| O    | 0.878954 | 2.870983 | -0.297878|
| N    | 1.408483 | 3.087956 | -2.500056|
| C    | 2.862520 | 3.228383 | -2.286014|
| O    | 3.384243 | 4.627988 | -2.586030|
| C    | 2.615953 | 5.579904 | -3.263398|
| N    | 3.138141 | 6.848325 | -3.532550|
| C    | 4.430444 | 7.176557 | -3.121112|
| O    | 5.195181 | 6.230907 | -2.431079|
| C    | 4.078836 | 4.962413 | -2.163394|
| H    | -2.346544| 1.403720 | -4.368382|
| H    | -1.886582| 0.701604 | -5.918770|
| H    | -1.871848| -3.086496| -2.590438|
| H    | -5.43267 | -1.673803| -5.592334|
| H    | -3.896069| -3.663794| -4.107723|
| H    | 1.680122 | -2.832228| 2.689389 |
| H    | 0.178684 | -1.411557| 1.216396 |
| H    | -1.140550| -2.542733| 1.525714 |
| H    | 2.499580 | -2.793739| 0.531169 |
| H    | 3.303446 | -4.402536| -1.202674|
| H    | 1.676941 | -5.665827| -2.574374|
| H    | -1.535542| -4.051356| -0.192945|
| H    | -0.754612| -5.492462| -2.083398|
| H    | 1.945515 | -0.962587| 3.717987 |
| H    | -0.487419| 0.336838 | 4.826824 |
| H    | 0.885553 | 1.628669 | 6.440995 |
| H    | 2.354040| 0.811785 | 5.876651 |
| H    | 1.518866 | -1.353753| 6.715626 |
| H    | -0.919056| -1.115060| 6.467968 |
| H    | -0.560774| -1.416813| 8.179407 |
| H    | -0.940907| 0.233304| 7.643817 |
| H    | 2.842084| 0.143782| 8.252575 |
| H    | 1.325575 | 0.869271 | 8.333965 |
| H    | 1.675673 | -0.841600| 9.165243 |
| H    | -0.677927| 2.613960| 4.244868 |
| H    | 0.165559 | 3.352415 | 1.836748 |
| H    | -0.257643| 5.728594 | 2.608767 |
| H    | -0.111033| 5.154193 | 4.285004 |
| H    | -3.734102| 5.036861 | 2.547977 |
Zero-point correction= 1.654286 (Hartree/Particle)
Thermal correction to Energy= 1.752108
Thermal correction to Enthalpy= 1.753052
Thermal correction to Free Energy= 1.520455

Sum of electronic and zero-point Energies= -5208.661140
Sum of electronic and thermal Energies= -5208.563317
Sum of electronic and thermal Enthalpies= -5208.562373

space group C2, model 3, reaction intermediate (proton of thiol on imidazole of H41)
Sum of electronic and thermal Free Energies = -5208.794970

| Atom | x     | y     | z     |
|------|-------|-------|-------|
| C    | -0.348053 | -2.271391 | 1.687179 |
| C    | 0.054126  | -3.275223  | 0.632795  |
| C    | 1.406716  | -2.4076209  | 0.002436  |
| C    | -0.911272 | -2.271391  | -0.967903  |
| O    | 0.054126  | -4.076209  | 1.687179  |
| C    | 1.788640  | -4.387595  | -1.295226  |
| C    | 0.819633  | -5.172093  | -1.295226  |
| C    | 1.845147  | -7.235088  | 8.365136  |
| N    | 1.357359  | -2.25812  | 5.945580  |
| C    | 0.800542  | 2.49333  | 7.113754  |
| C    | 0.530518  | -5.011263  | -0.967903  |
| O    | -0.911272 | -4.076209  | 1.687179  |
| N    | -0.530518 | 1.29393  | 7.405892  |
| O    | 1.040644  | 1.803772  | 3.537923  |
| N    | 0.090521  | 2.52012  | 2.771686  |
| O    | 0.548053  | 2.978506  | 3.537923  |
| C    | 0.690666  | 3.947514  | 2.427120  |
| N    | -0.122136 | 5.226703  | 2.720206  |
| O    | -1.648811 | 4.920274  | 2.734751  |
| N    | -2.101127 | 3.99312  | 3.432600  |
| C    | -2.382156 | 5.679666  | 1.909963  |
| O    | 2.189532  | 4.315722  | 2.414262  |
| N    | 2.790078  | 4.962481  | 3.426395  |
| C    | 2.718418  | 4.209023  | 1.163552  |
| O    | 4.155094  | 2.81114  | 0.931868  |
| N    | 4.738998  | 2.901518  | 0.574653  |
| C    | 5.822847  | 2.771740  | -0.030657 |
| N    | 3.970769  | 1.845228  | 0.980938  |
| C    | 4.494668  | 0.49270  | 0.851077  |
| O    | 4.257900  | -0.38219  | 2.112366  |
| N    | 3.862500  | -0.85859  | 2.139301  |
| O    | 3.903011  | -0.31042  | -0.293906 |
| C    | 4.865646  | -1.393490 | -0.607170 |
| N    | 2.776855  | 0.057537  | -0.909640 |
| C    | 2.256993  | -0.881006 | -1.924242 |
| O    | 0.974344  | -0.397999 | -2.595093 |
| S    | -0.334438 | -0.046415 | -1.365945 |
| C    | 3.344549  | -1.088801 | -2.991628 |
| O    | 4.030927  | -0.719039 | -3.471517 |
| C    | 3.464264  | -2.402461 | -3.362383 |
| O    | 4.672785  | -2.889706 | -4.030901 |
| N    | 5.463843  | -3.859401 | -3.123727 |
| O    | 6.246652  | -4.703233 | -3.621802 |
| N    | 5.210263  | -3.718735 | -1.801331 |
| C    | 5.866363  | -4.559508 | -0.768641 |
| N    | 5.602841  | -3.968947 | 0.631651  |
| C    | 6.257142  | -2.689968 | 0.842849  |
| O    | 5.247946  | -5.974765 | -0.833883 |
| S    | 3.816355  | -6.344716 | -0.018057 |
| C    | 5.719175  | -6.725833 | -1.861856 |
| N    | 5.545726  | -2.260319 | 2.702675  |
| O    | -4.659657 | -2.513499 | 1.882342  |
| S    | -3.659927 | -3.436699 | 2.029390  |
| C    | -3.682266 | -3.466389 | 3.236758  |
| O    | -4.990891 | -5.168000 | 3.205902  |
| C    | -2.473035 | -5.267980 | 2.983776  |
| O    | -3.526459 | -3.535340 | 4.513457  |
| N    | -4.534065 | -1.890442 | 0.663612  |
| C    | -5.413301 | -0.942067 | 0.148543  |
| N    | -3.823234 | -0.803605 | -1.617397 |
| C    | -6.857662 | -0.489958 | 0.703133  |
| O    | -7.315512 | 0.534337 | 0.046593  |
| C    | -6.853747 | 1.065369 | -1.124853 |
| N    | -5.688166 | 0.297234 | -1.692219 |
| C    | -5.111464 | 1.946618 | -2.944924 |
| C    | -6.165492 | 1.712004 | -3.915495 |
| N    | -7.140225 | 0.640109 | -4.410284 |
| O    | -6.730085 | -0.252941 | -5.578953 |
| S    | -6.833323 | -0.852156 | -4.185318 |
| C    | -4.139299 | 2.324269 | -2.514086 |
| O    | -4.427972 | 3.527375 | -2.629919 |
| N    | -2.991822 | 1.810864 | -2.002217 |
| C    | -1.916588 | 2.646366 | -1.458609 |
| O    | -1.752384 | 2.590348 | 0.089924  |
| C    | -2.625420 | 1.466955 | 0.808048  |
| C    | -1.827857 | 0.859804 | 1.974057  |
| O    | -0.589588 | 0.675964 | 1.978770  |
|     | H       | 3.490398 | 0.539258 |
|-----|---------|----------|----------|
|     | H       | 2.226767 | 0.293463 |
|     | H       | 3.616018 | -1.462587|
|     | H       | 0.201941 | -3.042709|
|     | H       | 0.872154 | -3.984229|
|     | H       | 2.526211 | -4.017188|
|     | C       | 2.939718 | -3.933918|
|     | C       | 4.440988 | -3.327121|
|     | C       | 5.362077 | -2.771738|
|     | C       | 5.567961 | -2.926548|
|     | C       | 3.797918 | -4.440988|
|     | C       | 2.939718 | -3.933918|
|     | C       | 5.362077 | -2.771738|
|     | C       | 5.567961 | -2.926548|
|     | C       | 3.797918 | -4.440988|
|     | C       | 5.362077 | -2.771738|
|     | C       | 5.567961 | -2.926548|
|     | C       | 3.797918 | -4.440988|
|     | C       | 5.362077 | -2.771738|
|     | C       | 5.567961 | -2.926548|
|     | C       | 3.797918 | -4.440988|
|     | C       | 5.362077 | -2.771738|
|     | C       | 5.567961 | -2.926548|
|     | C       | 3.797918 | -4.440988|
|     | C       | 5.362077 | -2.771738|
|     | C       | 5.567961 | -2.926548|
|     | C       | 3.797918 | -4.440988|

**space group C2, model 3, reaction intermediate (proton of thiol on imidazole of H41) isomer**

| Energy Type                              | Value                            |
|------------------------------------------|----------------------------------|
| Zero-point correction                   | 1.656171                         |
| Thermal correction to Energy             | 1.753828                         |
| Thermal correction to Enthalpy           | 1.754773                         |
| Thermal correction to Gibbs Free Energy  | 1.523363                         |
| Sum of electronic and zero-point Energies| -5208.673550                     |
| Sum of electronic and thermal Energies   | -5208.575892                     |
| Sum of electronic and thermal Enthalpies | -5208.574948                     |
| Sum of electronic and thermal Free Energies| -5208.806058                    |

**SOLVENT:** -5238.8292108
| X         | Y         | Z         |
|-----------|-----------|-----------|
| H 3.480363| 7.362856  | -1.237711 |
| H 2.339762| 7.837930  | -2.516871 |
| H 2.246311| 8.602798  | -0.914869 |
| H 0.110866| 3.116718  | -3.642530 |
| H 1.126737| 0.556907  | -3.575860 |
| H 1.22352  | 0.802055  | -6.072239 |
| H 1.279998 | 2.569076  | -5.868069 |
| H -2.32248 | 0.788197  | -6.197279 |
| H -0.820158| 0.027522  | -6.654780 |
| H 2.989749 | -0.371991 | -3.404920 |
| H 5.404009 | -0.69740  | -4.032601 |
| H 5.453468 | 1.176979  | -4.128747 |
| H 3.605266 | 1.208405  | -1.628538 |
| H 5.940210 | 1.171719  | 0.185889  |
| H 4.294354 | 3.210942  | -0.095056 |
| H 4.731108 | 2.704610  | 1.583932  |
| H 1.234713 | 1.896056  | 0.211578  |
| H 1.284138 | -0.534696 | -0.059639 |
| H 2.400465 | -0.732333 | 2.653429  |
| H 0.901716 | -2.540312 | 0.812572  |
| H 1.644781 | -3.050199 | 0.812572  |
| H 2.400465 | -2.040202 | 4.217676  |
| H 5.459148 | 2.960571  | 4.175268  |
| H 4.388823 | -3.674675 | 5.430826  |
| H 7.199557 | -0.484750 | 3.826679  |
| H 4.441719 | 1.170839  | 6.234719  |
| H 3.657193 | 2.849575  | 4.638826  |
| H 3.313254 | 1.631388  | 3.396534  |
| H 5.534678 | 1.384859  | 3.100869  |
| H 0.812735 | 1.421499  | 6.357099  |
| H 2.321839 | 2.216908  | 6.739559  |
| H 6.958155 | 1.032194  | 0.547536  |
| H -7.595496 | 0.963043  | 2.958573  |
| H -6.360875 | -0.099065 | 2.650597  |
| H -4.016257 | -3.630961 | 0.968994  |
| H -5.411286 | -9.05714  | 2.345524  |
| H -4.450393 | -5.722411 | 1.139443  |
| H -7.122231 | -4.310131 | -0.463027 |
| H -6.259062 | -7.302168 | -0.492146 |
| H -7.876611 | -6.655303 | 0.065421  |
| H -6.072566 | -5.262887 | 1.838475  |
| H -5.087872 | -5.908350 | 1.261286  |
| H -2.343274 | -2.222369 | -0.521688 |
| H -1.145705 | -2.796802 | -3.185788 |
| H -0.634855 | -0.560860 | -3.578846 |
| H -0.191158 | -0.306757 | 1.994770  |
| H -2.640218 | -0.330407 | 1.151360  |
| H -2.438213 | 3.359985  | 1.392880  |
| H -4.594637 | 2.169608  | -2.334431 |
| H -3.994335 | 2.617546  | 3.688224  |
| H -2.849542 | 0.431429  | 4.065535  |
| H -4.158537 | -0.103723 | 2.984531  |
| H -2.284164 | -3.895638 | -0.917699 |
| H 4.057588 | -1.634009 | 1.660101  |
| H 4.442682 | 2.918822  | 0.519933  |
| H 3.198759 | -4.745408 | -3.182212 |
| H 4.050724 | -5.852200 | 4.976560  |
| H 6.834218 | -5.113842 | 5.449553  |
| H 7.836395 | 3.272281  | 4.118033  |
| H 6.523327 | 2.161143  | 2.339542  |
| H -1.062150 | 2.365399  | 1.249771  |
| H -5.237342 | 4.891480  | 0.704683  |
| H -3.560975 | 5.962610  | -0.189094 |
| H -4.753015 | 6.306032  | 0.252938  |
| H -0.001459 | 4.258551  | 3.359808  |
| H -4.012030 | 5.931039  | 2.732074  |
| H -2.873299 | 4.734463  | 2.051050  |
| H -6.490034 | 4.062974 | 2.776316  |
| H -6.538059 | 5.701227  | 2.075917  |
| H -7.021121 | 4.298467  | 1.083099  |
| H -4.264875 | 0.665304  | 0.953384  |
| H -2.639255 | 5.820571  | 0.729763  |
| H -0.842699 | 3.821231  | 2.849656  |

**space group C2, model 3, product**

Zero-point correction= 1.653548 (Hartree/Particle)
| Property                                      | Value          |
|----------------------------------------------|----------------|
| Thermal correction to Energy                | 1.751821       |
| Thermal correction to Enthalpy              | 1.752766       |
| Thermal correction to Gibbs Free Energy     | 1.517996       |
| Sum of electronic and zero-point Energies   | -5208.669960   |
| Sum of electronic and thermal Energies      | -5208.571687   |
| Sum of electronic and thermal Enthalpies    | -5208.570743   |
| Sum of electronic and thermal Free Energies | -5208.805513   |
| SOLVENT:                                    | -5238.835376   |

RXsimpli2TSFFHMINRX SCF Done: -5210.323084 A.U.

C      5.449932    -3.585362     4.406214
C      4.155175    -2.962906     3.988368
N      3.299519    -3.594772     3.068874
C      2.268333    -2.772411     2.918007
N      2.393881    -1.645124     3.694334
C      3.608998    -1.759170     4.374864
C     -1.404105    -2.118529    -3.266818
C     -0.675511    -1.986982    -1.889955
N     -1.167228    -2.974486    -0.835437
C     -2.537729    -3.202146    -0.655435
C     -2.973612    -4.163912     0.262582
C     -2.042006    -4.826892     1.072014
C     -0.239762    -3.659504    -0.050626
C     -0.674802    -4.554878     0.930257
C     -0.851070    -1.009232    -4.134915
O      0.300196    -1.074630    -4.654441
N     -1.627837     0.096410    -4.206008
C     -2.074723    -1.403906    -5.721401
C     -1.734117    -1.203213    -5.993763
C     -2.431794    1.963205     -8.142159
C     -0.295589    0.806514     -7.398654
N     -1.201778    2.302249     -3.289097
O     -2.122048    2.115150    -2.448875
N     -3.626644    3.339586    -3.214832
C     -0.320665    4.149277    -1.983661
C     -0.714936    5.275504    -2.172392
C     -1.096622    4.711085    -2.425758
O     -2.308341    3.760402    -3.221348
N      3.118477    5.286947    -1.726517
N     -1.693574    4.791355    -1.705215
O     -2.341073    5.408846    -2.562246
N     -2.058151    4.623093    -0.401482
C     -3.410249    4.914599     0.057706
C     -4.180463    3.617673     0.367396
N     -5.138419    3.383673    -1.165839
N     -3.722412    2.519033    -0.307614
C     -4.670084    1.271132    -0.234600
C     -4.692370    0.603373    -1.619406
O     -3.461917   -0.090891    -2.032996
C     -3.382372    0.188114     0.617766
O     -4.353269   -0.825648     0.892799
N     -2.554821    0.258468     1.028011
C     -2.065234   -0.922388     1.774914
C     -0.646679   -0.786752     2.334499
S      0.611038   -0.237521     1.119498
C     -2.983251   -1.123024     3.002912
O     -3.328117   -1.831877     3.740443
C     -3.323925   -2.452309     3.205196
C     -4.143372   -2.780198     4.116654
C     -5.646928   -3.321256     3.361680
C     -6.514680   -3.997155     3.965244
C     -5.678012   -3.017483     2.045768
C     -6.769295   -3.475969     1.153385
C     -6.673395   -2.760604    -0.209235
C     -6.916447   -1.331771    -0.122525
C     -6.591442   -4.993937     0.927056
C     -6.032821   -5.435495    -0.098998
N     -7.054442   -5.757147     1.946584
C     -4.435856   -3.069285    -3.281906
C     -3.702718   -3.148478    -2.283608
O     -2.487682   -3.772954    -2.213038
C     -2.097004   -4.716320    -3.351163
C     -3.176278   -5.802444    -3.464112
C     -0.775122   -5.304013    -2.856665
C     -1.932260   -3.918821    -4.649451
N     -4.005909   -2.583555    -1.067270
C     -5.122392   -1.797533    -0.806930
C     -5.002983   -1.123666     0.462963
O     -3.978699   -1.307516     1.197426
C     -6.287443   -1.569934    -1.619819
C     -7.187992   -0.625991    -1.217157
C     -7.061721    0.042228   -0.033594
N     -5.997111   -0.219402     0.809975
C     -5.791916    0.516781     2.111578
C     -7.082797    1.081342     2.705902
C     -8.087747   -0.004279     3.034151
O     -8.970496    0.161686     4.264645
| H      | 7.406862 | 1.857522 | 2.049725 |
|--------|-----------|-----------|-----------|
| H      | 6.972733  | 1.596510  | 3.630792  |
| H      | 8.572063  | -0.514935 | 2.184456  |
| H      | 8.841806  | 1.063913  | 4.217661  |
| H      | 8.085585  | -1.906694 | 4.225928  |
| H      | 8.502200  | -6.284988 | 4.859792  |
| H      | 3.452491  | 0.124664  | 1.757121  |
| H      | 2.446105  | 2.967184  | 1.850816  |
| H      | 3.056740  | 3.028594  | -0.330977 |
| H      | 1.354676  | 2.528598  | -0.427119 |
| H      | 4.153032  | -0.678603 | -3.099850 |
| H      | 4.044573  | 0.763492  | -4.131771 |
| H      | 3.926511  | 1.063913  | -5.299850 |
| H      | 2.446105  | 1.954727  | -5.931755 |
| H      | 2.586972  | 2.187310  | -6.555028 |
| H      | -1.356573 | 1.602311  | 0.935043  |
| C      | -1.720466 | 0.696868  | -0.442514 |
| C      | 0.678625  | 0.311193  | -1.321054 |
| C      | 0.643596  | 0.172085  | -0.622709 |
| N      | 1.693049  | 0.931339  | 0.237204  |
| C      | 2.695001  | 0.234560  | 0.750096  |
| N      | 2.356184  | 0.250701  | 0.231518  |
| C      | 1.088356  | 0.907152  | -0.628240 |

**space group P2₁2₁2₁ (protomer A), H₄₁ simplified (tautomer)**

Zero-point correction= 0.154427 (Hartree/Particle)
Thermal correction to Energy= 0.163766
Thermal correction to Enthalpy= 0.164710
Thermal correction to Gibbs Free Energy= 0.119329

Sum of electronic and zero-point Energies= -470.747720
Sum of electronic and thermal Energies= -470.738382
Sum of electronic and thermal Enthalpies= -470.737437
Sum of electronic and thermal Free Energies= -470.782819

**SOLVENT:** -473.5595497

**space group P2₁2₁2₁ (protomer A), H₄₁ simplified protonated**

Zero-point correction= 0.168168 (Hartree/Particle)
Thermal correction to Energy= 0.176970
Thermal correction to Enthalpy= 0.177914
Thermal correction to Gibbs Free Energy= 0.133948

Sum of electronic and zero-point Energies= -471.155465
Sum of electronic and thermal Energies= -471.146663
Sum of electronic and thermal Enthalpies= -471.145719
Sum of electronic and thermal Free Energies= -471.189685

19

pentilRX2A SCF Done: -470.902147268 A.U.
N   -1.356573  1.602311  0.935043
C   -1.720466  0.696868 -0.442514
C   0.678625  0.311193 -1.321054
C  -0.643596  0.172085 -0.622709
N  -0.854487 -0.910505  0.359120
C  -2.087825 -0.849411  0.750896
O  -1.952004 -1.735930  0.000066
H  -2.609305  1.117424 -0.656751
H  -0.493584  1.299018 -1.863324
H  -0.974208 -0.413646 -1.861184
H  3.612837  0.698295  0.676140
H  0.543331 -2.099765 -0.507811
H  1.713466  1.902603 -0.587900
H  -0.465664  1.339105  1.363557
H  -2.731586 -0.452174  1.410931
H  -1.359075  2.567422  0.666582

20

pentilRX2AH+ SCF Done: -471.32633059 A.U.
N   1.581723 -1.641291  0.002444
C   1.837553 -0.214672 -0.442514
C   0.678625  0.311193 -1.321054
C  -0.643596  0.172085 -0.622709
N  -0.854487 -0.910505  0.359120
C  -2.087825 -0.849411  0.750896
N  -2.648824  0.250701  0.231518
C  -1.797247  0.901152 -0.628240
SOLVENT: -474.028082

space group P2₁₂₁₁(protomer A), H41 simplified (tautomer), transition state of rotation

Zero-point correction= 0.153946 (Hartree/Particle)
Thermal correction to Energy= 0.162710
Thermal correction to Enthalpy= 0.163655
Thermal correction to Gibbs Free Energy= 0.119597
Sum of electronic and zero-point Energies= -470.744744
Sum of electronic and thermal Energies= -470.735980
Sum of electronic and thermal Enthalpies= -470.735035
Sum of electronic and thermal Free Energies= -470.779093

SOLVENT: -473.558316

19 pentIRXATS SCF Done: -470.898689961 A.U.

N  -1.587248  1.749024  0.432837
C  -1.503830  0.451200 -0.249758
C  -0.515770 -0.587882  0.328010
C   0.919807 -0.231311  0.104374
N   1.948585 -1.167631  0.226604
C   3.145348 -0.520968 -0.039373
N   2.940552  0.759615 -0.318787
C   1.554681  0.946167 -0.227943
C  -2.916251  0.946167 -0.227943
O  -3.169734 -1.344038 -0.186653
H  -1.233210  0.649251 -1.297368
H  -0.754278 -1.557074 -0.127280
H  -0.725977 -0.688796  1.403772
H   4.096030 -1.024287  0.652577
H   1.112843  1.909414 -0.403907
H   1.824630 -2.146705  0.455563
H  -1.601689  1.664466  1.450907
H   3.684734  0.648818 -0.355236
H  -0.892871  2.428721  0.129878

space group P2₁₂₁₁(protomer A), H41 simplified (tautomer)

Zero-point correction= 0.155021 (Hartree/Particle)
Thermal correction to Energy= 0.164221
Thermal correction to Enthalpy= 0.165165
Thermal correction to Gibbs Free Energy= 0.119597
Sum of electronic and zero-point Energies= -470.744744
Sum of electronic and thermal Energies= -470.735980
Sum of electronic and thermal Enthalpies= -470.735035
Sum of electronic and thermal Free Energies= -470.779093

SOLVENT: -473.558316

19 pentIRXATS SCF Done: -470.898689961 A.U.

N  -1.560024 -1.405428 -1.061386
C  -1.780147 -0.626922  0.169392
C  -0.611966 -0.627481  1.194471
C   0.700940 -0.298428  0.558339
N   1.034508  0.901838  0.148520
C   2.285693  0.931648 -0.432024
N   2.760078 -0.308424 -0.415692
C   1.776849 -1.083963  0.198971
C  -2.141349  0.780014 -0.432024
O   1.594785  1.830318  0.484085
H  -2.686561 -1.020023  0.652577
H  -0.541268 -1.625163  1.639515
H  -0.842547  0.875484  1.993455
H   2.780067  1.798369 -0.837520
H   1.902961 -2.140741  0.361490
H   0.373505  1.762073  0.216321
H  -0.614922 -1.252553 -1.426305
H  -2.950376  0.758772 -1.054241
H  -1.740835 -2.403447 -0.941081

space group P2₁₂₁₁(protomer A), H41 simplified (tautomer), transition state of rotation

Zero-point correction= 0.153918 (Hartree/Particle)
Thermal correction to Energy= 0.162526
Thermal correction to Enthalpy= 0.163471
Thermal correction to Gibbs Free Energy= 0.118536
Sum of electronic and zero-point Energies= -470.740369
Sum of electronic and thermal Energies= -470.731360
Sum of electronic and thermal Enthalpies= -470.730416
Sum of electronic and thermal Free Energies= -470.775350

SOLVENT: -473.558316

19 pentIRXATS SCF Done: -470.898689961 A.U.

N  -1.517405  1.702309  0.584208
C  -1.469787  0.459364 -0.203523
C  -0.527759 -0.656722  0.301936
C   0.939477 -0.394928  0.118899
N   1.189642  0.806318 -0.359797
C   2.088166  0.653094 -0.371502
N   3.221448 -0.557061  0.031848
SOLVENT: -473.5554753

SOLVENT: -473.559278

space group P2\(1\)2\(1\)2\(1\)(protomer A), H41 simplified (tautomer), transition state of rotation (isomer)

Zero-point correction= 0.153512 (Hartree/Particle)
Thermal correction to Energy= 0.163935
Thermal correction to Enthalpy= 0.164789
Thermal correction to Gibbs Free Energy= 0.119938
Sum of electronic and zero-point Energies= -470.754137
Sum of electronic and thermal Energies= -470.744937
Sum of electronic and thermal Enthalpies= -470.743993
Sum of electronic and thermal Free Energies= -470.788935

SOLVENT: -473.5554758

space group P2\(1\)2\(1\)2\(1\)(protomer A), H41 simplified

Zero-point correction= 0.154736 (Hartree/Particle)
Thermal correction to Energy= 0.163935
Thermal correction to Enthalpy= 0.164789
Thermal correction to Gibbs Free Energy= 0.119938
Sum of electronic and zero-point Energies= -470.754137
Sum of electronic and thermal Energies= -470.744937
Sum of electronic and thermal Enthalpies= -470.743993
Sum of electronic and thermal Free Energies= -470.788935

SOLVENT: -473.5592788

space group P2\(1\)2\(1\)2\(1\)(protomer A), H41 simplified, transition state of rotation

Zero-point correction= 0.153512 (Hartree/Particle)
Thermal correction to Energy= 0.162386
Thermal correction to Enthalpy= 0.163330
Thermal correction to Gibbs Free Energy= 0.118979
Sum of electronic and zero-point Energies= -470.743633
Sum of electronic and thermal Energies = -470.734759
Sum of electronic and thermal Enthalpies = -470.733815
Sum of electronic and thermal Free Energies = -470.778166

SOLVENT: -473.5576842

C     -0.917549     0.286943     0.115835
N     -1.897558     1.280903     0.285599
C     -3.061681     0.698356     0.026346
N     -2.890251    -0.632056    -0.304330
C     -1.520900    -0.897634    -0.244528
C      2.927681     0.120343    -0.268360
O      3.209756     1.315623    -0.215085
H      1.234279    -0.653761    -1.286832
H      0.757687     1.573828    -0.134124
H      0.735226     0.723669     1.400047
H     -4.028088     1.170768     0.057023
H     -1.119524    -1.870896    -0.453948
H     -3.613413    -1.296463    -0.549653
H      1.550041    -1.636445     1.477330
H      3.678865    -0.689910    -0.326991
H      0.883875    -2.424661     0.151008

space group P2_1_2_1 (protomer A), 13b

Zero-point correction = 0.689078 (Hartree/Particle)
Thermal correction to Energy = 0.729441
Thermal correction to Enthalpy = 0.730385
Thermal correction to Gibbs Free Energy = 0.615946

Sum of electronic and zero-point Energies = -1993.618161
Sum of electronic and thermal Energies = -1993.577798
Sum of electronic and thermal Enthalpies = -1993.576853
Sum of electronic and thermal Free Energies = -1993.691293

SOLVENT: -2005.3834574

O      1.809236     5.245410     0.206946
C      2.036558     4.198781    -0.423778
N      1.780363     4.037283    -1.755110
C      1.847457     2.762651    -2.497900
C      0.496427     2.041049    -2.566528
C     -0.707226     2.751748    -2.654434
C     -1.930584     2.076355    -2.712074
C     -1.963738     0.682978    -2.665977
C     -0.767239    -0.030507    -2.575670
C      0.456725     0.693008    -2.520912
C      2.610715     2.964659     0.294419
O      3.776799     2.871796     0.664900
N      1.514551     1.950975     0.594851
O      0.619910     2.475189     1.741009
C     -0.652380     1.632669     1.889530
C     -1.657603     1.574775     0.726154
C     -3.034514     1.516168     1.413589
C     -2.795726     1.990727     2.788302
C     -1.451434     2.092647     3.123087
C     -0.981016     2.482888     4.201968
C      2.065243     0.648444     0.963413
C      2.821106    -0.073284     1.12407
O      3.240193     0.314486    -1.001385
C     -3.029073    -1.534857     0.570674
C     -4.02102     -2.055543     0.146695
C      4.619100    -3.507194     0.521414
O      4.983144    -3.823574     1.968452
C      6.029280    -3.969643     0.863032
C      1.871302    -2.261941    -0.063809
C      0.631569    -2.085356     0.565564
C      0.536456    -1.532990     1.703207
C      1.993337    -2.851455    -1.303108
C      0.901403    -3.337848    -1.960110
C     -0.388659    -3.162070    -1.399816
C     -0.524023    -2.520823    -1.93817
N     -1.732802    -2.158052     0.407690
C     -2.925280    -2.017553    -0.255158
C     -3.107122    -2.235293    -1.463278
C     -3.880829    -1.584916     0.638746
C     -5.318911    -1.466673     0.191404
C     -5.434466    -0.408724    -0.913890
C     -6.015616    -1.019223     1.480118
C     -5.812532    -2.842469    -0.270548
H      2.575035     2.100824    -2.018333
H     -0.692269     3.853588    -2.658880
H     -2.835707     2.644247    -2.773495
H     -2.895864     0.138454    -2.671619
H     -0.797960    -1.106085    -2.502971
H      1.382786     0.080003    -2.414856
H      0.899253     1.850652    -0.303650
H      1.178474     2.461329     2.683188
H      0.355609     3.517532     1.531984
H     -0.403683     0.572675     2.035354
H     -1.478536     1.045551    -0.081350
H     -1.619421    -2.768621     0.319396
H     -2.296923     0.458449     1.394010
space group P2₁2₁2₁ (protomer A), model 1, Mpro (heteroatoms frozen, free hydrogens)

Zero-point correction= 1.586256 (Hartree/Particle)
Thermal correction to Energy= 1.657805
Thermal correction to Enthalpy= 1.658749
Thermal correction to Gibbs Free Energy= 1.471531
Sum of electronic and zero-point Energies= -5036.484781
Sum of electronic and thermal Energies= -5036.413232
Sum of electronic and thermal Enthalpies= -5036.412287
Sum of electronic and thermal Free Energies= -5036.599506

SOLVENT:
space group $P2_12_12_1$(protomer A), model 1, Mpro

Zero-point correction= 1.603950 (Hartree/Particle)
Thermal correction to Energy= 1.701211
Thermal correction to Enthalpy= 1.702156
Thermal correction to Gibbs Free Energy= 1.467832

Sum of electronic and zero-point Energies= -5036.862382
Sum of electronic and thermal Energies= -5036.765121
Sum of electronic and thermal Enthalpies= -5036.764177
Sum of electronic and thermal Free Energies= -5036.998501

SOLVENT: -5065.6995283

RX2AsimpliPartSci SCF Done: -5038.466332 A.U.

N      2.843108    -6.382100    -1.903359
C      1.871368    -6.147864    -2.931756
C      1.204201    -4.768555    -2.689735
N      2.829586    -3.485780    -2.491365
C      3.669713    -2.037730    -2.746530
C      2.768740    -2.691711    -1.803273
C      2.561361    -6.167952    -4.288121
O      2.364768    -5.349563    -5.187285
C     -2.080365    -2.877864    -3.876324
H     -0.407727    -6.274331    -3.530203
| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| C    | -2.09683  | -1.14774  | -4.65672  |
| C    | -1.51339  | -0.35343  | -3.46709  |
| S    | 0.17728   | -0.87911  | -2.94113  |
| C    | -1.51339  | -0.35343  | -3.46709  |
| O    | -0.23489  | -1.86375  | -1.44298  |
| S    | 7.46373   | 4.95971   | 0.73181   |
| C    | 6.80494   | 5.78241   | -0.42113  |
| C    | 5.32054   | 5.92239   | -0.26432  |
| N    | 4.49030   | 4.79400   | -0.16594  |
| C    | 3.24648   | 5.23398   | 0.00780   |
| N    | 3.23452   | 6.60934   | 0.02220   |
| C    | 4.55173   | 7.05437   | -0.14655  |
| C    | 7.57432   | 3.44838   | 0.46489   |
| O    | 8.65935   | 2.84157   | 0.59805   |
| N    | 6.41474   | 2.82843   | 0.10278   |
| C    | 6.77994   | 0.54139   | 1.03523   |
| C    | 6.92993   | -0.98373  | 0.77459   |
| N    | 5.46796   | -1.58907  | 0.10922   |
| C    | 5.10886   | 0.00105   | -0.78298  |
| O    | 0.57574   | 0.07903   | -1.71736  |
| N    | 4.00983   | 1.35259   | -0.11963  |
| C    | 2.68753   | 0.75517   | -0.30341  |
| C    | 2.39601   | -0.31164  | 0.79655   |
| C    | 2.66801   | 0.22789   | 2.09919   |
| S    | 2.52606   | -1.01285  | 3.49293   |
| O    | 1.36375   | 1.84051   | -0.14390  |
| O    | 1.81467   | 2.81027   | 0.64260   |
| N    | 0.48734   | 1.61329   | -0.08947  |
| C    | -0.68225  | 2.48204   | -0.66429  |
| C    | -1.10375  | 3.05117   | -2.25762  |
| C    | -2.63300  | 3.05117   | -2.25762  |
| C    | -3.12062  | 3.97492   | -3.32943  |
| O    | -3.99434  | 3.78249   | -4.16437  |
| O    | -2.48986  | 5.23943   | -3.26354  |
| N    | -1.81437  | 1.68870   | 0.01600   |
| O    | -2.22224  | 0.58289   | -0.42991  |
| C    | -2.33310  | 2.31849   | 1.08866   |
| C    | -3.52923  | 1.88157   | 1.80470   |
| C    | -3.43023  | 2.44795   | 3.24280   |
| C    | -2.34211  | 1.71726   | 4.06071   |
| C    | -2.64628  | 0.21292   | 4.25306   |
| C    | -4.79287  | 2.36398   | 1.06159   |
| C    | -4.77457  | 3.09348   | 0.02250   |
| N    | -5.58090  | 1.93976   | 1.52605   |
| C    | -7.22579  | 2.30490   | 0.78046   |
| C    | -8.55589  | 1.68698   | 1.63381   |
| C    | -7.67670  | 0.47686   | 2.32491   |
| C    | -6.62626  | 1.01190   | 2.66165   |
| C    | 0.53876   | 5.16077   | 2.21484   |
| C    | -0.54532  | 5.19112   | 1.20736   |
| N    | -1.86007  | 5.11217   | 1.47176   |
| C    | -2.56598  | 5.35063   | 0.35131   |
| N    | -1.76210  | 5.87854   | -0.62190  |
| C    | -0.47229  | 5.96861   | -0.08730  |
| C    | 1.51022   | -5.46241  | 5.74634   |
| C    | 1.41489   | -4.74804  | 4.40153   |
| O    | 0.67272   | -3.75495  | 4.21751   |
| N    | 2.20260   | -5.26312  | 3.42274   |
| C    | 2.37766   | -4.62593  | 2.08679   |
| C    | 3.60787   | -5.11412  | 1.39602   |
| C    | 1.10032   | -4.96584  | 1.22911   |
| O    | 1.08725   | -5.84283  | 0.33380   |
| N    | 0.00933   | -4.23114  | 1.54717   |
| O    | -1.24379  | -4.42234  | 0.82230   |
| C    | -1.92737  | -5.75737  | 1.21030   |
| C    | -2.16408  | -3.25610  | 1.16929   |
| C    | -2.03048  | -2.58422  | 2.23528   |
| N    | -3.15102  | -3.03723  | 0.28496   |
| O    | -4.00369  | -1.82960  | 0.38190   |
| C    | -4.87130  | -1.47865  | -1.01722  |
| C    | -5.19334  | -0.12945  | -1.07863  |
| C    | -5.20002  | 0.39077   | -2.51096  |
| C    | -4.94269  | -0.32339  | -3.49847  |
| N    | -5.46816  | 1.73443   | -2.58450  |
| C    | -5.17196  | -2.04849  | 1.35668   |
| O    | -6.36492  | -2.01694  | 0.99955   |
| N    | -4.76008  | -2.22026  | 2.64304   |
space group P2₁2₁2₁ (protomer A), model 1, product (heteroatoms frozen, free hydrogens)

| X   | Y   | Z       |
|-----|-----|---------|
| -3.603971 | -1.413702 | -1.645247 |
| -5.172200 | -2.269742 | -1.400015 |
| -4.632920  | 0.584322  | -0.479077 |
| -6.207009  | -0.217911 | -0.680526 |
| -5.464844  | 2.194245  | -3.471107 |
| -5.452226  | 2.299853  | -1.732739 |
| -5.451904  | -2.442690 | 3.351753  |
| -3.752223  | -2.309144 | 2.834231  |
| 3.261970   | -7.004205 | -4.373835 |
| 3.573308   | -6.200720 | 1.213106  |
| 7.620866   | -1.433576 | 1.345011  |

Zero-point correction= 3.034132 (Hartree/Particle)
Thermal correction to Energy= 3.171895
Thermal correction to Enthalpy= 3.172839
Thermal correction to Gibbs Free Energy= 2.857544
Sum of electronic and zero-point Energies= -9547.621890
Sum of electronic and thermal Energies= -9547.484128
Sum of electronic and thermal Enthalpies= -9547.483183
Sum of electronic and thermal Free Energies= -9547.798479

SOLVENT: -9602.829254

RX2AsimpleP SCF Done: -9550.65590050 A.U.
| Atoms | X      | Y      | Z     |
|-------|--------|--------|-------|
| S     | -1.797951 | -3.436865 | -0.869555 |
| C     | -4.474553 | -6.037876 | -2.620155 |
| O     | -5.090571 | -6.831495 | -1.918037 |
| N     | -4.296171 | -6.147868 | -3.942333 |
| C     | -4.823388 | -7.259147 | -4.751764 |
| C     | -3.375857 | -2.389297 | -6.286209 |
| C     | -4.630080 | -1.986047 | -5.520552 |
| N     | -3.324991 | -0.902305 | -4.532133 |
| C     | -3.717024 | 0.267323  | -4.904276 |
| N     | -3.976934 | 0.350919  | -2.778216 |
| C     | -4.481858 | -0.845205 | -3.965885 |
| N     | -0.202126 | -2.322354 | -6.029028 |
| C     | 0.182452  | -1.278315 | -3.207736 |
| O     | 0.595092  | -1.701119 | -2.105934 |
| N     | -0.079910 | 0.018179  | -3.404342 |
| C     | 0.401042  | 1.005055  | 1.827511 |
| C     | -1.919882 | 1.177272  | -2.533300 |
| C     | 2.370106  | 1.609224  | -3.884703 |
| S     | 4.187078  | 1.720486  | -4.079585 |
| N     | 4.662112  | 2.543289  | -2.557977 |
| N     | -0.873110 | 2.762977  | -3.454744 |
| C     | -0.534788 | 4.500410  | -1.138792 |
| C     | -1.412708 | 4.686221  | 0.093661 |
| O     | -2.155101 | 6.014613  | 0.022605 |
| C     | -3.296339 | 6.223319  | 0.992860 |
| O     | -3.106914 | 7.140922  | 1.827511 |
| C     | -4.386528 | 5.518490  | 0.876306 |
| O     | 0.753791  | 5.533674  | -1.031885 |
| C     | 1.724421  | 4.922626  | -0.399531 |
| N     | 0.736380  | 6.532790  | -1.643181 |
| C     | 1.853983  | 7.507512  | -1.748618 |
| C     | 2.075521  | 7.634647  | -3.231320 |
| C     | 2.659826  | 6.707224  | -4.079555 |
| O     | 4.150816  | 6.552258  | -3.849899 |
| C     | 1.490739  | 8.743786  | -0.921919 |
| O     | 0.313883  | 8.972614  | -0.626017 |
| C     | 2.471428  | 9.574003  | -0.496463 |
| O     | 2.230830  | 10.530303 | 0.586172 |
| C     | 3.580196  | 11.234703 | 0.824804 |
| O     | 4.608266  | 10.422140 | 0.050300 |
| C     | 3.856639  | 9.620826  | -0.988125 |
| O     | 3.716992  | 4.547791  | -5.135042 |
| C     | 0.446412  | 4.988852  | -3.927043 |
| N     | -5.490356 | 5.809612  | -3.99241 |
| C     | -5.934983 | 6.131554  | -2.774214 |
| N     | -5.234426 | 5.379825  | -1.910889 |
| C     | -4.300573 | 4.683236  | -2.614959 |
| O     | 4.875483  | -0.065294 | -6.518299 |
| C     | 7.986551  | -0.579459 | 5.312607 |
| N     | 7.591913  | 0.225898  | 4.141237 |
| N     | 8.782418  | -1.904924 | -5.231446 |
| C     | 7.212933  | -2.590820 | -0.73284 |
| C     | 6.527553  | -3.907990 | -4.450525 |
| C     | 8.234187  | -2.790384 | -2.943218 |
| O     | 8.454794  | -3.809417 | -2.472738 |
| N     | 8.680328  | -1.576843 | -2.412452 |
| C     | 9.307893  | -1.511799 | -1.068819 |
| O     | 10.026595 | -1.835437 | -1.173838 |
| O     | 9.013675  | -0.167893 | -0.387562 |
| C     | 8.639338  | 0.796924  | 1.077453 |
| N     | 9.121997  | -0.124397 | 0.939423 |
| C     | 8.785336  | 1.065138  | 1.761852 |
| C     | 8.440272  | 0.616696  | 3.184323 |
| C     | 8.023483  | 1.757723  | 4.108731 |
| C     | 7.776806  | 1.299410  | 5.521524 |
| C     | 7.956016  | 0.132850  | 5.870120 |
| N     | 7.342972  | 2.255978  | 6.348177 |
| C     | 9.936649  | 2.092589  | 1.808421 |
| O     | 10.123979 | 2.477716  | 2.883673 |
| N     | 10.639928 | 2.391572  | 0.712415 |
| O     | -3.773815 | -3.460450 | 0.985324 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -2.695255 | -3.77395  | 1.430106  |
| N    | -2.697840 | -4.701260 | 2.252738  |
| C    | -1.851977 | -5.431094 | 3.100778  |
| C    | -2.261135 | -5.056064 | 4.513735  |
| C    | -3.167996 | -5.846996 | 5.207084  |
| C    | -3.491049 | -5.518144 | 6.527829  |
| C    | -2.913398 | -4.399746 | 7.163053  |
| C    | -2.010287 | -3.611420 | 6.457491  |
| C    | -1.679167 | -3.933767 | 5.143197  |
| C    | -1.458084 | -3.176130 | 0.891403  |
| O    | -0.361381 | -4.077364 | 1.233447  |
| C    | -1.310449 | -1.704019 | 1.315321  |
| C    | -2.391969 | -0.785358 | 0.713794  |
| C    | -2.361516 | 0.660216  | 1.259155  |
| C    | -2.652854 | 0.762099  | 2.753168  |
| N    | -3.715608 | 1.877767  | 2.904864  |
| C    | -4.034147 | 2.270811  | 1.525891  |
| O    | -3.589055 | 1.646221  | -0.660730 |
| C    | 0.042818  | -1.373946 | 0.789945  |
| O    | 0.861169  | -0.995363 | 2.853091  |
| C    | 2.374800  | -0.860476 | 0.909403  |
| N    | 3.147301  | -2.173837 | 0.741443  |
| C    | 4.531350  | -1.982277 | 0.118874  |
| C    | 4.617035  | -1.457997 | -1.314280 |
| C    | 4.935962  | -2.939354 | -1.017692 |
| N    | 3.060775  | 0.155764  | 1.674123  |
| C    | 2.484596  | 1.429603  | 1.505428  |
| O    | 1.497306  | 1.653343  | 0.702215  |
| C    | 4.056908  | -0.106799 | 2.535802  |
| C    | 4.669742  | 0.892755  | 3.293914  |
| C    | 4.142128  | 2.196015  | 3.196477  |
| C    | 3.097351  | 2.508355  | 2.319513  |
| N    | 2.549983  | 3.724154  | 2.194497  |
| C    | 2.928295  | 4.808993  | 2.771056  |
| O    | 3.838225  | 4.805359  | 3.587319  |
| C    | 2.180233  | 5.994366  | 2.482121  |
| C    | 1.845961  | 6.884724  | 3.473609  |
| N    | 1.530251  | 6.117675  | 4.767327  |
| C    | 0.582612  | 7.642634  | 3.102190  |
| C    | 3.057845  | 7.814169  | 3.583066  |
| H    | 5.722554  | -8.875269 | -0.812823 |
| H    | 5.191215  | -6.593469 | -1.822141 |
| H    | 5.912048  | -6.715414 | -0.531165 |
| H    | 0.960781  | -4.585843 | -2.702833 |
| H    | 2.346694  | -6.758857 | 1.034538  |
| H    | 0.471186  | -5.312064 | 0.085847  |
| H    | 3.678358  | -8.465993 | -2.897102 |
| H    | 9.062834  | -4.528779 | 3.121189  |
| H    | 10.713633 | -4.514537 | 4.509559  |
| H    | 8.846114  | -2.124798 | 4.993983  |
| H    | 8.345231  | -3.694093 | 5.611636  |
| H    | 7.288838  | -2.330180 | 3.094127  |
| H    | 6.494151  | -2.406890 | 4.668964  |
| H    | 7.660969  | -4.451296 | 1.423876  |
| H    | 6.118845  | -5.343276 | 1.271252  |
| H    | 6.121646  | -3.579407 | 1.253681  |
| H    | -9.804178 | 3.241108  | -2.743026 |
| H    | -10.394177| 4.429231  | -1.576447 |
| H    | -8.194717 | 4.155373  | -0.896943 |
| H    | -8.757545 | 1.277238  | -0.682484 |
| H    | -6.264819 | 2.839776  | -1.414029 |
| H    | -6.278145 | 1.111523  | -1.067165 |
| H    | -7.616458 | -0.437925 | -2.501162 |
| H    | -8.180123 | -0.998059 | -4.828768 |
| H    | -7.924183 | 0.702386  | -6.592952 |
| H    | -6.745672 | 3.544105  | -3.657352 |
| H    | -7.223531 | 2.989219  | -5.982583 |
| H    | -8.512976 | 0.491293  | 1.347315  |
| H    | -7.658134 | 2.084652  | 3.377390  |
| H    | -9.423170 | 0.149834  | 3.616224  |
| H    | -8.620475 | 0.812695  | 5.021301  |
| H    | -10.757787| 1.952173  | 4.493899  |
| H    | -10.885589| 2.508680  | 2.952586  |
| H    | -9.916939 | 4.278956  | 4.763318  |
| H    | -8.893748 | 3.182936  | 5.712413  |
| H    | -8.330204 | 3.810496  | 4.141837  |
| H    | -6.495713 | 0.329085  | 5.283042  |
| H    | -4.570047 | -1.546728 | 4.416459  |
| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| H    | -6.226134    | -1.444226    | 6.961530     |
| H    | -4.941656    | -6.17847     | 6.649461     |
| H    | -3.71027     | 0.220725     | 8.474363     |
| H    | -7.50590     | -5.768099    | 3.417212     |
| H    | -6.29538     | -2.957436    | 1.544062     |
| H    | -8.14358     | -4.200117    | -0.367583    |
| H    | -8.000118    | -2.003630    | -1.475454    |
| H    | -4.56588     | -6.874637    | -5.50376     |
| H    | -4.013408    | -7.855332    | -4.983704    |
| H    | -5.387511    | -1.642462    | -6.239024    |
| H    | -3.030628    | 1.962274     | -3.796243    |
| H    | -4.935474    | -1.521985    | -2.487340    |
| H    | -3.931560    | 0.702561     | -1.820783    |
| H    | -1.243688    | -1.102702    | -5.635116    |
| H    | -0.300542    | -3.240933    | -3.795295    |
| H    | -1.384190    | -1.637513    | -5.756624    |
| H    | -2.083914    | -2.932444    | -4.473600    |
| H    | -1.325364    | -3.417140    | -7.070604    |
| H    | -2.297371    | -5.174315    | -4.939915    |
| H    | -0.618503    | 0.394232     | -4.182886    |
| H    | 0.219837     | 0.585218     | -1.404692    |
| H    | 2.334408     | 0.198881     | -2.349837    |
| H    | 2.224908     | 1.835961     | -1.722424    |
| H    | 1.950229     | 2.687711     | -4.069798    |
| H    | 2.001945     | 1.024586     | -4.672864    |
| H    | 5.379896     | 2.725229     | -2.625797    |
| H    | 4.144640     | 3.501826     | -2.428614    |
| H    | 4.483145     | 1.919421     | -1.676760    |
| H    | 0.364051     | 2.681057     | -0.547686    |
| H    | -1.101348    | 4.770218     | -2.036796    |
| H    | -0.799102    | 4.618852     | 1.001079     |
| H    | -2.137307    | 3.866086     | 0.100472     |
| H    | -1.408614    | 6.681896     | 0.162919     |
| H    | -2.895433    | 6.079093     | -0.988169    |
| H    | -1.018177    | 6.846070     | -2.019177    |
| H    | -2.271368    | 7.005050     | -1.310101    |
| H    | -1.102914    | 8.153519     | -3.63509     |
| H    | 2.733365     | 8.712026     | -3.306896    |
| H    | 2.469888     | 6.929549     | -5.137427    |
| H    | 2.133794     | 5.771948     | -3.847584    |
| H    | 4.561667     | 5.723070     | -4.436866    |
| H    | 4.367933     | 6.342065     | -2.794376    |
| H    | 4.685436     | 7.468401     | -4.129787    |
| H    | 1.890542     | 9.980142     | 1.470032     |
| H    | 3.817905     | 11.284776    | 1.889710     |
| H    | 3.531401     | 12.258760    | 0.440470     |
| H    | 5.382095     | 11.047276    | -0.402883    |
| H    | 5.106670     | 9.724563     | 0.733978     |
| H    | 4.265053     | 8.615751     | -1.126194    |
| H    | 3.879396     | 10.123900    | -1.974409    |
| H    | -4.220384    | 3.695798     | -5.612846    |
| H    | -3.661535    | 5.368284     | -5.855203    |
| H    | -6.724789    | 6.806283     | -2.496012    |
| H    | -3.683500    | 3.938781     | -2.134514    |
| H    | -5.280076    | 5.351966     | -6.894042    |
| H    | 8.545790     | 0.997610     | -6.628323    |
| H    | 9.828408     | -0.196026    | -6.321152    |
| H    | 8.502700     | -0.594089    | -7.442847    |
| H    | 8.220464     | -2.498122    | -5.956067    |
| H    | 6.448840     | -1.887388    | -3.713400    |
| H    | 6.036957     | -4.318109    | -3.565903    |
| H    | 5.773884     | -3.725886    | -5.222087    |
| H    | 8.369483     | -0.671849    | -2.795859    |
| H    | 8.858614     | -2.311830    | -0.462657    |
| H    | 11.253877    | -1.881595    | -0.178456    |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| N    | 2.089755| -3.096826| 4.423864|
| C    | 1.495686| -3.340970| 3.078218|
| C    | 0.365931| -2.308540| 2.857895|
| C    | -0.804378| -2.578165| 3.782993|
| C    | -1.743710| -3.561703| 3.440574|
| C    | -2.836281| -3.815946| 4.265995|
| C    | -3.004843| -3.093043| 5.452205|
| C    | -0.965087| -1.879223| 4.985019|
| C    | -2.064387| -2.126045| 5.810557|
| C    | 2.558363| -3.211243| 1.975796|
| O    | 3.727913| -2.814976| 2.210723|
| N    | 2.085061| -3.567061| 0.758139|
| C    | 2.858510| -3.447058| -0.473246|
| C    | 3.074807| -4.833418| -1.132529|
| C    | 3.856504| -5.793069| -0.206232|
| C    | 5.183668| -2.917017| 0.783632|
| C    | 2.116265| -2.518055| -1.441866|
| O    | 0.936369| -2.07832| -1.240370|
| N    | 2.320398| -1.165010| -3.509914|
| C    | 3.474009| -0.535695| -4.342089|
| C    | 4.797450| -0.605251| -3.615196|
| O    | 5.390410| -1.737399| -3.512505|
| N    | 5.257287| 0.504396| -3.040417|
| C    | 1.685979| -2.295362| -5.858536|
| O    | 0.128195| -2.111957| -3.903424|
| N    | -0.862761| -2.956103| -4.565438|
| C    | -1.695524| -3.770681| -3.583620|
| O    | -2.810111| -4.230825| -3.927902|
| N    | -1.197641| -3.961323| -2.324628|
| C    | -2.009354| -4.389491| -1.332170|
| C    | -1.280126| -5.248856| -0.215792|
| O    | -0.536754| -4.230524| 0.536439|
| C    | -2.972344| -3.440307| -0.795417|
| O    | -2.658539| -2.814924| 0.269080|
| N    | -3.961133| -3.107350| -1.596765|
| C    | -4.793348| -1.901312| -1.426743|
| C    | -5.525444| -0.897936| -2.579596|
| S    | -2.738656| -0.670247| -2.947773|
| C    | -6.281239| -2.312558| -1.516664|
| O    | -6.613145| -3.410178| -2.004814|
| N    | -7.143155| -1.356743| -1.103859|
| C    | -8.591351| -1.392157| -1.234139|
| C    | -5.566816| -0.021753| 2.070911|
| C    | -4.479378| -1.020035| 2.579128|
| C    | -3.221950| -0.298162| 2.926493|
| N    | -3.173174| 0.718910| 3.900072|
| C    | -1.935812| 1.233688| 3.817976|
| N    | -2.123532| 0.641961| 2.820834|
| C    | -2.034202| -0.351101| 2.245609|
| C    | -0.902280| 0.840720| 0.916164|
| C    | -5.608424| 0.780352| -0.238594|
| N    | -4.171704| 1.741377| 1.181705|
| C    | -3.728543| 2.741878| 0.180058|
| C    | -3.236166| 4.019371| 0.893336|
| C    | -4.398371| 6.470081| 1.689885|
| N    | -5.500247| 5.226077| 0.865055|
| C    | -2.673390| 2.256025| -0.827028|
| O    | -2.865501| 2.416139| -2.065480|
| N    | -1.525609| 1.759745| -0.319589|
| C    | -0.343724| 1.489303| -1.164231|
| C    | 0.067841| 2.725249| -1.957905|
| C    | 0.496987| 3.895177| -1.016946|
| S    | 1.025630| 5.417696| -1.888882|
| C    | 2.489520| 4.777703| -2.795608|
| C    | 0.738962| 1.019302| -0.232721|
| C    | 0.579927| 0.588662| 0.925520|
| N    | 2.046134| 1.152847| -0.705497|
| C    | 3.183621| 1.040387| 0.223673|
| C    | 3.767410| -0.383583| 0.175382|
| C    | 5.212277| -0.624386| 0.744300|
| O    | 6.908945| -0.891002| -0.438254|
| O    | 6.919594| -0.948825| -0.918341|
| O    | 5.765485| -2.065363| -1.049823|
| C    | 4.189943| 2.108212| -0.156411|
| C    | 4.353605| 2.482410| -1.366429|
| N    | 4.860711| 2.581186| 0.890851|
| C    | 6.053927| 3.426419| 0.721649|
| C    | 6.075226| 4.512206| 1.812496|
space group P2₁2₁2₁ (protomer A), model 1, reactant complex

Zero-point correction=                           2.514777 (Hartree/Particle)
Thermal correction to Energy=                    2.662379
Thermal correction to Enthalpy=                  2.663324
Thermal correction to Gibbs Free Energy=         2.327889

Sum of electronic and zero-point Energies=          -7729.062047
Sum of electronic and thermal Energies=             -7728.914445
Sum of electronic and thermal Enthalpies=           -7728.915012
Sum of electronic and thermal Free Energies=        -7729.248935

SOLVENT: -7773.6587654

RX2Asimpl2REACTANT SCF Done: -7731.57682433 A.U.
| X       | Y       | Z       |
|---------|---------|---------|
| 2.117699 | -3.053530 | 4.20917 |
| 1.732023 | -2.716714 | 5.652583 |
| 0.250277 | -2.372857 | 5.747751 |
| -0.629766 | -3.219955 | 5.419070 |
| 3.428141 | -3.964656 | 4.287889 |
| 3.457693 | -4.942540 | 5.051589 |
| 4.438777 | -3.599824 | 3.448596 |
| 5.533519 | -4.228808 | 3.149499 |
| 5.651095 | -4.848428 | 1.646800 |
| 6.637583 | -5.452910 | 1.202414 |
| 4.600109 | -4.415527 | 0.878149 |
| 4.379888 | -4.710708 | -0.554437 |
| 5.379184 | -5.575595 | -0.944824 |
| 5.393550 | -5.651118 | -2.015903 |
| 5.817159 | 0.014892 | -0.893860 |
| 3.430652 | 0.946057 | -0.311422 |
| 6.644415 | -1.706269 | -2.519924 |
| 7.269549 | -2.729899 | -2.201503 |
| 6.938348 | -0.882406 | -3.555007 |
| 8.089178 | -1.158567 | -4.425570 |
| 4.153631 | 0.005596 | -5.549677 |
| 3.737020 | -1.429238 | -5.090713 |
| 2.383581 | -1.343158 | -4.472954 |
| 1.327889 | -0.738981 | -5.176281 |
| 0.291589 | -0.721602 | -4.326440 |
| 0.654823 | -1.244801 | -3.102216 |
| 1.798469 | -1.641784 | -3.191899 |
| 4.508067 | 0.976987 | -4.383488 |
| 5.078780 | 1.189440 | -3.633087 |
| 2.881681 | 1.584673 | -4.158704 |
| 2.760623 | 2.526783 | -3.038907 |
| 2.923154 | 4.009172 | -3.481234 |
| 4.378804 | 4.307024 | -3.955706 |
| 4.789630 | 5.722168 | -3.757258 |
| 1.556609 | 2.420340 | -2.107110 |
| 1.653587 | 3.062731 | -0.999955 |
| 0.426162 | 1.775002 | -2.398379 |
| 0.698451 | 1.876017 | -1.442082 |
| 1.465393 | 3.216726 | -1.616533 |
| 2.236741 | 3.263762 | -2.870843 |
| 2.207201 | 4.873846 | -3.05107 |
| 4.010635 | 4.917783 | -1.447842 |
| 1.701953 | 0.745044 | -1.638103 |
| 1.798837 | 0.119408 | -2.716595 |
| 2.353515 | 0.598064 | -0.586890 |
| 3.796718 | -0.141551 | -0.732708 |
| 4.142272 | -0.872348 | 0.590001 |
| 4.930947 | -2.189057 | 0.356339 |
| 5.131947 | -2.918970 | 1.652600 |
| 6.709998 | -3.327575 | 2.155398 |
| 3.904112 | -3.120426 | 2.303972 |
| 4.894442 | 0.887834 | -0.982475 |
| 4.877325 | 1.992093 | -0.353482 |
| 5.863304 | 0.319046 | -1.816984 |
| 7.114706 | 1.263042 | -1.926456 |
| 7.392915 | 1.559059 | -3.420811 |
| 6.493343 | 2.700401 | -3.945725 |
| 6.938250 | 4.084110 | -3.427970 |
| 8.205667 | 0.385843 | -1.296765 |
| 8.006709 | -0.811357 | -0.986117 |
| 9.406109 | 0.983831 | -1.072478 |
| 10.509193 | 0.192623 | -0.455833 |
| 11.704979 | 1.705859 | -0.493185 |
| 11.028834 | 2.561665 | -0.371336 |
| 9.770528 | 2.414072 | -1.258101 |
| 4.069005 | 0.030114 | -4.651393 |
| 4.208527 | -1.306681 | -4.004192 |
| 5.398605 | -1.713123 | -3.356880 |
| 5.124203 | -2.921805 | -2.828826 |
| 3.833656 | -3.299915 | -3.084935 |
| 3.250081 | -2.275691 | -3.830001 |
| 4.277948 | -1.345760 | 1.905359 |
| 4.393356 | -0.337862 | 2.662030 |
| 4.980099 | -0.435428 | 3.872369 |
| 5.177161 | 0.629508 | 4.903021 |
| X     | Y     | Z     |
|-------|-------|-------|
| 5.001054 | -2.221846 | 0.146101 |
| 4.624039 | -0.910403 | -2.428006 |
| 6.441365 | -0.362698 | -4.353394 |
| 8.839675 | -1.328751 | -2.242776 |
| 6.367596 | 0.690004 | -1.548089 |
| 6.346644 | -0.054530 | -3.722463 |
| 8.839675 | -0.362698 | -4.353394 |
| 3.877073 | -1.257364 | -5.467408 |
| 5.179598 | 0.006359 | -5.925793 |
| 3.465569 | 0.312029 | -6.340820 |
| 4.448210 | -1.660793 | -4.385728 |
| 3.702960 | -2.072230 | -5.978354 |
| -0.696570 | -0.357748 | -4.525073 |
| 2.489449 | -2.130294 | -2.386677 |
| 0.097232 | -1.328751 | -2.242776 |
| 2.089461 | 1.297842 | -4.735876 |
| 3.609083 | 2.296533 | -2.393807 |
| 2.189632 | 4.250710 | -4.25917 |
| 2.762984 | 4.635558 | -2.609128 |
| 4.499660 | 4.039492 | -5.008237 |
| 4.722419 | 6.357052 | -4.375669 |
| 4.625246 | 5.957233 | -2.761237 |
| 0.327052 | 1.140895 | -3.191210 |
| -0.298731 | 1.851186 | -0.434351 |
| -0.742616 | 4.033825 | -1.624158 |
| -2.097858 | 3.322710 | -0.737364 |
| -3.081839 | 2.465019 | -2.856033 |
| -1.726952 | 3.136834 | -3.775853 |
| -4.913253 | 5.644506 | -1.555505 |
| -4.525060 | 3.936375 | -1.209660 |
| -3.434061 | 5.236403 | -0.636137 |
| -2.428276 | 1.221511 | 0.227933 |
| -3.677112 | -0.831209 | -1.565838 |
| -4.701882 | -0.204992 | 1.252068 |
| -3.196998 | -1.123156 | 1.049198 |
| -5.904779 | -1.975336 | -0.096389 |
| -4.527799 | -2.830374 | -0.289479 |
| -5.832069 | -0.395730 | -2.338271 |
| -6.997508 | 2.184720 | -1.351251 |
| -7.204284 | 0.629121 | -3.969820 |
| -8.444978 | 1.826286 | -3.566222 |
| -6.509572 | 2.699452 | -5.042391 |
| -5.458435 | 2.516096 | -3.639732 |
| -6.250017 | 4.857899 | -3.781617 |
| -6.930504 | 4.110626 | -2.332253 |
| -7.952089 | 4.319526 | -3.738128 |
| -10.232195 | -0.072997 | 0.568844 |
| -12.419737 | 0.977746 | 0.310098 |
| -12.220444 | 1.094165 | -1.456604 |
| -11.671999 | 3.381089 | -0.701868 |
| -10.724891 | 2.733458 | 0.665546 |
| -8.956317 | 3.071169 | -0.942729 |
| -10.008489 | 2.623052 | -2.306960 |
| -3.157629 | 0.669422 | -5.253154 |
| -4.933012 | 0.247977 | -2.586406 |
| -5.815548 | -3.509788 | -2.253418 |
| -2.222856 | -2.282821 | -4.136705 |
| -3.319796 | -4.180185 | -2.760539 |
| 5.360183 | 1.561940 | 4.377166 |
| 4.754252 | -0.609545 | 7.311589 |
| 2.818535 | -0.558894 | 8.836817 |
| 0.938862 | 1.149968 | 8.229334 |
| 0.980426 | 2.339108 | 6.066658 |
| 2.926422 | 2.156465 | 4.568919 |
| 1.850280 | 0.747567 | 3.059585 |
| 1.819204 | -0.016671 | 0.096467 |
| 2.123421 | -1.189963 | 1.371498 |
| -0.360092 | 0.599339 | 1.134716 |
| -0.376273 | 0.276395 | 3.470670 |
| 0.575240 | -2.172887 | 3.341353 |
| -2.405822 | -0.913117 | 2.846580 |
| -1.525501 | -2.287669 | 3.557115 |
| -1.975351 | -2.856812 | 1.089750 |
| 1.704531 | 2.429905 | 0.619192 |
| 0.012063 | 3.813975 | 0.736231 |
| 1.328817 | 5.642899 | 2.800993 |
| 2.071501 | 4.984162 | 1.357288 |
| -0.296196 | 6.906149 | 1.336312 |
| -0.331719 | 6.566557 | -1.152899 |
| 0.970083 | 5.285223 | -0.950819 |
space group P2₁2₁2₁ (protomer A), model 1, transition state

Zero-point correction=  2.512756 (Hartree/Particle)
Thermal correction to Energy= 2.659035
Thermal correction to Enthalpy= 2.659979
Thermal correction to Gibbs Free Energy= 2.329843

Sum of electronic and zero-point Energies=  -7729.022331
Sum of electronic and thermal Energies=  -7728.876052
Sum of electronic and thermal Enthalpies=  -7728.875108
Sum of electronic and thermal Free Energies=  -7729.206144

SOLVENT: -7773.6080514
space group P2₁2₁2₁ (protomer A), model 1, product

Zero-point correction = 2.520078 (Hartree/Particle)
Thermal correction to Energy = 2.665898
Thermal correction to Enthalpy = 2.666842
Thermal correction to Gibbs Free Energy = 2.337182

Sum of electronic and zero-point Energies = -7729.098476
Sum of electronic and thermal Energies = -7728.952656
Sum of electronic and thermal Enthalpies = -7728.951712
Sum of electronic and thermal Free Energies = -7729.281372

SOLVENT: -777 3.688685

RX2asimpl2 SCF Done: -7731.61855343 A.U.
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| H    | -9.29159 | 2.732469 | 0.171307 |
| H    | -10.290029 | 2.887074 | -1.274268 |
| H    | -2.656007 | 2.590129 | -0.018765 |
| H    | -3.881784 | 2.914368 | -5.282048 |
| H    | -5.709923 | -1.756758 | -4.250744 |
| H    | -1.894251 | 0.027916 | -4.677031 |
| H    | -3.142129 | -2.232855 | -4.537336 |
| H    | 3.369779 | 0.104933 | 4.894696 |
| H    | 4.026779 | -3.170216 | 6.622601 |
| H    | 4.225261 | -4.274438 | 8.149624 |
| H    | 0.179123 | -3.273134 | 8.530041 |
| H    | -0.475471 | -1.206969 | 7.299662 |
| H    | 1.063733 | -0.189633 | 5.667084 |
| H    | 1.387303 | 0.029499 | 2.498011 |
| H    | 1.712090 | -1.511990 | 1.020656 |
| H    | -0.947163 | -1.026482 | 3.402279 |
| H    | 0.056409 | -2.349383 | 2.759724 |
| H    | -2.896368 | -1.853083 | 2.102570 |
| H    | -2.068333 | -3.406755 | 2.383378 |
| H    | -2.153478 | -3.086703 | -0.142737 |
| H    | 1.539499 | 2.217819 | 1.711621 |
| H    | -0.205369 | 3.469676 | 2.193338 |
| H    | 0.928763 | 4.234939 | 4.921979 |
| H    | 1.800978 | 4.151556 | 3.389016 |
| H    | -0.554367 | 6.085680 | 3.872270 |
| H    | -0.070844 | 6.776148 | 1.486431 |
| H    | 1.206944 | 5.461348 | 1.387747 |
| H    | 1.220754 | 7.826364 | 3.433491 |
| H    | 2.481893 | 6.304990 | 3.276025 |
| H    | -1.030508 | 4.295600 | 5.581009 |
| H    | -3.313720 | 4.056469 | 6.526118 |
| H    | -5.071013 | 2.829317 | 5.190031 |
| H    | 3.254006 | 1.823239 | 3.261127 |
| H    | -8.256969 | 0.888512 | 3.270594 |
| H    | -8.641737 | 0.672116 | 1.495393 |
| H    | -9.481948 | -0.458953 | 2.584882 |
| H    | -7.401541 | -1.198733 | 0.340528 |
| H    | -8.142392 | -2.411265 | 1.396369 |
| H    | -6.369283 | -2.264119 | 1.309702 |
| H    | -7.153614 | -0.802720 | 4.637966 |
| H    | -6.231856 | -2.058327 | 3.767933 |
| H    | -8.000294 | -2.209961 | 3.905674 |
| H    | 4.640100 | -0.823070 | 5.684327 |
| H    | 8.887529 | 3.571037 | -2.093658 |
| H    | 6.356399 | 5.956957 | -1.906033 |
| H    | 5.227577 | -4.924473 | -1.077191 |
| H    | -4.506667 | 1.787298 | 1.712829 |
| H    | 4.134360 | -2.640489 | 4.017677 |
| H    | -10.421778 | -0.721509 | -1.856479 |
| H    | -4.355125 | 2.831414 | -3.580475 |
| H    | -3.801330 | -4.622221 | -3.403973 |
| H    | 4.402678 | 5.392676 | -3.023814 |

Space group P2₁2₁2₁(protomer A), model 1, product (with a H-bond of OH with imidazole of H41)

Zero-point correction= 2.520059 (Hartree/Particle)
Thermal correction to Energy= 2.665033
Thermal correction to Enthalpy= 2.665977

RX2Asimpli2noRX SCF Done: -7731.64763362

A.U.

N 7.166273 -4.702740 -2.497195
Thermal correction to Gibbs Free Energy = 2.338696
Sum of electronic and zero-point Energies = -7729.127575
Sum of electronic and thermal Energies = -7728.982601
Sum of electronic and thermal Enthalpies = -7728.981657
Sum of electronic and thermal Free Energies = -7729.308937

SOLVENT: -7773.693982

C     -8.291665    -4.834269    -1.529882
C     -7.836597    -5.380988    -0.164016
C     -6.743388    -4.590945     0.479549
C     -5.388003    -4.808092     0.222246
C     -4.673251    -3.949230     1.001494
C     -5.497102    -1.918122     1.743122
C     -6.799580    -3.586605     1.421296
C     -8.979544    -3.482409    -1.364795
C      3.402110     5.449667    -3.509705
C      2.419724     4.388218    -3.922840
C      1.130336     4.314618    -3.161787
C      0.356594     3.064399    -3.509705
C     -0.222367     3.064399    -4.897591
C      1.328418     4.444021    -1.644992
O      2.439400     4.302060    -1.064992
N      0.179428     4.748925    -0.992503
C      0.155216     5.153013     0.411566
C      0.220085     6.600342     0.514996
C      0.706522     7.556177    -0.259718
C      2.232915     7.928855     0.216922
C      -0.852389     4.352539    1.240091
O      -1.803289     3.670472     0.738630
N      -0.071226     4.498566     2.557890
C      -1.659624     3.931057     3.544942
C      -1.033786     4.683324     4.958991
C      -0.469016     3.839284     4.961416
O      -1.234060     4.597673     4.298508
C      -0.825561     2.788228     5.663691
C      -2.931916     4.815786     3.513511
C      -2.896981     5.981619     3.948362
N      -4.022176     4.215773     2.974723
C      -5.193572     5.010756     2.608576
C      -5.463609     5.021603     1.091188
O      -6.495233     5.542100     0.634636
N      -5.01602     4.422503     0.328872
C      -6.494316     4.316119    -1.117919
C      -3.848146     4.819787    -1.912731
C      -2.319947     3.919619    -1.812973
C      -5.061398     2.908484    -1.620989
O      -5.290115     2.739933    -2.831552
N      -5.955567     1.926365    -0.698191
C      -5.675398     0.635767    -1.041107
C      -5.508105     0.362659     0.121618
S      -3.724634     0.762023     0.269508
C      -7.181743     0.809217    -1.348882
O      -7.816163     1.831923    -1.053326
N      -7.721295    -0.286418    -1.959419
C      -9.168165    -0.312558    -2.222487
C      -5.048127    -1.278994    -4.417765
C      -4.501462     0.189386    -4.435515
C      -3.076619     0.221596    -3.998374
N      -2.121357    -0.586671    -4.643206
C      -0.971872    -0.380676    -3.983896
O      -1.159564     0.477443    -2.921949
C      -2.492903     0.871597    -2.933319
C      -4.719337    -2.074768    -3.159249
C      -5.601570    -2.314910    -2.272004
N      -3.453977    -2.557064    -3.076085
C      -3.044203    -3.465284    -1.999984
C      -2.682866    -4.869453    -2.576088
C      -3.907178    -5.397252    -3.152415
N      -4.796926    -6.138361    -2.073293
C      -1.843564    -3.082930    -1.130748
C      -1.794988    -3.586183     0.044103
N      -0.787570    -2.439260    -1.638354
C      -0.472912    -2.416936    -0.862702
C      1.130507    -3.825914    -0.829766
C      1.866242    -4.214746    -2.119655
S      2.760081     5.811829    -1.928581
O      3.748347    -5.421153    -0.423580
C      1.476563    -1.437496    -1.473635
N      1.350323    -0.983414    -2.636163
N      2.537226    -1.210251    -0.675535
C      3.727388    -0.502896    -1.149024
space group P2_12_12_1(protomer A), model 1, product (with a H-bond of OH with imidazole of H41) (heteroatoms frozen, free hydrogens)

Zero-point correction= 2.498386 (Hartree/Particle)
Thermal correction to Energy= 2.607728
Thermal correction to Enthalpy= 2.608673
Thermal correction to Gibbs Free Energy= 2.355947
Sum of electronic and zero-point Energies= -7728.589550
Sum of electronic and thermal Energies= -7728.480207
Sum of electronic and thermal Enthalpies= -7728.479263
Sum of electronic and thermal Free Energies= -7728.731988

SOLVENT: -7773.4774294

| H  | 9.312371  | -2.069930  | -0.140490 |
| H  | 10.33517  | -2.640169  | -1.597770 |
| H  | 2.688035  | -1.939732  | -4.544232 |
| H  | 5.780134  | 2.366100   | 6.915489  |
| H  | 1.938497  | 0.716351   | 8.614938  |
| H  | 3.224526  | 2.916961   | 3.032311  |
| H  | -3.375927 | -1.014315  | 4.621502  |
| H  | -4.146798 | 1.877235   | 6.915489  |
| H  | -2.590086 | 2.780105   | 8.614938  |
| H  | -0.305099 | 0.004586   | 0.142206  |
| H  | -1.314352 | 1.380532   | 1.683515  |
| H  | 0.874674  | -0.323239  | 3.432452  |
| H  | 2.175544  | 3.175423   | 4.324522  |
| H  | -1.678961 | 1.663207   | 2.347556  |
| H  | 2.008567  | 3.103977   | 3.860392  |
| H  | -1.46813  | -0.150205  | 3.192506  |
| H  | -0.553396 | 0.004586   | 0.142206  |
| H  | 0.874674  | -0.323239  | 3.432452  |

SOLVENT: -7773.4774294

| H  | 3.276623  | -5.018703  | 5.497654  |
| H  | 0.988410  | 0.527996   | 3.432452  |
| H  | -0.053396 | 1.825194   | 8.837672  |
| H  | 0.433272  | 0.019457   | 7.284042  |
| H  | -1.055564 | -0.771045  | 5.495213  |
| H  | -1.546813 | -0.150205  | 3.192506  |
| H  | 0.938497  | 0.716351   | 8.614938  |
| H  | 3.224526  | 2.916961   | 3.032311  |
| H  | -3.375927 | -1.014315  | 4.621502  |
| H  | -4.146798 | 1.877235   | 6.915489  |
| H  | -2.590086 | 2.780105   | 8.614938  |
| H  | -0.305099 | 0.004586   | 0.142206  |
| H  | -1.314352 | 1.380532   | 1.683515  |
| H  | 0.874674  | -0.323239  | 3.432452  |
| H  | 2.175544  | 3.175423   | 4.324522  |
| H  | -1.678961 | 1.663207   | 2.347556  |
| H  | 2.008567  | 3.103977   | 3.860392  |
| H  | -1.46813  | -0.150205  | 3.192506  |
| H  | -0.553396 | 0.004586   | 0.142206  |
| H  | 0.874674  | -0.323239  | 3.432452  |

SOLVENT: -7773.4774294

Zero-point correction= 2.498386 (Hartree/Particle)
Thermal correction to Energy= 2.607728
Thermal correction to Enthalpy= 2.608673
Thermal correction to Gibbs Free Energy= 2.355947
Sum of electronic and zero-point Energies= -7728.589550
Sum of electronic and thermal Energies= -7728.480207
Sum of electronic and thermal Enthalpies= -7728.479263
Sum of electronic and thermal Free Energies= -7728.731988

SOLVENT: -7773.4774294

| N  | 5.859556  | 9.749443  | -0.716943 |
| C  | 5.409207  | 9.522712  | 0.684422  |
| C  | 4.023018  | 8.460689  | 0.726520  |
| C  | 4.008143  | 7.666690  | 0.471034  |
| N  | 3.540913  | 6.380533  | -0.708368 |
| C  | 3.601617  | 5.154159  | -0.654951 |
| C  | 4.101869  | 5.165900  | 0.596770  |
| C  | 4.377045  | 6.306842  | 1.227478  |
| C  | 6.486778  | 8.796943  | 1.530461  |
| C  | 6.261114  | 8.543193  | 2.747040  |
| C  | 2.249655  | -8.254911  | -3.236181 |
| N  | -0.082193 | -7.398560  | -2.284518 |
| C  | 0.773005  | -6.304130  | -1.751540 |
| C  | 0.415217  | -4.968457  | -2.400764 |
| C  | 0.779833  | -4.819946  | -3.855045 |
| C  | 2.080592  | -4.597024  | -4.237470 |
| Atoms | Coordinates |
|-------|-------------|
| C     | 2.423864, -4.482112, -5.574061 |
| C     | 1.449841, -4.522933, -6.531560 |
| C     | -0.180667, -4.896597, -4.835652 |
| C     | 0.149435, -4.759816, -6.170393 |
| C     | 0.543296, -6.236078, -0.242725 |
| O     | -0.635465, -6.091065, 0.165754 |
| N     | 1.615216, -6.389482, 0.529534 |
| C     | 1.581834, -6.390922, 2.341855 |
| O     | 1.637413, -6.238111, 2.002457 |
| C     | 2.308101, -7.484058, 2.567732 |
| C     | 1.581834, -8.810729, 2.341855 |
| C     | 0.264742, -8.873706, 3.120565 |
| C     | 2.427403, -4.980350, 2.382513 |
| O     | 2.923610, -4.280683, 1.493499 |
| N     | 2.530611, -4.693654, 3.677538 |
| C     | 3.599258, -3.643539, 2.436444 |
| C     | 3.406036, -3.684173, 5.767799 |
| C     | 2.116661, -3.169905, 6.373548 |
| O     | 1.305035, -2.532219, 5.705060 |
| N     | 1.914688, -3.457820, 7.647174 |
| C     | 4.810496, -3.803702, 3.644489 |
| O     | 5.368780, -4.919825, 3.698695 |
| N     | 5.344260, -3.741692, 3.045922 |
| C     | 6.736007, -2.737948, 2.560655 |
| C     | 6.834451, -2.855235, 1.049691 |
| O     | 7.397876, -2.742942, 0.545252 |
| N     | 7.170418, -2.305957, 0.357553 |
| C     | 5.655374, -3.559520, -1.091390 |
| O     | 5.481612, -2.554240, -1.403349 |
| N     | 5.362021, -1.664413, -0.999953 |
| C     | 5.657239, -2.082268, -1.941832 |
| C     | 5.941093, -2.188957, -3.142154 |
| C     | 5.381155, -0.910560, -1.356496 |
| C     | 5.373420, -0.405217, -2.046558 |
| C     | 5.079812, 1.564532, -1.104695 |
| S     | 3.333437, 1.613691, -0.600457 |
| C     | 6.697312, 0.608688, -2.761181 |
| O     | 7.074587, 0.537201, -2.169823 |
| N     | 6.661419, 1.073675, -4.016019 |
| C     | 7.693431, 0.370733, -8.475631 |
| O     | 8.144873, -0.094614, -4.783228 |
| N     | 5.090808, -0.097263, -6.054909 |
| C     | 0.191594, 1.134930, -4.071922 |
| C     | 0.642025, -1.477440, -3.083533 |
| C     | 1.918354, -1.366961, -3.505742 |
| C     | 2.741257, 1.855832, -5.092024 |
| O     | 3.823492, 2.086344, -4.540971 |
| N     | 1.571922, 2.435395, -4.747250 |
| C     | 1.432631, 3.483100, -3.658158 |
| C     | 1.100023, 4.080778, -2.227400 |
| O     | 2.166480, 5.491213, -5.028679 |
| N     | 2.691004, 6.705496, -4.624166 |
| C     | 0.450927, 2.981599, -2.567149 |
| C     | 0.748134, 3.270236, -1.398216 |
| O     | 0.640855, 2.265758, -2.857466 |
| N     | 1.686683, 2.101324, -1.810258 |
| C     | 2.457729, 3.417357, -1.643644 |
| C     | 3.173979, 3.381605, -2.894145 |
| S     | 1.717374, 5.533231, -2.721303 |
| C     | 4.805048, 5.327428, -1.164854 |
| O     | 2.673211, 0.948767, -2.041648 |
| C     | 0.239016, 0.465387, -3.161499 |
| C     | 3.276453, 0.515141, -0.941570 |
| C     | 4.450179, -0.386481, -0.886544 |
| C     | 4.208699, -1.489865, 0.137311 |
| C     | 5.315181, -2.672652, -0.127464 |
| C     | 4.818796, -3.968884, 0.586177 |
| O     | 5.693187, -4.332459, 1.409372 |
| C     | 3.743726, -4.683504, 0.277790 |
| C     | 5.740811, 0.402785, -0.553903 |
| O     | 5.702797, 1.318900, 0.275944 |
| N     | 6.843422, 0.035132, -1.195976 |
| C     | 8.187370, 0.664721, -1.108766 |
| O     | 8.650249, 1.023069, -2.527348 |
| C     | 7.891963, 2.167115, -3.201249 |
| C     | 8.334360, 3.517586, -2.671746 |
| C     | 9.133998, 0.319388, -0.415296 |
| C     | -8.877564, 1.529299, -0.367890 |
| N     | -10.263859, 0.140777, 0.169197 |
|   | C    | O     | N     | C     | H     | C     | O     | N     |
|---|------|-------|-------|------|-------|------|-------|-------|
| 1 | -10.986656 | -6.71947 | 1.14753 | -12.161781 | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 |
| 2 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
| 3 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
| 4 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
| 5 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
| 6 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
| 7 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
| 8 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
| 9 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
|10 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
|11 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
|12 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |
|13 | -3.421062  | -2.462611 | -5.440455 | -3.462853 | -3.547323 | -4.421701 | -5.350934 | -5.209347 | -6.328272 |

S164
| H | 2.067281 | -5.310571 | 4.349358 |
| H | 2.974407 | -2.675306 | 3.950794 |
| H | 3.66489 | -6.934414 | 6.109047 |
| H | 4.209793 | -3.010371 | 8.095617 |
| H | 2.573140 | -3.982630 | 8.211049 |
| H | 6.929341 | -3.855496 | -1.355487 |
| H | 4.468993 | -2.488638 | 2.359871 |
| H | 3.567063 | 1.134920 | -6.91118 |
| H | 1.797984 | -6.816447 | 5.296771 |
| H | 2.861781 | -1.255447 | -6.637900 |
| H | -1.258125 | -1.075408 | -3.899092 |
| H | 2.754396 | -2.880733 | 2.101553 |
| H | 0.737546 | 2.089548 | -5.214622 |
| H | 2.410361 | 3.448189 | -3.167767 |
| H | 0.168862 | 4.704679 | -4.803162 |
| H | 0.845050 | 5.453971 | -3.369794 |
| H | 1.792326 | 5.59215 | -6.060041 |
| H | 2.067843 | 7.506945 | -4.627740 |
| H | 3.371602 | 6.707217 | -3.855991 |
| H | -1.179620 | 1.915415 | -0.858560 |
| H | -1.732172 | 4.178097 | -1.339062 |
| H | -3.147290 | 3.282873 | -0.805237 |
| H | -3.933850 | 3.149853 | -3.194442 |
| H | -2.457432 | 3.973027 | -3.717571 |
| H | -5.887250 | 6.176426 | -1.054242 |
| H | -5.400288 | 4.405937 | -1.151731 |
| H | -4.124147 | 5.317655 | -0.307802 |
| H | -3.104974 | 1.021747 | -0.060514 |
| H | -4.156317 | -0.825575 | -1.888067 |
| H | -4.347806 | -1.093263 | 1.151052 |
| H | -3.167944 | -1.810426 | 0.028337 |
| H | -6.178061 | -2.437794 | 0.151111 |
| H | -5.066165 | -2.887120 | -1.206620 |
| H | -6.833201 | -0.818098 | -1.750357 |
| H | -8.052282 | 1.554493 | -0.486331 |
| H | -8.570640 | 0.106391 | -3.127366 |
| H | -9.718271 | 1.275383 | -2.500087 |
| H | -8.068952 | 2.118777 | -4.282650 |
| H | -6.814038 | 2.025280 | -3.047373 |
| H | -7.776756 | 4.334273 | -3.144412 |
| H | -8.166945 | 3.991610 | -1.591313 |
| H | -9.402947 | 3.678303 | -2.860832 |
| H | -10.306236 | -0.929699 | 1.963739 |
| H | -12.249694 | 0.187556 | 2.716078 |
| H | -13.098669 | -0.173030 | 1.205794 |
| H | -12.771272 | 2.133837 | 0.793339 |
| H | -11.394951 | 2.195643 | 1.897355 |
| H | -10.134009 | 2.253007 | -0.052191 |
| H | -11.402051 | 1.472994 | -1.014740 |
| H | -2.472334 | -2.484433 | -5.993113 |
| H | -4.239910 | -2.596993 | -6.152736 |
| H | -4.155299 | -6.579875 | -3.537866 |
| H | -2.724715 | -2.783052 | -2.473338 |
| H | -3.328487 | -5.016541 | -1.627199 |
| H | 4.699414 | 2.432264 | 3.331874 |
| H | 7.342929 | 0.214389 | 4.648941 |
| H | 7.155437 | -1.016991 | 6.794562 |
| H | 5.000554 | -1.100990 | 8.025002 |
| H | 2.987707 | 0.017735 | 7.053366 |
| H | 3.171122 | 1.239277 | 4.913032 |
| H | 1.628517 | 0.753731 | 2.653875 |
| H | 1.091297 | 0.051482 | -0.304221 |
space group P2_12_12 (protomer A), model 1, product (heteroatoms frozen, free hydrogens)

Zero-point correction=                           2.500377 (Hartree/Particle)
Thermal correction to Energy=                    2.609355
Thermal correction to Enthalpy=                  2.610299
Thermal correction to Gibbs Free Energy=         2.359451
Sum of electronic and zero-point Energies=          -7728.592471
Sum of electronic and thermal Energies=             -7728.483493
Sum of electronic and thermal Enthalpies=           -7728.482549
Sum of electronic and thermal Free Energies=        -7728.733998

SOLVENT: -7773.4788064
space group P2₁2₁2₁ (protomer A), model 3, Mpro

Zero-point correction= 0.909142 (Hartree/Particle)
Theoretical correction to Energy= 0.965010
Theoretical correction to Enthalpy= 0.965954
Theoretical correction to Gibbs Free Energy= 0.818493

Sum of electronic and zero-point Energies= -2988.278849
Sum of electronic and thermal Energies= -2988.222981
Sum of electronic and thermal Enthalpies= -2988.222037
Sum of electronic and thermal Free Energies= -2988.369498

SOLVENT: -3005.433981

RX2Asimpl22REACTANT0 SCF Done: -2989.18799073 A.U.

H     -1.076246     5.227346     3.969666
H     -3.851833     5.474138     5.437802
H     -4.865532     3.815101     5.002183
H     -9.217357     0.720746     5.010104
H     -9.305682     -0.042229     5.013840
H     -8.099199     -1.981750     2.436401
H     -8.133838     -2.125060     4.064255
H     -6.602579     -1.978750     3.165401
H     -6.327107     -0.566312     5.829696
H     -5.479748     -0.708902     4.917101
H     -6.903838     -1.115095     5.902504
H     -8.473849     1.529543     4.803999
H     -9.217357     0.720746     5.437802
H     -9.305682     -0.042229     5.437802
H     -8.099199     -1.981750     3.969666
H     -8.133838     -2.125060     5.437802
H     -6.602579     -1.978750     3.969666
H     -6.327107     -0.566312     5.437802
H     -5.479748     -0.708902     5.437802
H     -6.903838     -1.115095     5.437802
H     -8.473849     1.529543     5.437802
H     -9.217357     0.720746     5.437802
H     -9.305682     -0.042229     5.437802
H     -8.099199     -1.981750     5.437802
H     -8.133838     -2.125060     5.437802
H     -6.602579     -1.978750     5.437802
H     -6.327107     -0.566312     5.437802
H     -5.479748     -0.708902     5.437802
H     -6.903838     -1.115095     5.437802
H     -8.473849     1.529543     5.437802
H     -9.217357     0.720746     5.437802
H     -9.305682     -0.042229     5.437802
H     -8.099199     -1.981750     5.437802
H     -8.133838     -2.125060     5.437802
H     -6.602579     -1.978750     5.437802
H     -6.327107     -0.566312     5.437802
H     -5.479748     -0.708902     5.437802
H     -6.903838     -1.115095     5.437802
H     -8.473849     1.529543     5.437802
H     -9.217357     0.720746     5.437802
H     -9.305682     -0.042229     5.437802
H     -8.099199     -1.981750     5.437802
H     -8.133838     -2.125060     5.437802
H     -6.602579     -1.978750     5.437802
H     -6.327107     -0.566312     5.437802
H     -5.479748     -0.708902     5.437802
H     -6.903838     -1.115095     5.437802
H     -8.473849     1.529543     5.437802
H     -9.217357     0.720746     5.437802
H     -9.305682     -0.042229     5.437802
| Atom | x      | y      | z      |
|------|--------|--------|--------|
| C    | 0.2529 | 1.8309 | -2.2497 |
| C    | 0.6651 | 0.7398 | -1.2505 |
| C    | 2.7021 | 2.9424 |  1.0055 |
| O    | 3.3462 | 2.8513 | -2.0769 |
| N    | 3.1351 | 3.5655 |  0.1079 |
| C    | 4.4640 | 4.1820 |  0.1456 |
| H    | 5.5345 |-0.9321 | -4.0402 |
| H    | 4.9196 |-3.3068 | -3.7303 |
| H    | 3.4719 |-2.3622 | -4.1835 |
| H    | 3.6485 |-4.0682 |  0.9057 |
| H    | 1.3567 |-2.5168 | -2.9127 |
| H    | 1.3120 |-3.4260 | -1.3552 |
| H    | 5.6442 | 3.5339 |
| H    | 2.9689 | 2.4917 |
| H    | 0.7471 |-1.0941 |  3.3089 |
| H    | 1.2272 |-0.9349 |  0.3025 |
| H    | 0.5889 | 0.2931 |  1.4403 |
| H    | 2.2215 | 1.2679 |
| H    | 4.5269 | 3.4799 |
| H    | 6.3166 | 1.8734 |
| H    | 3.5188 |-0.9613 | -0.2595 |
| H    | 5.7634 |-0.0128 | -0.0627 |
| H    | -1.3976 | 1.7354 |
| H    | -2.3723 | 0.6943 |
| H    | -4.1154 | 2.8112 |
| H    | -6.4677 | 1.6062 |
| H    | -4.3530 | 3.8101 |
| H    | -2.6709 | 3.8638 |
| H    | -2.9021 | 3.1517 |
| H    | -3.7751 | 1.7025 |
| H    | -2.0676 | 1.9379 |
| H    | -4.2582 | -0.7245 |
| H    | -3.5591 | -2.3255 |
| H    | -6.4098 | -1.3735 |
| H    | -5.9485 | 3.0053 |
| H    | -6.2798 | -4.0651 |
| H    | -6.6563 | -4.3601 |
| H    | -3.0197 | 1.8555 |
| H    | -5.0625 | -0.3153 |
| H    | -4.1086 | -1.6146 |
| H    | -2.4743 | 0.4549 |
| H    | -1.3436 | 0.2033 |
| H    | -0.6731 | 3.7014 |
| H    | -2.4224 | 3.3455 |
| H    | -1.5987 | 1.7387 |
| H    | -0.6125 | -0.3640 |
| H    | 1.5798 | 0.9280 |
| H    | 0.6016 | -2.8185 |
| H    | 1.6152 | 2.1580 |
| H    | 2.5850 | 4.3593 |
| H    | 4.3985 | 0.4867 |
| H    | 5.1191 | 0.8130 |
| H    | 4.8652 | -0.8694 |
| H    | -0.5601 | -3.3904 |
| H    | 4.7356 | 2.3688 |
| H    | 6.8952 | -2.3298 |
| H    | 1.0049 | 2.3808 |

**Space group P2₁2₁2₁ (Protomer A), model 3, reactant complex**

Zero-point correction= 1.603132 (Hartree/Particle)
Thermal correction to Energy= 1.699184
Thermal correction to Enthalpy= 1.700128
Thermal correction to Gibbs Free Energy= 1.469375
Sum of electronic and zero-point Energies= -4982.004981
Sum of electronic and thermal Energies= -4981.908929
Sum of electronic and thermal Enthalpies= -4981.907985
Sum of electronic and thermal Free Energies= -4982.138739

SOLVENT: -5010.8574576
| Atom | X    | Y    | Z     |
|------|------|------|-------|
| C    | -4.695898 | -1.279881 | -2.475991 |
| C    | -4.877143 | -2.761750 | -2.739268 |
| C    | -5.020502 | -3.635467 | -1.649755 |
| C    | -5.065122 | -5.016836 | -1.838885 |
| C    | -4.967653 | -5.549914 | -3.128745 |
| C    | -4.767798 | -3.306279 | -4.027047 |
| C    | -4.819822 | -4.690465 | -4.221543 |
| O    | -5.311673 | 1.802084 | -1.857537 |
| O    | -4.952600 | 1.652867 | -2.489977 |
| N    | -5.112590 | 0.527143 | 0.063146 |
| C    | -4.354800 | 1.500789 | 0.837320 |
| C    | -5.222349 | 2.155060 | 1.944740 |
| C    | -6.392698 | 2.969201 | 1.353490 |
| C    | -5.906462 | 4.109933 | 0.414765 |
| O    | -1.375902 | 0.261460 | -1.789321 |
| C    | -0.370906 | 4.341358 | 1.795581 |
| N    | -0.749965 | -1.969339 | 0.949338 |
| C    | -3.309603 | -4.341358 | 1.376851 |
| O    | -4.049621 | -5.343258 | 1.189953 |
| N    | -2.241049 | -0.039976 | 0.611091 |
| C    | -1.764900 | -5.060023 | -0.353114 |
| O    | -0.933299 | -4.849438 | -1.512349 |
| O    | -1.436589 | -2.830881 | -2.131357 |
| N    | -1.491587 | -5.790485 | 0.571347 |
| O    | 0.269531 | -1.618959 | -1.789321 |
| N    | -1.647408 | -6.513847 | 0.315382 |
| C    | -1.706248 | -7.341796 | 2.581423 |
| O    | -0.035588 | -2.128666 | 0.774278 |
| N    | 1.120494 | -2.381552 | 0.297252 |
| C    | -1.719250 | -3.563393 | 0.410339 |
| C    | 3.120616 | -3.944089 | 0.087309 |
| C    | 4.110585 | -3.471163 | 1.149220 |
| C    | 5.249782 | -4.237306 | 1.425041 |
| C    | 6.238840 | -3.748346 | 2.279182 |
| C    | 7.216263 | -2.473681 | 2.844899 |
| C    | 8.498337 | -1.703070 | 2.563921 |
| C    | 9.382412 | -2.213964 | 1.741512 |
| C    | 10.778035 | -1.275200 | -0.521864 |
| C    | 11.260667 | -1.516528 | -1.389932 |
| C    | 12.225230 | 0.125659 | -0.286905 |
| C    | -0.099471 | 0.215291 | -1.120724 |
| C    | -0.497139 | -1.599303 | -1.647330 |
| C    | -0.732972 | 2.712795 | -0.615454 |
| C    | -1.928826 | 3.524199 | -1.189106 |
| C    | -2.648970 | 2.500855 | -1.969967 |
| C    | -1.901257 | 1.404039 | -2.279074 |
| C    | -2.265387 | 0.392270 | -2.899946 |
| C    | 2.227114 | 1.104934 | -0.698341 |
| C    | 3.332517 | 1.286020 | 0.075837 |
| C    | 3.552932 | 0.635589 | 1.118660 |
| C    | 4.293354 | 2.578034 | -0.446329 |
| C    | 5.778721 | 2.883394 | -0.032475 |
| C    | 6.724880 | 3.129991 | -0.519779 |
| C    | 6.863980 | 3.376447 | -2.019866 |
| C    | 7.984518 | 2.678005 | -1.256517 |
| C    | 8.708773 | 3.696544 | 0.060183 |
| C    | 2.685032 | 4.233744 | -6.353767 |
| C    | 2.203875 | 3.665981 | -1.666379 |
| C    | 4.257233 | 4.281669 | 1.197763 |
| C    | 3.785811 | 5.425197 | 1.675692 |
| C    | 2.651117 | 6.050113 | 1.022136 |
| C    | 2.103786 | 5.446607 | -0.808003 |
| C    | 0.955450 | 5.820614 | -0.750191 |
| C    | -0.055661 | 6.077991 | -0.229997 |
| O    | 0.044189 | 7.225715 | 0.862301 |
O  -1.153026  6.576020  -1.017293
C  -2.386631  7.393331  -0.643573
C  -2.834023  7.102116   0.796751
C  -3.411518  6.890291  -1.664107
C  -2.026859  8.866902  -0.855984
H   8.875434 -3.914707  -1.057085
H   8.731738 -1.498631  -0.396981
H   7.368590 -2.443773   0.265376
H   5.827506  0.592455  -3.873020
H   4.899837 -1.606261  -0.360314
H   3.923817 -0.310779  -2.276698
H   8.419639 -1.978698  -3.219156
H   6.879305 -1.652191  -4.449719
H   -8.395866  0.723640  -4.320809
H   -6.610234  0.690228  -3.432007
H   -6.456197 -1.204328  -1.93120
H   -5.465437  0.742633  -3.359516
H   -3.898848 -1.169969  -1.731916
H   -5.030689 -3.218822  -0.650422
H   -5.123008  5.653878  -0.964396
H   -4.994177  6.232335  -3.280869
H   -6.423466 -2.643194  -4.874005
H   -7.300072 -5.096202  -5.223226
H   -5.265359 -0.405193  -0.488485
H   -0.018102  2.271473  0.142258
H   -5.598121  1.361916  2.602836
H   -4.599395  2.825962  2.546108
H   -6.966560  3.392267  2.187032
H   -7.056408  2.296308  0.799393
H   -6.721591  4.801533  0.203817
H   -5.080948  4.660603  0.874619
H   -5.576314  3.669212  -0.534066
H   -2.828265  2.720169  2.159952
H   -0.339117  1.227580  1.788009
H   -1.035953  2.745050  4.326067
H   0.564812  2.639915  3.571763
H   0.024823  5.854388  2.117403
H   1.098294  4.758205  2.949341
H   -0.293796  0.988562  2.118528
H   -0.387354  1.804505  4.973248
H   0.663642  2.370512  3.740739
H   -2.404046  1.632014  2.490894
H   -3.775564 -0.095671  3.411028
H   -5.693352  3.296930  2.008851
H   -5.019177  1.873682  3.061808
H   -3.844408 -1.508854  0.866578
H   -1.609864 -3.253545  0.803740
H   -2.645593 -5.580020  -0.726511
H   0.102370 -4.382691  -1.190929
H   -0.942024 -5.214488  -2.330772
H   -2.669598  6.750959  -1.237993
H   -1.100145 -6.545211  3.334194
H   -1.661686 -8.202364  2.908915
H   -0.041988 -7.635178  2.398581
H   3.418929  3.543893  -0.888057
H   5.375299  5.196983  0.940213
H   7.131356 -4.353871  2.490844
H   6.898681  2.086404  3.487437
H   4.885415  0.692760  2.937743
H   3.137727 -1.377031  1.530371
H   1.014893  0.245509  0.778604
H   -0.014947  0.436801  1.993841
H   -0.887757 -0.196021  -0.498043
H   0.190370  1.954005  -2.426298
H   -0.144024  3.279495  -0.483333
H   -1.064869  2.267054  0.316926
H   -1.577380  4.357402  1.813280
H   -2.542079  3.925467  -0.378792
H   -3.665351  2.492417  -2.133253
H   -2.022334  1.814949  -1.407611
H   2.210560  2.437493  1.531515
H   5.785514  1.930450  1.050860
H   5.978281  1.112645  -0.468534
H   6.828858  4.012850  0.102814
H   7.016642  4.395257  -2.355294
H   6.275186  2.752277  -2.681782
H   8.901144  3.228366  -1.08099
H   8.091771  1.616980  -1.454137
H   5.909898  3.770275  1.675682
H   4.192370  5.911989  2.552157
|   | H  | 2.197227 | 6.950948 | 1.403527 |
|---|----|----------|----------|----------|
|   | H  | -2.557922 | -3.233993 | -2.769233 |
|   | H  | -1.222881 | 9.146649 | -0.170636 |
|   | H  | -1.704586 | 9.486470 | -0.651372 |
|   | H  | -3.011302 | 6.992846 | -2.676387 |
|   | H  | -4.329262 | 7.479195 | -1.575401 |
|   | H  | -3.644775 | 5.839011 | -1.476558 |
|   | H  | -2.223442 | 7.657429 | 1.508397 |
|   | H  | -2.735693 | 6.039808 | 1.030543 |
|   | H  | -3.882370 | 7.401426 | 0.899775 |
|   | H  | 3.119465 | -5.034572 | 0.030395 |
|   | H  | 7.168380 | -4.636908 | -2.895040 |
|   | H  | 9.862990 | -2.660995 | -2.717629 |
|   | H  | 0.759732 | 5.299961 | -1.611145 |
|   | H  | 1.134055 | -4.361865 | 0.756521 |
|   | H  | -7.980825 | -1.941879 | -3.098732 |

### space group P2_1212_1 (protomer A), model 3, product (heteroatoms frozen, free hydrogens)

|   | RX2Asimpli22F SCF Done: -4983.23745115 A.U. |
|---|-----------------------------------------------|
|   | N  | 9.455607 | -5.394931 | -1.630718 |
|   | C  | 9.480170 | -4.431672 | -0.496759 |
|   | C  | 8.862685 | -3.072438 | -0.899373 |
|   | C  | 7.368106 | -3.072438 | -0.899373 |
|   | N  | 6.667531 | -2.976887 | -2.113255 |
|   | O  | 5.369809 | -2.886230 | -1.856007 |
|   | N  | 5.202946 | -2.876511 | -0.553308 |
|   | C  | 6.436488 | -2.966995 | 0.048925 |
|   | C  | 8.869217 | -5.032265 | 0.793233 |
|   | C  | 8.827066 | -4.346544 | 1.847610 |
|   | C  | 8.513199 | 0.546237 | -3.579024 |
|   | N  | 7.499829 | 1.128913 | -2.958843 |
|   | C  | 6.362247 | 0.436970 | -2.296479 |
|   | N  | 5.141352 | 0.399149 | -3.213609 |
|   | C  | 5.248559 | -0.504020 | -4.418500 |
|   | C  | 5.137512 | -1.867838 | -4.294388 |
|   | C  | 5.257909 | -2.697871 | -5.395923 |
|   | C  | 5.425388 | -2.158332 | -6.639584 |
|   | C  | 5.454218 | 0.018737 | -5.673294 |
|   | C  | 5.552344 | -0.801479 | -6.789918 |
|   | O  | 6.036808 | 1.210705 | -1.02006 |
|   | C  | 5.785518 | 2.436793 | -1.124573 |
|   | N  | 6.096692 | 0.528830 | 0.120333 |
|   | N  | 5.703772 | 1.049873 | 1.449987 |
|   | C  | 6.866934 | 0.763256 | 2.399240 |
|   | C  | 8.180901 | 1.474155 | 2.097830 |
|   | C  | 8.065371 | 2.981702 | 2.306188 |
|   | C  | 4.428317 | 0.344658 | 1.926222 |
|   | O  | 3.903432 | -0.515057 | 1.210320 |
|   | N  | 3.933750 | 0.727571 | 3.099393 |
|   | C  | 2.836476 | 0.019647 | 3.805388 |
|   | C  | 2.622634 | 0.594196 | 5.208733 |
|   | C  | 1.970880 | 1.961213 | 5.189418 |
|   | O  | 1.425459 | 2.396064 | 4.176661 |
|   | N  | 2.036257 | 2.654801 | 6.312120 |
|   | C  | 3.141235 | -1.488506 | 3.834515 |
|   | O  | 4.250534 | -1.875765 | 4.256153 |
|   | C  | 2.212332 | -2.307426 | 3.347058 |
|   | C  | 2.370995 | -3.772906 | 3.443111 |
|   | O  | 2.076888 | -4.421792 | 2.120944 |
|   | O  | 2.719321 | -5.676917 | 2.088703 |
|   | C  | 2.908064 | -3.220399 | 1.080563 |
|   | C  | 3.516648 | -0.923463 | -0.216917 |
|   | C  | 4.413024 | -3.044579 | -0.829674 |
|   | O  | 3.721575 | -1.823778 | -1.017811 |
|   | C  | 2.401182 | -4.338501 | -1.169259 |
|   | O  | 2.715342 | -5.242162 | -1.238222 |
|   | N  | 1.139780 | -4.175620 | -0.906771 |
|   | C  | 0.042633 | -4.554411 | -1.722771 |
|   | C  | 1.351677 | -0.393968 | -1.140481 |
|   | S  | 1.543968 | -2.245589 | -1.364214 |
|   | C  | 0.078993 | -0.625984 | -1.889735 |
|   | O  | -0.223578 | -6.732556 | -0.908756 |
|   | N  | 0.330333 | -6.547102 | -3.112365 |
|   | C  | 0.278665 | -7.978442 | -3.454247 |
|   | O  | -0.343811 | -2.341888 | 0.578095 |
H  -4.725979    -3.431967    -1.803588
H  -5.313075    -2.942842    -0.196452
H  -3.847854    -1.214525    -0.234489
H  -0.970595    -3.487354    -0.181368
H  -0.074599    -4.100352    -2.721245
H   1.434378    -4.350517    -0.092308
H   2.184924    -4.494047    -1.684924
H   0.404871    -5.894651    -3.886663
H  -0.521674    -8.172803    -4.175388
H   1.235814    -8.322555    -3.861251
H   0.058000    -8.505659    -2.522839
H   2.967908    -2.104772     2.664532
H   0.898113    -3.828415     5.168251
H   0.052692    -2.729243     7.221817
H   0.241959    -0.270696     7.520505
H   1.244848    1.110651     5.700216
H   2.093811    0.021228     3.651433
H   1.290925    0.639025     1.059628
H   0.080000    0.090826    -1.742242
H  -0.794486   -0.288409    -0.278249
H   0.208548    2.485539    -1.108984
H  -0.190328   0.3041491    1.127751
H  -0.978882   1.503651    -4.455080
H  -2.299430   4.051224     0.822101
H  -3.027232   2.515799     1.317129
H  -3.690344   2.856123    -1.088692
H   2.453789   0.622197    -1.672063
H   4.100255   2.066001    -1.998336
H   5.316619   0.076868    -1.095857
H   7.441929   2.411269    -1.083248
H   7.305620   2.408040    -3.585055
H   5.585669   1.297711    -3.518998
H   8.691670   0.651808    -2.372835
H   7.338331   -0.457685    -2.316675
H   6.304135   3.166431     0.563230
H   5.662095   5.544664     1.414133
H   4.921805   7.209345     0.270127
H   3.621062   -0.824622     0.394065
H   2.765632   10.678410    -1.00963
H   1.765296   10.919138    -2.454673
H   1.281771   11.673091    -0.911268
H  -0.512565   9.758606    -2.604892
H  -0.978605  10.418488    -1.017642
H  -1.000320   8.655602    -1.302778
H   1.906672   9.109098     0.898248
H   0.467537   8.181105     0.576583
H   0.285198   9.905560     0.972664
H   2.372724   3.679697     3.238448
H   8.546610   -6.082001    -0.709333
H  10.224787  -5.226580    -2.282313
H   2.120433   6.079882    -1.870081
H   0.298636  -3.201102     2.385000
H  -8.915974  -0.310121   -3.005243

space group P2_12_121(protomer A), model 3, product

Zero-point correction=  1.605177 (Hartree/Particle)
Thermal correction to Energy=  1.700650
Thermal correction to Enthalpy=  1.701594
Thermal correction to Gibbs Free Energy=  1.470072
Sum of electronic and zero-point Energies= -4981.988268
Sum of electronic and thermal Energies= -4981.892795
Sum of electronic and thermal Enthalpies= -4981.891851
Sum of electronic and thermal Free Energies= -4982.123373

SOLVENT: -5010.8606759
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -1.639918 | -5.098369 | -5.554090 |
| C       | -4.432449 | -0.570677 | -2.921470 |
| C       | -8.217942 | -1.294670 | -0.543298 |
| C       | -6.212159 | -0.614747 | -0.027342 |
| C       | -7.265556 | -0.392121 | -1.147291 |
| C       | -7.525885 | 0.828773  | -1.705443 |
| C       | -3.887094 | 3.440855  | 2.785594  |
| C       | -4.151654 | 3.489812  | 1.604858  |
| N       | -5.544997 | 4.568516  | 3.461109  |
| C       | -3.708448 | -0.320791 | 3.672970  |
| C       | -4.833045 | -0.348428 | 4.206971  |
| N       | -2.758850 | -1.279217 | 3.819321  |
| C       | -3.085477 | -2.541820 | 4.495923  |
| C       | -3.030367 | -3.778161 | 3.574682  |
| C       | -0.310978 | -4.924715 | 4.042114  |
| N       | -2.915097 | -3.494442 | 2.242404  |
| N       | -3.697580 | -2.431359 | 0.012967  |
| O       | -3.059021 | -3.159502 | -0.751553 |
| C       | -3.847911 | -0.144104 | 0.629519  |
| C       | -2.978482 | -1.045975 | 0.825455  |
| C       | -2.043465 | -3.489812 | 1.604858  |
| O       | -1.477844 | -5.008978 | 0.821459  |
| N       | -1.356098 | -5.959207 | -0.006724 |
| C       | -0.438918 | -4.373971 | 1.384945  |
| C       | 0.945549  | -7.866623 | 1.072048  |
| C       | 1.931798  | -6.666774 | 4.123348  |
|       | 1.630095  | -2.168899 | 0.341813  |
|        | 1.321701  | -6.042602 | 1.904045  |
| C       | 2.157321  | -5.984602 | 2.826413  |
| N       | 0.655437  | -7.156334 | 1.501973  |
| O       | 0.826654  | -8.425709 | 2.228557  |
| N       | -0.422178 | -1.758143 | 2.457084  |
| C       | 0.563866  | -0.980814 | 2.635816  |
| C       | 0.660526  | -0.229158 | 3.754093  |
| N       | 1.599624  | 0.773455  | 4.212238  |
| C       | 1.345161  | 2.151104  | 3.611716  |
| C       | 0.061578  | 2.710156  | 3.640885  |
| C       | -0.190279 | 3.934208  | 3.020075  |
| C       | 0.839442  | 4.614255  | 2.362214  |
| C       | 2.122887  | 4.065273  | 2.349512  |
| C       | 2.377634  | 2.844459  | 2.976613  |
| C       | 1.663063  | -0.837414 | 1.551971  |
| C       | 2.937780  | -0.756711 | 2.244769  |
| C       | 1.293056  | 0.462954  | 0.743338  |
| C       | 0.067036  | 0.283455  | 0.044642  |
| C       | 0.069902  | 1.485574  | -0.729836 |
| C       | -1.383648 | 2.575194  | 0.037292  |
| C       | -2.654695 | 1.844053  | -1.827773 |
| C       | -1.654967 | 0.936043  | -1.724075 |
| N       | -1.563905 | -0.164970 | -2.302525 |
| C       | 2.302159  | 0.801311  | -0.30376 |
| C       | 3.544892  | 1.252240  | -0.059214 |
| C       | 4.134480  | 1.154279  | 1.056591  |
| C       | 4.227313  | 1.989448  | -1.222862 |
| C       | 5.737542  | 1.762589  | -1.220348 |
| C       | 6.426164  | 2.461592  | -2.372372 |
| C       | 6.287657  | 1.830869  | -3.755986 |
| C       | 7.622668  | 1.768112  | -3.015744 |
| C       | 3.811239  | 3.427459  | -1.034367 |
| C       | 2.517627  | 3.740413  | -1.463998 |
| C       | 1.882921  | 2.907072  | -2.125627 |
| C       | 4.600961  | 4.323460  | -0.349168 |
| C       | 4.140637  | 5.573603  | -0.053164 |
| C       | 2.810242  | 5.933761  | -0.393291 |
| C       | 2.010800  | 5.038171  | -1.057784 |
| C       | 0.664371  | 5.220664  | -1.392348 |
| C       | -0.177135 | 6.133019  | -0.808249 |
| C       | 0.143074  | 6.917830  | 0.102928  |
| C       | -1.425247 | 6.027695  | -1.373204 |
| C       | -2.559363 | 6.886183  | -0.858093 |
| C       | -2.855406 | 6.501686  | 0.601167  |
| C       | -3.711670 | 6.495293  | -1.787588 |
| C       | -2.189364 | 8.367525  | -1.015431 |
| H       | 10.276483 | 1.441538  | -1.294992 |
| Atom | X         | Y          | Z         |
|------|-----------|------------|-----------|
| H    | 8.624179  | 0.149558   | -0.402462 |
| H    | 9.028032  | -1.587484  | 5.39804   |
| H    | 4.010611  | -1.890108  | 1.149963  |
| H    | 6.651344  | -1.443663  | 5.380174  |
| H    | 4.226392  | -1.758074  | 1.395804  |
| H    | 7.617354  | -1.891008  | -1.149904 |
| H    | -4.828771 | -2.514861  | -6.615030 |
| H    | -6.591868 | -2.370638  | -6.380074 |
| H    | -5.561036 | -0.559557  | -5.127991 |
| H    | -4.334134 | -2.649070  | -3.470811 |
| H    | -3.070537 | -1.278634  | -5.751273 |
| H    | -2.289121 | -0.819832  | -4.213529 |
| H    | -1.764933 | -2.649070  | -2.209890 |
| H    | -0.868419 | -5.514030  | -4.062919 |
| H    | -0.856620 | -1.944215  | -3.122543 |
| H    | -4.073434 | 0.888057   | -0.23050 |
| H    | -6.088415 | -1.636020  | 0.356573  |
| H    | -5.237171 | 0.024774   | 0.808074  |
| H    | -8.207488 | 1.602152   | -0.376664 |
| H    | -6.954401 | 1.243774   | -1.968125 |
| H    | -8.402036 | 0.827716   | -2.363017 |
| H    | -7.094253 | 1.542270   | -0.891729 |
| H    | -6.64885  | 1.156344   | -2.294917 |
| H    | -4.330875 | 1.707703   | 1.271058  |
| H    | -2.220890 | 0.912301   | 2.619915  |
| H    | -4.971012 | 1.874781   | 3.933995  |
| H    | -3.149590 | 2.278305   | 4.459996  |
| H    | -3.661221 | 4.569576   | 3.000035  |
| H    | -3.222303 | 4.552538   | 4.421247  |
| H    | -1.909667 | -1.301772  | 3.237646  |
| H    | -4.101865 | -2.444823  | 4.888430  |
| H    | -2.405547 | -2.736245  | 5.330008  |
| H    | -2.903240 | -2.354357  | 1.909103  |
| H    | -3.320944 | -5.462224  | 1.751797  |
| H    | -3.705040 | -5.102159  | -0.642939 |
| H    | -4.722157 | -3.970037  | 0.309721  |
| H    | -2.806672 | -2.389034  | -0.134189 |
| H    | -0.751836 | -3.505640  | 1.910693  |
| H    | 0.987621  | -5.040130  | 0.006481  |
| H    | 1.821630  | -3.393599  | 2.474881  |
| H    | 2.952648  | -4.027842  | 1.289531  |
| H    | -0.058058 | -7.055113  | 0.779512  |
| H    | -0.106219 | -8.730124  | 2.716982  |
| H    | 1.148481  | -9.218193  | 1.544484  |
| H    | 1.595666  | -8.261587  | 2.986370  |
| H    | 2.575705  | 0.986312   | 3.924474  |
| H    | -0.745599 | 2.172352   | 4.128560  |
| H    | -1.192517 | 4.341613   | 3.026139  |
| H    | 0.641019  | 5.259373   | 1.834471  |
| H    | 2.917197  | 4.569000   | 1.810920  |
| H    | 3.360246  | 2.399177   | 2.392463  |
| H    | 1.721131  | 1.285557   | 1.458834  |
| H    | 0.020330  | -0.526080  | -0.689834 |
| H    | -0.815398 | -0.062796  | 0.759007  |
| H    | 0.168355  | 1.968632   | -1.305023 |
| H    | -0.751443 | 3.397792   | 0.371923  |
| H    | -1.880834 | 2.134778   | 0.901854  |
| H    | -2.112891 | 3.893365   | -1.564611 |
| H    | -3.914344 | 3.116668   | -0.471674 |
| H    | -3.457994 | 1.607272   | -2.451257 |
| H    | 1.923077  | 1.009393   | -1.228268 |
| H    | 3.800265  | 1.832323   | -2.178892 |
| H    | 6.157821  | 2.023631   | -0.243595 |
| H    | 5.881015  | 0.681812   | -1.326006 |
| H    | 6.450875  | 3.546210   | -2.340499 |
| H    | 6.207592  | 2.488078   | -4.613342 |
| H    | 5.722818  | 0.908834   | -3.823104 |
| H    | 8.435641  | 2.388021   | -3.379420 |
| H    | 7.908931  | 0.801704   | -2.617813 |
| H    | 5.581048  | 3.977610   | -0.655111 |
| H    | 4.779503  | 6.271292   | 0.469280  |
| H    | 2.396043  | 6.880509   | -0.084014 |
| H    | 3.474822  | 0.053817   | 1.865654  |
| H    | -1.340000 | 8.613122   | -0.373421 |
| H    | -1.942415 | 8.568442   | -2.058174 |
| H    | -3.054282 | 8.981851   | -7.461833 |
| H    | -3.343015 | 6.697484   | -2.825623 |
space group $P_2_1_2_1$ (protomer A), model 3, product (H-bond with the free N of the imidazole of H41)

Zero-point correction= 1.606055 (Hartree/Particle)
Thermal correction to Energy= 1.701342
Thermal correction to Enthalpy= 1.702286
Thermal correction to Gibbs Free Energy= 1.472109
Sum of electronic and zero-point Energies= -4981.993590
Sum of electronic and thermal Energies= -4981.898304
Sum of electronic and thermal Enthalpies= -4981.897360
Sum of electronic and thermal Free Energies= -4982.127536

SOLVENT: -5010.866130

RX2Asimpli22noRX SCF Done: -4983.59964578 A.U.
|   |   |   |   |
|---|---|---|---|
| C  | 2.284723 | 1.098268 | 3.974168 |
| C  | 1.592159 | 1.650081 | 5.063571 |
| C  | 1.707493 | 3.006391 | 5.397377 |
| C  | 2.531853 | 3.830685 | 4.596660 |
| C  | 3.227216 | 3.285812 | 3.512070 |
| C  | 3.101478 | 1.929033 | 3.197377 |
| O  | 1.027871 | -1.711606 | 1.087021 |
| C  | 2.146589 | -2.369388 | 1.644325 |
| C  | 1.340516 | -0.359229 | 0.316456 |
| C  | 0.143424 | 0.038374 | -0.555601 |
| C  | 0.252106 | 1.347618 | -1.346289 |
| N  | -0.045231 | 2.639600 | -0.570734 |
| C  | -1.488123 | 2.493352 | -2.447461 |
| O  | -0.884113 | 1.282899 | -2.390651 |
| N  | -1.182578 | 0.247217 | -3.014978 |
| C  | 2.559943 | -0.422483 | -0.513628 |
| O  | 3.791913 | -0.253493 | 1.215014 |
| O  | 4.869145 | -2.23122 | -1.004014 |
| N  | 3.687697 | 4.463913 | -1.561428 |
| C  | 2.017554 | 5.946369 | -1.116722 |
| O  | 2.269333 | 1.72022 | -0.036697 |
| O  | 1.063356 | 5.971545 | -2.01041 |
| C  | 0.334486 | 7.297775 | -1.843692 |
| C  | -0.316195 | 7.249900 | -0.460234 |
| C  | -0.715199 | 7.203958 | -2.954387 |
| C  | 1.365138 | 8.401926 | -2.103394 |
| C  | 8.155299 | 5.863871 | -2.276454 |
| H  | 6.301130 | 4.838828 | -3.440043 |
| H  | 7.157111 | 3.555245 | -2.565456 |
| H  | 1.995138 | 3.527029 | -1.753527 |
| H  | 5.647662 | 3.516813 | 0.344275 |
| H  | 3.853832 | 4.301738 | -3.384893 |
| H  | 5.718289 | -6.456888 | -0.713464 |
| H  | -6.088889 | -1.227958 | 5.749026 |
| H  | -7.537228 | -0.182691 | 5.673343 |
| H  | -5.853736 | 1.139402 | 4.846801 |
| H  | -5.488600 | -0.823405 | -2.680443 |
| H  | -3.837138 | -0.578598 | -5.189996 |
| H  | -2.868771 | -0.547078 | -3.719842 |
| H  | -3.962394 | -2.402574 | -1.860401 |
| H  | -4.113951 | -4.810695 | -1.632889 |
| H  | -4.151548 | -6.280079 | -3.677702 |
| H  | -3.921666 | -2.764502 | -6.146650 |
| H  | -4.054859 | -5.227846 | -5.927659 |
| H  | -4.776012 | 0.087744 | -0.914736 |
| H  | -3.601043 | 2.841378 | -0.996638 |
| H  | -5.885850 | 1.88256 | 0.826913 |
| H  | -5.122758 | 3.497622 | 0.888182 |
| H  | -7.305992 | 3.553144 | 0.316222 |
| H  | -6.712420 | 2.363083 | -1.483666 |
| H  | -6.611727 | 4.785054 | -2.324904 |
| H  | -5.379784 | 5.114717 | -1.083397 |
| H  | -5.067251 | 3.922996 | -2.392076 |
| H  | -2.670964 | 3.314993 | 1.224756 |
| H  | -1.021346 | 1.459101 | 2.256635 |
| H  | -1.911329 | 3.989687 | 3.686215 |
| H  | -0.315447 | 3.211570 | 3.814121 |
| H  | 1.081164 | 5.336879 | 1.318996 |
| H  | 1.300430 | 4.287466 | 2.692803 |
| H  | -1.924996 | -0.329226 | 3.253640 |
| H  | -4.096438 | 0.194212 | 5.212617 |
| H  | -2.821305 | -0.945211 | 5.678981 |
| H  | -3.564427 | -0.869696 | 2.268477 |
| H  | -5.407368 | -3.163856 | 2.644036 |
| H  | -6.057147 | -2.796587 | 0.297088 |
| H  | -6.183911 | 1.240360 | 1.215484 |
| H  | -3.313136 | -0.923777 | 0.254379 |
### Table

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| H    | -2.082561| -2.860195| 1.985037 |
| H    | -1.953322| -4.990850| 0.046042 |
| H    | 0.195168 | -4.017269| 2.043481 |
| H    | 0.484026 | -5.087831| 0.694030 |
| H    | -3.618689| -6.219980| 1.316974 |
| H    | -3.935090| -7.673019| 3.400603 |
| H    | -3.423836| -8.709634| 2.041112 |
| H    | -2.211582| -8.098267| 3.203841 |
| H    | 2.760299 | -0.675307| 2.801600 |
| H    | 0.970335 | 1.014437 | 5.687576 |
| H    | 3.870223 | 3.911096 | 2.904917 |
| H    | 3.655911 | 1.499468 | 2.373379 |

### Space group

- Space group: P2₁2₁2₁ (protomer A), model 3, product (H-bond with the free N of the imidazole of H41; heteroatoms frozen, free hydrogens)

### Calculation Details

- Zero-point correction: 1.595874 (Hartree/Particle)
- Thermal correction to Energy: 1.670394
- Thermal correction to Gibbs Free Energy: 1.671338

### Solvent

- Solvent correction: -5010.6998918

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190

RX2Asimpl22norXF SCF Done: -4983.23696592

A.U.

| N   |    |    |
|-----|----|----|
| 9.480564 | -5.351905 | -1.596344 |
| 9.497956 | -4.385817 | -0.463896 |
| 8.875029 | -3.030170 | -0.870022 |
| 7.380334 | -2.973833 | -0.905619 |
| 6.682382 | -2.946724 | -2.089070 |
| 5.383638 | -2.861693 | -1.834981 |
| 5.212962 | -2.850477 | -0.534271 |
| 6.446252 | -2.934645 | 0.072559 |
| 8.866602 | -4.986685 | 0.825534 |
| 8.839048 | -4.300421 | 1.879134 |
| 8.511324 | 0.503226 | -3.595242 |
| -7.502106 | 1.091586 | -2.974616 |
| -6.362833 | 0.405978 | -2.307572 |
| -5.139650 | 0.367502 | -3.221815 |
| -5.239878 | -0.330406 | -4.425563 |
| -5.122732 | -1.896141 | -4.299092 |
| -5.256724 | -2.728413 | -5.399620 |
| -5.402044 | -2.191560 | -6.644943 |
| -5.545073 | -0.013177 | -5.681634 |

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S181
C  -5.536806  -0.835539  -6.788216
C  -6.043981  -1.381891  -1.031548
C  -6.873914  -0.737121  -2.386479
C  -8.196485  -1.067995  -2.080928
C  -8.091502  -2.955158  -2.287213
C  -4.438281  -0.328571  -1.919715
O  -3.907734  -0.529180  -1.206352
N  -3.948214  0.714366  3.093437
C  -2.849290  -0.014478  -3.803045
C  -2.641381  -0.592167  -5.205993
C  -1.995973  -1.962183  -5.186070
O  -1.452046  -2.380028  1.739044
N  -2.067183  -2.657180  6.307552
C  -3.147075  -1.495035  3.837373
O  -4.255524  -0.868827  2.453472
N  -3.713375  -0.737121  -1.137423
C  -6.103317  0.502778  0.109705
C  -5.715907  1.026789  1.439454
C  -6.873914  0.737121  2.386479
C  -8.196485  1.441384  2.080928
C  -8.091502  2.955158  2.287213
C  -4.438281  0.328571  1.919715
O  -3.907734  0.529180  1.206352
N  -3.948214  0.714366  3.093437
C  -2.849290  0.014478  3.803045
C  -2.641381  0.592167  5.205993
C  -1.995973  1.962183  5.186070
O  -1.452046  2.380028  2.453472
C  -2.067183  2.657180  6.307552
C  -3.147075  1.495035  3.837373
O  -4.255524  0.868827  2.453472
N  -3.713375  0.737121  -1.137423
C  -6.103317  -0.502778  -0.109705
C  -5.715907  -1.026789  -1.439454
C  -6.873914  -0.737121  -2.386479
C  -8.196485  -1.441384  -2.080928
C  -8.091502  -2.955158  -2.287213
C  -4.438281  -0.328571  -1.919715
O  -3.907734  -0.529180  -1.206352
N  -3.948214  -0.714366  -3.093437
C  -2.849290  -0.014478  -3.803045
C  -2.641381  -0.592167  -5.205993
C  -1.995973  -1.962183  -5.186070
O  -1.452046  -2.380028  -2.453472
C  -2.067183  -2.657180  -6.307552
C  -3.147075  -1.495035  -3.837373
O  -4.255524  -0.868827  -2.453472
N  -3.713375  -0.737121  -1.137423
C  -6.103317  0.502778  -0.109705
C  -5.715907  1.026789  -1.439454
C  -6.873914  0.737121  -2.386479
C  -8.196485  1.441384  -2.080928
C  -8.091502  2.955158  -2.287213
C  -4.438281  0.328571  -1.919715
O  -3.907734  0.529180  -1.206352
N  -3.948214  0.714366  -3.093437
C  -2.849290  0.014478  -3.803045
C  -2.641381  0.592167  -5.205993
C  -1.995973  1.962183  -5.186070
O  -1.452046  2.380028  -2.453472
C  -2.067183  2.657180  -6.307552
C  -3.147075  1.495035  -3.837373
O  -4.255524  0.868827  -2.453472
N  -3.713375  0.737121  -1.137423
C  -6.103317  -0.502778  0.109705
C  -5.715907  -1.026789  1.439454
C  -6.873914  -0.737121  2.386479
C  -8.196485  -1.441384  2.080928
C  -8.091502  -2.955158  2.287213
C  -4.438281  -0.328571  1.919715
### space group P2₁2₁2₁ (protomer A), model 3, Mpro

Zero-point correction = 0.909138 (Hartree/Particle)
Thermal correction to Energy = 0.964765
Thermal correction to Enthalpy = 0.965709
Thermal correction to Gibbs Free Energy = 0.818664

Sum of electronic and zero-point Energies = -2988.279889
Sum of electronic and thermal Energies = -2988.224261
Sum of electronic and thermal Enthalpies = -2988.223317
Sum of electronic and thermal Free Energies = -2988.370362

SOLVENT: -3005.4426009

### RX2Aisimpl22REACTANT0 SCF Done: -2989.18902609 A.U.

### Geometrical Coordinates for Mpro

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| H    | -1.029173 | 10.414199| -1.031484|
| H    | -1.041389 | 8.650818 | -1.314441|
| H    | 1.857918  | 9.192987 | 0.892306 |
| H    | 0.424444  | 8.186240 | 0.569194 |
| H    | 0.232743  | 9.910406 | 0.962571 |
| H    | 2.382440  | -3.657777| 3.253295 |
| H    | 8.574028  | -6.038688| 0.741359 |
| H    | 10.216278 | -5.182793| -2.281328|
| H    | 2.090873  | 6.086139 | -1.866243|
| H    | 0.301302  | -3.191059| 2.393628 |

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S184
space group P2_12_12_1(protomer A), model 3, reactant complex

Zero-point correction= 1.603715 (Hartree/Particle)
Thermal correction to Energy= 1.700439
Thermal correction to Enthalpy= 1.701383
Thermal correction to Gibbs Free Energy= 1.470204

Sum of electronic and zero-point Energies= -4981.978334
Sum of electronic and thermal Energies= -4981.881611
Sum of electronic and thermal Enthalpies= -4981.880667
Sum of electronic and thermal Free Energies= -4982.111845

SOLVENT: -5010.8631068

RX2Assimp22REACTANT SCF Done: -4983.58204938 A.U.
H  3.836279  -0.637668  -0.235882
H  0.118625  -6.542342  -0.480995
H  -1.100245  -5.558191  1.176402
H  -0.337010  -3.12125  -1.762472
H  -0.373719  -2.675113  -1.094495
H  0.853389  -2.426187  1.291078
H  3.154846  -2.492465  2.126768
H  4.845245  -4.014187  1.077042
H  1.882653  -3.749442  -1.789768
H  4.195797  -3.65789  -0.908750
H  -2.073873  -1.989691  1.229926
H  -4.117951  -1.471773  -0.891446
H  -4.394680  -0.725135  2.073336
H  -5.572073  -0.336300  0.809474
H  -6.298775  -2.286568  2.183787
H  -4.822418  -3.164266  1.755600
H  -5.495486  -3.310547  -0.607010
H  -4.120334  0.879501  -1.654481
H  -1.910726  2.411893  -1.197213
H  -4.802919  3.421196  -1.96508
H  -3.403961  4.339173  -1.804975
H  -4.072194  3.142380  -5.095469
H  -3.522116  4.456620  -4.086464
H  -1.074281  3.659461  0.519312
H  -2.72698  3.737944  2.958714
H  -1.521490  4.974041  2.668085
H  -1.056132  1.627737  1.751833
H  0.961502  1.377411  3.928102
H  -0.735298  -0.371118  4.112066
H  -1.320740  -0.490140  1.728033
H  1.312554  2.792184  1.473948
H  2.663943  1.315368  -0.501199
H  3.137646  4.287737  -0.071323
H  3.141349  3.342700  -1.562887
H  4.005800  0.428458  1.705473
H  6.362060  0.428050  2.573354
H  6.344721  -0.152063  0.869070
H  6.755761  1.547790  1.231993
H  0.449102  2.736220  -1.314853
H  5.559213  1.150941  -1.721801
H  4.511276  -2.090159  -0.723388
H  -0.165060  -6.364435  1.256298

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H  8.140416  -1.003192  -2.974533
C  7.706666  -1.125218  -1.581893
C  7.15323  0.163983  -0.899399
C  6.183191  0.879134  -1.795073
N  6.885076  2.010899  -2.566050
C  5.322614  2.388867  -3.223255
N  4.362060  1.560348  -2.920480
C  4.861967  0.612080  -2.036888
C  6.659188  2.241929  -1.531316
O  5.734256  -2.305831  -0.718484
C  6.537552  3.005047  -1.566423
N  6.129797  2.388866  -0.295529
C  -5.064888  1.385632  -0.385113
C  -3.600277  1.802484  -0.730939
C  -3.498965  2.291705  -2.173469
C  -3.643282  3.497974  -3.185653
C  -3.430305  1.678883  -4.528222
C  -2.974030  2.958222  -4.866825
C  -2.921207  3.560339  -2.517997
C  -2.708691  3.892418  -3.858436
C  -4.912119  0.715570  0.978938
O  -4.656179  1.395324  2.017268
N  -5.092676  -0.629642  0.974661
C  -4.466075  -1.439305  2.067562
C  -5.554251  -2.520996  2.729489
|   |   |   |   |
|---|---|---|---|
| C | -6.47099 | -1.491594 | 3.284370 |
| C | -6.329701 | -0.415581 | 4.276504 |
| C | -3.345996 | -2.715542 | 0.305983 |
| N | -2.493879 | -2.842493 | 2.369923 |
| C | -1.407555 | -3.691023 | 1.883036 |
| C | -0.501760 | -4.125727 | 3.056668 |
| C | 0.042782 | -2.903935 | 3.787955 |
| C | -1.973219 | -6.139068 | -0.953009 |
| C | -2.760130 | -6.046992 | -3.254439 |
| O | -2.818688 | -4.09644 | -2.011109 |
| C | -1.542136 | -1.509628 | -1.669492 |
| C | -2.177205 | -2.170621 | -3.643536 |
| C | -0.339010 | -1.422260 | -4.500735 |
| N | -1.487200 | -1.956018 | -3.128614 |
| C | -0.800360 | -0.701020 | -3.459168 |
| C | 0.565072 | -0.612551 | -2.646692 |
| S | 0.955399 | 1.142864 | -2.335021 |
| C | -0.186833 | -0.646564 | -4.948367 |
| O | 0.136417 | -1.596694 | -5.522251 |
| N | -0.640387 | 0.372254 | -5.509412 |
| C | -0.281749 | 0.833302 | -6.905416 |
| O | 0.373093 | -3.112275 | -0.577012 |
| C | 1.574113 | -3.153422 | -0.181268 |
| N | 2.183976 | -2.480078 | 0.217046 |
| C | 3.651017 | -4.418777 | 0.488234 |
| C | 4.013851 | -4.000182 | 1.902680 |
| C | 3.785619 | -4.855120 | 2.993271 |
| C | 4.066217 | -4.432844 | 4.292233 |
| C | 4.578474 | -3.139781 | 4.513142 |
| O | 4.795632 | -2.284868 | 3.430117 |
| C | 4.540913 | -2.724235 | 2.128099 |
| C | 3.374109 | -1.835973 | -0.231141 |
| O | 3.147019 | -1.699899 | -1.184066 |
| C | 2.102282 | -0.805920 | 0.851194 |
| C | 0.579619 | -0.706477 | 1.115238 |
| C | 0.050308 | 0.580994 | 1.750044 |
| C | 0.313363 | 0.878504 | 3.243828 |
| C | -0.974513 | 1.647383 | 3.702415 |
| N | -1.997075 | 1.155596 | 2.760426 |
| C | -1.482273 | 0.465551 | 1.712019 |
| C | -2.116921 | -0.165404 | 0.833684 |
| N | 2.680335 | 0.477602 | 0.475706 |
| C | 3.873042 | 0.917349 | 0.945498 |
| O | 4.694505 | 0.226371 | 1.592579 |
| C | 4.103100 | 2.418184 | 0.674844 |
| C | 5.557080 | 2.822656 | 0.905018 |
| C | 5.771268 | 4.315583 | 0.763898 |
| C | 5.625218 | 4.917665 | -0.629873 |
| C | 7.022392 | 4.800506 | 0.409094 |
| N | 3.146460 | 3.154437 | 1.562985 |
| C | 1.906369 | 3.453375 | 1.001926 |
| O | 1.631526 | 3.149858 | -0.192477 |
| C | 3.443608 | 3.143707 | 2.886628 |
| C | 2.532116 | 4.026768 | 3.693338 |
| C | 1.248530 | 4.368751 | 3.185813 |
| C | 0.932059 | 4.072941 | 1.883590 |
| N | -0.293932 | 4.259850 | 1.242984 |
| C | -1.409484 | 4.699521 | 1.855545 |
| O | -1.525937 | 4.938374 | 3.073685 |
| C | -2.451114 | 4.832888 | 0.939500 |
| C | -3.744613 | 5.040244 | 1.392789 |
| C | -4.421667 | 4.639898 | 2.462989 |
| C | -4.556018 | 5.561337 | 0.097990 |
| C | -3.413662 | 6.915860 | 1.898428 |
| H | 8.535518 | -1.501619 | -0.993589 |
| H | 7.996770 | 0.818720 | -0.643965 |
| H | 6.629986 | -0.105089 | 0.024976 |
| H | 5.271585 | 3.238025 | -3.881614 |
| H | 4.269297 | -0.190520 | -1.641842 |
| H | 7.376904 | 2.490408 | -2.595904 |
| H | 7.440718 | -0.537277 | -3.557496 |
| H  | -5.772125 | 3.619112 | -2.062692 |
| H  | -7.423396 | 3.621012 | -1.379361 |
| H  | -5.950011 | 3.647032 | -0.513134 |
| H  | -3.955454 | 0.346463 | -2.940303 |
| H  | -5.676177 | 0.903465 |  0.053381 |
| H  | -2.090931 | 3.216068 | -5.073959 |
| H  | -2.692634 | 4.264766 | -1.724721 |
| H  | -2.329732 | 4.875250 | -4.117566 |
| H  | -5.165492 | -1.091809 |  0.069588 |
| H  | -4.033982 | -0.737932 |  2.799665 |
| H  | -5.897666 | -3.035406 |  1.988007 |
| H  | -5.884322 | -2.875269 |  3.553384 |
| H  | -7.471304 | -2.181062 |  3.699994 |
| H  | -7.234222 | -1.007697 |  2.394751 |
| H  | -7.215476 |  0.046591 |  4.726666 |
| H  | -5.731094 | -0.861817 |  5.081210 |
| H  | -5.746933 |  0.370715 |  3.787365 |
| H  | -2.253547 | -2.421678 |  3.317621 |
| H  | -0.845436 | -3.120987 |  1.148971 |
| H  | -1.120689 | -4.716357 |  3.740274 |
| H  |  0.303038 | -4.751523 |  2.662539 |
| H  |  1.807684 | -1.968917 |  4.246880 |
| H  |  2.018575 | -3.469071 |  3.408043 |
| H  | -0.731352 | -4.498034 | -0.367143 |
| H  | -2.790544 | -6.645085 | -0.426726 |
| H  | -1.265266 | -6.891645 | -1.309547 |
| H  | -2.789641 | -3.702562 | -1.065426 |
| H  | -3.774648 | -4.038287 | -3.845575 |
| H  | -5.390225 | -2.308789 | -3.347998 |
| H  | -5.397988 | -3.437142 | -1.946426 |
| H  | -3.855872 | -1.305565 | -0.963411 |
| H  | -1.085979 | -2.600160 | -2.454151 |
| H  | -1.467733 |  0.126414 | -3.206863 |
| H  |  0.348226 | -1.096140 | -1.685639 |
| H  |  1.302408 | -1.149413 | -3.169535 |
| H  | -1.145737 |  1.282477 | -4.988785 |
| H  | -1.169695 |  1.071713 | -7.502729 |
| H  |  0.453886 |  1.658259 | -6.981991 |
| H  |  0.172759 | -0.085804 | -7.282314 |
| H  |  4.204001 | -3.090711 | -0.229532 |
| H  |  3.391261 |  5.852769 |  2.825038 |
| H  |  3.920907 | -5.101192 |  5.129052 |
| H  |  4.791185 | -2.809346 |  5.523297 |
| H  |  5.153181 | -1.271376 |  3.566056 |
| H  |  4.759852 | -2.062806 |  1.303035 |
| H  |  2.607572 | -1.151140 |  1.760443 |
| H  |  0.018737 | -0.819767 |  0.188069 |
| H  |  0.302798 | -1.344507 |  1.750233 |
| H  |  0.313654 |  1.442353 |  1.126638 |
| H  |  1.218251 |  1.462056 |  3.418351 |
| H  |  0.332418 | -0.065921 |  3.792369 |
| H  | -0.881853 |  2.730260 |  3.614587 |
| H  | -1.244434 |  1.388495 |  4.729633 |
| H  | -3.008825 |  1.325968 |  2.788061 |
| H  |  2.142176 |  1.056998 | -0.183747 |
| H  |  3.791611 |  2.651178 | -0.348866 |
| H  |  5.911237 |  2.438346 |  1.866895 |
| H  |  6.124977 |  2.299397 |  0.134485 |
| H  |  5.410876 |  4.924791 |  1.585367 |
| H  |  5.216035 |  5.904351 | -0.724023 |
| H  |  5.428580 |  4.231937 | -1.437255 |
| H  |  7.499556 |  5.709299 |  0.387317 |
| H  |  7.003332 |  4.038267 | -0.330124 |
| H  |  4.419534 |  3.104707 |  3.227524 |
| H  |  2.781325 |  4.236304 |  4.723678 |
| H  |  0.499984 |  4.821535 |  3.815233 |
| H  |  2.198874 |  1.177021 | -2.879061 |
| H  | -2.793063 |  6.858135 |  2.792777 |
| H  | -2.885274 |  7.474301 |  1.118728 |
| H  | -4.438828 |  7.433705 |  2.134051 |
| H  | -4.008279 |  6.176064 | -0.667545 |
| H  | -5.510395 |  6.906874 |  0.292533 |
| H  | -4.749391 |  4.555338 | -0.269352 |
| H  | -3.824062 |  4.653126 |  3.374990 |
| H  | -4.522720 |  3.603049 |  2.129413 |
| H  | -5.415445 |  5.051432 |  2.672199 |
| H  |  3.893764 | -5.471389 |  0.321337 |
space group \textit{P2}_1/\textit{2}_1/\textit{2}_1\textit{(protomer A)}, model 3, transition state of deprotonation of the thiol by the imidazole of H41)

Zero-point correction= 1.604157 (Hartree/Particle)
Thermal correction to Energy= 1.697766
Thermal correction to Enthalpy= 1.698710
Thermal correction to Gibbs Free Energy= 1.477521
Sum of electronic and zero-point Energies= -4982.027730
Sum of electronic and thermal Energies= -4981.934121
Sum of electronic and thermal Enthalpies= -4981.933176
Sum of electronic and thermal Free Energies= -4982.154365
SOLVENT: -5010.848793

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RX2Aissimpl22TSFFl SCF Done: -4983.63188677 A.U.
C  -2.366142  -2.088669  -0.081545
O  -3.139735  -3.126907  -0.375848
C  -0.972752  -2.492565   0.490672
C  -0.136691  -1.287137   0.940702
C   1.384247  -1.444081   0.966561
C   2.059868  -2.409311   1.968279
C   3.436441  -1.724528   2.273070
N   3.135882  -0.295568   2.021263
C   1.960481  -0.091090   1.394853
O   1.408908   1.014617   1.174093
N  -0.283604  -3.321941  -0.488069
C  -0.271173  -4.672373  -0.424529
O  -0.859515  -5.380523   0.417423
C   0.669412  -5.283493  -1.061684
C   0.391643  -6.773117  -1.691062
C   1.343323  -7.413388  -2.680681
C   1.087444  -7.185786  -4.166522
C   0.842307  -8.561244  -3.544031
N   2.069853  -4.909708  -1.021407
C   2.594171  -3.747348  -1.374836
O   1.931995  -2.902772  -2.079490
C   2.726853  -5.852796  -0.167523
C   3.956428  -5.535158   0.327718
C   4.558709  -2.496416  -0.099191
C   3.895896  -3.416377  -0.832109
N   4.321803  -2.140347  -1.209268
C   5.432639  -1.506904  -0.698504
O   6.124066  -1.977745   0.222698
C   5.654805  -3.200324  -1.339336
C   6.984809  -0.397917  -1.061684
C   7.003814   0.875983   0.393935
C   6.942318  1.572294  -2.037835
C   8.134522  -0.563798  -1.396400
H  -6.913145  3.107713  -2.058675
H  -8.144839   0.948281  -2.203537
H  -7.427415  1.160002  -0.581378
H  -4.268851  -2.026326  -3.525275
H  -6.259545  -1.343214   0.146968
H  -5.772573  3.010797  -3.642655
H  -9.491281  2.306436  -3.756363
H   4.965430  5.734055   0.179692
H   6.526017  5.042655  -0.326424
H   4.885129  3.959485  -1.670471
H   2.835161  4.209685  -0.409099
H   3.822716  1.567876  -0.871571
H   2.137888  1.796001  -0.519140
H   1.186534  3.770792  -2.031341
H   0.678429  4.234953  -4.381770
H   2.019685  3.122582  -6.203519
H   4.303857  1.061031  -3.177180
H   3.812631  1.517603  -5.865955
H   1.870666  4.237645   1.394297
H   2.553735  2.155137   3.396596
H   1.326129  4.874992  -4.102788
H   1.647298  3.551033   5.236311
H   3.402812  5.306544   5.403849
H   3.747262  5.156330   3.672432
H   5.433344  3.923998   5.147256
H   4.126916  2.841940   5.671926
H   4.632423  2.877956   3.959303
H   0.608753  1.000403   4.215302
H  -1.312669  0.763767   2.361663
H  -1.701772  0.440367   5.377502
H  -2.624427  0.431950   4.122460
H  -0.337132  3.106043   4.139076
H  -1.985660  2.572716   4.062899
H  -3.133832  1.545750  -1.681371
H  -4.183458  3.943741   3.113149
H  -5.288878  2.971141   2.026838
H  -1.774859  3.662977   1.436733
H  -2.573434  5.286743  -0.674113
H  -0.243333  6.164887  -0.843279
H  -0.580153  6.035485   0.918258
H   0.287241  3.780424   0.685547
H  -2.203816  2.244001  -0.527701
H  -0.626122  1.398693  -2.578515
H  -3.210464  0.576408  -1.446330
H  -3.250608  0.310811  -3.178836
H  -0.262780  2.085591  -4.619996
H  -0.928289  3.724201  -6.337555
| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| H    | -1.310967 | 2.091480 | -6.958011 |
| H    | -2.583447 | 3.083748 | -6.176764 |
| H    | -4.877078 | -2.997479 | 1.024796 |
| H    | -4.751771 | -2.458312 | 6.163890 |
| H    | -1.986910 | -5.921512 | 5.185058 |
| H    | -1.641268 | -5.969411 | 2.687849 |
| H    | -2.898232 | -4.632926 | 1.250493 |
| H    | -1.890438 | -3.134956 | 1.351207 |
| H    | -0.343466 | -0.433080 | 0.295262 |
| H    | -0.466374 | -1.024700 | 2.250493 |
| H    | 1.754352  | -1.636222 | 0.047433 |
| H    | 2.181248  | -3.421706 | 1.580959 |
| H    | 1.486136  | -2.408256 | 2.896573 |
| H    | 4.240763  | -2.067931 | 1.621490 |
| H    | 3.728655  | 0.494269  | 2.174795 |
| H    | 0.273051  | -2.864943 | -1.221087 |
| H    | 0.568570  | -4.742082 | -2.433439 |
| H    | 0.385669  | -7.282418 | -0.721832 |
| H    | -0.636463 | -6.843870 | -2.078999 |
| H    | 2.382731  | -7.449577 | -2.372938 |
| H    | 1.942968  | -7.070283 | -4.820993 |
| H    | 0.218936  | -6.594668 | -4.436715 |
| H    | 1.537371  | -9.351619 | -3.780645 |
| H    | -0.186447 | -8.875581 | -3.407791 |
| H    | 2.212993  | -6.768112 | 0.077820 |
| H    | 8.190580  | -0.921305 | -2.432011 |
| H    | 9.808132  | -0.021784 | -1.294770 |
| H    | 6.765829  | 1.217786  | -3.059363 |
| H    | 7.906590  | 2.091680  | -2.002699 |
| H    | 6.157916  | 2.262612  | -1.722683 |
| H    | 7.044297  | 0.017653  | 1.065340 |
| H    | 6.148434  | 1.473242  | 0.612741 |
| H    | 7.893819  | 1.493558  | 0.541780 |
| H    | -5.583386 | -2.188962 | 2.435322 |
| H    | -4.373538 | 2.992529  | -1.714272 |
| H    | -6.568437 | 2.377526  | -4.245247 |
| H    | 3.725365  | -1.671160 | -1.892132 |
| H    | -4.523994 | -0.380501 | 2.143462 |
| H    | 5.722137  | 4.330683  | 1.130537 |

**space group P212121 (protomer A), model 2, reactant complex**

Zero-point correction= 1.444078 (Hartree/Particle)
Thermal correction to Energy= 1.530754
Thermal correction to Enthalpy= 1.531698
Thermal correction to Gibbs Free Energy= 1.416790

Sum of electronic and zero-point Energies= -4511.164827
Sum of electronic and thermal Energies= -4511.078151
Sum of electronic and thermal Enthalpies= -4511.077207
Sum of electronic and thermal Free Energies= -4511.289231

SOLVENT: -4537.2651363

| XYZ | XYZ |
|-----|-----|
| C   | 6.473641 | 3.699758 | 0.446266 |
| N   | -5.308051 | 3.335797 | 2.852414 |
| O   | -4.415655 | 2.996164 | 0.720218 |
| C   | -3.995909 | 2.608173 | -0.681261 |
| C   | -4.617731 | 2.089717 | -1.848369 |
| C   | -4.733282 | 0.715486 | -1.963728 |
| C   | -5.628310 | 0.215999 | -3.029481 |
| C   | -6.112936 | 1.082792 | -4.015129 |
| C   | -5.104950 | 2.984181 | -2.847419 |
| C   | -5.842986 | 2.451314 | -3.222929 |
| C   | -3.326271 | 2.100657 | 1.755285 |
| O   | -2.602501 | 3.069272 | 2.126256 |
| N   | -3.228794 | 0.851220 | 2.242689 |
| C   | -2.163533 | 0.438132 | 3.205502 |
| C   | -2.809261 | -0.042134 | 4.521952 |
| C   | -3.812342 | 1.043339 | 5.117075 |
| C   | -3.067963 | 2.563392 | 5.410780 |
| C   | -1.344291 | -0.944888 | 2.647508 |
| O   | -1.610999 | -1.349285 | 1.929907 |
| N   | -0.275938 | -0.949414 | 3.395985 |
| C   | 0.630361 | -2.115967 | 3.070538 |
| C   | 1.800810 | -2.099660 | 4.084705 |
| C   | 2.345181 | -0.697366 | 4.319791 |
| O   | 1.612666 | 0.212619 | 4.794245 |
| N   | 3.630104 | -0.489625 | 3.965619 |
| C   | -0.128616 | -3.454778 | 3.267226 |
| O   | -0.468166 | -3.833198 | 4.409037 |

TX1141
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| N       | -0.358847    | -4.144140    | 2.114552     |
| C       | -1.284225    | -5.281603    | 2.095797     |
| C       | -2.462266    | -5.07544     | 2.114552     |
| O       | -3.202619    | -6.022137    | 0.814889     |
| N       | -2.623824    | -3.789180    | 0.684283     |
| C       | -3.825976    | -3.430128    | -0.060805    |
| C       | -4.645375    | -2.360990    | 0.686019     |
| O       | -4.012435    | -1.041717    | 0.566485     |
| C       | -3.618834    | -2.884088    | -1.479181    |
| O       | -4.630115    | -2.488844    | -2.099149    |
| N       | -2.37496     | -2.791331    | -4.279576    |
| C       | -2.00265     | -4.003407    | -4.507681    |
| N       | -1.794980    | -4.933717    | -5.849947    |
| C       | -2.93803     | -3.268394    | -0.381812    |
| C       | -1.521464    | -3.528520    | -0.531104    |
| O       | -1.233728    | 1.418668     | 0.502780     |
| N       | -1.233728    | 1.416333     | -0.089302    |
| N       | 0.063871     | -0.266037    | -1.856593    |
| C       | 4.373966     | -0.042126    | -1.848309    |
| O       | 5.020143     | -0.636161    | -1.127037    |
| C       | 4.798790     | 1.164984     | -2.79171     |
| C       | 6.225034     | 1.060208     | -3.236418    |
| C       | 6.716837     | 2.247606     | -3.959985    |
| C       | 6.225782     | 2.495475     | -5.372790    |
| C       | 7.677809     | 2.087607     | -5.121363    |
| N       | 4.627009     | 2.228403     | -1.770647    |
| C       | 3.338859     | 2.862429     | -1.702711    |
| C       | 2.414809     | 2.451943     | -2.473334    |
| C       | 5.625460     | 2.746601     | -0.881765    |
| C       | 5.392961     | 3.062126     | 0.089121     |
| C       | 4.107106     | 4.186637     | 0.219689     |
| C       | 3.098521     | 3.852537     | -0.643332    |
| N       | 1.709919     | 4.246673     | -0.585893    |
| C       | 1.222024     | 5.007396     | 0.426114     |
| C       | 1.878280     | 5.479021     | 1.376771     |
| C       | 0.114926     | 5.544683     | 0.227641     |
| C       | 0.894557     | 6.149839     | 1.061675     |
| C       | 0.833560     | 5.796940     | 2.555440     |
| C       | 2.310655     | 5.965642     | 0.514350     |
| C       | 0.316789     | 7.540051     | 0.770011     |
| H       | -6.221355    | 4.076732     | -0.556995    |
| H       | -7.074135    | 4.451666     | 0.968986     |
| H       | -4.735557    | 4.170382     | 1.520121     |
| H       | -5.026598    | 1.381007     | 0.636740     |
| H       | 3.656617     | 3.906206     | -0.761933    |
| H       | -2.95460     | 2.131885     | -0.699008    |
| H       | -4.50087     | 0.026952     | -1.211379    |
| H       | -5.810343    | -0.849471    | -3.067764    |
| H       | -6.700070    | 0.690761     | -4.841738    |
| H       | -4.095144    | 4.012979     | -2.771784    |
| H       | -6.211702    | 3.131637     | -4.682505    |
| H       | -3.974364    | 0.110287     | 1.789422     |
| H       | -1.575763    | 1.293367     | 3.415351     |
| H       | -3.467662    | -0.950339    | 4.303062     |
| H       | -2.107291    | -0.306477    | 5.241856     |
| H       | -4.251188    | 0.647966     | 6.041305     |
| H       | -6.628925    | 1.227618     | 4.413669     |
| H       | -3.715934    | 3.058909     | 5.960482     |
| H       | -2.168094    | 2.180588     | 6.011093     |
Space group P2₁2₁2₁ (protomer A), model 3, reactant complex

Zero-point correction= 1.445975 (Hartree/Particle)
Thermal correction to Energy= 1.531956
Thermal correction to Enthalpy= 1.532900
Thermal correction to Gibbs Free Energy= 1.327750

Sum of electronic and zero-point Energies= -4511.193410
Sum of electronic and thermal Energies= -4511.104730
Sum of electronic and thermal Enthalpies= -4511.106486
Sum of electronic and thermal Free Energies= -4511.315636
| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| H     | -4.76012 | -0.926138 | 4.470565 |
| C     | -5.935339 | -0.349900 | 4.975186 |
| C     | -2.192256 | -3.674449 | 1.651929 |
| O     | -1.176449 | -4.360298 | 1.951080 |
| N     | -2.518394 | -3.397247 | 0.359631 |
| C     | -1.556007 | -3.560442 | -0.726130 |
| C     | -2.073057 | -4.534249 | -1.818426 |
| C     | -2.411839 | -5.922933 | -1.237428 |
| C     | -2.073057 | -5.922933 | -1.818426 |
| O     | -2.073057 | -5.922933 | -1.818426 |
| N     | -2.073057 | -5.922933 | -1.818426 |
| C     | -0.276640 | -0.917836 | -2.827511 |
| C     | 1.643491 | -1.189948 | -3.596608 |
| S     |  -2.850195 | 0.043541 | -0.149097 |
| C     | -5.671699 | 3.910415 | -0.061139 |
| O     | -0.628954 | 0.126654 | -2.795294 |
| C     | -3.040776 | -0.089215 | -2.122133 |
| O     | -4.446644 | -1.695638 | -0.474208 |
| C     | -5.601741 | 0.876172 | -0.963183 |
| N     | -6.753071 | 0.833550 | -0.448020 |
| C     | -4.888101 | 2.697977 | 0.519949 |
| O     | -3.582332 | 3.211996 | 1.128233 |
| S     | -2.849401 | 1.961581 | 2.268931 |
| C     | -5.671699 | 3.910415 | -0.061139 |
| O     | -5.165851 | 5.045341 | -0.249077 |
| N     | -6.939565 | 3.593075 | -0.432174 |
| C     | -7.812733 | 4.593558 | -1.052776 |
| O     | -1.665239 | 1.741434 | -1.166651 |
| C     | 0.099230 | 2.423254 | -1.156781 |
| N     | 0.902142 | 2.705711 | -2.272985 |
| C     | 1.312905 | 3.539762 | -2.381435 |
| O     | 2.414306 | 2.768678 | -3.097244 |
| C     | 2.220622 | 2.326813 | -4.414727 |
| O     | 3.222724 | 1.623328 | -5.084506 |
| C     | 4.439544 | 1.361749 | -4.444132 |
| O     | 4.639149 | 1.804857 | -3.128848 |
| C     | 3.630753 | 2.905085 | -2.458154 |
| O     | 0.088979 | 2.837110 | 0.189296 |
| C     | 0.527507 | 3.782669 | 0.861999 |
| O     | 1.057134 | 1.813283 | 0.623798 |
| C     | 0.338983 | 0.581454 | 1.238335 |
| O     | 1.322143 | -0.540752 | 1.605768 |
| C     | 1.904293 | -1.296614 | 0.400409 |
| O     | 2.003936 | -2.775824 | 0.882633 |
| C     | 0.986982 | -2.837568 | 1.944795 |
| O     | 0.560896 | -1.631245 | 2.388006 |
| C     | -0.302291 | 1.144146 | 3.262737 |
| O     | 1.980648 | 2.359658 | 1.611744 |
| O     | 2.859941 | 3.336947 | 1.291260 |
| O     | 2.809584 | 4.017440 | 0.240571 |
| O     | 4.081997 | 3.441017 | 2.223174 |
| C     | 4.579406 | 4.880502 | 2.349102 |
| C     | 5.868202 | 4.908446 | 3.138874 |
| C     | 5.782415 | 4.897876 | 4.659623 |
| C     | 6.115739 | 6.225618 | 3.979855 |
| O     | 5.055586 | 2.513878 | 1.538250 |
| C     | 4.872928 | 1.149245 | 1.802042 |
| O     | 4.091171 | 0.754980 | 2.715604 |
| C     | 5.885088 | 2.972262 | 0.536739 |
| C     | 6.591020 | 2.100998 | -0.238148 |
| C     | 6.421420 | 0.702035 | -0.060287 |
| C     | 5.586428 | 0.236406 | 0.923761 |
| C     | 5.295788 | -1.037075 | 1.196903 |
| O     | 5.576586 | -2.164498 | 0.375921 |
| O     | 6.106646 | -2.063680 | -0.752289 |
| O     | 5.163280 | -3.320674 | 0.956671 |
| O     | 5.471688 | -4.663017 | 0.301916 |
| O     | 4.975802 | -4.714442 | -1.149514 |
| O     | 4.689888 | -5.022565 | 1.202442 |
| O     | 6.968550 | -4.869160 | 0.403710 |
| X       | Y       | Z       |
|---------|---------|---------|
| -3.720871 | -5.013747 | 4.569849 |
| -2.304686 | -4.716157 | 5.590665 |
| -1.684865 | -2.871693 | 4.146549 |
| -4.115549 | -3.527008 | 2.619700 |
| -2.388039 | -1.056228 | 2.952542 |
| -3.244145 | -1.288078 | 1.442769 |
| -5.366026 | -0.528687 | 1.164275 |
| -7.401007 | 0.542054  | 2.022902 |
| -7.788235 | 0.655181  | 4.510555 |
| -4.027437 | -1.374489 | 5.122017 |
| -6.099856 | -0.320095 | 6.047249 |
| -3.419522 | -2.942051 | 0.393233 |
| -0.637776 | -3.949637 | -0.280579 |
| -2.966606 | -4.089086 | -2.276386 |
| -1.304060 | -4.628225 | -2.596923 |
| -2.762359 | -5.650102 | -2.058713 |
| -3.236306 | -5.812793 | -0.524755 |
| -1.440853 | -7.621432 | -0.267899 |
| -0.327124 | -6.586933 | -1.185644 |
| -0.968164 | -6.044772 | 0.393233 |
| 0.353688  | -0.116684 | 2.087548  |
| 1.421639  | -1.793086 | -4.380140 |
| 2.034521  | -0.215572 | -3.857840 |
| 4.803210  | -1.740020 | -1.940425 |
| 4.003714  | -0.378769 | -2.849237 |
| -1.613785 | 0.862438  | -2.696721 |
| -2.524580 | 0.243063  | -5.458815 |
| -2.473747 | 1.947308  | -4.961819 |
| -3.189204 | -0.306357 | -2.41424 |
| -6.093961 | 0.081268  | -2.860395 |
| -6.393195 | -1.652277 | -1.412800 |
| -5.228629 | -2.237025 | -2.382190 |
| -3.577700 | -1.320243 | -0.720450 |
| -3.689766 | 1.669944  | -0.958586 |
| -5.505575 | 2.200966  | 1.274557 |
| -2.808537 | 3.460144  | 0.344164 |
| -3.806456 | 4.126821  | 1.677317 |
| -7.234077 | 2.613626  | -0.351220 |
| -8.742461 | 4.707841  | -0.484184 |
| -7.645256 | 5.540063  | 1.046931 |
| -8.056703 | 4.322049  | -2.086197 |
| 1.647401  | 3.826734  | -1.382409 |
| 1.286292  | 2.538741  | -4.929543 |
| 3.059379  | 1.284690  | -6.101459 |
| 5.224464  | 0.825968  | -4.965396 |
| 5.577776  | 1.615650  | -2.627721 |
| 3.793244  | 2.869125  | -1.453374 |
| 1.613964  | 1.501096  | -0.271480 |
| -0.199910 | 0.891055  | 2.136615 |
| -0.414910 | 0.213151  | 0.532001 |
| 2.140306  | -0.180673 | 2.238128 |
| 2.860794  | -0.910462 | 0.052272 |
| -1.185458 | -1.260153 | -0.415497 |
| -2.998035 | 3.005492  | 1.267721 |
| 1.780035  | 3.463580  | 0.066803 |
| 0.415963  | -0.667400 | 2.146604 |
| 2.185075  | -1.966442 | 2.436478 |
| 3.809463  | 3.003260  | 3.202212 |
| 4.652831  | 5.329856  | 1.353358 |
| 3.788072  | 5.432966  | 2.872691 |
| 6.777370  | 4.251367  | 2.680979 |
| 6.576183  | 4.359094  | 5.188896 |
| 4.795662  | 4.793739  | 5.097382 |
| 7.132352  | 6.591584  | 4.057459 |
| 5.350164  | 6.993177  | 3.972695 |
| 5.932677  | 4.040842  | 0.407679 |
| 7.261683  | 2.479479  | -0.995964 |
| 6.915015  | -0.007295 | -0.705732 |
| -1.780087 | 2.730522  | 2.561667 |
| 7.499467  | -0.099263 | -0.178537 |
| 7.304875  | -4.813496 | 1.448917 |
| 7.243756  | -5.537311 | 0.001363 |
| 4.939263  | -5.486818 | 2.243913 |
| 4.890240  | -6.537788 | 0.897113 |
| 3.618019  | -5.424006 | 1.116062 |
| 5.651982  | -4.105211 | -1.802438 |
| 3.975491  | -4.286156 | -1.250889 |
| 4.947499  | -5.763447 | -1.46587 |
| 1.063804  | 4.446363  | -2.945169 |

S194
space group P2₁,₂,₂₁ (protomer A), model 3, Mpro

| Atom | Coordinates | Thermal correction to Energy | Thermal correction to Enthalpy | Thermal correction to Gibbs Free Energy | Sum of electronic and zero-point Energies | Sum of electronic and thermal Energies | Sum of electronic and thermal Enthalpies | Sum of electronic and thermal Free Energies |
|------|-------------|------------------------------|-----------------------------|----------------------------------------|------------------------------------------|----------------------------------------|------------------------------------------|-------------------------------------------|
| C    | 0.156438    | 0.145583                    | 0.265812                    | 0.315497                               | 0.749583                                 | 0.795997                               | 0.796941                                 | -2517.462206                              |
| N    | 0.284543    | 0.389454                    | 0.483454                    | 0.507454                               | 0.795343                                 | 0.775343                               | 0.775343                                 | -2517.45791                               |
| C    | -2.087865   | -5.380082                   | 3.946724                    | 0.786015                               | 2.478427                                 | 2.478427                               | 2.478427                                 | -2517.41847                               |

SOLVENT: -2531.850794

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RX2/RSimpl/Part1/3SH SCF Done: -2518.21178850 A.U.

C      0.156438     6.142456    -0.175220
C      0.478778     5.003957     0.726750
C      2.904555     3.698875     0.076031
C      0.975343     2.591268     0.932486
C      2.478427     2.421300     0.786015
C      3.099212     1.836989    -0.181558
C      4.481410     1.847879    -0.333211
C      5.263991     2.685660     0.465599
C      3.261331     3.506832     1.559169
C      4.649102     3.534388     1.401749
C      1.197047     3.332691    -0.044063
O      0.280961     3.932839     0.622856
O      1.448481     2.264104    -0.857192
C      -2.070904    1.537162    -0.734814
C      -3.464263    1.435293    -2.084054
C      -3.708287    2.828783    -2.702034
C      -4.501382    3.769321    -1.765259
C      -2.556655    0.129274    -0.219772
O      -1.331113    -0.463018    -0.274803
N      -3.509367    -0.473329     0.359059
C      -3.412340    -1.818546     0.961757
C      -4.834246    -2.256164     1.395366
C      -5.624931    -1.182256     2.135180
C      -5.711784    -0.006698     1.703895
C      -6.263886    -1.581849     3.259827
C      -2.959065    -2.847288    -0.104825
N      -3.709673    -3.152255    -1.046075
N      -1.735717    -3.409544     0.110405
C      -1.875799    -4.361268    -0.860596
C      -0.032271    -3.799749    -1.714328
O      -0.674152    -4.530207    -2.422538
C      -0.132112    -2.443478    -1.594962
C      -1.210834    -1.753639    -2.302516
O      -0.747885    -0.383493    -2.840936
N      -0.554830    -0.506536    -1.737788
C      -2.412239    -1.452632    -1.380515
O      -0.393604    -0.794413    -1.805173
N      -2.269251    -1.888154    -0.138866
C      -3.099070    -4.077757    1.017264
C      -2.353223    -1.677768    2.336735
C      -0.675752    -3.100016     2.199865
C      -0.472928    -2.113855     1.078551
O      -0.806618    -2.814952     2.054162
N      -5.238356    -1.862864    -0.009685
C      -6.575290    -2.544548    -0.140361
O      -0.868783     1.642204     1.006432
H      0.278543     0.707472     0.379982
H      -0.158484     0.513156     1.535197
H      0.758311     3.710975    -0.913468
H      0.672451     2.740563     1.975380
H      0.612241     1.611274     0.616962
H      2.473250     1.226406    -0.824566
H      0.928740     1.194412    -1.071753
H      0.324784     2.693420     0.359482
H      2.772305     4.175298     2.256846
H      0.525197     4.192125     2.007488
H      -0.688259    1.836461    -1.407759
H      -3.308437     2.093865    -0.010670
H      -2.870566     0.816241    -2.769952
H      -4.193355     0.924849    -1.099354
H      -4.278681     2.049763    -3.646149
H      -2.738259     3.281228    -2.934794
H      -4.764713     4.694016    -2.290721
H      -5.415035     3.289412    -1.435304
H      -3.968639     4.034993    -0.884958
H      -4.390746     0.024444     0.586700
H      -2.715501    -1.793820    1.805746
H      -5.539389    -2.480314     0.458063
H      -4.728365    -3.179834     1.974035

4.769519 -1.260098 2.057746
-0.285648 2.310321 -3.138112
-2.087865 -5.380082 3.946724

S195
space group P2₁2₁2₁ (protomer A), model 3, reactant complex deprotonated

| Atom | X  | Y  | Z  |
|------|----|----|----|
| H    | -6.838136 | -0.905518 | 3.753949 |
| H    | -6.211158 | -2.509663 | 3.613692 |
| H    | -1.120870 | -3.033293 | 0.837535 |
| H    | -2.011844 | -4.624455 | -1.530508 |
| H    | -0.823722 | -5.268635 | -0.371630 |
| H    | -0.539539 | -1.885946 | -1.060213 |
| H    | 1.545627  | -2.484713 | -3.118874 |
| H    | 1.547880  | 0.027601  | -3.455552 |
| H    | -0.164673 | -0.517001 | -3.436154 |
| H    | -0.080196 | 0.140945  | -1.058286 |
| H    | 1.470746  | -2.484713 | 0.078907  |
| H    | 3.247376  | -0.334962 | 0.869500  |
| H    | 2.441552  | -2.736441 | 2.586543  |
| H    | 2.832264  | -1.096574 | 3.125765  |
| H    | 4.823847  | -1.321376 | -0.778611 |
| H    | 7.336364  | -1.673771 | -0.246197 |
| H    | 6.762638  | -3.025233 | 0.771404  |
| H    | 6.625632  | -3.123350 | -1.007107 |
| H    | 0.296133  | -1.398621 | 3.503446  |
| H    | -0.867599 | 6.102650  | -0.580824 |

Zero-point correction= 1.432913 (Hartree/Particle)
Thermal correction to Energy= 1.518506
Thermal correction to Enthalpy= 1.519450
Thermal correction to Gibbs Free Energy= 1.312537
Sum of electronic and zero-point Energies= -4510.648361
Sum of electronic and thermal Energies= -4510.562768
Sum of electronic and thermal Enthalpies= -4510.561823
Sum of electronic and thermal Free Energies= -4510.768737

SOLVENT: -4536.7925751

RX2Aisimpl22REACTANT- SCF Done: -4512.08127371 A.U.

S196
| Atom | x   | y   | z   |
|------|-----|-----|-----|
| C    | -6.317135 | -2.910320 | -2.704153 |
| C    | -6.160664 | -2.047337 | -1.616377 |
| C    | -5.639876 | -2.523285 | -0.412707 |
| C    | -3.078063 | -1.817220 | 1.206554  |
| O    | -3.924076 | -1.686676 | 2.098411  |
| C    | -2.842274 | -0.760705 | 0.125418  |
| C    | -1.428927 | -0.774379 | -0.473689 |
| C    | -1.043416 | 0.455139  | -1.295559 |
| C    | -4.229500 | 1.049754  | 0.534210  |
| O    | -5.407572 | 0.507027  | -0.040266 |
| C    | -4.716717 | 2.513124  | 1.065227  |
| C    | -5.863331 | 2.976689  | 1.353980  |
| C    | -5.944576 | 4.476573  | 1.552415  |
| C    | -5.349138 | 5.050444  | 2.829498  |
| C    | -6.653700 | 5.057867  | 2.618528  |
| N    | 0.336002  | 3.265451  | -0.153263 |
| C    | -2.87472  | 3.769003  | 0.015035  |
| O    | -2.044272 | 3.864997  | 1.136573  |
| C    | -3.920084 | 3.712173  | -2.494008 |
| C    | -5.658899 | 4.153755  | -2.423921 |
| N    | -1.901305 | 4.122018  | -1.226898 |
| C    | -0.544163 | 4.384712  | -1.000148 |
| C    | 0.375187  | 4.633258  | -1.976941 |
| O    | 0.108588  | 4.713834  | -3.192622 |
| C    | 1.631948  | 4.785443  | -1.433509 |
| C    | 2.742442  | 5.298162  | -3.313897 |
| C    | 3.027528  | 4.268490  | -3.449949 |
| C    | 3.919580  | 5.419514  | -1.362002 |
| C    | 2.334607  | 6.671434  | -2.883417 |
| H    | 5.514320  | 3.317332  | 0.622956  |
| H    | 6.078370  | 3.420956  | -0.400535 |
| H    | 5.092930  | 2.780665  | -1.795938 |
| H    | 4.800380  | 0.518250  | 0.078563  |
| H    | 2.709432  | 2.628952  | -0.689174 |
| H    | 2.336300  | 1.057507  | 0.005703  |
| H    | 3.870826  | 0.453361  | 2.165218  |
| H    | 3.867589  | 1.155687  | 4.493058  |
| H    | 3.293623  | 3.227489  | 5.101766  |
| H    | 2.496371  | 4.330169  | 0.942406  |
| H    | 2.599454  | 5.109590  | 3.310757  |
| H    | 4.322215  | 1.292159  | -0.923013 |
| H    | 2.568443  | 0.108115  | -3.313156 |
| H    | 4.505845  | -3.406740 | -2.829349 |
| H    | 3.342159  | -3.282493 | -4.158577 |
| H    | 5.837975  | -2.708112 | -4.932167 |
| H    | 5.761490  | -1.452623 | -3.688042 |
| H    | 5.200480  | -0.520177 | -6.000296 |
| H    | 3.651786  | -1.389729 | -5.936642 |
| H    | 4.012900  | -0.096479 | -5.740819 |
| H    | 0.718867  | -2.683596 | -3.256162 |
| H    | -0.161046 | -3.204999 | -0.742483 |
| H    | -0.603963 | -3.966530 | -3.197971 |
| H    | -1.694562 | -4.876386 | -1.784226 |
| H    | -3.475712 | -2.096004 | -3.059431 |
| H    | -3.400775 | -3.514508 | -2.069211 |
| H    | 0.019638  | -4.232227 | 0.826560  |
| H    | 2.034383  | -6.97453  | 0.526922  |
| H    | 0.778314  | -6.831309 | 1.781967  |
| H    | 2.214805  | -3.711188 | 0.951321  |
| H    | 3.866511  | -3.886032 | 3.410842  |
| H    | 5.362582  | -2.301658 | 2.386578  |
| H    | 4.976734  | -3.522299 | 1.110808  |
| H    | 3.290886  | -1.859219 | 0.448595  |
| H    | 0.958070  | -2.442371 | 2.648466  |
| H    | 1.557927  | 0.322755  | 2.943965  |
| H    | -0.639038 | -0.996334 | 2.151870  |
| H    | -1.166103 | -0.888866 | 3.082682  |
| H    | 0.564975  | 1.758503  | 4.490252  |
| H    | 1.588684  | 2.427925  | 6.766545  |
| H    | -0.137116 | 2.000131  | 6.927043  |
| H    | 1.119144  | 0.770445  | 7.256428  |
| H    | -4.837960 | -3.745120 | 1.825354  |
| H    | -5.036425 | -5.747979 | -1.319966 |

S197
### Table

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | -6.042072  | -4.924238  | -3.430108  |
| H    | -6.732402  | -2.546710  | -3.637189  |
| H    | -6.415126  | -0.995290  | -1.666478  |
| H    | -5.543615  | -1.823127  | 0.404506   |
| H    | -3.574171  | -0.997856  | -0.661020  |
| H    | -0.675673  | -0.850069  | 0.307822   |
| H    | -1.339104  | -1.656428  | -1.103935  |
| H    | -1.106357  | 1.344233   | -0.654298  |
| H    | -2.440797  | 0.964403   | 1.336507   |
| H    | -3.776280  | 2.683121   | 1.829860   |
| H    | -6.582209  | 2.636483   | 0.579429   |
| H    | -6.173001  | 2.464622   | 2.281644   |
| H    | -5.803873  | 5.061791   | 0.650176   |
| H    | -4.818901  | 5.992644   | 2.764485   |
| H    | -4.937247  | 4.344384   | 3.541813   |
| H    | -7.345553  | 6.009626   | 2.417107   |
| H    | -7.458888  | 4.359457   | 3.199645   |
| H    | -5.549573  | 2.749971   | -1.377001  |
| H    | -4.440865  | 3.703134   | -3.441293  |
| H    | -2.035199  | 4.469498   | -3.308755  |
| H    | 1.461724   | 6.565765   | -3.528419  |
| H    | 2.099134   | 7.346376   | -2.053845  |
| H    | 3.169313   | 7.087413   | -3.457057  |
| H    | 3.658988   | 3.630599   | -0.534752  |
| H    | 4.787321   | 5.823137   | -1.895389  |
| H    | 4.170379   | 4.441500   | -0.954829  |
| H    | 2.170491   | 4.235596   | -4.121782  |
| H    | 3.212222   | 3.283765   | -3.049441  |
| H    | 3.912461   | 4.615797   | -4.005867  |
| H    | 4.757695   | -5.389609  | 1.148945   |
| H    | -0.259016  | 4.286779   | -0.020361  |
| H    | -2.490152  | -5.116847  | 0.821515   |
| H    | 6.551011   | 2.104398   | 0.710769   |

### Additional Information

- **Zero-point correction**: 1.448708 (Hartree/Particle)
- **Thermal correction to Energy**: 1.533323
- **Thermal correction to Enthalpy**: 1.534267
- **Thermal correction to Gibbs Free Energy**: 1.328412
- **Sum of electronic and zero-point Energies**: -4511.197373
- **Sum of electronic and thermal Energies**: -4511.112758
- **Sum of electronic and thermal Enthalpies**: -4511.111814
- **Sum of electronic and thermal Free Energies**: -4511.317669

**SOLVENT**: -4537.2840139
O     -3.925394     0.880935    -0.456827
C     -5.061155    -1.448196     0.866300
O     -5.968292    -1.751932     0.043527
N     -4.078049    -2.283596     1.246168
C     -3.985320    -3.653490     0.695171
C     -2.568116    -4.201192     0.881884
S     -1.398968    -3.329904    -0.229995
C     -4.949978    -4.614738     1.444287
O     -4.524179    -5.522709     2.183769
N     -6.262620    -4.363645     1.229672
C     -7.278543    -5.159955     1.929017
O     -1.490533    -1.543536     2.245066
C     -0.380215    -2.143711     2.137448
N      0.570440    -1.972194     3.079480
C      1.949815    -2.542142     3.213065
C      2.957730    -1.406456     3.196292
C      2.936029    -0.441050     4.213285
C      3.806614     0.646772     4.172254
C      4.696537    0.787977    3.103392
C      2.570735    -0.187389     2.301392
C     -0.890135     1.289205     2.538181
O      0.666573     4.969450     0.830104
O     -1.363013    -0.070721     0.096771
N     -0.531504    -0.080071     0.441436
C     -1.268430    -0.187403    -1.317909
C     -2.091360    1.156175    -0.258532
C     -2.087818    2.493807    -1.072849
N      0.885082    2.365138    -1.917314
C      0.364140    1.112175    -1.958271
O      0.674638    0.754986    -2.532207
N      0.694809    -2.804706    -1.017064
C      1.785267    -3.512633    -0.823475
O      3.225145    -3.839187     0.304022
C      3.629882    -3.809650    -2.071654
C      3.924032    -5.303558    -2.215933
C      4.868050    -5.882343    -3.366842
C      4.293820    -5.571224    -4.779838
C      7.180711    -6.892351    -4.138285
N      4.841268    -2.970526    -1.810180
C      4.652180    -1.601239    -2.062494
O      3.648216    -1.186491    -2.704054
C      5.894713    -3.449083    -1.061001
C      6.843686    -2.603236    -0.572399
C      6.708152    -1.203750    -0.766303
C      5.635591    -0.713906    -1.467796
N      5.303710    0.631413    -1.651415
C      5.839559    1.682652    -0.955225
O      6.756668    1.581199    -0.119611
O      5.211531    2.644590    -1.328315
C      5.629448    1.674122    -0.720102
C      5.444515    4.120933     0.804958
C      4.643983    5.140757    -1.373253
C      7.075825    4.662753    -1.134751
H      5.504339    4.736031    -3.945368
H      4.303586    5.562309    -5.063864
H      2.741725    3.784646    -4.901962
H      4.432065    2.828263    -2.691748
H      2.788009    1.289109    -4.681701
H      2.791928    0.736099    -3.004314
H      4.724607    -0.343859    -2.052272
H      6.976759    -1.258663    -2.627518
H     -8.348967    -0.745273    -4.315582
H      5.906072    1.650491    -5.819321
H     -7.390044    0.706123    -6.087236
H     -3.195922    2.278487    -0.878876
H     -6.691756    3.668217    -0.560870
H     -3.166117    4.204710    1.231151
H     -1.617165    5.029672    1.457522
H      3.291023    6.527219    0.400189
H     -3.560927    5.382076    -0.931497
H     -1.968696    7.337232    -1.517457
H     -0.811968    6.739569    -0.310516
H     -1.221246    5.746369    -1.748388
H      0.358014    5.538247    1.602516
H      0.458440    0.982092    2.696683
H      0.449465    3.472506    4.418517
H      1.427735    2.003701    4.632628
H      3.945404    4.391204    3.659783
H      3.601967    3.823871    5.056562
| X         | Y         | Z         |
|-----------|-----------|-----------|
| H         | -1.484303 | -0.224430 | 3.310868 |
| H         | -3.199569 | 1.274086  | 5.238137 |
| H         | -5.558696 | 0.819927  | -5.228339|
| H         | -5.155963 | 1.997561  | 0.864812 |
| H         | -3.071665 | 0.802280  | 0.082171 |
| H         | -3.282451 | -1.937237 | 1.787887 |
| H         | -4.269772 | -3.605882 | -0.362534|
| H         | -2.258435 | -4.072092 | 1.919797 |
| H         | -2.569422 | -5.269820 | 0.667800 |
| H         | -6.515529 | -3.554287 | 0.651669 |
| H         | -8.266238 | -4.801400 | 1.633387 |
| H         | -7.179965 | -6.219718 | 1.670149 |
| H         | -7.167124 | -5.068628 | 3.015350 |
| H         | -2.113838 | -3.249796 | 2.402486 |
| H         | -2.249608 | -0.553257 | 5.048730 |
| H         | 3.789287  | 1.387519  | 4.962207 |
| H         | 5.351691  | 1.648655  | 3.049010 |
| H         | 5.461924  | -0.074011 | 1.884182 |
| H         | 3.942946  | -2.066433 | 1.405078 |
| H         | 1.808023  | -1.792664 | 0.781151 |
| H         | -0.423490 | -1.084156 | -1.186978|
| H         | -0.222303 | -0.313306 | 0.360145 |
| H         | 1.948088  | -0.321804 | -1.824991|
| H         | 3.107968  | 0.810395  | -0.66789 |
| H         | 1.600167  | 1.333427  | 0.697138 |
| H         | 2.997100  | 2.607469  | -1.665671|
| H         | 2.011087  | 3.342408  | -0.393089|
| H         | 0.406771  | 3.121856  | -2.417856|
| H         | 1.380166  | -2.340146 | -1.966422|
| H         | 3.819794  | -3.407444 | -2.973342|
| H         | 4.296751  | -5.696428 | -2.162777|
| H         | 2.961512  | -5.799896 | -2.402666|
| H         | 5.873418  | -5.198969 | -3.248716|
| H         | 4.909595  | -5.171761 | -5.576360|
| H         | 3.230297  | -5.383536 | -4.883471|
| H         | 5.617445  | -7.368745 | -4.597171|
| H         | 3.935000  | -7.572958 | -3.823074|
| H         | 5.926528  | -4.315654 | -0.896670|
| H         | 7.679639  | -2.997713 | -0.013637|
| H         | 7.405474  | -5.097773 | -0.324878|
| H         | 0.970296  | -4.704167 | 0.700203 |
| H         | 7.739281  | 3.087874  | -0.710262|
| H         | 7.157409  | 4.449615  | -2.225990|
| H         | 7.363927  | 5.453161  | -0.767757|
| H         | 4.703851  | 5.049826  | -2.461084|
| H         | 4.891817  | 6.165680  | -1.080678|
| H         | 3.623097  | 4.912207  | -1.057031|
| H         | 6.149654  | 3.408350  | 1.233546 |
| H         | 4.420486  | 3.827733  | 1.054464 |
| H         | 5.636802  | 5.124843  | 1.202487 |
| H         | 1.992301  | -3.091386 | 4.160220 |
| H         | 4.511297  | 0.785495  | -2.276414|
| H         | 0.285437  | -1.358777 | 3.843459 |
| H         | -3.897028 | 5.464837  | -3.333847|

**space group P2_12_1 (protomer A), model 3, product (heteroatoms frozen, free hydrogens)**

| Component | Value                  |
|-----------|------------------------|
| Zero-point correction | 1.440173 (Hartree/Particle) |
| Thermal correction to Energy | 1.505804 |
| Thermal correction to Enthalpy | 1.506748 |
| Thermal correction to Gibbs Free Energy | 1.341604 |
| Sum of electronic and zero-point Energies | -4510.878105 |
| Sum of electronic and thermal Energies | -4510.812473 |
| Sum of electronic and thermal Enthalpies | -4510.811529 |
| Sum of electronic and thermal Free Energies | -4510.976673 |

**SOLVENT:** -4537.1361219
space group $P2_12_12_1$ (protomer B), His41 imidazole
Space group P2_12_12_1 (protomer B), His41 imidazole protonated

Zero-point correction = 0.187849 (Hartree/Particle)
Thermal correction to Energy = 0.197864
Thermal correction to Enthalpy = 0.198808
Thermal correction to Gibbs Free Energy = 0.152133
Sum of electronic and zero-point Energies = -526.214296
Sum of electronic and thermal Energies = -526.204282
Sum of electronic and thermal Enthalpies = -526.203337
Sum of electronic and thermal Free Energies = -526.250013

SOLVENT: -529.4267972

Space group P2_12_12_1 (protomer B), 13b

Zero-point correction = 0.690203 (Hartree/Particle)
Thermal correction to Energy = 0.730116
Thermal correction to Enthalpy = 0.731060
Thermal correction to Gibbs Free Energy = 0.616904
Sum of electronic and zero-point Energies = -1993.623252
Sum of electronic and thermal Energies = -1993.583339
Sum of electronic and thermal Enthalpies = -1993.582395
Sum of electronic and thermal Free Energies = -1993.696550

SOLVENT: -2005.3813133

21
pentil2 SCF Done: -525.996025732 A.U.
N -1.108716 1.687280 0.797907
C -1.363570 0.866788 -0.425295
C -0.143925 0.679863 1.362694
C 1.012413 0.107556 -0.605081
N 2.071950 0.869170 -0.096408
C 2.904010 0.008386 0.607419
N 2.427041 -1.747705 0.592915
C 1.244990 -1.747705 -0.158476
C -1.901440 -1.747705 -0.025264
O -1.787115 -1.499627 -0.777285
N -2.498137 -0.499655 1.187159
H -2.166315 1.383641 -0.982472
H 0.126021 1.632548 -1.833485
H -0.450903 -0.027656 -2.137045
H 3.809272 0.338961 0.974585
H 0.613944 -2.027647 -0.329000
H 2.232755 1.851144 -0.285165
H -0.208979 -2.027647 1.238625
H -2.887928 -1.348728 1.576518
H -2.426133 0.372204 -0.329000
H -1.082236 2.092049 0.603766

22
pentil2H+ SCF Done: -526.402145605 A.U.
N -1.472243 1.641983 0.844663
C -1.471788 0.859667 -0.389023
C -0.158370 0.829856 1.235552
C 1.000196 0.232591 -0.503306
N 2.116572 0.958255 0.053936
C 3.005140 0.139997 0.547366
N 2.476676 -1.096988 0.500608
C 1.237713 -1.069787 -0.141955
C -1.892766 -0.604950 -0.091344
O -1.443110 -1.556364 -0.766122
N -2.764264 -0.692593 0.926940
H -2.250912 1.276446 -1.039449
H 0.082864 1.846653 -1.560775
H -0.356561 0.212269 -2.115734
H 3.949191 0.421619 0.976718
H 0.597268 -1.918780 -0.297866
H 2.248735 1.956904 0.19143
H -0.736172 1.391838 1.505487
H -3.166160 -1.596451 1.182579
H -2.990366 0.150501 1.433027
H -1.570199 2.649050 0.723536
H 2.919224 -1.933683 0.871625

82
RX2B-13 SCF Done: -1994.31345475 A.U.
O 2.310484 -3.602425 1.373981
C 2.987287 -3.247730 0.386868
N 4.277999 -3.612824 0.187873
C 5.225378 -3.079117 -0.821696
C 5.893398 -1.777330 -0.384012
C 7.520623 -1.560624 0.617274
C 7.841822 -3.332257 -0.298820
C 7.067989 0.690736 0.260443
C 5.707103 0.478066 0.496003
C 5.131415 -0.751980 0.183813
C 2.328108 -2.911666 -0.620563
O 2.657263 -2.159717 -1.800163
C 1.92432 -1.506853 0.031437
C -1.032756 -2.088949 -0.034924
C -1.314438 -1.471276 1.477497
C -1.133562 -0.893499 1.900629
C -2.564136 -0.915489 2.513468
N -3.220800 -1.994456 1.747578
H -2.605311 -2.309196 0.560546
O -3.037008 -3.085477 -0.309575
space group P2₁2₁2₁ (protomer B), model 0, product (H-bond between the hydroxyl and the imidazole; heteroatoms frozen, free hydrogens)

GAS: -11387.2832919
SOLVENT: -11449.7545585
| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| N     | -11.06519 | -0.638492 | -2.718132 |
| C     | -11.49881 | -1.715851 | -1.786834 |
| C     | -12.22397 | -2.808868 | -1.557059 |
| C     | -12.24903 | -4.150230 | -0.969539 |
| O     | -9.264665| -2.541419 | 0.342412  |
| N     | -10.46649 | -2.453553 | 1.221438  |
| C     | -9.420829 | -3.050491 | -0.965939 |
| C     | -3.495288 | -3.040281 | -2.606074 |
| C     | -4.913239 | -3.086584 | 2.166743  |
| N     | -4.479756 | -3.347642 | 3.222630  |
| C     | -3.111222 | 3.963543  | 3.248276  |
| C     | -5.425531 | 2.698405  | 3.018273  |
| N     | -3.929757 | 2.361605  | 1.834892  |
| C     | -4.584699 | 3.487468  | 1.326110  |
| C     | -7.389900 | 5.469312  | 1.723161  |
| O     | -7.376503 | 5.713849  | 0.513592  |
| N     | -8.338093 | 4.759255  | 2.310254  |
| C     | -2.799601 | 9.931616  | -3.33920  |
| C     | -2.621371 | 8.566542  | -4.011968 |
| C     | -1.972063 | 7.503133  | -3.123240 |
| S     | -3.125009 | 6.787313  | -1.910268 |
| C     | -3.027691 | 8.002789  | -0.601309 |
| C     | -1.469667 | 10.708542 | -3.331421 |
| O     | -0.639857 | 10.535113 | -2.399740 |
| C     | 2.708356 | -10.317620 | 1.644085 |
| C     | 2.631947 | -9.261762 | 0.825377  |
| C     | 1.445833 | -8.346434 | 0.714406  |
| C     | 1.613283 | -7.150007 | 1.599900  |
| C     | 1.501348 | -7.578971 | 3.084833  |
| C     | 0.334817 | -7.863668 | 3.648510  |
| C     | 0.216416 | -8.020623 | 5.020911  |
| C     | 1.269481 | -6.699904 | 5.849122  |
| C     | 2.563650 | -7.103379 | 3.924854  |
| C     | 2.447823 | -7.266562 | 5.299462  |
| C     | 1.270168 | -7.964241 | -0.742798 |
| O     | 2.241226 | -7.452601 | -1.321564 |
| N     | 0.078106 | -8.176855 | -1.300073 |
| C     | -0.261663 | -7.790804 | -2.689671 |
| O     | -0.723340 | -9.043828 | -3.447111 |
| C     | 0.280994 | -10.201779 | -3.556941 |
| C     | 1.585821 | -9.767880 | -4.213439 |
| C     | -1.348949 | -6.707747 | -2.630454 |
| O     | -1.776748 | -6.324504 | -5.127187 |
| N     | -1.766404 | -6.203616 | -3.802529 |
| C     | -2.905013 | -5.250283 | -3.909455 |
| C     | -3.247077 | -4.885746 | -5.365054 |
| C     | -2.128699 | -4.172481 | -6.109940 |
| C     | -2.143019 | -4.136783 | -7.343524 |
| N     | -1.146328 | -6.325626 | -5.398228 |
| C     | 4.098362 | -5.881254 | -3.178089 |
| O     | -3.453516 | -7.099549 | -3.406607 |
| N     | 0.758232 | -5.105224 | -2.310810 |
| C     | -0.972745 | -5.132601 | -1.519388 |
| C     | -5.558455 | -5.963496 | -0.115083 |
| C     | -6.285638 | -6.300105 | 0.640909  |
| C     | -6.265569 | -6.031292 | 0.240481  |
| O     | -3.754432 | -6.525998 | 1.554785  |
| C     | -3.232824 | -6.907948 | 1.461384  |
| O     | -1.461091 | -5.908888 | 1.157319  |
| C     | -3.922895 | -5.472403 | 2.663600  |
| O     | 0.451153  | -5.863492 | 3.855485  |
| C     | -5.793357 | -4.200186 | 2.279290  |
| C     | -4.115409 | -3.039239 | 3.176866  |
| C     | -2.427988 | -3.710383 | 2.400001  |
| S     | -2.659463 | -1.113719 | 1.790775  |
| C     | -5.281196 | -3.201593 | 4.119108  |
| O     | -6.627478 | -3.710735 | 3.657980  |
| N     | -5.604637 | -3.036022 | 5.411357  |
| C     | -0.798094 | -4.089850 | 6.178707  |
| C     | 0.095321  | -3.970490 | 4.988845  |
| C     | 1.428112  | -3.631040 | 5.113104  |
| C     | 1.969749  | 3.558245  | 3.908347  |
| Atom | X Position | Y Position | Z Position |
|------|------------|------------|------------|
| N    | 1.032541   | -3.816584  | 3.016457   |
| C    | -0.146278  | -4.078912  | 3.664600   |
| C    | -1.250223  | -1.576516  | 6.115111   |
| O    | -2.595966  | -0.748845  | 5.671987   |
| N    | -0.552088  | 0.429143   | 4.793093   |
| C    | -0.240029  | 1.734885   | 5.530590   |
| C    | -1.198130  | 2.086244   | 6.620429   |
| N    | -2.022684  | 3.182852   | 6.553339   |
| C    | 0.248597   | 0.407612   | 3.479590   |
| O    | -0.276577  | 0.931406   | 2.524571   |
| N    | 1.501790   | -0.070524  | 3.425429   |
| C    | 2.316193   | 0.219383   | 2.222801   |
| C    | 2.835239   | 1.68912    | 2.30655    |
| C    | 3.388274   | 1.885463   | 3.384071   |
| S    | 3.686955   | 3.528915   | 3.273283   |
| C    | 3.389136   | 4.493805   | 4.019006   |
| C    | 3.491668   | -0.757008  | 2.024198   |
| O    | 3.911952   | -1.495210  | 2.965611   |
| N    | 4.055371   | -0.751356  | 0.820249   |
| C    | 3.736710   | -1.385006  | 0.564662   |
| C    | 5.331372   | -2.508419  | -0.462036  |
| C    | 4.810190   | -2.103143  | -1.816503  |
| C    | 4.917891   | -3.215830  | -2.857280  |
| O    | 5.562638   | -4.295600  | -2.546472  |
| C    | 6.800723   | 0.226246   | 0.243030   |
| C    | 9.538216   | 0.302965   | 1.60046    |
| C    | 8.767786   | 1.116134   | 2.632575   |
| C    | 8.644326   | 2.064683   | 2.298251   |
| C    | 9.692807   | -0.392167  | -0.859708  |
| O    | 9.518208   | -1.560278  | -1.219914  |
| N    | 10.642103  | 0.380904   | -1.432230  |
| C    | 11.32954   | -0.003412  | -2.664617  |
| C    | 12.340755  | 1.141938   | -2.871157  |
| C    | 11.696032  | 2.311020   | -2.182245  |
| C    | 11.09445   | 1.688286   | -0.834979  |
| C    | 12.075649  | -1.350989  | -2.645220  |
| C    | 12.203810  | -1.936922  | -3.721130  |
| N    | 12.502934  | -1.840645  | -1.478412  |
| C    | 13.253174  | -3.127894  | -1.378647  |
| C    | 12.334185  | -4.327125  | -1.035903  |
| N    | 11.014472  | -4.249121  | -1.296294  |
| C    | 10.041414  | -5.335984  | -1.053147  |
| C    | 9.821350   | -5.638797  | 0.455540   |
| C    | 9.898852   | -6.069969  | 1.316012   |
| C    | 6.374668   | -3.293393  | 4.505947   |
| C    | 5.454686   | -5.147877  | 4.615416   |
| C    | 5.576927   | -5.382641  | 3.409688   |
| C    | 6.184861   | -6.467464  | 3.367281   |
| C    | 6.367313   | -7.050592  | 2.170115   |
| C    | 5.545866   | -6.302525  | 1.432945   |
| C    | 5.060847   | -5.264886  | 2.166233   |
| C    | 4.974462   | 1.290303   | 5.795447   |
| C    | 3.713522   | 0.917369   | 5.722732   |
| C    | 2.778190   | 8.205528   | 4.733871   |
| N    | 3.310572   | 5.724065   | 3.804880   |
| N    | 1.458688   | 8.336451   | 4.905442   |
| C    | 0.494552   | 7.648820   | 4.011505   |
| C    | 0.751660   | 7.178979   | 4.744382   |
| C    | 1.453717   | 8.225019   | 5.579441   |
| C    | -0.902453  | 9.358249   | 5.761211   |
| C    | -2.551592  | 8.688824   | 6.084542   |
| C    | 0.203569   | 8.543654   | 2.796568   |
| C    | -0.867213  | 9.147429   | 2.719365   |
| N    | 1.136022   | 8.555486   | 1.857216   |
| C    | 1.101707   | 9.636555   | 0.613508   |
| C    | 1.518179   | 10.780613  | 1.040191   |
| C    | 2.393139   | 11.542355  | 0.054774   |
| C    | 1.960572   | 8.655012   | -0.469631  |
| C    | 2.908207   | 7.924864   | -0.101572  |
| C    | 1.634150   | 8.812413   | -1.759715  |
| C    | 2.607632   | 8.524059   | -2.860337  |
| C    | 1.957956   | 8.396761   | -4.236837  |
| C    | 2.940451   | 7.910873   | -5.297548  |
| C    | 3.213261   | 7.347577   | -6.492346  |
| C    | 0.994133   | 7.178866   | -6.468472  |
| Atoms | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-------|--------------|--------------|--------------|
| N     | 2.957527     | 7.052198     | -7.544736    |
| C     | 3.673352     | 9.629543     | -2.895267    |
| O     | 3.399072     | 10.760841    | -3.496806    |
| N     | 4.830465     | 9.311941     | -2.316800    |
| O     | -3.656885    | -2.970865    | -0.157315    |
| C     | -3.831829    | -1.845965    | -0.496806    |
| N     | -4.815618    | -1.748225    | -1.214939    |
| C     | -5.496148    | -2.545782    | -5.168682    |
| O     | -3.453152    | 0.959674     | -0.559869    |
| C     | -2.902478    | 0.524663     | -0.391556    |
| C     | -1.505981    | -0.950830    | -0.687251    |
| C     | -0.775424    | -2.299819    | -0.437849    |
| C     | 0.495145     | -2.432646    | -1.285405    |
| N     | 1.743050     | -2.675370    | -2.754773    |
| C     | 1.065962     | -3.954825    | -3.190794    |
| C     | 0.209064     | -2.765370    | -2.754773    |
| C     | 0.495145     | -2.432646    | -1.285405    |
| N     | 0.740530     | 1.210099     | -0.209389    |
| C     | -0.345112    | 1.136384     | -1.107710    |
| O     | -0.575252    | 0.959674     | -0.559869    |
| C     | 1.021966     | 3.781588     | -2.678335    |
| C     | 1.959082     | 4.082916     | -3.667994    |
| C     | 1.704888     | 3.390307     | -3.784614    |
| O     | 1.494778     | 2.732111     | -2.871359    |
| N     | 5.675599     | 1.715854     | -3.753461    |
| C     | 5.709646     | 2.507856     | -4.666186    |
| O     | 8.150086     | 0.864599     | -3.622084    |
| H     | -12.748465   | 2.476771     | -6.307525    |
| H     | -11.948450   | 3.280909     | -4.343027    |
| H     | -10.544688   | 1.991194     | -4.161611    |
| H     | -10.963187   | 2.814873     | -1.797740    |
| H     | -9.615353    | 4.566902     | -2.571547    |
| H     | -8.556583    | 2.849046     | -1.227726    |
| H     | -9.049499    | 1.171366     | -1.553440    |
| H     | -8.169243    | 2.103821     | -2.795414    |
| H     | -10.281042   | -0.888070    | -3.315642    |
| H     | -12.213616   | -1.219306    | -1.126878    |
| H     | -13.231755   | -2.447424    | -2.809875    |
| H     | -11.700606   | -2.922825    | -3.538781    |
| H     | -12.832610   | -4.879209    | -2.448712    |
| H     | -11.231138   | -4.540408    | -1.765915    |
| H     | -12.690862   | -0.075158    | -0.875860    |
| H     | -11.340621   | -2.187195    | 0.788116     |
| H     | -6.931531    | -3.851756    | 0.654401     |
| H     | 7.605218     | -2.428970    | 2.266284     |
| H     | 7.789265     | -1.837469    | 0.608221     |
| H     | -0.949556    | -0.020259    | 1.235381     |
| H     | 10.681185    | -4.502133    | 2.100189     |
| H     | 7.058754     | 0.594183     | 1.264515     |
| H     | 7.983759     | 1.351264     | 2.436654     |
| H     | 6.904793     | -0.019650    | 2.987614     |
| H     | -9.781528    | 0.308042     | 3.731714     |
| H     | -10.606624   | -1.144024    | 3.180639     |
| H     | 9.072066     | -1.274423    | 4.064540     |
| H     | 8.817391     | 3.293277     | 3.998396     |
| H     | 8.603875     | -4.795089    | 3.353899     |
| H     | 6.528355     | 7.217493     | 2.438171     |
| H     | 4.234977     | 6.454135     | 2.796920     |
| H     | 4.828353     | 6.223793     | 1.132439     |
| H     | -2.802021    | 2.050539     | 3.605837     |
| H          | X         | Y         | Z         |
|----------|----------|----------|----------|
| -5.95116 | 3.419933 | 0.378708 |
| -3.857212 | 1.472829 | 1.337983 |
| -5.91164 | 5.141812 | 4.379751 |
| -9.93051 | 4.367929 | 1.762347 |
| -8.22518 | 4.720510 | 3.329256 |
| -3.545202 | 10.51631 | -3.883859 |
| -3.27276 | 9.813391 | -2.303729 |
| -3.603495 | 8.771188 | -0.676884 |
| -3.802690 | 8.771188 | -0.676884 |
| 3.570237 | -10.955806 | 1.391799 |
| 2.791264 | -10.105515 | 2.733642 |
| 3.480867 | -8.751115 | 0.599548 |
| 0.590847 | -8.963760 | 1.052572 |
| 2.569870 | -6.681114 | 1.346126 |
| 0.823126 | -6.427853 | 1.338403 |
| -0.499662 | -8.125241 | 3.014410 |
| -0.718151 | -8.380667 | 5.437496 |
| 1.170468 | -7.806741 | 6.923697 |
| 3.492214 | -6.731662 | 3.512746 |
| 3.296144 | -7.019013 | 5.931040 |
| -0.690914 | -8.521879 | -0.735894 |
| 0.659074 | -7.377435 | -3.113415 |
| 1.649731 | -9.396077 | -2.972447 |
| -1.006812 | -8.475863 | -4.676064 |
| -0.195407 | -10.001612 | -4.135604 |
| 0.486055 | -10.593627 | -2.553675 |
| 2.247709 | -10.624926 | -4.377275 |
| 1.398233 | -9.294755 | -5.181272 |
| 2.118743 | -9.054689 | -3.571359 |
| -1.427272 | -6.601355 | -4.673639 |
| -2.624571 | -4.338362 | -3.365978 |
| -4.171092 | -4.222328 | -5.346940 |
| -3.513634 | -5.786884 | -5.922955 |
| -0.425404 | -3.120968 | -5.904295 |
| -1.668459 | -3.597894 | -4.399118 |
| -4.031888 | -4.258278 | -1.974675 |
| -6.656592 | -4.714088 | -1.439295 |
| -6.383479 | -6.372493 | -2.039121 |
| -3.550155 | -5.828836 | -0.455709 |
| -4.398105 | -7.350387 | -1.874983 |
| -2.062946 | -7.366487 | -2.450229 |
| -2.254530 | -7.811174 | -0.736207 |
| -1.370853 | -5.872065 | 0.161124 |
| -3.811525 | -3.963363 | 1.296634 |
| -3.211643 | -2.952747 | 3.790408 |
| -6.389500 | -9.780830 | 3.043777 |
| -4.994272 | -1.844847 | 1.610386 |
| -5.784110 | -3.239967 | 6.082567 |
| -4.161988 | -2.635304 | 5.730906 |
| 2.962025 | -3.243366 | 6.671130 |
| -1.014118 | -4.380461 | 3.106286 |
| -0.907522 | -2.152827 | 6.955825 |
| 1.167319 | -3.834616 | 1.990177 |
| -0.950325 | -5.169631 | 6.358225 |
| -1.796141 | -3.687788 | 6.038743 |
| -0.278157 | -3.735646 | 7.067319 |
| 0.653965 | 0.975555 | 5.997827 |
| -1.604422 | 0.360845 | 4.513776 |
| 0.797625 | 1.667926 | 5.887613 |
| -0.252977 | 2.534727 | 4.773406 |
| -0.629241 | 2.158274 | 7.557697 |
| -1.755317 | 4.049092 | 6.648845 |
| -2.723316 | 3.212810 | 5.809894 |
| 1.904069 | -0.715268 | 4.105031 |
| 1.674951 | 0.147481 | 1.330959 |
| 1.960822 | 2.310961 | 2.459668 |
| 3.256942 | 1.911032 | 1.328510 |
| 3.455439 | 1.759561 | 4.338359 |
| 4.689377 | 1.143374 | 3.283291 |
| 3.929737 | 4.272719 | 5.089092 |
| 3.595820 | 5.558828 | 3.890113 |
| 2.429496 | 4.293364 | 3.535792 |
| 3.723696 | -0.082753 | 0.107132 |
| 0.566315 | -1.820464 | 1.528815 |
| 6.340625 | -2.92635 | -0.568435 |
| Atom Index | x       | y       | z       |
|------------|---------|---------|---------|
| H          | 4.691228| -3.301927| -0.060225 |
| H          | 3.757809| -1.808946| -1.778629 |
| H          | 5.373522| -1.249455| -2.222748 |
| H          | 7.863809| -1.572175| 0.726660  |
| H          | 8.452242| 1.198043 | -0.084703 |
| H          | 9.686957| -0.730458| 1.945285  |
| H          | 10.539150| 0.735998| 1.480398  |
| H          | 9.194969| 0.936600 | 3.626306  |
| H          | 7.724221| 0.781566 | 2.661113  |
| H          | 8.278248| 3.201356 | 3.021927  |
| H          | 8.414976| 2.813034 | 1.311279  |
| H          | 9.853563| 2.950279| 2.304667  |
| H          | 10.635010| -0.073338| -3.494929 |
| H          | 12.590268| 1.300121| -3.929924 |
| H          | 13.278069| 0.878083| -2.365094 |
| H          | 9.853563| 2.950279| 2.304667  |
| H          | 10.635010| -0.073338| -3.494929 |
| H          | 12.590268| 1.300121| -3.929924 |
| H          | 13.278069| 0.878083| -2.365094 |
| H          | 10.635010| -0.073338| -3.494929 |
| H          | 12.590268| 1.300121| -3.929924 |
| H          | 13.278069| 0.878083| -2.365094 |
| H          | 10.635010| -0.073338| -3.494929 |
| H          | 12.590268| 1.300121| -3.929924 |
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| H          | 13.278069| 0.878083| -2.365094 |
| H          | 10.635010| -0.073338| -3.494929 |
| H          | 12.590268| 1.300121| -3.929924 |
| H          | 13.278069| 0.878083| -2.365094 |
| H          | 10.635010| -0.073338| -3.494929 |
| H          | 12.590268| 1.300121| -3.929924 |
| H          | 13.278069| 0.878083| -2.365094 |
| H          | 10.635010| -0.073338| -3.494929 |
| H          | 12.590268| 1.300121| -3.929924 |
| H          | 13.278069| 0.878083| -2.365094 |
| H          | 10.635010| -0.073338| -3.494929 |
| H          | 12.590268| 1.300121| -3.929924 |
| H          | 13.278069| 0.878083| -2.365094 |
space group P2₁2₁2₁ (protomer B), model 0, product (heteroatoms frozen, free hydrogens)

GAS: -11387.2830860

SOLVENT: -11449.752171
| H         | 2.259490 | -10.627504 | -4.371526 |
|-----------|----------|------------|-----------|
| H         | 1.040693 | -9.298741  | -5.181742 |
| H         | 2.127855 | -9.05897    | -3.566959 |
| H         | -1.414449| -6.602075  | -4.672883 |
| H         | -2.619056| -4.344898  | -3.366780 |
| H         | -4.109777| -2.420696  | -5.344142 |
| H         | -5.06502  | -5.795234  | -5.923497 |
| H         | -0.423915| -3.120671  | -5.905781 |
| H         | -1.71353 | -3.518933  | -4.401272 |
| H         | -4.29493 | -4.263615  | -1.973641 |
| H         | -6.649390| -4.720719  | -1.449991 |
| H         | -3.77782 | -6.380464  | -2.040026 |
| H         | -3.545445| -5.819682  | -0.452434 |
| H         | -4.392625| -7.554530  | 1.874734  |
| H         | -2.057335| -7.362747  | 2.452016  |
| H         | -2.247970| -7.814727  | 0.732198  |
| H         | -1.373782| -5.865101  | 0.161482  |
| H         | -3.803672| -3.959475  | 1.297181  |
| H         | -3.209590| -2.955576  | 3.794065  |
| H         | -4.614345| -0.978589  | 3.084326  |
| H         | -4.893912| -1.852819  | 1.604060  |
| H         | -5.780338| -3.241323  | 6.080423  |
| H         | -4.158934| -2.643893  | 5.726283  |
| H         | 2.963361 | -3.229701  | 3.667493  |
| H         | -1.012363| -4.576084  | 3.099189  |
| H         | -0.905659| -2.156929  | 6.948099  |
| H         | 1.168105 | -3.827674  | 1.997794  |
| H         | -0.947833| -5.167623  | 6.359735  |
| H         | -1.795930| -3.688336  | 6.037010  |
| H         | -0.277507| -3.732979  | 7.067495  |
| H         | 0.658576 | -0.942310  | 5.962502  |
| H         | -1.064645| 0.369924   | 4.503373  |
| H         | 0.789813 | 1.682173   | 5.889370  |
| H         | -0.267559| 2.531157   | 4.763377  |
| H         | -0.609151| 2.060687   | 7.559929  |
| H         | -1.602294| 4.096045   | 6.740152  |
| H         | -2.925194| 3.092235   | 7.014966  |
| H         | -1.901549| -0.722308  | 4.095294  |
| H         | 1.671378 | 0.149341   | 1.338296  |
| H         | 1.965080 | 2.312367   | 2.454057  |
| H         | 3.253965 | 1.911921   | 1.324941  |
| H         | 3.453907 | 1.762800   | 4.381374  |
| H         | 4.487731 | 1.148558   | 3.280786  |
| H         | 3.284385 | 4.274995   | 5.085052  |
| H         | 3.956353 | 5.562184   | 3.887515  |
| H         | 2.425898 | 4.299074   | 3.527406  |
| H         | 3.717955 | -0.091080  | 0.102999  |
| H         | 5.667411 | -1.816172  | 1.526761  |
| H         | 6.343484 | -2.922359  | -0.565833 |
| H         | 4.692856 | -3.298458  | -0.059030 |
| H         | 3.760137 | -1.810035  | -1.778439 |
| H         | 5.375053 | -2.47525   | -2.222477 |
| H         | 7.865279 | -1.567384  | 0.724886  |
| H         | 8.451274 | 1.203249   | -0.085221 |
| H         | 9.686614 | -0.722473  | 1.947316  |
| H         | 10.538586| 0.744071   | 1.481993  |
| H         | 9.928188 | 0.945203   | 3.626958  |
| H         | 7.722906 | 0.788238   | 2.660439  |
| H         | 8.275153 | 3.209085   | 3.020770  |
| H         | 8.411896 | 2.819193   | 1.310385  |
| H         | 9.882412 | 2.958523   | 2.303281  |
| H         | 10.636857| -0.068477  | -3.492853 |
| H         | 12.551664| 1.360378   | -3.928205 |
| H         | 13.278864| 0.886042   | -2.362721 |
| H         | 12.394825| 3.125208   | -1.947801 |
| H         | 10.888707| 2.723389   | -2.804240 |
| H         | 10.26762 | 2.280200   | -0.527005 |
| H         | 11.853858| 1.572368   | -0.154511 |
| H         | 12.257249| -1.355350  | -0.614970 |
| H         | 13.701704| -3.245012  | -2.363269 |
| H         | 14.037843| -3.019926  | -0.618739 |
| H         | 12.807419| -5.181208  | -1.575071 |
| H         | 10.603211| -3.334317  | -1.482849 |
| H         | 10.355258| -6.256104  | -1.533730 |
| H         | 9.109973 | -4.902839  | -1.483156 |
| H         | 10.557080| -6.440927  | 0.702236  |
| H         | 9.307208 | -4.578664  | 2.139313  |
| H         | 10.154209| -3.694561  | 0.926591  |
| H         | 4.420174 | -4.200731  | 4.776683  |
| H         | 5.758379 | -5.118743  | 5.476982  |
space group P2_12_1,(protomer B), model 1, product

Zero-point correction = 2.705923 (Hartree/Particle)
Thermal correction to Energy = 2.864477
Thermal correction to Enthalpy = 2.865421
Thermal correction to Gibbs Free Energy = 2.505958

Sum of electronic and zero-point Energies = -8180.315252
Sum of electronic and thermal Energies = -8180.156698
Sum of electronic and thermal Enthalpies = -8180.155754
Sum of electronic and thermal Free Energies = -8180.515217

SOLVENT: -8227.660279

RX2Bsimpliz SCF Done: -8183.02117474 A.U.

N  5.074624   8.095335  -2.499991
C  4.415109  8.534185  -1.244172
C  3.458281  7.523400  -0.554670
C  4.124078  6.206838  -0.339615
N  4.416322  5.365365  -1.426307
C  5.034082  4.293246  -0.925786
N  5.173444  4.408795  0.429103
C  4.602797  5.631369  0.814442
C  5.492237  8.977728  -0.203921
O  5.270785  8.927785  1.020992
N  6.647216  9.303587  -0.807283
C  -0.549777  -7.008823  -3.973172
N  -0.786307  -5.948765  -2.966978
C   0.421733  -5.353179  -2.398628
C   0.855520  -3.986123  -3.011362
C   1.035368  -4.074493  -4.054443
C   2.283960  -4.415490  -5.038138
C   2.454915  -4.545504  -6.416933
C   1.373112  -3.396727  -7.277701
C  -0.042968  -3.850683  -5.350835
C   0.126551  -3.900483  -6.752778
C   0.267360  -5.133462  -0.885242
O  -0.848207  -4.939202  -0.305467
N   1.444178  -5.138957  -0.222354
C   1.555360  -5.204512  -2.228499
C   2.118482  -6.010932  -1.650209
C   1.249584  -7.759069  1.120855
C  -0.217046  -7.681318  1.605202
C   2.518065  -4.163722  -1.782776
O   3.340802  -3.509381  1.080029
C   2.519660  -4.063776  3.126853
C   3.684817  -3.500408  3.842579
C   3.571422  -3.803643  5.350835
C   2.253608  -3.583115  6.106175
C   2.107539  -4.041531  7.245946
N   1.276739  -2.873970  5.454115
C    4.913139  -4.311488  3.345666
O    4.873690  -5.553882  3.398081
C    5.984336  -3.584139  2.936260
C    7.167975  -4.297505  2.443528
C    7.230859  -4.424264  0.913181
C    8.199445  -4.991438  0.367724
N    6.160417  -3.923898  0.229999
C    6.314539  -4.019358  -1.229146
C    4.944529  -4.829346  -1.744197
C    3.655476  -4.165277  -4.850055
C    6.171249  -2.660410  -1.947648
C    5.920085  -2.593568  -3.169323
C    6.964445  -1.602443  -1.777335
C    6.632734  -0.286665  -1.763201
C    6.377894  0.795946  -0.686605
S    4.570305  0.868052  -0.404338
C    8.034765  -0.060359  -2.390843
O    8.994363  -0.815544  -2.205152
N    8.043015  1.074113  -3.148428
C    4.304534  -1.565866  -5.582139
C    3.129429  -1.042674  -4.708798
C    2.981275  -0.321565  -5.197061
C    1.108967  -0.371080  -4.185011
N    1.615388  -1.024016  -3.087549
C    2.897920  -1.459437  -3.413874
C    4.517333  1.705630  -3.811014
O    5.413603  2.265596  -3.118920
N    3.216982  2.040284  -3.861519
C    2.639924  3.193798  -3.156010
C    1.795586  4.043804  -4.149775
C    2.638381  5.186854  -4.782245
N    2.976881  6.270400  -3.827020
C    1.778152  2.842474  -1.931042
O    1.988456  3.392395  -0.807100
N    0.715011  2.044753  -2.131412
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | -0.361869    | 1.956058     | -1.137197    |
| C       | -1.167237    | 3.290305     | -1.070411    |
| C       | -1.783288    | 3.697493     | -2.418450    |
| S       | -2.365885    | 5.447225     | -2.387279    |
| C       | -0.768400    | 6.320157     | -2.608504    |
| C       | -1.325847    | 0.841657     | -1.532361    |
| O       | -1.347735    | 0.391030     | -2.704036    |
| N       | -2.180151    | 0.511763     | -0.545504    |
| C       | -3.464919    | -0.151290    | -0.805531    |
| C       | -3.673624    | -1.391879    | 0.086138     |
| C       | -3.655297    | -1.031801    | 1.577617     |
| O       | -3.789911    | -2.221732    | 2.474786     |
| O       | -4.589074    | -3.196450    | 1.906279     |
| C       | -5.563652    | 0.164711     | -1.052297    |
| C       | -6.868579    | 1.564221     | -0.707241    |
| C       | -7.384274    | 2.222426     | -2.09564     |
| C       | -6.252939    | 2.903048     | -2.876903    |
| C       | -5.546389    | 4.027676     | -2.072221    |
| O       | -7.902821    | 0.775323     | -0.080299    |
| O       | -9.063051    | 1.463182     | 0.377021     |
| N       | -10.114547   | 0.724417     | 1.135153     |
| C       | -11.22452    | 1.843356     | 1.487288     |
| C       | -10.206450   | 3.686363     | 1.715492     |
| C       | -9.178312    | 2.943650     | 0.565215     |
| O       | -11.284235   | -1.368417    | 1.058329     |
| O       | -10.080722   | -0.354908    | -0.957751    |
| C       | -11.249323   | -1.505071    | -1.770373    |
| O       | -10.066566   | -2.116841    | -2.548890    |
| C       | -9.030237    | -2.551742    | -1.610970    |
| C       | -7.823749    | -3.193651    | -2.161786    |
| C       | -7.158563    | -2.431442    | -3.333800    |
| C       | -6.954250    | -0.999908    | -2.910595    |
| C       | -3.097574    | -0.128829    | -4.538715    |
| C       | -3.477647    | -1.546409    | -4.996004    |
| C       | -3.325034    | -2.523395    | -3.862545    |
| C       | -4.023189    | -3.616424    | -3.722535    |
| C       | -3.766947    | -4.305479    | -2.665598    |
| C       | -2.653832    | -3.714118    | -2.109734    |
| C       | -2.369997    | -2.573629    | -2.867400    |
| O       | 5.625573     | -1.191250    | 1.588134     |
| C       | 5.097487     | -0.202090    | 2.166182     |
| N       | 5.997766     | -0.130735    | 3.517268     |
| C       | 4.622653     | 0.917137     | 4.476380     |
| C       | 4.132611     | 0.209687     | 5.724766     |
| C       | 5.030353     | -0.483806    | 6.548893     |
| C       | 4.563237     | -1.205720    | 7.649177     |
| C       | 3.195878     | -1.223489    | 7.944606     |
| C       | 2.306750     | -0.500294    | 7.146362     |
| C       | 2.766854     | 0.206298     | 6.032442     |
| C       | 4.362410     | 0.900241     | 1.394878     |
| C       | 4.761391     | 2.163941     | 2.026607     |
| C       | 2.815979     | 0.709276     | 1.645247     |
| C       | 2.133476     | -0.331613    | 0.742771     |
| C       | 0.715026     | -0.635684    | 1.253717     |
| C       | 0.696371     | -1.222777    | 2.681655     |
| C       | -0.374367    | -2.349884    | 2.647174     |
| N       | -0.511179    | -2.632350    | 1.190070     |
| C       | 0.081244     | -1.728343    | 0.387866     |
| C       | 0.121056     | -1.789555    | -0.865289    |
| C       | 2.173515     | 2.023295     | 1.543971     |
| C       | 1.348943     | 2.481410     | 2.555751     |
| C       | 1.283928     | 1.910845     | 3.678249     |
| C       | 0.590653     | 3.647192     | 2.119335     |
| C       | 1.319903     | 4.964740     | 2.006524     |
| C       | 0.720959     | 5.860804     | 0.937214     |
| C       | 0.470867     | 7.338959     | 1.188267     |
| C       | -0.709213    | 6.377425     | 1.084693     |
| C       | -0.700817    | 3.695731     | 2.974840     |
| C       | -1.701591    | 2.775027     | 2.640525     |
| C       | -1.493319    | 1.938871     | 1.702601     |
| C       | -0.767048    | 4.482909     | 4.101372     |
| C       | -1.884173    | 4.481610     | 4.880671     |
| C       | -2.989694    | 3.678025     | 4.517248     |
| C       | -2.926786    | 2.860828     | 3.409175     |
| N       | -3.953497    | 2.019719     | 2.965368     |
|     | X          | Y          | Z          |
|-----|------------|------------|------------|
|     | -5.003076  | 1.619469   | 3.757116   |
| O   | -5.255258  | 2.649103   | 4.893200   |
| O   | -5.741137  | 0.641965   | 3.107261   |
| C   | -6.233722  | 0.176367   | 3.936847   |
| C   | -7.162533  | 1.285591   | 2.986179   |
| C   | -7.888149  | 0.744994   | 3.326021   |
| O   | -5.987763  | -0.768560  | 5.157870   |
| C   | 3.844939   | 9.444222   | -1.474335  |
| C   | 2.567927   | 7.382699   | -1.77505   |
| O   | 3.161283   | 7.849716   | 0.404906   |
| C   | 5.333883   | 3.446677   | -1.51622   |
| C   | 5.611222   | 3.642949   | 1.043948   |
| C   | 5.104888   | 7.177380   | -2.337992  |
| H   | 7.454770   | 9.600523   | -0.261440  |
| C   | 6.667334   | 9.186752   | -1.823087  |
| C   | -1.516212  | -7.357125  | -4.341387  |
| H   | 0.099773   | -6.654801  | -4.831660  |
| C   | 1.079390   | -6.957577  | -2.542767  |
| H   | 3.123278   | -4.548713  | -4.363552  |
| H   | 3.428098   | -4.801711  | -6.819507  |
| C   | 1.505047   | -4.242144  | -8.34950   |
| H   | -1.005524  | -3.562775  | -4.963814  |
| H   | -0.711483  | -3.801041  | -7.416858  |
| C   | 3.147540   | -4.860632  | 1.278278   |
| H   | 2.183015   | -6.646443  | 2.742710   |
| C   | 1.702093   | -8.699863  | 1.456498   |
| H   | 0.058648   | -6.681436  | -4.831660  |
| H   | 1.431084   | -5.238266  | -3.309395  |
| H   | -1.247207  | -6.060796  | -2.542222  |
| C   | 1.743007   | -7.754568  | 0.025706   |
| C   | -0.757518  | -8.594801  | 1.332237   |
| H   | -0.256955  | -7.577009  | 2.697130   |
| H   | -0.737959  | -6.836749  | 1.143528   |
| H   | 3.149342   | -4.588224  | 3.679138   |
| C   | 3.774799   | -2.432646  | 3.636191   |
| H   | -0.631989  | -3.226581  | 5.882237   |
| H   | 3.811579   | -4.868704  | 5.480344   |
| C   | 0.436175   | -2.669935  | 5.984725   |
| H   | 1.504039   | -2.253503  | 4.689938   |
| C   | 5.867311   | -2.616412  | 2.598025   |
| H   | 8.082307   | -3.768855  | 2.761488   |
| C   | 7.151873   | -5.302211  | 2.865846   |
| H   | 5.356923   | -3.543469  | 0.723586   |
| C   | 7.058478   | -4.349199  | -1.496040  |
| H   | 5.024889   | -4.900128  | -2.829020  |
| C   | 4.965141   | -5.827218  | -1.290639  |
| H   | 3.614226   | -3.761735  | -0.556016  |
| C   | 6.541395   | -1.701726  | -0.168093  |
| H   | 5.809779   | -0.193551  | -2.567638  |
| C   | 6.727851   | 1.762772   | -1.040514  |
| H   | 6.898648   | 0.533511   | 0.237107   |
| C   | 8.903702   | 1.339749   | -3.611367  |
| H   | 7.187042   | 1.625173   | -3.282838  |
| C   | 0.099884   | -0.038856  | -4.213590  |
| H   | 3.491652   | -2.078550  | -2.766965  |
| C   | 4.750895   | 0.857620   | -4.454914  |
| H   | 1.099499   | -1.232634  | -2.217376  |
| C   | 4.034615   | -2.177365  | -6.259124  |
| H   | 5.148870   | -1.673099  | -4.966958  |
| C   | 4.576453   | -0.496549  | -6.209399  |
| H   | 2.624166   | 1.446111   | -4.462838  |
| C   | 3.448039   | 3.800830   | -2.759639  |
| C   | 1.374502   | 3.384292   | -4.919616  |
| H   | 0.986774   | 4.902026   | -3.615596  |
| C   | 2.084945   | 5.612373   | -5.627429  |
| C   | 2.120080   | 6.700268   | -3.458256  |
| C   | 3.546912   | 5.916412   | -3.036541  |
| C   | 0.580848   | 1.529663   | -2.998244  |
| C   | 0.053093   | 1.757982   | -0.153529  |
| H   | -0.475691  | 4.063630   | -0.735914  |
| H   | 1.957518   | 3.181587   | -0.326599  |
| H   | -1.067785  | 3.576104   | -3.235388  |
| H   | -2.662019  | 3.084508   | -2.642527  |
| H   | -0.397880  | 6.211639   | -3.631387  |
| H   | -0.950834  | 7.379728   | -2.405894  |
| C   | -0.016373  | 5.955330   | -1.903078  |
| H   | -2.105337  | 1.022948   | 0.340991   |
H  -3.491499  -0.461102  -1.848993
H  -4.632583  -1.850229  -0.169275
H  -2.882982  -2.105146  -0.142487
H  -2.755730  -0.480078   1.862637
H  -4.513665  -0.396050   1.829770
H  -5.981037  -0.170309  -1.692781
H  -6.476418   2.324132  -0.089666
H  -7.868370   1.454671  -2.694508
H  -8.142747   2.969373  -1.827962
H  -6.680530   3.316191  -3.798828
H  -5.514399   2.146722  -3.164750
H  -4.869104   4.581057  -2.708848
H  -5.002997   3.619716  -1.225365
H  -6.307801   4.739248  -1.692215
H   9.685406   0.294719   2.041754
H  -11.725083   1.576454   2.356227
H  -11.791122   2.016918   0.627368
H  -10.742665   4.019462   1.683809
H   9.693730   2.970345   2.677707
H   8.207448   3.378106   0.813305
H   9.562598   3.413802  -0.344999
H  -10.346601   4.283333  -1.409184
H  -11.631405  -2.233720  -1.053010
H  -12.045638  -1.201665  -2.458653
H  -10.432910  -2.918025  -3.117503
H  -8.821142  -1.875240  -0.874864
H  -8.606773  -4.207781  -2.506917
H  -7.102442  -3.273139  -1.341282
H  -7.815477  -0.390221  -3.730966
H  -7.788978  -0.723565  -2.378595
H  -2.530428  -1.469126  -5.545453
H  -4.262722  -1.965720  -5.675857
H  -4.193905  -5.214691  -2.281641
H  -1.570700  -1.900230  -2.626915
H  -4.802578  -0.199761  -3.912454
H  -3.103347   0.320852  -3.957107
H  -4.127085   0.508457  -5.401933
H  -2.060557  -4.135929  -1.375098
H   5.596069  -0.899548   3.972067
H   3.812343   1.487739   4.038948
H   5.451395   1.598976   4.689120
H   6.095702  -0.452690   6.336223
H   5.259541  -1.750320   8.276271
H   2.825280  -1.820582   8.767100
H   1.249019  -0.501865   7.381260
H   2.081470   0.759077   5.398978
H   2.951515   0.403323   2.638398
H   2.077542   0.020502  -0.291209
H   2.723382  -1.255522   0.755832
H   0.075914   0.251302   1.217940
H   0.492362  -0.450277   3.424542
H   1.678034  -1.603262   2.869082
H  -0.028394  -3.240185   3.175805
H  -1.321338  -2.040357   3.084233
H  -0.873809  -3.512428   0.801202
H   2.094826   2.480305   0.607114
H   0.157624   3.422955   1.118690
H   2.334077   4.705719   1.685985
H   1.403632   5.474673   2.969598
H   1.051917   5.753999  -0.055148
H   0.719037   7.730349   2.168830
H   0.646371   8.022493   0.367988
H  -1.328021   6.403340   0.195679
H  -1.235258   6.133422   1.998664
H   0.093058   5.803737   4.320817
H  -1.924072   5.102701   5.767799
H  -3.886923   3.661477   5.114355
H  -3.972772   1.798891   1.952491
H   3.909775   2.704756   1.980451
H  -5.604292   0.021485   5.843527
H  -5.115953  -1.322112   4.824059
H  -6.608652  -1.457215   5.667517
H  -7.530105   1.333197   4.987317
H  -8.302105   1.191431   3.417201
H  -8.667680   0.158599   4.823488
H  -6.349624  -1.946705   2.729313
H  -7.574405  -0.882089   2.057195
H  -7.954852  -1.875635   3.481747
H   4.389355   7.949676  -3.258273
space group P2₁2₁2₁ (protomer B), model 1, product (H-bond of the hydroxyl with the imidazole)

Zero-point correction= 2.706216 (Hartree/Particle)
Thermal correction to Energy= 2.864091
Thermal correction to Enthalpy= 2.865036
Thermal correction to Gibbs Free Energy= 2.506132
Sum of electronic and zero-point Energies= -8180.361862
Sum of electronic and thermal Energies= -8180.203987
Sum of electronic and thermal Enthalpies= -8180.203043
Sum of electronic and thermal Free Energies= -8180.561947

SOLVENT: -8227.6690997
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| C    | 2.638381 | 5.188854 | -4.782245 |
| N    | 2.976881  | 6.270400  | -3.827020  |
| C    | 1.778152  | 2.842474  | -1.931042  |
| O    | 1.988456  | 3.392395  | -0.807100  |
| N    | 0.715011  | 2.044753  | -2.131412  |
| C    | -0.361869 | 1.956058  | -1.137197  |
| C    | -1.167237 | 3.290305  | -1.070411  |
| C    | -1.783288 | 3.697493  | -2.418450  |
| S    | -2.365885 | 5.447225  | -2.387279  |
| C    | -0.768400 | 6.320157  | -2.698594  |
| C    | -1.325847 | 0.841657  | -1.532361  |
| N    | -1.347735 | 0.391030  | -2.704036  |
| C    | -2.180151 | 0.517163  | -0.545504  |
| N    | -3.464919 | -0.151290 | -0.805531  |
| C    | -3.673624 | -1.391879 | 0.086138   |
| C    | -3.655297 | -1.031801 | 1.577617   |
| C    | -3.899176 | -2.221732 | 2.474786   |
| O    | -4.589074 | -3.196450 | 1.906279   |
| O    | -3.30219  | -2.352240 | 3.612234   |
| C    | -4.556758 | 0.882073  | -0.510484  |
| C    | -4.126279 | 1.880195  | 0.238992   |
| N    | -5.576362 | 0.648471  | -1.052297  |
| C    | -6.868579 | 1.564221  | -0.770241  |
| C    | -7.384274 | 2.222426  | -2.079564  |
| O    | -6.252939 | 2.903048  | -2.876903  |
| N    | -5.564389 | 4.026767  | -2.072221  |
| C    | -7.900281 | 0.775323  | -0.080229  |
| N    | -9.003051 | 1.461382  | 0.377021   |
| C    | -10.114547 | 0.724417 | 1.135153   |
| N    | -11.122452 | 1.843536 | 1.487288   |
| C    | -10.206450 | 3.068636 | 1.715492   |
| C    | -9.178312 | 2.943684  | 0.565215   |
| O    | -10.776289 | -0.445597 | 0.404543   |
| O    | -11.284235 | -1.368417 | 1.058329   |
| N    | -10.807220 | -0.354908 | -0.957751  |
| C    | -11.249323 | -1.505071 | -1.770373  |
| C    | -10.086566 | -2.116841 | -2.548090  |
| N    | -9.030237 | -2.551742 | -1.610970  |
| C    | -7.823749 | -3.193651 | -2.161786  |
| C    | -7.158563 | -2.431442 | -3.338000  |
| N    | -6.954250 | -0.999908 | -2.910595  |
| C    | -3.909754 | -0.128829 | -4.538715  |
| C    | -3.477647 | -1.546409 | -4.996004  |
| C    | -3.325034 | -2.523295 | -3.862545  |
| N    | -4.403219 | -3.616424 | -3.722535  |
| C    | -3.769647 | -4.305479 | -2.665598  |
| N    | -2.653832 | -3.714118 | -2.109734  |
| C    | -2.369997 | -2.573629 | -2.867400  |
| N    | 5.625573 | -1.192550 | 1.588134   |
| C    | 5.097487 | -0.202808 | 2.166182   |
| N    | 5.097706 | -0.130735 | 3.517268   |
| C    | 4.622653 | 0.917137  | 4.476380   |
| C    | 4.132611 | 0.209887  | 5.724766   |
| C    | 5.030353 | -0.483806 | 6.548893   |
| C    | 4.563257 | -1.205720 | 7.649177   |
| C    | 3.915878 | -2.223489 | 7.944606   |
| C    | 2.306730 | -0.500294 | 7.146362   |
| C    | 2.768654 | 0.206298  | 6.033442   |
| C    | 4.362410 | 0.900241  | 1.394878   |
| C    | 4.761391 | 2.163941  | 2.026607   |
| C    | 2.815979 | 0.709276  | 1.645247   |
| C    | 2.133476 | -0.331613 | 0.742771   |
| C    | 0.715026 | -0.635684 | 1.253717   |
| C    | 0.696371 | -1.222777 | 2.681655   |
| C    | 0.374367 | -2.349884 | 2.647174   |
| N    | -0.511179 | -2.632350 | 1.190070   |
| C    | 0.081244 | -1.728343 | 0.387866   |
| C    | 0.121056 | -1.789555 | -0.865289  |
| C    | 2.173515 | 2.023295  | 1.543971   |
| C    | 1.348943 | 2.448140  | 2.557551   |
| C    | 1.283928 | 1.910445  | 3.678249   |
| C    | 0.596563 | 3.647192  | 2.193335   |
| C    | 1.319903 | 4.964740  | 2.006524   |
| C    | 0.728959 | 5.860804  | 0.937214   |
| C    | 0.470867 | 7.338959  | 1.188267   |
| C    | -0.792913 | 6.777425 | 1.084693   |
| C    | -0.700817 | 3.695731  | 2.974840   |
| C    | -1.701591 | 2.775067  | 2.640525   |
| C    | -1.489319 | 1.938871  | 1.702601   |
|   |   |   |   |
|---|---|---|---|
| H | -2.662019 | 3.084508 | -2.642527 |
| H | -0.397880 | 6.211639 | -3.631387 |
| H | -0.950834 | 7.379728 | -2.405894 |
| H | -0.016373 | 5.955330 | -1.903078 |
| H | -2.103537 | 1.022948 | 0.346991 |
| H | -3.491499 | -0.461102 | -1.848993 |
| H | -4.632583 | -1.850229 | -0.169275 |
| H | -2.882982 | -2.105146 | -0.142487 |
| H | -2.755730 | -0.480078 | 1.862637 |
| H | -4.513665 | -0.396050 | 1.829770 |
| H | -5.981037 | -0.170309 | -1.692781 |
| H | -6.476418 | 2.324132 | -0.089666 |
| H | -7.868370 | 1.456671 | -2.694508 |
| H | -8.142747 | 2.969373 | -1.827962 |
| H | -6.680530 | 3.316191 | -3.798828 |
| H | -5.514399 | 2.146722 | -3.164750 |
| H | -4.869104 | 4.581057 | -2.708848 |
| H | -5.002997 | 3.619716 | -2.223365 |
| H | -6.307801 | 4.739248 | -1.992215 |
| H | -9.685406 | 0.294719 | 2.041754 |
| H | -11.720083 | 1.576545 | 2.356227 |
| H | -11.779122 | 2.016918 | 0.627368 |
| H | -10.742665 | 4.019462 | 1.683809 |
| H | -9.693730 | 2.970345 | 2.677707 |
| H | -8.207448 | 3.378106 | 0.813505 |
| H | -9.562598 | 3.413802 | -0.344999 |
| H | -10.346601 | 0.428333 | -1.239844 |
| H | -11.631405 | -2.237370 | -1.053010 |
| H | -12.045638 | -1.201665 | -2.458653 |
| H | -10.432910 | -2.981625 | -3.117503 |
| H | -8.821142 | -1.875240 | -0.874864 |
| H | -8.060773 | -4.207781 | -2.509617 |
| H | -7.102442 | -2.371369 | -1.341282 |
| H | -7.815474 | -2.486131 | -4.214359 |
| H | -8.663477 | -0.390221 | -3.739666 |
| H | -7.788978 | -0.723565 | -2.378959 |
| H | -2.304248 | -1.469126 | -5.545453 |
| H | -4.226722 | -1.965720 | -5.675857 |
| H | -4.193905 | -5.214691 | -2.281641 |
| H | -1.570700 | -1.900230 | -2.626915 |
| H | -4.802578 | -0.199761 | -3.912454 |
| H | -3.103347 | 0.320858 | -3.957107 |
| H | -4.127085 | 0.508457 | -5.404193 |
| H | -2.060557 | -4.135929 | -1.375098 |
| H | 5.590609 | -0.899548 | 3.972067 |
| H | 3.812343 | 1.487379 | 4.038948 |
| H | 5.451395 | 1.589876 | 4.689120 |
| H | 6.095702 | -0.452690 | 6.336223 |
| H | 5.259541 | 1.750302 | 8.276271 |
| H | 2.825200 | -1.820582 | 8.767100 |
| H | 1.249019 | -0.301865 | 7.381260 |
| H | 2.081470 | 0.759077 | 5.398978 |
| H | 2.695115 | 0.403323 | 2.683898 |
| H | 2.077542 | 0.020502 | -0.291209 |
| H | 2.723382 | 1.255522 | 0.755832 |
| H | 0.075914 | 0.251392 | 1.217940 |
| H | 0.492362 | -0.450277 | 3.424542 |
| H | 1.678034 | 1.669126 | 2.869082 |
| H | -0.028394 | -3.240185 | 3.175805 |
| H | -1.321338 | -2.040357 | 3.084233 |
| H | -0.873809 | -3.512428 | 0.801202 |
| H | 2.094826 | 2.480305 | 0.607114 |
| H | 0.157624 | 3.429555 | 1.118690 |
| H | 2.334027 | 4.705719 | 1.685985 |
| H | 1.403632 | 5.474673 | 2.969598 |
| H | 1.051917 | 5.573999 | -0.055148 |
| H | 0.719037 | 7.730349 | 2.168830 |
| H | 0.646371 | 8.022493 | 0.367088 |
| H | -1.328021 | 6.403340 | 0.195679 |
| H | -1.235258 | 6.133422 | 1.998664 |
| H | 0.093058 | 5.927377 | 4.320817 |
| H | -1.924972 | 5.102701 | 5.767799 |
| H | -3.886923 | 3.661477 | 5.114355 |
| H | -3.972772 | 1.798981 | 1.952491 |
| H | 3.909775 | 2.704756 | 1.980451 |
| H | -5.649292 | 0.021495 | 5.843527 |
| H | -5.115953 | -1.322112 | 4.824059 |
| H | -6.680652 | -1.457215 | 5.667517 |
| H | -7.530105 | 1.533197 | 4.987317 |
| H | -8.302105 | 1.191431 | 3.417201 |
space group P2_12_12_1 (protomer B), model 1, product (heteroatoms frozen, free hydrogens)

| Zero-point correction= | 2.691285 (Hartree/Particle) |
|------------------------|-------------------------------|
| Thermal correction to Energy= | 2.809530                     |
| Thermal correction to Enthalpy= | 2.810474                     |
| Sum of electronic and zero-point Energies= | -8179.769669 |
| Sum of electronic and thermal Energies= | -8179.651424 |
| Sum of electronic and thermal Enthalpies= | -8179.650480 |
| Sum of electronic and thermal Free Energies= | -8179.921673 |

SOLVENT: -822 7.3967724
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| N       | -0.099670| 4.308802 | 2.748795 |
| C       | -1.321110| 3.630158 | 2.531053 |
| O       | -1.418413| 4.597625 | 4.582093 |
| C       | -2.237784| 2.759310 | 3.469432 |
| N       | -3.605373| 3.058528 | 3.202424 |
| C       | -4.724102| 3.044442 | 3.937459 |
| O       | -4.885060| 3.601799 | 4.960610 |
| O       | -5.866642| 2.273462 | 3.511218 |
| C       | -7.389847| 0.355280 | 3.392711 |
| C       | -7.407064| 1.965992 | 5.308774 |
| C       | -5.300326| 0.460335 | 4.981319 |
| H       | 8.268084 | 9.056745 | 0.424901 |
| H       | 6.024589 | 8.452069 | -0.357185|
| H       | 6.385226 | 7.924293 | 1.305013 |
| H       | 4.647673 | 4.314024 | -2.102582|
| H       | 6.515843 | 5.018666 | 1.580999 |
| H       | 5.380993 | 3.143878 | 0.144459 |
| H       | 7.913036 | 7.377490 | -1.914517|
| H       | 10.665621| 6.037443 | 0.917147 |
| H       | 10.119943| 6.676213 | -0.653183|
| H       | -2.16423 | -8.629560| -3.09118 |
| H       | -1.203538| -7.566884| -4.100301|
| H       | -2.148312| -6.954714| -1.867766|
| H       | 0.782738 | -8.40106 | -1.976549|
| H       | -1.114699| -4.460475| -2.117460|
| H       | 0.619358 | -4.282011| -1.840004|
| H       | 2.127956 | -5.71529  | -3.604147|
| H       | 2.663005 | -5.538781| -5.986029|
| H       | 0.999825 | -4.665859| -7.578449|
| H       | -1.739857| -4.103733| -4.358677|
| H       | -1.225942| -3.980271| -6.744308|
| H       | 1.810972 | -6.759974| 0.010141 |
| H       | 0.175104 | -5.987577| 2.358790 |
| H       | 2.450869 | -8.039968| 2.164500 |
| H       | 1.623727 | -7.632368| 3.655658 |
| H       | 0.829999 | -9.764601| 2.830602 |
| H       | 0.371306 | -9.964173| 1.271019 |
| H       | -1.617861| -9.341145| 2.817826 |
| H       | -0.863990| -8.205559| 3.951878 |
| H       | -1.358295| -7.660927| 2.325750 |
| H       | 2.048449 | -5.734996| 4.285992 |
| H       | 3.442221 | -3.166078| 3.560853 |
| H       | 4.659592 | -3.451749| 5.705245 |
| H       | 3.959370 | -5.065830| 5.916747 |
| H       | 0.939151 | -2.324344| 5.967915 |
| H       | 1.862001 | -2.507784| 4.518217 |
| H       | 5.279671 | -2.923191| 2.408052 |
| H       | 7.681146 | -3.354154| 2.126874 |
| H       | 7.317455 | -5.081579| 2.393426 |
| H       | 4.722274 | -4.173428| 0.576040 |
| H       | 5.851767 | -5.297951| 1.855283 |
| H       | 3.614532 | -5.123578| -2.720109|
| H       | 3.565712 | -5.867373| -1.095739|
| H       | 2.646071 | -4.020917| -0.312199|
| H       | 5.243320 | -2.043345| -0.775880|
| H       | 4.996140 | -0.592111| -3.110085|
| H       | 6.341840 | 1.174070 | -1.902741|
| H       | 6.490792 | 0.505742 | -0.555324|
| H       | 7.851938 | -0.574327| -5.055134|
| H       | 6.208792 | 0.017650 | -4.825826|
| H       | -1.141656| -0.658650| -3.828751|
| H       | 2.706479 | -2.034313| -2.964985|
| H       | 3.148857 | -0.826637| -6.351988|
| H       | 0.406821 | -1.605165| -2.075425|
| H       | 3.065731 | -2.248626| -6.292107|
| H       | 3.883153 | -0.877600| -5.610024|
| H       | 2.515824 | -0.689920| -6.818864|
| H       | 1.493095 | 1.938915 | -5.401323|
| H       | 3.553215 | 2.853021 | -3.437896|
| H       | 1.375821 | 4.466285 | -4.858799|
| H       | 2.279532 | 0.990349 | -3.483290|
| H       | 3.012215 | 5.183888 | -6.218294|
| H       | 3.850156 | 6.890008 | -4.850758|
| H       | 4.876265 | 5.833885 | -4.056444|
| H       | 0.099739 | 1.846281 | -3.672558|
| H       | -0.124704| 2.223281 | -0.796068|
|   H   |       X       |       Y       |       Z       |
|-------|--------------|--------------|--------------|
|  X    |  Y           |  Z           |
|  -0.231462 | 4.355605 | -1.549338 |
|  -1.665804 | 4.015678 | -0.680274 |
|  -1.694100 | 4.074381 | -2.739057 |
|  -0.552937 | 6.831279 | -2.209634 |
|  -2.321411 | 1.857793 | 0.101932 |
|  -8.048165 | 0.471236 | -1.836979 |
|  -5.048842 | -0.948353 | -0.072345 |
|  -3.542211 | -1.298638 | -0.424616 |
|  -2.632575 | -0.159897 | 1.635480 |
|  -2.844246 | 0.377557 | 1.959302 |
|  -6.364235 | 0.662156 | -1.295242 |
|  -7.014473 | 3.273674 | -0.094652 |
|  -7.997172 | 1.770856 | -2.571988 |
|  -8.879102 | 3.167820 | -1.969449 |
|  -7.259316 | 3.681782 | -3.856672 |
|  -5.932156 | 3.306284 | -2.754077 |
|  -6.399845 | 5.772973 | -2.755310 |
|  -6.762113 | 3.102340 | -1.166862 |
|  -8.089928 | 5.461187 | -2.296762 |
|  -9.694436 | 1.517766 | 2.731512 |
|  -11.584216 | 2.869399 | 3.151600 |
|  -12.10446 | 2.730709 | 1.457092 |
|  -11.139735 | 4.993112 | 1.555678 |
|  -9.768661 | 4.395094 | 2.514551 |
|  -8.855873 | 4.325436 | 0.294344 |
|  -10.389955 | 3.750614 | -0.390694 |
|  -10.894401 | 0.806419 | -0.510152 |
|  -12.582977 | -1.300894 | 0.681558 |
|  -12.681835 | -0.768066 | -1.025261 |
|  -11.620394 | -3.105435 | -0.311453 |
|  -9.396359 | -1.352708 | 0.200250 |
|  -9.200489 | -4.248499 | -0.225384 |
|  -7.941221 | -3.032754 | 0.107107 |
|  -9.106250 | -4.040639 | -2.466359 |
|  -7.665867 | -2.011388 | -3.399113 |
|  -8.638832 | -1.312222 | -2.157085 |
|  -2.451226 | -1.366936 | -5.266739 |
|  -6.398020 | -2.100087 | -6.282024 |
|  -5.364577 | -5.386084 | -3.364096 |
|  -2.762068 | -2.262235 | -2.386770 |
|  -5.456619 | -0.756747 | -5.001375 |
|  -4.101725 | 0.097501 | -4.191629 |
|  -4.332614 | 0.255369 | -5.940011 |
|  -3.932840 | -4.298093 | -1.566174 |
|  6.395800 | -1.244421 | 2.192216 |
|  5.988748 | 1.443664 | 3.235074 |
|  7.578930 | 0.663371 | 3.009701 |
|  8.281122 | -1.170071 | 4.435055 |
|  7.970091 | -2.483369 | 6.521159 |
|  5.805062 | -2.326674 | 7.752403 |
|  3.987009 | -0.918831 | 6.875303 |
|  4.294333 | 0.398631 | 4.783543 |
|  2.723519 | 0.653056 | 2.490267 |
|  1.894457 | -0.448886 | -0.255402 |
|  2.675114 | -1.458418 | 0.946912 |
|  0.103639 | 0.138794 | 1.461978 |
|  0.535820 | -0.649092 | 3.639855 |
|  1.783640 | -1.718487 | 3.002011 |
|  0.346885 | -3.292923 | 2.358690 |
|  -1.019485 | -2.488664 | 3.674893 |
|  -1.159663 | -3.531414 | 1.280114 |
|  1.986744 | 2.231188 | 0.050250 |
|  0.477739 | 4.067528 | 0.756792 |
|  3.034457 | 4.614193 | 1.959802 |
|  1.938902 | 5.766170 | 2.641224 |
|  2.934960 | 5.610232 | -0.178689 |
|  1.906453 | 7.817431 | 1.768593 |
|  2.866203 | 8.100293 | 0.230815 |
|  1.070072 | 6.929959 | -1.102450 |
|  0.079711 | 6.695028 | 0.481177 |
|  0.990929 | 5.554207 | 4.041523 |
|  -0.846778 | 5.879070 | 5.696354 |
|  -0.340739 | 4.718040 | 5.291896 |
|  -3.676627 | 2.880465 | 2.245904 |
|  4.000898 | 2.756146 | 1.680379 |
|  -4.733908 | 1.114590 | 5.654254 |
|  -4.621750 | 0.026065 | 4.250195 |
space group P2_12_12_1 (protomer B), model 1, product

Zero-point correction = 2.706216 (Hartree/Particle)
Thermal correction to Energy = 2.864091
Thermal correction to Enthalpy = 2.865036
Thermal correction to Gibbs Free Energy = 2.506132
Sum of electronic and zero-point Energies = -8180.361862
Sum of electronic and thermal Energies = -8180.203987
Sum of electronic and thermal Enthalpies = -8180.203043
Sum of electronic and thermal Free Energies = -8180.561947

SOLVENT: -8227.6690997

RX2Bisimpl2 SCF Done: -8183.06807831 A.U.
C      2.964234    -2.267008    -2.895576
C      4.486339     0.694382    -4.373713
O      5.473573     1.418803    -4.042655
N      3.190896     1.043825    -4.245293
C      2.838438     2.317803    -3.609651
C      2.566931     3.444614    -4.641115
C      3.797368     3.736528    -5.544554
N      4.189666     5.189627    -5.419706
C      1.701282     2.345535    -2.585346
O      1.662023     3.369390    -1.835507
N      0.767723     1.386960    -2.531796
C     -0.389570     1.544259    -1.626364
C     -1.294383     2.737015    -2.060174
C     -1.831571     2.572307    -3.492781
S     -2.364210     4.181537    -4.212472
N     -0.715090     4.897164    -4.558408
C     -1.251833     3.017333    -1.664047
O     -1.243681    -0.495498    -2.635150
N     -2.151653     0.271731    -0.642717
C     -3.423086     0.463919    -0.692130
C     -3.604328    -1.387605     0.530867
C     -3.606328    -0.593808     1.845554
C     -3.719957    -1.454221     3.062424
O     -4.478724    -2.585455     2.815602
N     -7.622522    -0.584111    -0.259863
C     -7.917322    -0.593231     0.163160
N     -9.037265     1.381813     0.008870
C     -10.98677     0.867655     0.921299
C     -11.08961     2.053847     0.985734
C     -10.15855     3.286298     0.900667
C     -9.129311     2.693792    -0.175406
C     -10.781590    -0.432190     0.489255
O     -11.316112    -1.158985     1.339328
N     -10.800124    -0.671111    -0.855446
C     -11.250934    -1.975996    -1.370603
C     -10.666581    -2.774596    -1.957713
N     -9.060083    -2.992683    -0.917085
C     -7.856712    -3.766435    -1.273318
C     -7.166981    -3.347989    -2.591799
N     -6.932142    -1.847520    -2.543431
C     -3.844143    -1.355684    -4.298132
C     -3.885098    -2.862867    -4.372775
C     -3.394443    -5.310318    -3.023895
N     -4.225858    -4.523475    -2.603562
C     -3.800225    -4.905886    -1.395629
C     -2.690058    -4.192697    -1.009497
C     -2.388263    -3.304001    -2.044037
O     -5.331110    -0.947034     1.460005
C     -5.063946     0.244340     1.825775
N     -5.302212     0.603171     3.105966
C     -5.161154     1.935507     3.759232
C     -4.456502     1.814836     5.097017
C     -5.142164     1.305553     6.209123
C     -4.523932     1.235456     7.459507
C     -3.214745     1.703152     7.614406
C     -2.524790     2.212263     6.507436
C     -3.133068     2.290457     5.246737
C     -4.392096     1.256311     0.882622
C     -5.031776     2.492296     1.134047
C     -2.865590     1.234646     1.273903
C     -2.152790    -0.041102     0.772748
C     -0.769503    -0.249490     1.395834
C     -0.789345    -0.468803     2.924317
C     -0.294672    -1.554055     3.184726
N     -0.414955    -2.219061     1.858071
C     -0.169318     1.550048     0.842079
C     -0.230627    -1.956132    -0.349667
C     -2.175542     2.443768     0.818623
C     -3.399227     3.109744     1.654270
C     -1.229661     2.885574     2.879947
C     -0.432412     4.116666     0.922796
C     -1.125649     5.391351     0.400842
C  0.276061  6.039980  -0.679132
C  0.238651  7.558908  -0.834482
C -0.989014  6.811337  -0.323699
N -0.744021  4.351294  1.793533
C -1.739064  3.374699  1.740451
O -1.560879  2.336189  1.026160
C -0.755238  5.367221  2.717015
C -1.834466  5.551208  3.529549
C -2.952059  4.690736  3.410708
N -3.961583  2.706965  2.330608
C -4.998786  2.526826  3.203006
O -5.253441  3.242666  4.190302
O -5.729455  1.401290  2.848989
C -6.706920  0.830808  3.866468
C -7.134869  -0.506418  3.254640
C -7.885813  1.306593  3.975346
C -5.994194  0.609421  5.210337
H  3.683097  9.406306  -1.611879
H  3.444948  7.471998  -3.088747
H  2.458263  7.226884  -1.629897
H  5.635180  3.221410  -2.685239
H  4.149102  5.648211  0.442782
H  4.574130  5.293344  -3.795803
H  6.086941  7.097972  -1.591325
H  5.061504  8.938262  -1.896718
H  5.821045  9.238202  0.300240
H -1.605392  -8.161043  -2.392430
H  0.020597  -7.749942  -2.997861
H -1.408105  -5.840344  -2.039182
H  1.226713  -6.508983  -1.060218
H  0.083711  -3.832912  -1.941893
H  1.727252  -4.181128  -1.577092
H  3.167430  -5.469821  -3.024884
H  3.593239  -6.368124  -5.312186
H  1.746830  -6.419291  -6.979265
H -0.916742  -4.706142  -4.062008
H -0.506650  -5.583442  -6.353831
H  2.362524  -5.216570  0.387320
H  0.716487  -4.454546  2.768061
H  3.124437  -6.354071  2.765999
H  2.255524  -5.809214  4.210182
H  1.542836  -8.085081  3.567417
H  1.087912  -7.328009  1.952587
H -0.894040  -7.784160  3.564297
H -0.221878  -6.452742  4.529033
H -0.761125  -6.170739  2.849744
H  2.060531  -3.563021  4.571074
H  3.729496  -1.407141  3.694620
H  3.718527  -0.889863  6.067549
H  3.643236  -2.627082  6.463700
H  0.157645  -0.393310  6.300825
H  1.709931  0.222236  6.309850
H  5.666203  -2.003306  2.716072
H  8.079857  -2.795529  3.447869
H  7.188319  -4.219000  4.099850
H  5.316177  -3.484608  1.454499
H  7.134478  -4.916624  -0.406343
H  5.133100  -5.669116  -1.593377
H  5.010791  -6.093961  0.147571
H  3.679785  -3.901746  0.195512
H  6.065253  -1.744188  -0.001637
H  5.678464  -1.007294  -2.736504
H  6.578773  1.258918  -1.860250
H  6.780811  0.469818  -0.281694
H  8.793625  -0.029389  -4.132863
H  7.117640  0.494471  -3.931062
H  0.163979  -1.098724  -4.066742
H  3.549227  -2.096169  -2.102488
H  4.622236  -0.291772  -4.811541
H  1.158906  -1.750052  -1.802970
H  4.059111  -3.720345  -5.476399
H  5.193328  -2.990379  -4.317488
H  4.700185  -2.109508  -5.808540
H  2.506779  0.354469  -4.587761
H  3.700171  2.614074  -3.018659
H  1.697706  3.172160  -5.246698
H  2.317247  4.333186  -4.054316
H  3.580012  3.462992  -6.844988
H  3.412987  5.801389  -5.700649
| H | 5.004183 | 5.400057 | -6.010492 |
| H | 0.854538 | 0.513637 | -3.048542 |
| H | -0.036779 | 1.727227 | -0.615937 |
| H | -0.692447 | 3.639293 | -1.985143 |
| H | -2.123448 | 2.812753 | -1.354147 |
| H | -1.074685 | 2.125042 | -4.144848 |
| H | -2.710560 | 1.920280 | -3.506214 |
| H | -0.210699 | 4.341967 | -5.354361 |
| H | -0.868316 | 5.931215 | -4.881213 |
| H | -0.088575 | 4.894837 | -3.662129 |
| H | -2.103708 | 1.035939 | 0.050420 |
| H | -3.447250 | -1.069735 | -1.596253 |
| H | -5.45777 | -1.932967 | 0.425390 |
| H | -2.78308 | -2.108986 | 0.526543 |
| H | -2.721437 | 0.039130 | 1.946281 |
| H | -4.480097 | 0.067840 | 1.890922 |
| H | -5.954820 | -0.745737 | -1.557943 |
| H | -6.454105 | 2.073725 | -0.647858 |
| H | -7.785277 | 0.381431 | -2.987328 |
| H | -8.144161 | 2.238676 | -2.493997 |
| H | -6.437166 | 2.206244 | -4.460542 |
| H | -5.478882 | 1.260807 | -3.563252 |
| H | -4.923308 | 3.770583 | -3.642751 |
| H | -5.039582 | 3.134539 | -1.995680 |
| H | -6.389873 | 4.069722 | -2.695348 |
| H | -9.675537 | 0.663264 | 1.906219 |
| H | -11.691813 | 2.019785 | 1.894591 |
| H | -11.748784 | 2.016271 | 0.110895 |
| H | -10.683491 | 4.204072 | 0.626952 |
| H | -9.649243 | 3.429162 | 1.85551 |
| H | -8.152896 | 3.32018 | -0.035425 |
| H | -9.504018 | 3.100857 | -1.176000 |
| H | -11.660215 | -2.505166 | -0.513403 |
| H | -12.028744 | -1.835084 | -2.134598 |
| H | -10.440375 | -3.743117 | -1.315065 |
| H | -8.840138 | -2.157472 | -0.371116 |
| H | -8.106088 | -4.832485 | -1.359956 |
| H | -7.144534 | -3.643933 | -0.452587 |
| H | -7.817724 | -3.598326 | -3.439158 |
| H | -6.975632 | -1.474380 | -3.482010 |
| H | -7.772165 | -1.420040 | -2.135239 |
| H | -2.551312 | -2.974880 | -4.939499 |
| H | -4.268527 | -3.410878 | -4.907971 |
| H | -4.233608 | -5.681008 | -0.789542 |
| H | -1.586466 | -2.593196 | -1.992643 |
| H | -4.727016 | -1.215529 | -3.668543 |
| H | -3.006959 | -0.810067 | -3.859026 |
| H | -4.048850 | -0.954722 | -5.298150 |
| H | -2.070059 | -4.426239 | -0.211559 |
| H | 5.754296 | -0.115782 | -3.673614 |
| H | 4.649992 | 2.589414 | 3.058979 |
| H | 6.168605 | 2.343603 | 3.906226 |
| H | 6.172201 | 0.977960 | 6.100598 |
| H | 5.603290 | 0.836741 | 8.310289 |
| H | 2.739342 | 1.675349 | 8.588173 |
| H | 1.515319 | 2.594995 | 6.622255 |
| H | 2.570038 | 2.692797 | 4.390206 |
| H | 2.814487 | 1.268151 | 2.363529 |
| H | 2.036154 | 0.005979 | -0.313604 |
| H | 2.778786 | -0.913798 | 0.995806 |
| H | 0.091526 | 0.576737 | 1.154107 |
| H | 0.633741 | 0.464556 | 3.460212 |
| H | 1.767123 | -0.863095 | 3.209745 |
| H | 0.014517 | -2.272936 | 3.944075 |
| H | -1.242466 | -1.155981 | 3.490365 |
| H | -0.722215 | -3.170682 | 1.700112 |
| H | 2.195656 | 2.710998 | -0.170913 |
| H | 0.055485 | 3.602019 | 0.047561 |
| H | 2.056846 | 5.064236 | -0.063015 |
| H | 1.396739 | 6.976061 | 1.187203 |
| H | 0.251236 | 4.545327 | -1.591043 |
| H | 0.844233 | 8.116090 | -0.131418 |
| H | 0.191033 | 7.962761 | -1.840533 |
| H | -1.835230 | 6.710674 | -0.993797 |
| H | -1.242252 | 6.908639 | 0.723915 |
| H | 0.116191 | 6.000996 | 2.742504 |
| H | -1.836568 | 6.356346 | 4.250908 |
| H | -3.824569 | 4.816773 | 4.031049 |
| H | -3.971961 | 2.207641 | 1.424561 |
|                |                |
|----------------|----------------|
| Space group    | P2_1_2_1       |
| Protomer       | B              |
| Model          | 1              |
| Product        | (heteroatoms frozen, free hydrogens) |

Zero-point correction= 2.690987 (Hartree/Particle)
Thermal correction to Energy= 2.809229
Thermal correction to Enthalpy= 2.810174
Thermal correction to Gibbs Free Energy= 2.537905
Sum of electronic and zero-point Energies= -8179.770358
Sum of electronic and thermal Energies= -8179.652115
Sum of electronic and thermal Enthalpies= -8179.651171
Sum of electronic and thermal Free Energies= -8179.923440

SOLVENT: -8227.3940938

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| Element | Atomic Number | Coordinates |
|---------|---------------|-------------|
| C       | 6             | 8.528225, 7.996905, -1.333937 |
| N       | 7             | 8.094136, 8.024667, 0.086547 |
| O       | 8             | 8.830411, 7.189121, 2.183624 |

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| Element | Atomic Number | Coordinates |
|---------|---------------|-------------|
| C       | 6             | 8.094136, 8.024667, 0.086547 |
| N       | 7             | 8.830411, 7.189121, 2.183624 |
| O       | 8             | 8.830411, 7.189121, 2.183624 |

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| Element | Atomic Number | Coordinates |
|---------|---------------|-------------|
| C       | 6             | 8.094136, 8.024667, 0.086547 |
| N       | 7             | 8.830411, 7.189121, 2.183624 |
| O       | 8             | 8.830411, 7.189121, 2.183624 |

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| Element | Atomic Number | Coordinates |
|---------|---------------|-------------|
| C       | 6             | 8.094136, 8.024667, 0.086547 |
| N       | 7             | 8.830411, 7.189121, 2.183624 |
| O       | 8             | 8.830411, 7.189121, 2.183624 |
| Atom | x-coordinate | y-coordinate | z-coordinate |
|------|--------------|--------------|-------------|
| N    | 0.568425     | -0.844562    | -5.110443   |
| C    | -0.128983    | -0.961796    | -3.992431   |
| N    | 0.675313     | -0.844562    | -5.110443   |
| C    | -0.128983    | -0.961796    | -3.992431   |
| N    | 0.675313     | -0.844562    | -5.110443   |
| C    | 1.926003     | -1.601942    | -3.573938   |
| C    | 3.391327     | 1.243537     | -5.374427   |
| O    | 4.539090     | 1.196091     | -4.847637   |
| N    | 2.400197     | 2.018895     | -4.917825   |
| C    | 2.554594     | 3.013824     | -2.634299   |
| C    | 0.196009     | 3.122597     | -1.550313   |
| S    | -0.635480    | 2.468791     | -1.79472    |
| C    | -1.14045     | 3.796828     | -2.75977    |
| S    | -2.79038     | 6.095907     | -2.459103   |
| C    | -1.85073     | 7.036516     | -2.845891   |
| C    | -1.843135    | 1.526381     | -1.851205   |
| O    | -2.14457     | 1.017083     | -2.949215   |
| N    | -2.563433    | 1.344303     | -0.748796   |
| C    | -3.917600    | 0.729652     | -0.783576   |
| O    | -4.029615    | -0.556808    | 0.023080    |
| N    | -3.685557    | -0.415877    | 1.483998    |
| C    | -3.953912    | -1.688072    | 2.286507    |
| O    | -4.569066    | -2.669955    | 1.707115    |
| N    | -3.552684    | -1.696698    | 3.488064    |
| C    | -4.994988    | 1.757360     | -0.339401   |
| C    | -6.957301    | 3.686556     | -2.792525   |
| C    | -7.053083    | 5.097723     | -2.210488   |
| O    | -8.623804    | 0.412674     | 0.390800    |
| N    | -9.373270    | 2.330660     | 0.798566    |
| C    | -10.229923   | 1.764237     | 1.842373    |
| O    | -11.256937   | 2.896518     | 2.118185    |
| N    | -10.485879   | 4.140989     | 1.738413    |
| C    | -9.732940    | 3.721394     | 0.490902    |
| C    | -10.986683   | 0.472839     | 1.486766    |
| C    | -11.267289   | -0.286486    | 2.415087    |
| N    | -11.260469   | 0.212279     | 0.206079    |
| C    | -12.012007   | -1.008339    | -0.218164   |
| C    | -11.079983   | -2.166495    | -0.630220   |
| O    | -9.801725    | -2.185444    | -0.209167   |
| C    | -8.820793    | -3.248355    | -0.532127   |
| C    | -8.407403    | -3.294619    | -0.01735    |
| N    | -8.351130    | -2.125027    | -2.67595    |
| C    | -4.408460    | -0.418632    | -5.097749   |
| C    | -3.502771    | -1.638256    | -6.030459   |
| C    | -3.800573    | -2.697789    | -4.298590   |
| N    | -4.683030    | -3.738455    | -4.559642   |
| C    | -4.777639    | -4.478660    | -3.481346   |
| C    | -4.051097    | -3.950232    | -2.530727   |
| O    | -3.454500    | -2.820149    | -2.997785   |
| O    | 4.098936     | -1.321681    | 0.805871    |
| N    | 5.055521     | -0.281430    | 1.360532    |
| C    | 5.935315     | -0.350536    | 2.025693    |
| C    | 6.501571     | 0.464677     | 3.210122    |
| C    | 6.289713     | 0.346025     | 4.483151    |
| C    | 7.325023     | -1.162848    | 4.979044    |
| C    | 7.154378     | -1.891012    | 6.149979    |
| C    | 5.947235     | -1.809302    | 6.835953    |
| C    | 4.914626     | -1.001274    | 6.337617    |
| C    | 5.082339     | -0.267620    | 5.163575    |
| C    | 4.217012     | 0.918779     | 0.973353    |
| C    | 4.756970     | 2.083518     | 1.635225    |
| C    | 2.740563     | 0.659881     | 1.405313    |
| C    | 2.027609     | -0.594119    | 0.826636    |
| C    | 0.652561     | -0.821281    | 1.465263    |
| C    | 0.732834     | -1.147271    | 2.876043    |
| C    | -0.194780    | -2.629012    | 2.978086    |
| O    | -0.703437    | -2.691688    | 1.620046    |
| C    | -0.195255    | -1.829004    | 0.736031    |
| O    | -0.379710    | -1.813737    | -0.478536   |
| N    | 2.065972     | 1.918503     | 1.047896    |
| C    | 1.589842     | 2.686662     | 2.038028    |
| H | 2.300117 | 5.088470 | -3.455747 |
| H | 3.007542 | 5.092227 | -6.222401 |
| H | 3.905118 | 5.074393 | -3.656439 |
| H | -0.118031 | 2.224238 | -0.786418 |
| H | -0.223298 | 4.558322 | -1.529483 |
| H | -0.223298 | 4.558322 | -1.529483 |
| H | -2.830865 | 3.667494 | -2.894121 |
| H | -1.666070 | 6.902559 | -3.886581 |
| H | -1.675284 | 7.083368 | -2.707569 |
| H | -0.540158 | 6.832599 | -2.186436 |
| H | -2.314116 | 1.852497 | 0.111619 |
| H | -0.082707 | 0.481052 | -1.836248 |
| H | -5.051240 | -0.943518 | -0.077905 |
| H | -3.355617 | -1.293577 | -0.428053 |
| H | -2.635417 | -0.164027 | 1.635412 |
| H | -4.286132 | 0.376075 | 1.959845 |
| H | -6.363547 | 0.672467 | -1.293083 |
| H | -7.009837 | 3.282406 | -0.887567 |
| H | -7.992255 | 1.589466 | -2.571180 |
| H | -8.873271 | 3.185747 | -1.965453 |
| H | -7.520215 | 3.703115 | -3.849093 |
| H | -5.925236 | 3.217708 | -2.745342 |
| H | -6.388880 | 5.789705 | -2.740434 |
| H | -6.753360 | 5.114064 | -1.156091 |
| H | -8.078889 | 5.479193 | -2.858657 |
| H | -9.690638 | 1.522232 | -2.729486 |
| H | -11.583826 | 2.875712 | 3.152272 |
| H | -11.02394 | 2.763286 | 1.456792 |
| H | -11.134310 | 5.003873 | 1.563621 |
| H | -9.763358 | 4.400147 | 2.251874 |
| H | -8.850138 | 4.336201 | 0.302645 |
| H | -10.384509 | 3.766467 | -0.392355 |
| H | -10.891487 | 0.821880 | -0.515394 |
| H | -12.588886 | -1.284934 | 0.608820 |
| H | -12.683408 | -0.746635 | -1.037335 |
| H | -11.626729 | -3.088015 | -0.330909 |
| H | -9.400638 | -1.341689 | 0.192551 |
| H | -9.208473 | -2.435360 | -0.244815 |
| H | -7.947649 | -3.022734 | 0.092645 |
| H | -9.111927 | -4.019844 | -2.485495 |
| H | -7.653173 | -1.987462 | -3.396861 |
| H | -8.363184 | -1.295093 | -2.161693 |
| H | -2.449311 | -1.349929 | -5.269490 |
| H | -3.695966 | -2.076959 | -6.289065 |
| H | -5.370788 | -5.703707 | -3.383464 |
| H | -2.763843 | -2.253793 | -2.393246 |
| H | -5.543813 | -0.736761 | 0.004647 |
| H | -4.097142 | 0.115151 | -4.192833 |
| H | -4.328499 | 0.278184 | -5.940841 |
| H | -3.937575 | -2.489889 | -1.580488 |
| H | 6.389600 | -1.265034 | 2.195173 |
| H | 5.975584 | 1.417208 | 3.232139 |
| H | 7.567987 | 0.640178 | 3.024369 |
| H | 8.272531 | -1.201197 | 4.441907 |
| H | 7.957375 | -2.521232 | 6.524872 |
| H | 5.918537 | -2.364465 | 7.754187 |
| H | 3.977007 | -0.949093 | 6.880032 |
| H | 4.289615 | 0.379797 | 4.790038 |
| H | 2.726956 | 0.645048 | 2.498204 |
| H | 1.892418 | -0.453188 | -0.251063 |
| H | 2.699760 | -1.469531 | 0.948251 |
| H | 0.106263 | 0.133998 | 1.465585 |
| H | 0.532243 | -0.662377 | 3.640516 |
| H | 1.776646 | -1.734112 | 2.990317 |
| H | 0.336784 | -3.544747 | 3.251540 |
| H | -1.028434 | -2.462325 | 3.696950 |
| H | -1.166712 | -3.536979 | 1.271518 |
| H | 2.047439 | 2.248288 | 0.074245 |
| H | 0.479322 | 0.409887 | 0.775163 |
| H | 3.026797 | 4.567676 | 1.955155 |
| H | 1.961627 | 5.476288 | 2.671344 |
| H | 2.923728 | 5.826565 | -0.153680 |
| H | 1.919390 | 7.082239 | 1.800553 |
| H | 2.868875 | 8.104905 | 0.271578 |
| H | 1.077743 | 6.932773 | -1.075655 |
| H | 0.089747 | 6.687366 | 0.443155 |
| H | 0.996942 | 5.531726 | 4.063867 |
**space group P2_12_1_21 (protomer B), model 3, Mpro (imidazole tautomer)**

| Zero-point correction | 0.899646 (Hartree/Particle) |
|-----------------------|-----------------------------|
| Thermal correction to Energy | 0.954609 |
| Thermal correction to Enthalpy | 0.955554 |
| Thermal correction to Gibbs Free Energy | 0.810289 |
| Sum of electronic and zero-point Energies | -3004.267348 |
| Sum of electronic and thermal Energies | -3004.212384 |
| Sum of electronic and thermal Enthalpies | -3004.211440 |
| Sum of electronic and thermal Free Energies | -3004.356704 |

**SOLVENT:** -3021.5170532
space group P2\(_1\)2\(_1\)2\(_1\) (protomer B), model 3, reactant complex (imidazole tautomer)

|          | Energy            | Enthalpy           | Free Energy         |
|----------|-------------------|--------------------|---------------------|
| Zero-point correction | 1.593118 (Hartree/Particle) | | |
| Thermal correction to Energy | 1.688579 | | |
| Thermal correction to Enthalpy | 1.689524 | | |
| Thermal correction to Gibbs Free Energy | 1.460891 | | |
| Sum of electronic and zero-point Energies | -4998.016624 | | |
| Sum of electronic and thermal Energies | -4997.921162 | | |
| Sum of electronic and thermal Enthalpies | -4997.920128 | | |
| Sum of electronic and thermal Free Energies | -4998.148850 | | |

SOLVENT: -5026.9533040
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -0.29336  | 4.422206  | -6.42706  |
| C    | -0.176359 | 5.804286  | -4.439766 |
| C    | -0.261973 | 5.664533  | -5.829158 |
| C    | -1.198398 | 4.011525  | -0.091683 |
| O    | -0.512514 | 4.742864  | 0.678954  |
| N    | -2.093469 | 4.919443  | 1.413616  |
| C    | -2.453958 | 2.941205  | 1.740859  |
| C    | -3.889717 | 3.504619  | 2.098766  |
| C    | -4.075328 | 4.919443  | 1.413616  |
| C    | -3.176562 | 5.973843  | 2.098766  |
| O    | -0.993416 | 1.726989  | 5.647474  |
| N    | -0.078346 | -0.410317 | 5.430469  |
| N    | -1.056062 | 1.469578  | 6.114632  |
| S    | -3.946765 | -0.876894 | 3.436978  |
| O    | -4.924093 | -0.562137 | 4.137082  |
| N    | -3.974015 | -1.757778 | 2.406317  |
| C    | -5.323551 | -2.332817 | 1.925114  |
| C    | -5.710506 | -1.735864 | 0.589618  |
| O    | -6.559450 | -2.311577 | -0.116532 |
| N    | -5.134269 | -0.552706 | 0.247175  |
| C    | -5.448092 | 0.025284  | -1.070013 |
| C    | -4.718450 | 1.362595  | -1.252560 |
| O    | -3.265805 | 1.224282  | -1.361115 |
| N    | -5.107440 | -0.976063 | -2.190062 |
| O    | -5.859872 | -1.135852 | -3.176857 |
| N    | -3.980219 | -1.701252 | -1.983346 |
| C    | -3.776669 | -2.932948 | -2.779699 |
| C    | -2.304801 | -3.156922 | -2.824810 |
| S    | -1.257536 | -1.861991 | -3.160894 |
| C    | -4.695182 | -3.948144 | -2.053275 |
| O    | -4.320255 | -4.677633 | -1.101988 |
| N    | -5.980036 | -3.866171 | -2.456229 |
| C    | -2.315292 | -2.104502 | 0.208782  |
| C    | -1.700762 | -3.199104 | 0.383586  |
| O    | -2.315441 | -4.362630 | 0.623425  |
| N    | -1.573457 | -5.01987 | 1.218424  |
| O    | -0.604548 | -4.956526 | 2.262298  |
| C    | -1.027886 | -3.984114 | 3.185096  |
| O    | -0.098684 | -3.364059 | 4.023967  |
| N    | 1.250025  | -3.727735 | 3.966546  |
| C    | 1.666289  | -4.723989 | 3.082823  |
| C    | 0.745238  | -5.526636 | 2.227602  |
| C    | 0.187986  | -3.264206 | 0.136925  |
| O    | 0.182659  | -4.102656 | -0.702180 |
| C    | 0.715125  | -2.258786 | 0.789073  |
| O    | 0.300119  | -0.803061 | 0.384901  |
| C    | 1.216080  | 0.227067  | 1.053557  |
| O    | 1.134036  | 0.273492  | 2.597269  |
| C    | 1.171957  | 1.790821  | 2.960014  |
| N    | 0.780047  | 2.439014  | 1.689938  |
| O    | 0.861081  | 1.639417  | 0.597411  |
| C    | 0.704176  | 2.014500  | -0.587713 |
| O    | 2.095342  | -2.511624 | 0.384019  |
| C    | 3.142169  | -3.310504 | 1.213926  |
| O    | 3.082890  | -1.240912 | 2.450621  |
| C    | 4.484386  | -2.195969 | 0.449747  |
| C    | 5.323102  | -3.747972 | 0.847070  |
| O    | 6.496394  | -3.433678 | -0.570811 |
| C    | 7.711599  | -4.187812 | -0.360977 |
| C    | 7.688679  | -2.597578 | -0.299382 |
| N    | 5.101572  | -0.971421 | 1.035982  |
| O    | 4.596016  | 0.222516  | 0.514333  |
| O    | 3.976838  | 0.257544  | -0.597083 |
| C    | 5.727109  | -1.027336 | 2.260293  |
| C    | 5.910500  | 0.100176  | 3.003802  |
| O    | 5.339836  | 1.321995  | 2.573277  |
| C    | 4.674304  | 1.385359  | 1.370134  |
| C    | 3.973961  | 2.492098  | 0.869851  |
| C    | 3.654487  | 3.603757  | 1.612233  |
| O    | 3.966351  | 3.735417  | 2.809466  |
| O    | 2.938556  | 4.496906  | 0.864032  |
| C    | 2.768013  | 5.911681  | 1.402911  |
| C    | 2.051933  | 6.012295  | 0.249111  |
| C    | 4.158100  | 6.005742  | 1.667346  |
| C    | 1.890187  | 5.809027  | 2.664376  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 2.365547| 5.280859| 3.423117|
| H    | 0.902094| 5.50316 | 2.410745|
| H    | 1.776223| 6.18753 | 3.026007|
| H    | 4.655400| 5.95978 | 2.470110|
| H    | 4.760332| 6.44779 | 0.754935|
| H    | 4.046791| 7.55676 | 1.952175|
| H    | 1.082097| 6.13539 | 0.110199|
| H    | 2.643554| 6.52547 | -0.666797|
| H    | 1.916669| 7.67028 | 0.497937|
| H    | 2.889495| -3.92162| -6.35153|
| H    | -3.047198| 2.82049| -3.059903|

Space group P2₁2₁2₁ (protomer B), model 3, reactant complex deprotonated (imidazole tautomer)

Zero-point correction= 1.403394 (Hartree/Particle)
Thermal correction to Energy= 1.487218
Thermal correction to Enthalpy= 1.488162
Thermal correction to Gibbs Free Energy= 1.285252
Sum of electronic and zero-point Energies= -4471.570975
Sum of electronic and thermal Energies= -4471.487151
Sum of electronic and thermal Enthalpies= -4471.486207
Sum of electronic and thermal Free Energies= -4471.689117

SOLVENT: -4497.4648771

RX2bismipl22REACTANT- SCF Done: -4472.97436930 A.U.
| Atom | x       | y       | z       |
|------|---------|---------|---------|
| C    | 1.231548| 1.471708| 1.572483|
| C    | 0.060197| 2.294051| 2.211747|
| N    | -1.099640| 1.939380| 1.372991|
| C    | -0.805117| 1.204749| 0.264866|
| O    | -1.645398| 0.795706| -0.563891|
| N    | 3.067884| 0.473630| -1.264360|
| C    | 4.182545| 1.165932| -1.002126|
| O    | 5.003056| 0.952930| -0.072382|
| C    | 4.272844| 2.462725| -2.193484|
| C    | 5.708176| 2.811653| -2.219348|
| C    | 5.811903| 4.120448| -2.974248|
| C    | 7.143580| 4.862492| -2.992207|
| C    | 5.958555| 5.462210| -0.896914|
| C    | 2.932600| 3.746643| 1.207355|
| O    | 1.670812| 3.118841| -1.202952|
| C    | 4.303584| 3.837728| 0.258239|
| C    | 3.681938| 4.597320| 1.203735|
| C    | 2.392924| 4.904245| 1.046557|
| C    | 1.625939| 4.493468| -0.035352|
| N    | 0.252334| 4.594050| -0.295243|
| C    | -0.673478| 5.483278| 0.583000|
| O    | -0.394414| 5.632776| 1.666721|
| H    | -1.938417| 4.854952| 0.106252|
| C    | -3.102725| 5.819200| 0.740000|
| O    | -4.277460| 5.070701| -0.976869|
| H    | -2.867080| 7.089010| 0.574188|
| H    | -3.268297| 5.180236| 2.214811|
| O    | -8.245995| 1.986829| -0.586040|
| H    | -7.143739| 2.101166| -1.965150|
| H    | -6.926658| 2.495631| 0.361822|
| H    | -5.131004| -0.030700| -0.805104|
| O    | -4.931832| 2.561829| -2.045204|
| C    | -3.333953| 2.193074| -1.369888|
| C    | -1.833030| 0.903709| -2.765615|
| O    | -1.428044| -0.700225| -4.519395|
| H    | -3.332784| -1.880090| -5.637026|
| H    | -6.082921| 0.453915| -3.287967|
| H    | -5.677867| -1.214261| -5.061022|
| H    | -3.618779| -0.912289| 0.497834|
| H    | -2.820515| 0.659110| 2.905275|
| H    | -4.231952| -2.059890| 3.126899|
| H    | -3.611594| -1.107415| 4.490090|
| H    | -6.084888| -0.840463| 4.237243|
| H    | -5.589684| -0.213009| 2.607936|
| O    | -6.243754| 1.571191| 4.392186|
| H    | -4.969695| 1.111046| 5.135323|
| H    | -4.743864| 1.777554| 3.474246|
| H    | -1.532659| -1.335694| 4.362095|
| H    | 0.725842| -2.040254| 2.571826|
| H    | 1.515356| -3.276909| 4.628707|
| H    | 0.010276| -2.855367| 5.436677|
| H    | 1.537263| 0.779042| 4.980595|
| H    | 0.283440| -0.030000| 4.042804|
| H    | 0.260417| -3.070678| 1.086853|
| H    | -0.370474| -6.262500| 1.816171|
| H    | -1.840004| -6.070800| 1.931435|
| H    | -1.835782| -3.103987| 0.082390|
| H    | -3.014406| -4.652251| -2.152729|
| H    | -3.899218| -2.287078| -2.776533|
| H    | -4.534539| -3.035558| -1.282498|
| H    | -2.531588| -0.926256| -1.301936|
| H    | -0.069139| -2.793056| -1.685851|
| H    | 0.179279| -2.608321| -4.634982|
| H    | 2.586949| -1.830427| -3.966488|
| H    | 1.981150| -1.749916| -2.354864|
| H    | 0.927293| -6.057897| -4.111755|
| H    | -0.290271| -4.867312| -4.574557|
| H    | 2.675907| -4.953332| 0.575838|
| H    | 5.175250| -3.655205| -0.291813|
| H    | 4.980959| -5.002925| 0.857233|
| H    | 4.100408| -4.493588| 3.205322|
| H    | 3.908367| -2.822477| 5.055015|
| H    | 4.574872| -0.471290| 4.645726|
| H    | 5.145810| 0.275582| 2.337335|
| H    | 5.369631| -1.334882| 0.562363|
| H    | 3.065930| -0.409268| 0.601983|
| H    | 0.544419| -0.628167| -1.152054|
| H    | 0.679926| -1.114183| 0.541897|
| H    | 1.037050| 1.679449| -0.607249|
space group P2_12_12_1 (protomer B), model 3, reactant complex

Zero-point correction= 1.594518 (Hartree/Particle)
Thermal correction to Energy= 1.689475
Thermal correction to Enthalpy= 1.690420
Thermal correction to Gibbs Free Energy= 1.464541

Sum of electronic and zero-point Energies= -4998.043884
Sum of electronic and thermal Energies= -4997.948927
Sum of electronic and thermal Enthalpies= -4997.947983
Sum of electronic and thermal Free Energies= -4998.173862

SOLVENT: -5026.9599338

RX2Bsimp22REACTANT180 SCF Done: -4999.63840228 A.U.
C  2.436996  2.526142  3.049695
O  1.507316  1.571501  2.452902
C  4.630829  1.124125  2.902576
O  5.463230  1.096825  3.833190
N  4.554788  -1.37016  -1.838254
C  5.522216  -0.936115  1.942910
C  5.087421  -2.294788  1.382029
S  4.458012  -3.451812  2.663926
C  6.545245  -0.206668  1.046643
O  6.515444  -0.220722  -0.216218
N  7.402387  0.562224  1.746145
O  3.105444  -0.082108  -0.404967
C  3.368515  -1.000448  -1.244126
N  4.554788  -1.137016  -1.838254
C  4.707725  -1.984691  -3.047176
C  3.489765  -1.781330  -3.945661
C  3.003709  -0.484321  -4.190009
C  1.788629  -0.302007  -4.854834
C  1.551333  -1.414503  -5.276963
O  0.938970  -1.818050  -1.852092
C  0.455261  -0.489067  -1.215710
C  -1.034758  -0.223496  -1.431802
C  -1.485243  0.266344  -2.826082
N  -2.250276  1.757417  -1.111254
C  -1.486827  0.853593  -0.469084
O  -1.95599  0.875831  0.753000
C  -0.504011  -2.920665  -1.491834
C  -1.054435  -3.162258  -2.233144
O  -1.238227  -2.750997  -3.408810
C  -2.145461  -3.908124  -1.425719
C  -2.184506  -5.422919  -1.685044
C  -2.927783  -6.121969  -0.566165
C  -3.732576  -7.381229  -0.851395
C  -4.489893  -6.066829  -0.534985
C  -3.408582  -3.175533  -1.729844
C  -3.755962  -2.143340  -0.840193
O  -3.182732  -2.018597  0.282483
C  -3.971280  -3.294251  -2.974964
C  -4.941268  -2.432144  -3.397058
C  -5.309224  -1.344827  -2.569160
C  -4.729003  -1.188410  -1.332131
C  -4.945860  -0.94847  -0.470076
C  -5.400188  1.126309  -0.892217
O  -5.746571  1.386077  -2.062405
C  -5.392402  2.038022  0.138377
C  -6.069584  3.382666  -0.971355
C  -5.985464  4.060115  1.278464
C  -7.528295  3.141895  -0.506642
C  -5.278165  4.176620  -1.142532
H  0.121042  6.516051  2.733297
H  -0.721054  4.661984  4.257546
C  -1.474170  4.651270  2.641571
H  2.039910  -0.631864  3.096690
H  -1.60968  2.136339  1.636324
H  -0.14500  -0.119483  1.768659
H  1.91569  4.468259  3.805231
H  2.404503  7.494074  0.014807
H  2.738830  5.305520  1.683968
H  -0.232638  2.011918  5.712404
H  -1.625206  0.984572  5.263414
H  -1.779272  3.493771  4.665548
H  -1.755502  1.475396  2.558485
H  -0.074095  2.977937  3.813455
H  -4.15546  2.325728  2.618984
H  -3.154464  -0.153648  1.910236
H  -3.876637  -2.397698  2.537601
H  -5.046018  -2.781989  4.722192
H  -4.904873  1.446968  5.495835
H  -5.536967  -0.845640  6.198272
H  0.083433  3.036015  2.135639
H  -1.009754  4.500068  -0.219437
H  1.703764  5.125081  1.090109
H  1.005758  5.972638  -0.299509
H  0.683302  7.280423  1.798934
H  -0.146643  5.903249  2.546056
H  -1.757556  7.681695  1.684047  
H  -1.181294  7.366554  0.036381  
H  -2.038932  6.094486  0.946510  
H   0.243382  4.350564 -2.239187  
H   1.649420  1.897426 -2.725343  
H   2.295173  2.973945 -4.836562  
H   2.030469  4.580972 -4.123716  
H  -1.488130  4.556619 -4.765271  
H  -0.048138  5.490806 -4.471372  
H   3.446262  1.491784 -1.310748  
H   5.906174  1.853504 -1.185542  
H   3.113843  2.035361  3.049669  
H   4.473036  2.926720  4.122287  
H   2.095326  3.559883  2.890944  
H   1.436433  1.726480  1.453606  
H   3.810713  0.151284  1.240585  
H   5.937873 -1.068514  2.941227  
H   5.972762 -2.786317  0.965618  
H   4.364323 -2.214248  0.574447  
H   7.841729  1.333460  2.468886  
H   7.203893  0.729024  2.734952  
H   5.378427 -0.718173 -1.343690  
H   4.789734 -3.038239 -2.763530  
H   5.630345 -1.671102 -3.545153  
H   3.545834  0.369132 -3.793428  
H   1.358590  0.684365 -4.987580  
H   0.066256 -1.297272 -5.703751  
H   0.951021 -3.559433 -5.356939  
H   3.117854 -3.885258 -4.189028  
H   0.897570 -1.715988 -2.939768  
H   0.654715 -0.232933 -0.147292  
H   1.035689  0.338234 -1.618905  
H  -1.587865 -1.105352 -1.119148  
H  -1.955007 -0.539723 -3.386880  
H  -0.634956  0.636812 -3.397698  
H  -2.194118  2.315787 -3.170955  
H  -3.511117  1.199662 -2.726296  
H  -2.737428  2.487114 -0.583939  
H  -0.160051 -3.462011 -0.616135  
H  -1.958232 -3.758092 -0.367823  
H  -1.141032 -5.753493 -1.671807  
H  -2.612591 -5.655638 -2.665900  
H  -2.394865 -6.056144  0.376394  
H  -3.762032 -7.735657 -1.876003  
H  -3.744463 -8.159335 -0.097247  
H  -4.934813 -5.972500  0.428968  
H  -4.944798 -5.552810 -1.349571  
H  -3.580703 -4.080707 -3.601456  
H  -5.384677 -2.556093 -4.374833  
H  -5.996347 -0.592787 -2.920274  
H  -4.455530 -0.207140  0.499031  
H  -3.221852 -2.922866  2.827294  
H  -5.277815  3.633273 -0.208737  
H  -4.258788  4.325084 -0.778770  
H  -5.543868  5.153790 -1.277789  
H  -7.568890  2.640170 -1.473224  
H  -8.025077  2.539272  0.248467  
H  -8.042498  4.106128 -0.569130  
H  -4.937433  4.229493  1.525085  
H  -6.468993  3.423994  2.038522  
H  -6.517777  5.016307  1.234686  
H  -1.792210 -6.096437  4.255349  
H  -0.172468  1.044337  4.220676  

space group P2_{1}2_{1}2_{1} (protomer B), model 3, reactant complex (isomer)

Zero-point correction=                             1.595739 (Hartree/Particle)
Thermal correction to Energy=                      1.690095
Thermal correction to Enthalpy=                    1.691039
Thermal correction to Gibbs Free Energy=           1.466655
Sum of electronic and zero-point Energies=          -4998.039795
Sum of electronic and thermal Energies=             -4997.945439
Sum of electronic and thermal Enthalpies=           -4997.944495
Sum of electronic and thermal Free Energies = -4998.168879

SOLVENT: -5026.9609615

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.467356| 2.249063| 2.146789|
| O    | 0.061961| 5.181722| 1.035908|
| O    | 0.141440| 4.765509| 0.567819|
| N    | -2.095524| 5.328641| 0.357496|
| C    | 1.211616| -3.021288| 4.019880|
| C    | 2.03916| -2.490045| 2.917143|
| O    | 3.521537| -2.186976| 3.184660|
| C    | 3.738738| -0.805691| 4.970311|
| N    | 3.751319| 1.603887| 3.431549|
| C    | 4.260951| 1.786608| 4.720086|
| C    | 4.247437| 0.610992| 5.058530|
| C    | 4.496748| 0.600755| 5.539555|
| C    | 1.852589| -3.566068| 1.669854|
| O    | 2.786758| -3.724537| 0.896135|
| N    | 0.555587| -3.560788| 1.416053|
| C    | -1.515799| -2.347964| -0.200662|
| C    | -0.973489| -3.629379| -1.982159|
| C    | -1.707248| -2.921146| -2.889420|
| C    | -1.524607| -3.446077| -4.315803|
| C    | -0.650692| -3.161480| -4.684994|
| O    | 0.517060| -2.778803| -4.899034|
| N    | -1.606479| -1.939197| -2.409292|
| O    | -4.695921| -1.491586| 2.788938|
| O    | -5.525739| -1.54239| 3.718262|
| N    | -4.417480| -0.352415| 2.090823|
| C    | -5.408771| 0.762162| 2.144725|
| C    | -4.780193| 2.145231| 1.878697|
| S    | -6.393098| 2.990866| 3.480918|
| C    | -6.545755| 0.271814| 1.126661|
| O    | -6.381489| 0.437245| -0.125250|
| N    | -7.404880| -0.506193| 1.684966|
| C    | -2.915753| 0.307140| -0.285995|
| C    | -3.215398| 1.135769| -1.263958|
| C    | -4.224111| 1.218433| -1.765449|
| O    | -4.640455| 1.946773| -3.041263|
| C    | -3.43503| 1.742591| -3.970340|
| C    | -2.805863| 0.462719| -4.159544|
| C    | -1.706144| 0.303238| -4.876280|
| O    | -1.061478| 1.419905| -5.417485|
| C    | -1.62835| 2.690369| -5.267000|
| C    | -2.808292| 2.848569| -4.546820|
| C    | -4.328797| 2.227444| -1.603335|
| C    | -6.605556| 3.397333| -1.545557|
| C    | -0.774276| 1.867535| -1.935552|
| C    | -0.336133| 0.484909| -1.398578|
| C    | 1.173919| 0.247545| -1.505076|
| C    | 1.736699| -0.173822| -2.885900|
| C    | 2.688674| -1.384460| -2.594241|
| C    | 2.387059| -1.733470| -1.176982|
| C    | 1.590639| -0.852605| -0.555149|
| C    | 0.756060| -0.910207| 0.662093|
| C    | 0.105097| 2.930051| 1.457991|
| C    | 1.255428| 3.244193| -2.139787|
| C    | 1.490199| 2.878193| -3.305995|
| C    | 2.242160| 4.016267| -1.256624|
| C    | 2.256887| 5.522945| -1.497823|
| C    | 2.918324| 6.232161| -0.330655|
| C    | 3.593040| 7.524019| -0.554459|
| C    | 1.683753| 6.320066| -0.226944|
| C    | 1.534399| 3.306210| -1.479246|
| C    | 0.974817| 2.231621| -0.611049|
| C    | 1.316572| 2.054420| 0.440467|
| C    | 1.001118| 3.477804| -2.667922|
| Atom  | X          | Y          | Z          |
|-------|------------|------------|------------|
| H     | 2.728024   | 5.789134   | -2.451499  |
| H     | 2.345245   | 6.129063   | 0.585073   |
| H     | 3.754900   | 7.892299   | -1.570026  |
| H     | 4.880590   | 6.135262   | 0.757480   |
| H     | 4.990197   | 5.748809   | -1.025096  |
| H     | 3.867267   | 4.293113   | -3.287130  |
| H     | 5.730521   | 2.790155   | -3.967850  |
| H     | 6.218901   | 0.775113   | -2.547293  |
| H     | 4.607743   | 0.249037   | 0.728211   |
| H     | -2.562137  | 2.472348   | 3.439893   |
| H     | 5.516664   | -3.502934  | -1.922247  |
| H     | 4.418172   | -4.251379  | -0.714224  |
| H     | 5.968472   | -5.031362  | -1.114393  |
| H     | 7.721513   | -3.758177  | 2.284757   |
| H     | 6.519033   | -4.977278  | 1.449502   |
| H     | -2.696358  | 6.311655   | 3.635318   |
| H     | -0.123322  | -1.429763  | 4.252100   |

**space group P212121 (protomer B), model 3, Mpro**

Zero-point correction= 0.900498 (Hartree/Particle)
Thermal correction to Energy= 0.954939
Thermal correction to Enthalpy= 0.955883
Thermal correction to Gibbs Free Energy= 0.813056

SOLVENT: -3021.5174858

| Atom  | X          | Y          | Z          |
|-------|------------|------------|------------|
| N     | 1.055751   | -4.522278  | 0.098368   |
| C     | 2.496316   | -4.463769  | -0.277546  |
| C     | 2.785499   | -3.795858  | -1.647213  |
| C     | 1.894992   | -2.622860  | -1.890290  |
| N     | 1.806194   | -1.530452  | -1.002477  |
| C     | 0.877260   | -0.718463  | -1.525693  |
| N     | 0.369775   | -1.219107  | -2.687243  |
| C     | 0.998334   | -2.437824  | -2.919130  |
| C     | 3.357926   | -3.751124  | 0.805654   |
| O     | 4.516770   | -3.565725  | 0.560638   |
| N     | 2.723799   | -3.697596  | 1.991599   |
| C     | 3.879605   | 0.988828   | -1.871387  |
| C     | 2.510208   | 2.088999   | -1.404046  |
| C     | 3.473957   | 2.542020   | 1.103634   |
| C     | 4.766700   | 1.744351   | 0.104365   |
| C     | 4.735131   | 0.362166   | 1.274543   |
| O     | 5.835419   | -0.447158  | 0.999050   |
| C     | 7.016201   | 1.138136   | 0.528658   |
| C     | 5.956735   | 2.319205   | 0.581408   |
| C     | 7.081226   | 1.521798   | 0.340747   |
| C     | 1.127429   | 2.705754   | 0.076389   |
| O     | 0.625835   | 3.237403   | 1.095150   |
| C     | 0.485634   | 2.587293   | -1.110806  |
| C     | -0.853893  | 3.122649   | -1.361393  |
| C     | -1.158723  | 3.152323   | -2.869492  |
| C     | -0.082142  | 3.909198   | -3.681915  |
| C     | 0.165991   | 5.343531   | -3.168621  |
| C     | -1.844042  | 2.212063   | -0.610934  |
| O     | -2.343176  | 1.171553   | -1.142390  |
| N     | -2.054076  | 2.530551   | 0.669216   |
| C     | -2.886744  | 1.710135   | 1.566736   |
| C     | -3.052234  | 2.449748   | 2.913892   |
| C     | -1.630102  | 2.595945   | 3.471897   |
| O     | -0.974905  | 1.611682   | 3.846449   |
| N     | -1.108466  | 3.853851   | 3.370786   |
| C     | -4.223310  | 1.328989   | 0.908510   |
| C     | -4.761445  | 1.952594   | -0.024132  |
| O     | -4.695166  | 1.156876   | 1.420234   |
| C     | -5.721828  | -0.586362  | 0.667545   |
| C     | -4.964246  | -1.598135  | -0.208811  |
| O     | -4.852032  | -2.804118  | 0.079207   |
| N     | -4.305322  | -1.042943  | -1.279467  |
| C     | -3.345173  | -1.909089  | -1.993893  |
| C     | -2.923988  | -1.309755  | -3.353155  |
| C     | -1.970259  | -0.203959  | -3.301094  |
| C     | -2.154324  | -2.292263  | -1.071051  |
| O     | -1.651887  | -3.440584  | -1.102588  |
| N     | -1.794497  | -1.332424  | -0.190019  |
| C     | -1.035956  | -1.664599  | 1.035924   |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| 1    | -0.298689 | -0.435138 | 1.619125 |
| 2    | 1.401762  | -0.815493 | 2.176613 |
| 3    | -2.161250 | -2.152540 | 1.951843 |
| 4    | -2.788421 | -1.359997 | 2.701494 |
| 5    | 2.898110  | -5.483358 | -0.313987 |
| 6    | 2.642846  | -4.519607 | -2.456411 |
| 7    | 3.837159  | -3.490775 | -1.617819 |
| 8    | 0.532714  | 0.205218  | 1.091478 |
| 9    | 0.765850  | -3.063650 | -3.761475 |
| 10   | -0.484575 | -0.809699 | -3.139203 |
| 11   | 3.134206  | -3.218493 | 2.783104 |
| 12   | 1.724082  | -3.906081 | 1.954363 |
| 13   | 3.83473   | 0.997333  | 2.966461 |
| 14   | 4.901902  | 1.082408  | 1.496933 |
| 15   | 3.394973  | 0.080222  | 1.587983 |
| 16   | 2.318403  | 0.062200  | 0.223135 |
| 17   | 3.668401  | 3.610826  | 0.951629 |
| 18   | 2.967746  | 2.418851  | 2.067108 |
| 19   | 3.818998  | -0.089269 | 1.628823 |
| 20   | 5.726219  | -1.322608 | 1.091478 |
| 21   | 7.876138  | -0.481561 | 0.301266 |
| 22   | 5.998541  | 3.387308  | 0.390695 |
| 23   | 7.997891  | 1.978320  | -0.016296 |
| 24   | 1.136191  | 2.260624  | 1.857452 |
| 25   | -0.925047 | 4.127251  | -0.932128 |
| 26   | -1.252432 | 2.127837  | -3.242653 |
| 27   | -2.130863 | 3.641007  | -3.007351 |
| 28   | -0.411133 | 3.942415  | -4.720402 |
| 29   | 0.860687  | 3.349396  | -3.664095 |
| 30   | 0.851335  | 5.879212  | -3.833670 |
| 31   | -0.747254 | 5.905129  | -3.119051 |
| 32   | 0.613409  | 5.322906  | -2.168597 |
| 33   | -1.364387 | 3.165276  | 1.097543 |
| 34   | -2.378542 | 0.776151  | 1.800584 |
| 35   | -3.632198 | 1.806393  | 3.577991 |
| 36   | -3.566028 | 3.401968  | 2.762628 |
| 37   | -0.999919 | 3.955571  | 3.436174 |
| 38   | -1.664181 | 4.565270  | 3.102686 |
| 39   | -4.133330 | -0.392894 | 2.074730 |
| 40   | -6.371878 | -1.136185 | 1.346761 |
| 41   | -6.281777 | 0.134526  | 0.069998 |
| 42   | -4.300172 | -0.031900 | -1.411775 |
| 43   | -3.837391 | -2.858006 | -2.187951 |
| 44   | -2.431155 | -2.105006 | -3.918548 |
| 45   | -3.833947 | -1.008708 | -3.887339 |
| 46   | -2.156346 | 0.409875  | -2.507472 |
| 47   | -2.186739 | -0.393269 | -0.292711 |
| 48   | -0.325818 | -2.469071 | 0.798772 |
| 49   | -0.811768 | -0.065148 | 2.508381 |
| 50   | -0.267892 | 0.374911  | 0.888174 |
| 51   | -3.465536 | -3.717128 | 1.995535 |
| 52   | -2.083778 | -3.942964 | 0.962596 |
| 53   | 1.816637  | 1.273286  | 0.954734 |
| 54   | 0.701272  | -5.481143 | 0.115519 |
| 55   | 3.466353  | 0.040459  | -1.527686 |

**space group P2₁2₁2₁ (protomer B), model 3, reactant complex**

| Property                        | Value                      |
|---------------------------------|----------------------------|
| Zero-point correction           | 1.593490 (Hartree/Particle)|
| Thermal correction to Energy    | 1.688558                   |
| Thermal correction to Enthalpy  | 1.689502                   |
| Thermal correction to Gibbs Free Energy | 1.464575                |
| Sum of electronic and zero-point Energies | -4998.040832            |
| Sum of electronic and thermal Energies  | -4997.345764            |
| Sum of electronic and thermal Enthalpies  | -4997.944819          |
| Sum of electronic and thermal Free Energies | -4998.169747          |

**SOLVENT:** -5026.9591822

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**Zero-point correction**: 1.593490 (Hartree/Particle)

**Thermal correction to Energy**: 1.688558

**Thermal correction to Enthalpy**: 1.689502

**Thermal correction to Gibbs Free Energy**: 1.464575

**Sum of electronic and zero-point Energies**: -4998.040832

**Sum of electronic and thermal Energies**: -4997.345764

**Sum of electronic and thermal Enthalpies**: -4997.944819

**Sum of electronic and thermal Free Energies**: -4998.169747
space group P2\textsubscript{1}2\textsubscript{1}2\textsubscript{1}(protomer B), model 3, product (imidazole tautomer; heteroatoms frozen, free hydrogens)

Zero-point correction= 1.586954 (Hartree/Particle)
Thermal correction to Energy= 1.659859
Thermal correction to Enthalpy= 1.660803
Thermal correction to Gibbs Free Energy= 1.479238

Sum of electronic and zero-point Energies= -4997.628942
Sum of electronic and thermal Energies= -4997.556038
Sum of electronic and thermal Enthalpies= -4997.555093
Sum of electronic and thermal Free Energies= -4997.736658

SOLVENT: -5026.7860733

RX2Bisimpl22F SCF Done: -4999.21589624 A.U.
Zero-point correction=                           1.596811 (Hartree/Particle)
Thermal correction to Energy=                    1.691140
Thermal correction to Enthalpy=                  1.692085
Thermal correction to Gibbs Free Energy=         1.466318
Sum of electronic and zero-point Energies=          -4997.981372
Sum of electronic and thermal Energies=             -4997.887043
Sum of electronic and thermal Enthalpies=           -4997.886098
Sum of electronic and thermal Free Energies=        -4998.111866

SOLVENT: -5026.9507137

RX2Bsimphili2RX SCF Done: -4999.57818311 A.U.

H     -0.324014     7.771145     0.050991
H      0.048712     7.664268    -1.692762
H     -1.386728     8.565523    -1.143245
H     -2.761092     5.312533    -2.467675
H     -1.386868     6.188978    -3.200659
H     -2.846307     7.087927    -2.690698
H      8.096527    -0.803662    -4.054564
H     -3.691001    1.872998    -5.897481

space group P2_12_12_1 (protomer B), model 3, product

N      7.766736    -2.290314    -3.464560
C      7.740543    -1.117047    -2.547994
C      6.374117    -0.384712    -2.537586
C      5.311298    -1.342173    -2.110351
N      4.603647    -2.135433    -3.036064
C      3.826066    -2.935708    -2.295267
N      4.018135    -2.715349    -0.952309
C      4.968718    -1.714338    -0.831362
N      8.057524    -1.572466    -1.099119
O      7.799108    -0.856059    -0.105453
N      8.614982    -2.793016    -1.077212
C      8.032132    4.006952    -5.399042
N      3.794203    3.723017    -3.980599
C      3.000209    2.623714    -3.367449
C      -1.495405    2.969452    -3.247550
C      -0.452978    1.859019    -3.259965
C      -0.734898    0.494414    -3.376658
C      1.507714    -0.031103    -3.340275
C      0.889698    2.262339    -1.378972
C      1.928143    1.30495    -3.205324
C      3.658410    2.473259    -1.996145
O      -3.711704    3.452266    -1.195609
N      -4.265732    1.290033    -1.753459
C      -4.805264    1.046375    -0.423678
C      -6.250150    0.481803    -0.505536
C      -7.181261    1.471420    -1.234969
C      -7.169047    2.885761    -0.680306
C      -3.973109    0.081415    -0.406393
O      -3.287912    -0.882365    -0.028947
N      -4.125955    0.251270    -1.749682
C      -3.562253    -0.845555    2.677023
C      -4.198406    -0.464665    4.097472
C      -3.571225    0.770484    4.749100
O      -3.573144    0.899199    5.986814
N      -3.040716    1.705150    3.913327
C      -4.620117    -2.058030    2.255154
C      -5.569795    -1.925254    2.180670
C      -3.942042    -3.206008    2.007043
C      -4.672948    -4.368259    1.501562
C      -4.613015    -4.531888    -0.028017
O      -5.058431    -5.549019    -0.582033
N      -4.061635    -3.475779    -0.703593
C      -3.999695    -3.528965    -2.160467
C      -4.343990    -2.195894    -2.841940
O      -3.326051    -1.157184    -2.659837
O      -2.660238    -0.402913    -2.690715
O      -2.511871    -4.258427    -3.925558
N      -1.704641    -4.287266    -1.778281
O      -0.376765    -4.767048    -2.200831
C      -0.648481    -4.441729    -1.112374
S      0.707214    -2.229992    -0.918964
C      -0.396403    -6.302851    -2.425649
O      0.235797    -7.079294    -1.682184
N      -1.135041    -6.657407    -3.490576
O      -1.258377    -3.326635    1.184980
C      -0.123481    -3.122482    1.694080
N      0.135793    -3.459513    2.979334
C      1.184278    -2.926009    3.920248
C      0.597846    -1.785634    4.742658
C      -0.636535    -1.945965    5.390909
C      -1.220776    -0.882661    6.072541
O      -0.579152    0.360816    6.112352
C      0.667261    0.514447    5.507939
C  1.259495  -0.554969   4.825468
C  1.031175  -2.509185   0.869282
O  2.298583  -3.175889   1.230992
C  1.164170  -0.993519   1.249078
C  -0.034802  -0.218370   0.689282
C  -0.001350   1.300078   0.894972
C  -0.043677   1.914407   2.311195
C  -0.854482   3.238905   2.104608
N  -1.749818   2.879612   0.974121
C  -1.268214   1.836244   0.238336
O  -1.771984   1.349320  -0.785348
N   2.437333  -0.413570   0.814602
C   3.475898  -0.284778   1.687327
O   3.542257  -0.860117   2.795050
C   4.516100   0.782629   1.274526
C   5.853076   0.631807   1.562369
C   7.390715   2.148121   0.510731
C   8.245224  -0.860117   2.795050
C   9.169210  -0.022728   2.916358
C   6.150831  -0.022728   2.916358
C   6.426797  -0.022728   2.916358
C   3.118025   -0.646671   2.679738
C   3.568449   -1.406355   0.111638
H   6.621315   -2.669330   -3.561406
H   8.869210  -3.240252  -0.205764
H   8.653592  -3.240252  -0.205764
H   4.199861   4.805975   -5.728101
H   -2.492241   4.309132   -5.633998
H   -3.779253   4.544763   -3.372214
H   -3.152191   1.726621   -3.972399
H   -1.253491   3.615078   -4.099993
H   -1.354227   3.777265  -2.349911
H   -1.749949   0.122688  -3.384527
H   -0.061730  -1.486864  -3.537466
H   -2.451066  -0.752353  -3.378442
H   -1.100944   3.226992  -3.096868
H   -2.951998   1.658407  -3.085089
H   -4.030101   0.461880  -2.326172
H   -4.804014   2.014003   0.800478
H   -6.214317  -0.472991  -1.039578
H   -6.611031   0.266688   0.512021
H   -8.199047   1.063604  -1.226095
H   -6.855988   1.540823  -2.277247
H   -7.938897   3.512164  -1.071469
H   -7.357771   2.834727   0.468807
H   -6.199690   3.737371  -0.762065
H   -4.838898   0.901812   2.068388
H   -2.691077  -1.040528   2.609343
H   -3.985397  -1.299563   4.769621
H   -5.290661  -0.348821   4.076557
H   -2.618904   2.516681   4.349523
H   -2.975382   1.602372  2.903910
H   -2.920219  -3.209542   1.887578
H   -4.301028  -5.923405   1.988071
H   -5.724226  -4.235388   1.772827
H   -3.728388  -2.642489  -0.217616
H   -4.737979  -4.271132  -2.471603
H   -4.390411  -2.383802  -3.915721
H   -5.326020  -1.865194  -2.478979
H   -3.087916  -1.079439  -1.674824
H   -1.837666  -4.025053  -0.809886
H   -0.136541  -4.273834  -3.150174
H   1.618931  -4.856690  -1.391417
space group P2₁2₁2₁ (protomer B), model 3, product (heteroatoms frozen, free hydrogens)

Zero-point correction= 1.587641 (Hartree/Particle)
Thermal correction to Energy= 1.661455
Thermal correction to Enthalpy= 1.662399
Thermal correction to Gibbs Free Energy= 1.477559

Sum of electronic and zero-point Energies= -4997.623891
Sum of electronic and thermal Energies= -4997.550078
Sum of electronic and thermal Enthalpies= -4997.549133
Sum of electronic and thermal Free Energies= -4997.733974

SOLVENT: -5026.7828272
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -8.351390 | 1.766447  | 2.040794  |
| C       | -4.442466 | -0.485134 | 5.149744  |
| O       | -3.387140 | -2.67596  | 1.223036  |
| C       | -2.753486 | -0.764116 | 3.721541  |
| C       | -2.466506 | -0.267596 | 5.149744  |
| C       | -2.178539 | 1.223036  | 5.247045  |
| O       | -2.273039 | 1.792898  | 6.337703  |
| N       | -3.969777 | -0.145599 | 3.125924  |
| C       | -3.993382 | -3.282227 | -1.209962 |
| O       | -4.061322 | -2.748899 | 4.034280  |
| N       | -1.925395 | -0.009082 | 3.187198  |
| C       | -1.915171 | -4.476705 | 3.061881  |
| C       | -2.106869 | -4.958646 | 1.669750  |
| O       | -2.655600 | -6.173177 | 1.455963  |
| N       | -2.672515 | -0.535815 | 0.745935  |
| C       | -3.146118 | -3.828267 | -0.632870 |
| O       | -3.240899 | -2.099824 | -1.394034 |
| C       | -1.974638 | -4.723843 | -1.570403 |
| C       | -1.575619 | -1.970864 | -1.573851 |
| O       | -0.785571 | -2.146624 | -1.256411 |
| C       | 0.455838  | -4.002121 | -2.027248 |
| C       | 1.657519  | -3.762091 | -1.332831 |
| O       | 0.949189  | -6.709086 | -1.335476 |
| N       | 0.960151  | -6.214189 | -3.550705 |
| C       | 1.120391  | -2.108246 | -1.023099 |
| O       | 1.411385  | -2.568270 | 2.117205  |
| C       | 2.458913  | -2.471292 | 3.059150  |
| O       | 1.759041  | -1.985309 | 4.321271  |
| C       | 1.351269  | -2.999803 | 5.290970  |
| O       | 0.723117  | -2.461160 | 6.470658  |
| C       | 0.505912  | -1.099329 | 6.654743  |
| C       | 0.902348  | -0.185005 | 5.667082  |
| O       | 1.528588  | -0.620069 | 4.499257  |
| O       | 1.958889  | -1.226395 | 0.121951  |
| C       | 3.294367  | -1.155965 | 0.686006  |
| C       | 1.303895  | 0.188331  | 0.053620  |
| O       | -0.160419 | 0.282450  | -0.458506 |
| O       | -0.733269 | 1.696706  | -0.309495 |
| C       | -1.128689 | 2.039416  | 1.131989  |
| N       | -2.549222 | 2.603091  | 1.156838  |
| N       | -2.903739 | 2.506050  | -0.247054 |
| O       | -2.621199 | 1.910984  | -1.058345 |
| O       | -2.187028 | 1.596188  | -2.234280 |
| N       | -2.251170 | 0.951203  | -0.775987 |
| C       | 2.925865  | 1.971733  | -0.209115 |
| C       | 2.693930  | 2.276717  | 0.945456  |
| C       | 3.996804  | 2.735789  | -0.971182 |
| C       | 5.334007  | 2.025248  | -0.743322 |
| O       | 6.080035  | 1.614498  | -2.008029 |
| O       | 7.507460  | 2.121539  | -2.142830 |
| C       | 6.446485  | 2.604562  | -3.114474 |
| N       | 4.011962  | 4.128374  | -0.470222 |
| C       | 2.974347  | 4.956740  | -0.957042 |
| O       | 2.154830  | 4.468386  | -1.749351 |
| C       | 4.899019  | 4.625825  | 0.419991  |
| C       | 4.818292  | 5.956104  | 0.834863  |
| C       | 3.811754  | 6.818025  | 0.391087  |
| C       | 2.842665  | 6.362542  | -0.525298 |
| N       | 1.799754  | 7.103833  | -1.029065 |
| C       | 1.517373  | 8.382238  | -0.747825 |
| O       | 2.160196  | 9.083555  | -0.002181 |
| C       | 0.395440  | 9.035333  | -1.377968 |
| O       | -0.661963 | 9.604070  | -0.625653 |
| C       | -1.852151 | 9.734401  | -1.566818 |
| C       | -0.171656 | 10.983195 | -0.194205 |
| C       | -1.003578 | 8.674163  | 0.540474  |
| H       | 10.836617 | -3.026656 | -0.639750 |
| H       | 9.502168  | -1.509333 | -2.012722 |
| H       | 9.278004  | -1.297133 | -0.222197 |
| H       | 4.998772  | -2.050227 | -2.238035 |
| H       | 6.592325  | -2.014466 | 0.642855  |
| H       | 4.493115  | -2.006960 | -0.707364 |
| H       | 8.914139  | -4.052156 | -2.551700 |
| H       | 8.767272  | -5.701345 | 1.284359  |
| H       | 9.048468  | -5.684067 | -0.474463 |
H     -9.438244     0.494907    -3.778351
H     -8.266257    -0.514080    -4.634334
H     -4.351358    -0.429565    -2.618446
H     -5.425332    -2.812543    -3.395025
H     -5.348180    -4.194748    -5.414469
H     -5.173488    -3.135113    -7.639103
H     -5.170725     0.706499    -5.771697
H     -5.128917    -0.674638    -7.806744
H     -6.155011    -1.355571     0.010009
H     -5.692858     1.212732     1.415110
H     -6.959298    -1.380083     2.465924
H     -6.679816     0.042167    3.452739
H     -9.022730    -0.103707     2.864710
H     -8.653376    -0.144099    1.133879
H     -9.371938     2.160503     1.904937
H     -7.953307    2.221633     2.966794
H     -7.750991    2.147381     1.195372
H     -4.539042     0.422828    3.746241
H     -1.902474    -0.510845     3.075073
H     -1.591891    -0.808299     5.526459
H     -3.12902     -0.496922     5.802000
H     -1.638678     2.864826     4.214978
H     -1.684858     1.421818     3.249562
H     -1.227233    -2.531531     2.618153
H     -0.926494    -4.877814     3.296676
H     -2.647655    -4.870216     3.770619
H     -2.763946    -3.073237     1.008145
H     -3.17071     -5.314020    -0.576655
H     -4.326914     -3.639256    -2.186642
H     -4.882592    -3.137367    -0.567008
H     -3.365787     -1.591175    -0.574780
H     -0.721126    -3.531241    -0.498781
H     0.335348    -3.901281    -3.003978
H     1.653084    -4.045538    -0.278520
H     1.021367    -7.209942    -3.780021
H     0.851782    -5.559471    -4.316207
H     0.680984    -3.190615     2.466633
H     3.210611    -1.767174     2.713520
H     2.930515    -3.446767     3.225557
H     1.552760    -9.573384     5.157634
H     0.419232    -3.175672     7.225842
H     0.026578    -0.732216     7.555477
H     0.716648     0.871256     5.822190
H     1.852696     0.092911     3.746833
H     1.390568     0.634205     1.047882
H     -0.202975     0.016593    -1.520440
H     -0.776322    -0.452443     0.064342
H     -0.003609     2.421796    -0.699512
H     -0.400517    2.705386     1.603446
H     -1.096066     1.088801     1.681741
H     -3.219529     2.011386     1.787437
H     -2.578320     3.642770     1.504957
H     -3.876183     2.582772    -0.554751
H     -2.224956     0.826993    -1.785558
H     3.750969     2.790441    -2.033766
H     5.187077     1.120808    -0.144105
H     6.004561     2.643911    -0.160177
H     5.919884     0.580014    -2.329731
H     7.854049     2.822591    -1.391372
H     8.259575     1.431927    -2.508145
H     6.468386     2.222573    -4.128554
H     6.097118     3.626722    -3.091590
H     5.651781     3.982905     0.837144
H     5.551379     6.307292     1.547834
H     3.753280     7.839047     0.733462
H     1.208452     6.938222    -1.674970
H     3.698598    -0.314308     0.317046
H     -0.151285     8.600555     2.223469
H     -1.240699     7.678449     0.150035
H     -1.865534     9.053134     1.097819
H     0.720535    10.872941     0.422869
H     0.097405    11.550248    -1.090456
H     -0.946338    11.528342     0.356673
H     -2.174504     8.746399    -1.912223
H     -1.568974    10.330883    -2.439375
H     -2.880373    10.225597    -1.047638
space group P2₁2₁2₁ (protomer B), model 2, Mpro

| Atomic Number | X          | Y          | Z          |
|---------------|------------|------------|------------|
| H             | 10.582644  | -4.162294  | -2.557831  |
| H             | -8.950339  | -1.045092  | -3.100789  |

Zero-point correction= 0.720699 (Hartree/Particle)
Thermal correction to Energy= 0.765783
Thermal correction to Enthalpy= 0.766727
Thermal correction to Gibbs Free Energy= 0.638819

Sum of electronic and zero-point Energies= -2478.374995
Sum of electronic and thermal Energies= -2478.329910
Sum of electronic and thermal Enthalpies= -2478.328966
Sum of electronic and thermal Free Energies= -2478.456875

SOLVENT: -2492.5363008
space group P2₁2₁2₁ (protomer B), model 2, reactant complex

Zero-point correction= 1.415378 (Hartree/Particle)
Thermal correction to Energy= 1.500584
Thermal correction to Enthalpy= 1.501528
Thermal correction to Gibbs Free Energy= 1.291274
Sum of electronic and zero-point Energies= -4472.090552
Sum of electronic and thermal Energies= -4472.005347
Sum of electronic and thermal Enthalpies= -4472.004402
Sum of electronic and thermal Free Energies= -4472.214657

SOLVENT: -4497.963382
|    |    |    |    |    |    |
|----|----|----|----|----|----|
| C  | 2.138430 | -1.651465 | -0.560278 |    |    |
| C  | 0.800855  | -0.890304  | -0.386004 |    |    |
| C  | 1.075166  | 0.476081   | 0.244656  |    |    |
| C  | 1.645171  | 0.443948   | 1.678642  |    |    |
| C  | 1.028692  | 1.705663   | 2.363586  |    |    |
| N  | -0.175632 | 1.960999   | 1.549490  |    |    |
| C  | -0.211997 | 1.289565   | 0.362104  |    |    |
| O  | -1.113566 | 1.332658   | -0.494221 |    |    |
| N  | 2.930122  | -0.999533  | -1.594903 |    |    |
| C  | 4.264589  | -1.185105  | -1.670917 |    |    |
| O  | 4.988275  | -0.592688  | -2.438241 |    |    |
| C  | 4.734078  | -0.497770  | -2.912777 |    |    |
| C  | 7.175652  | 0.623407   | -3.550777 |    |    |
| C  | 8.597781  | 0.325385   | -4.008077 |    |    |
| C  | 3.836483  | 1.872902   | -1.433059 |    |    |
| C  | 2.901557  | 1.696127   | -2.274949 |    |    |
| C  | 5.967877  | 1.181816   | -0.485234 |    |    |
| C  | 3.836483  | 1.872902   | -1.433059 |    |    |
| C  | 3.722793  | 2.826002   | -0.344270 |    |    |
| C  | 2.513626  | 3.527162   | -0.368839 |    |    |
| C  | 2.054040  | 4.548538   | 0.636967  |    |    |
| C  | 0.854362  | 5.859585   | 2.593340  |    |    |
| C  | 0.717596  | 1.694813   | 0.460924  |    |    |
| C  | 2.841993  | 4.418336   | -0.977718 |    |    |
| C  | 0.908084  | 0.945857   | 0.498274  |    |    |
| C  | 2.471285  | 1.635848   | 3.053379  |    |    |
| C  | -4.806290 | -0.286409  | 2.783556  |    |    |
| C  | -4.029869 | 0.119659   | 4.279929  |    |    |
| C  | 1.314853  | 1.414751   | 4.095754  |    |    |
| H  | 1.783342  | 2.524180   | 0.406774  |    |    |
| H  | 2.070996  | 3.687284   | 4.511168  |    |    |
| H  | 0.988765  | 2.549497   | 5.187570  |    |    |
| H  | 0.960207  | 2.101483   | 2.546516  |    |    |
| H  | -2.507997 | 3.687284   | 4.511168  |    |    |
| H  | 0.960207  | 2.101483   | 2.546516  |    |    |
| H  | -2.070733 | -1.738653  | -3.952616 |    |    |
| H  | 0.000000  | 0.000000   | 0.000000  |    |    |
| H  | -2.507997 | 3.687284   | 4.511168  |    |    |
| H  | -2.070733 | -1.738653  | -3.952616 |    |    |
| H  | 0.000000  | 0.000000   | 0.000000  |    |    |
| H  | -2.507997 | 3.687284   | 4.511168  |    |    |
### space group P2₁2₁2₁ (protomer B), model 2 + H₂O transition state

| Coordinates | 1.440943 (Hartree/Particle) | 1.524910 | 1.525855 | 1.326328 | -4548.112182 | -4548.028214 | -4548.027270 | -4548.226797 |
|-------------|----------------------------|----------|----------|---------|--------------|-------------|-------------|-------------|
| C           | -1.074067                  | -3.581138| -4.116695|
| N           | -0.966066                  | -4.220058| -2.777779|
| C           | -1.279198                  | -3.331460| -1.624662|
| C           | -2.613921                  | -2.576953| -1.626652|
| C           | -2.636832                  | -1.339904| -2.517797|
| C           | -1.511438                  | -0.517108| -2.687427|
| C           | -0.820865                  | 0.616859 | -3.492803|
| C           | -2.761153                  | 0.963612 | -4.132725|
| C           | -3.838331                  | -0.79407 | -3.151491|
| C           | -3.907031                  | 0.166630 | -3.949206|
| C           | -1.095161                  | -4.17036 | -0.353589|
| O           | -1.892666                  | -4.205194| 0.614470 |
| N           | -0.139764                  | -4.823658| -0.354867|
| C           | 2.877011                   | -4.891892| 0.885697 |
| C           | 1.491191                   | -6.280768| 1.136483 |
| O           | 0.402380                   | -7.377937| 1.125285 |
| C           | -0.740692                  | -7.097642| 2.128130 |
| C           | 1.938643                   | -3.789812| 0.790486 |
| O           | 2.308182                   | -3.311786| -0.316040|
| N           | 2.408892                   | -3.315554| 1.955997 |
| C           | 3.233432                   | -2.095062| 1.957602 |
| C           | 3.466429                   | -2.632282| 3.392047 |
| C           | 2.219658                   | -1.210174| 4.192709 |
| O           | 2.347450                   | -0.716242| 5.327889 |
| N           | 1.019039                   | -1.402660| 3.580396 |
| C           | 4.569319                   | -2.427612| 1.273489 |
| O           | 5.196333                   | -3.318257| 1.425205 |
| N           | 5.012494                   | -1.415937| 0.475986 |
| C           | 6.049120                   | -1.703136| -0.516448|
| C           | 5.458110                   | -1.605476| -1.931937|
| O           | 6.104183                   | -1.096737| -2.881180|
| N           | 4.176046                   | -2.013363| -2.053452|
| C           | 3.403312                   | -1.639559| -3.246643|
| C           | 1.905684                   | -1.877954| -2.964218|
| O           | 1.447038                   | -1.177764| -1.758144|
| N           | 3.661817                   | -0.158539| -3.613369|
| C           | 3.857865                   | 0.223648 | -4.775211|
| O           | 3.648723                   | 0.657071 | -2.519720|
| C           | 4.120612                   | 2.034426 | -2.593733|
| C           | 3.082316                   | 3.109670 | -2.393808|

S264
| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| S    | 1.433839  | 2.405795  | -1.836894 |
| C    | 5.228198  | 2.250403  | -1.525245 |
| O    | 5.140409  | 2.250403  | -1.715839 |
| N    | 3.95743   | 2.237639  | 1.804835  |
| C    | 3.410531  | 3.432344  | 2.682368  |
| C    | 2.902231  | 1.876680  | 3.70927   |
| C    | 2.098229  | 2.192301  | 4.458040  |
| C    | 0.921057  | 1.948277  | 5.166761  |
| C    | -0.191658 | 2.776793  | 4.976698  |
| C    | -0.119121 | 3.840110  | 4.074361  |
| C    | 1.064292  | 4.084617  | 3.370927  |
| C    | 1.738951  | 2.815237  | 0.272401  |
| O    | 2.003484  | 4.108347  | 0.374769  |
| C    | 0.360959  | 2.302852  | 0.807945  |
| C    | 0.306426  | 0.774876  | 0.856199  |
| O    | -1.892147 | 0.597221  | 2.311964  |
| C    | -2.749338 | -0.672878 | 2.640997  |
| N    | -1.933844 | -1.761046 | 2.028617  |
| C    | -0.940070 | -1.310537 | 1.233508  |
| O    | 0.000509  | -2.008662 | 0.769270  |
| N    | -0.759014 | 2.870070  | 0.047640  |
| C    | -3.852307 | 5.781054  | -0.279171 |
| C    | -2.239074 | 6.532742  | -1.316772 |
| C    | -2.730910 | 7.883888  | -1.803667 |
| C    | -3.813500 | 6.661085  | -2.723065 |
| N    | -3.684941 | 3.387844  | 0.297080  |
| C    | -3.762753 | 2.099298  | -0.232331 |
| O    | -0.994530 | 1.733342  | -1.742717 |
| C    | -4.391531 | 3.775355  | 1.414652  |
| C    | -5.253337 | 2.907722  | 2.019457  |
| C    | -5.430111 | 1.601538  | 1.493509  |
| C    | -7.174644 | 1.204883  | 0.385805  |
| N    | -7.702800 | -0.046338 | -0.241607 |
| C    | -5.141875 | -1.140359 | 0.281002  |
| O    | -5.873536 | -1.931000 | 1.436739  |
| O    | -5.454064 | -2.160531 | -0.635164 |
| C    | -6.061671 | -3.489020 | -0.215333 |
| C    | -5.553236 | -4.324444 | -1.494936 |
| C    | -7.537245 | -3.272948 | 0.169196  |
| C    | -5.521621 | -4.085603 | 0.928830  |
| H    | -0.728022 | -4.296045 | -4.869817 |
| H    | -2.088872 | -3.245837 | -4.371758 |
| H    | -1.562471 | -5.055934 | -2.741220 |
| H    | -0.466320 | -2.092521 | -1.563820 |
| H    | -3.412217 | -3.250605 | -1.926350 |
| H    | -2.837671 | -2.281160 | -0.596455 |
| H    | -0.563970 | -0.743173 | -2.209878 |
| H    | -0.699819 | 1.237169  | -3.607282 |
| H    | -2.828645 | 1.850698  | -4.753447 |
| H    | -4.719912 | -1.590313 | -2.991615 |
| H    | -4.842959 | 0.430895  | -4.429463 |
| H    | 0.633199  | -7.320066 | -1.223952 |
| H    | 0.190520  | -4.625469 | 1.689725  |
| H    | 2.243546  | -6.483569 | 0.364802  |
| H    | 2.004314  | -6.268361 | 2.107239  |
| H    | 0.875594  | -3.406046 | 1.352534  |
| H    | -0.013704 | -7.436587 | 0.113884  |
| H    | -1.418295 | -7.956739 | 2.182692  |
| H    | -0.337415 | -6.920364 | 3.133691  |
| H    | -1.322616 | -6.233996 | 1.817834  |
| H    | 2.162566  | -3.751871 | 2.838065  |
| H    | 2.712224  | -1.327619 | 1.376491  |
| H    | 4.118602  | -0.743581 | 3.370385  |
| H    | 3.998741  | -2.401387 | 3.951839  |
| H    | 0.183408  | -1.085386 | 4.059866  |
| H    | 0.914068  | -1.776095 | 2.640560  |
| H    | 4.447181  | -0.563211 | 0.360808  |
| H    | 6.881667  | -0.991128 | -0.465992 |
| H    | 6.408023  | -2.714766 | -0.308157 |
| H    | 3.673138  | -2.448071 | -1.275236 |
| H    | 3.700407  | -2.215512 | -4.127659 |
| H    | 1.280500  | -1.480018 | -3.801496 |
| H    | 1.710078  | -2.951561 | -2.870401 |
space group P2₁2₁2₁ (protomer B), model 2, product

Zero-point correction = 1.420198 (Hartree/Particle)

Thermal correction to Energy = 1.503392

Thermal correction to Enthalpy = 1.504336

Thermal correction to Gibbs Free Energy = 1.302187

Sum of electronic and zero-point Energies = -4472.136010

Sum of electronic and thermal Energies = -4472.052816

Sum of electronic and thermal Enthalpies = -4472.051872

Sum of electronic and thermal Free Energies = -4472.254021

SOLVENT: -4497.9850217

RXB simpli3 SCF Done: -4473.55620806 A.U.

C 0.647556 5.200978 3.835203
N -0.687494 4.956556 2.376222
O 0.634374 5.989671 -1.369273
C 2.650847 3.187249 -0.742664
C 4.156045 3.586616 -0.633406
C 4.351298 4.979739 -0.005536
C 3.673847 6.105034 -0.819831
C 2.636164 1.745116 -1.212651
O 2.564725 0.745005 -0.443494
N 2.879322 1.570230 -2.533814
C 3.285788 0.235655 -3.048823
C 3.114082 0.201852 -4.566788
space group P2₁,2₁,2₁(protomer B), model 2, product (isomer)

| Zero-point correction= 1.418637 (Hartree/Particle) |
|-----------------------|---------------------------------------------|
| Thermal correction to Energy= 1.502156 |
| Thermal correction to Enthalpy= 1.503100 |
| Thermal correction to Gibbs Free Energy= 1.298207 |
| Sum of electronic and zero-point Energies= -4472.112498 |
| Sum of electronic and thermal Energies= -4472.028035 |
| Sum of electronic and thermal Enthalpies= -4472.028035 |

H 5.428715 5.169240 0.075399
H 3.958034 4.962355 1.009231
H 3.935172 7.084886 -0.404692
H 4.010512 6.079482 -1.864253
H 3.630662 3.704101 -3.095659
H 2.664653 -0.302894 -2.546014
H 3.584267 -0.695665 -4.976289
H 3.646974 1.958311 -4.997674
H 3.705515 0.964149 -1.887076
H 4.221272 0.204539 0.247038
H 5.759799 0.677508 2.743719
H 3.720303 1.951025 3.686497
H 4.075374 2.389949 2.126934
H 2.405652 0.704518 1.263172
H 3.672589 -1.838486 1.417594
H 2.844538 -2.616433 4.094404
H 1.657832 -4.459665 2.886595
H 2.577930 -4.139191 1.430598
H 5.997643 -4.201012 4.671268
H 5.130486 -2.651457 4.747705
H 2.703901 -2.998083 -2.609542
H 0.589566 -4.832554 -1.839063
H 1.565128 -4.852414 -3.332818
H 1.034493 -2.438583 -4.754586
H -0.788875 -1.486527 -6.011499
H -3.167512 -2.175206 -5.518894
H -3.607180 -3.769328 -3.631212
H -1.735043 -4.666380 -2.322132
H -0.842190 -2.667495 -1.412815
H 0.048595 -0.246627 -0.039590
H 0.469658 -0.730802 -1.726721
H -1.938169 0.425295 -0.249886
H -3.149394 -1.030073 -1.775627
H -1.789942 -1.046516 -2.918283
H -3.082246 0.581796 -4.040238
H -3.839314 1.195912 -2.537821
H -1.812147 2.695083 -3.261630
H -1.949466 -1.394360 0.999648
H -3.507881 -2.570827 2.218726
H -3.897105 -5.048624 1.896897
H -4.944071 -4.754288 0.532957
H -5.858115 -3.710454 3.401444
H -6.817856 -5.985802 1.749061
H -7.300220 -5.449145 3.429355
H -7.759055 -3.109035 2.540384
H -7.296149 -3.660948 0.865126
H -5.597609 -3.287973 -0.742591
H -6.688251 -1.471380 -2.040464
H -6.130152 0.926247 -1.502442
H -3.812258 1.667228 1.345043
H -0.582464 -4.578887 0.132683
H -2.853052 4.282417 -1.978899
H -1.650891 4.904172 -0.794104
H -2.537967 6.027887 -1.859486
H -5.340807 5.023738 -1.728973
H -5.869752 5.631782 -1.040266
H -4.953284 6.700141 -2.122433
H -2.524551 5.640140 1.464959
H -4.221627 6.177610 1.617918
H -3.099113 7.089465 0.572539
H -0.371536 5.324724 1.241810

RXBismip3 SCF Done: -4473.5313476 A.U.

H 3.426755 6.062191 -2.246069
N -2.88731 5.479396 -1.013167
C -2.132468 4.197747 -1.236869
C -2.132468 4.197747 -1.236869
C -0.869992 4.244128 -2.175795
C -1.193352 3.505399 -3.466369
C -1.504841 2.137075 -3.401567
C -2.026217 1.467308 -4.508973

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S268
Sum of electronic and thermal Free Energies = -4472.232928

SOLVENT: -4497.96949

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
|     C | -2.176930 | 2.146792 | -5.723361 |
|     C | -1.346888 | 4.174311 | -4.685439 |
|     C | -1.817507 | 3.494062 | -5.814013 |
|     C | -1.832916 | 3.731879 | 0.181011 |
|     O | -1.115424 | 4.408357 | 0.978338 |
|     N | -2.490427 | 2.615099 | 0.537891 |
|     C | -2.623871 | 2.193610 | 1.921286 |
|     O | -4.080012 | 2.496657 | 2.399080 |
|     C | -4.405171 | 3.994112 | 2.239080 |
|     C | -3.548300 | 4.911529 | 3.116816 |
|     C | -2.363500 | 0.705277 | 2.062079 |
|     O | -2.167962 | -0.084414 | 1.094175 |
|     N | -2.255788 | 0.227004 | 3.341857 |
|     C | -4.195664 | -1.245925 | 3.551979 |
|     C | -1.901274 | -1.555312 | 5.039365 |
|     O | -5.184244 | -1.182164 | 5.575043 |
|     N | 0.149155 | -1.976799 | 6.262644 |
|     C | -0.992816 | 0.070378 | 5.252343 |
|     C | -3.520155 | -1.842811 | 3.187548 |
|     O | -4.531934 | -1.428682 | 3.783449 |
|     N | -3.506517 | -2.843602 | 2.238121 |
|     C | -1.282700 | -3.104931 | -2.272600 |
|     O | -3.202483 | -4.657144 | -3.901746 |
|     O | -3.177317 | -5.879760 | -3.744558 |
|     N | -4.307223 | -4.059106 | -6.178787 |
|     C | -1.585540 | -3.100905 | 0.271593 |
|     O | -0.938362 | -3.701799 | 0.472557 |
|     N | -0.066681 | -2.206142 | 1.687769 |
|     C | 1.199000 | -4.840403 | 2.186257 |
|     C | 2.147694 | -3.844249 | 2.835490 |
|     C | 1.821702 | -4.221284 | 4.054160 |
|     C | 2.680597 | -3.208054 | 6.439188 |
|     C | 3.868647 | -1.953166 | 3.994856 |
|     C | 4.201083 | -2.550054 | 2.775067 |
|     C | 3.354855 | -3.504654 | 2.205160 |
|     C | 0.715028 | -3.514375 | -0.580941 |
|     C | 1.550956 | -4.884410 | -0.541496 |
|     C | 1.480053 | -2.214083 | -1.338332 |
|     C | 0.569360 | -1.007517 | 0.118898 |
|     C | 1.317341 | 0.165452 | 0.755732 |
|     C | 1.457567 | 1.080395 | 2.290293 |
|     C | 1.450318 | 1.702264 | 2.635693 |
|     C | 0.619447 | 2.260784 | 1.546600 |
|     C | 0.581681 | 1.473440 | 0.438436 |
|     O | 0.069062 | 1.755698 | -0.660191 |
|     C | 2.461384 | -1.790877 | -1.164031 |
|     C | 3.629159 | -2.413066 | -1.406639 |
|     C | 3.911025 | -3.888868 | -1.047629 |
|     C | 4.652853 | -1.525783 | -2.137535 |
|     C | 5.883515 | -2.310821 | -2.592870 |
|     C | 6.799733 | -1.492450 | -3.478991 |
|     C | 8.245840 | -1.937318 | -3.656079 |
|     C | 7.928886 | -0.662614 | -2.877336 |
|     N | 4.941227 | -0.398848 | -1.191845 |
|     C | 4.064642 | 0.902908 | -1.268538 |
|     C | 3.119727 | 0.706965 | -2.119471 |
|     C | 5.879686 | -0.509660 | -0.881199 |
|     C | 6.016680 | 0.469004 | 0.750887 |
|     C | 5.180422 | 1.090909 | 0.722821 |
|     C | 4.212595 | 1.721356 | -0.298880 |
|     N | 3.255516 | 2.722947 | -0.391515 |
|     C | 3.057320 | 3.762579 | 0.497290 |
|     O | 3.727949 | 3.892752 | 1.551627 |
|     O | 2.889669 | 4.595167 | 0.054929 |
|     N | 1.980056 | 5.983438 | 0.678702 |
|     C | 0.886682 | 6.627006 | -0.173695 |
|     C | 3.331374 | 6.691941 | 0.517354 |
|     C | 1.549278 | 5.878035 | 2.148447 |
|   |   |   |   |
|---|---|---|---|
| H | -3.968494 | 6.976693 | -1.984926 |
| H | -2.681420 | 6.297925 | -3.023421 |
| H | -2.252747 | 6.129181 | -0.509133 |
| H | -2.847691 | 3.503937 | -1.681857 |
| H | -0.620556 | 5.289338 | -2.383037 |
| H | -0.028849 | 3.782632 | -1.655623 |
| H | -1.385063 | 1.615261 | -2.466389 |
| H | -2.360070 | 0.439031 | -4.404550 |
| H | -2.582935 | 1.633521 | -6.588033 |
| H | -1.137486 | 5.234010 | -4.748514 |
| H | -1.929531 | 4.023792 | -6.750466 |
| H | -1.952935 | 2.008488 | -0.218733 |
| H | -3.907383 | 4.288138 | 1.189418 |
| H | -3.971686 | 5.935373 | 3.093637 |
| H | -3.577373 | 4.569600 | 4.159885 |
| H | -2.527680 | 4.935471 | 2.750282 |
| H | -2.754368 | 0.738159 | 4.070654 |
| H | -1.345152 | -1.619528 | 2.920419 |
| H | -2.000127 | -2.631896 | 5.196298 |
| H | -2.696098 | -1.068506 | 5.618230 |
| H | 0.831723 | 0.359312 | 5.552696 |
| H | -0.596704 | 0.633936 | 4.575819 |
| H | -2.609176 | -3.002209 | 1.645920 |
| H | -4.750834 | -4.421238 | 1.638818 |
| H | -5.553877 | -3.054203 | 2.451026 |
| H | -3.545113 | -1.446464 | 0.428733 |
| H | -5.666135 | -1.439787 | -1.641611 |
| H | -4.763584 | 0.690416 | -2.421670 |
| H | -5.089340 | 0.770724 | -0.657470 |
| H | -2.598043 | 0.231742 | -0.540894 |
| H | -2.754190 | -3.020407 | -1.268448 |
| H | -2.016906 | -2.935352 | -4.071205 |
| H | -0.756523 | -5.101695 | -3.366234 |
| H | -1.462575 | -4.991300 | -1.763205 |
| H | -5.034304 | -6.385390 | -5.022812 |
| H | -4.364016 | -3.036562 | -4.655135 |
| H | -0.848999 | -4.223054 | 2.341858 |
| H | 1.654100 | -5.308385 | 1.320550 |
| H | 0.890196 | -5.539690 | 2.917156 |
| H | 0.906474 | -3.491701 | 4.576688 |
| H | 2.387951 | -1.873545 | 5.585943 |
| H | 4.532545 | -1.219826 | 4.439243 |
| H | 5.112322 | -2.266397 | 2.261048 |
| H | 3.614932 | -3.948368 | 1.251731 |
| H | 2.026086 | -2.472756 | 0.767124 |
| H | 0.159988 | -0.658985 | -0.840735 |
| H | -0.285544 | -1.278508 | 0.729316 |
| H | 2.306227 | 0.268603 | 0.306297 |
| H | 2.351635 | -0.327622 | 2.649070 |
| H | 0.583739 | -0.294347 | 2.741161 |
| H | 1.001503 | 1.908875 | 3.610229 |
| H | 2.453843 | 2.138826 | 2.606289 |
| H | 0.249070 | 3.216166 | 1.506056 |
| H | 2.313708 | -0.878592 | -1.624132 |
| H | 4.161676 | -1.052214 | -2.992109 |
| H | 5.501616 | -3.175840 | -3.148311 |
| H | 6.421953 | -2.726632 | -1.734898 |
| H | 6.314598 | -1.073718 | -4.355935 |
| H | 8.579971 | -2.803629 | -3.090114 |
| H | 8.692484 | -1.837475 | -4.637004 |
| H | 8.157965 | 0.287684 | -3.344357 |
| H | 8.057128 | -0.811156 | -1.802688 |
| H | 6.478078 | -1.406306 | -0.190378 |
| H | 6.762940 | 0.367779 | 1.525944 |
| H | 5.227289 | 2.372573 | 1.478356 |
| H | 2.605528 | 2.611297 | -1.173877 |
| H | 2.488771 | -4.421375 | -0.840002 |
| H | 2.290970 | 5.301526 | 2.706267 |
| H | 0.569810 | 5.395125 | 2.201381 |
| H | 1.472467 | 6.882664 | 2.565809 |
| H | 4.096388 | 6.183967 | 1.106896 |
| H | 3.622222 | 6.694091 | -0.538057 |
| H | 3.233522 | 7.726531 | 0.860448 |
| H | -0.026336 | 6.046409 | -0.031133 |
| H | 1.178645 | 6.618315 | -1.227214 |
| H | 0.729476 | 7.659277 | 0.155998 |
space group P2₁2₁2₁(protomer B), model 2, product (heteroatoms frozen, free hydrogens)

| Zero-point correction= | 1.411138 (Hartree/Particle) |
| Thermal correction to Energy= | 1.474762 |
| Thermal correction to Enthalpy= | 1.475706 |
| Thermal correction to Gibbs Free Energy= | -1.318548 |
| Sum of electronic and zero-point Energies= | -4471.790225 |
| Sum of electronic and thermal Energies= | -4471.726601 |
| Sum of electronic and thermal Enthalpies= | -4471.725656 |
| Sum of electronic and thermal Free Energies= | -4471.882815 |

SOLVENT: -4497.8138417

RX2Bsimp13F SCF Done: -4473.20136220 A.U.
|   | X          | Y          | Z          |
|---|------------|------------|------------|
| N | 5.940598   | -1.715769  | -1.213381  |
| C | 6.013953   | -0.395348  | -1.341444  |
| O | 5.124655   | -1.309348  | -1.748299  |
| C | 7.33348    | -1.670332  | 0.098453   |
| C | 8.052956   | -2.080384  | 0.094024   |
| N | 1.02114    | 0.468633   | -0.713906  |
| C | 1.01110    | 1.333341   | -0.868539  |
| C | 1.94307    | 2.695989   | -0.368538  |
| O | 8.955946   | 2.368825   | 0.296290   |
| O | 0.781883   | 4.108382   | -0.638079  |
| C | 7.52418    | 5.063864   | 0.401146   |
| C | 7.14617    | 6.319039   | -0.220564  |
| C | 9.174497   | 5.334902   | 0.833578   |
| C | 6.824182   | 4.151571   | 1.484926   |
| H | -4.810480  | 7.718177   | -1.829361  |
| H | -4.999291  | 6.444818   | -3.041078  |
| H | -2.861148  | 6.502909   | -1.417362  |
| H | -4.666219  | 4.193282   | -1.082414  |
| H | -1.938961  | 4.444052   | -2.414632  |
| H | -2.636620  | 2.890537   | -1.973866  |
| H | -5.22043   | 2.609384   | -2.786517  |
| H | -6.362470  | 2.301389   | -4.931348  |
| H | -5.450129  | 3.322283   | -6.982621  |
| H | -2.251576  | 4.988832   | -4.686688  |
| H | -3.411859  | 4.713833   | -6.838354  |
| H | -4.355746  | 3.108919   | 0.851217   |
| H | -1.953186  | 3.817162   | 2.434871   |
| H | -7.766745  | 3.096180   | 3.404351   |
| H | -3.425254  | 3.413619   | 4.475320   |
| H | -9.900799  | 5.331419   | 4.420715   |
| H | -7.66657   | 5.466147   | 2.660678   |
| H | -3.267937  | 7.119021   | 3.866128   |
| H | -2.378953  | 5.758248   | 4.574674   |
| H | -2.370379  | 6.091925   | 2.809509   |
| H | -1.884637  | 1.861310   | 4.323089   |
| H | -1.156218  | -0.562405  | 2.957548   |
| H | -1.157671  | -1.608600  | 5.204772   |
| H | -1.882793  | -0.153583  | 5.910670   |
| H | -1.91884   | 0.814949   | 4.430479   |
| H | 0.564525   | 3.11097    | 3.323563   |
| H | -2.473130  | -2.107366  | 2.102999   |
| H | -4.171739  | -3.825444  | 2.386547   |
| H | -5.139088  | -2.588548  | 3.235780   |
| H | -3.798428  | -0.780697  | 0.824053   |
| H | -6.224592  | -0.864354  | -0.774834  |
| H | -5.240830  | 0.967322   | -1.976484  |
| H | -5.107323  | 1.267212   | -0.222383  |
| H | -2.927051  | 0.959518   | -0.368036  |
| H | -3.047397  | -2.253020  | -1.150179  |
| H | -2.809874  | -2.639999  | -3.855459  |
| H | -1.744822  | -4.877774  | -3.213458  |
| H | -2.103309  | -4.468434  | -1.543761  |
| H | -5.143705  | -4.818526  | -5.188582  |
| H | -3.906337  | -6.361228  | -5.452412  |
| H | -1.891868  | -3.937292  | 1.435477   |
| H | 0.729487   | -5.194329  | 1.280142   |
| H | -0.793430  | -6.950870  | 1.625226   |
| H | -1.952745  | -5.749619  | 3.738695   |
| H | -1.908011  | -4.956512  | 6.093242   |
| H | -0.122194  | -3.369688  | 6.814296   |
| H | 1.544672   | -2.569911  | 5.190714   |
| H | 1.502247   | -3.360210  | 2.827643   |
| H | 1.613722   | -1.979716  | 0.397344   |
| H | 0.128265   | -0.417386  | -1.798328  |
| H | -0.538261  | -0.633717  | -0.194655  |
| H | 2.238723   | 0.555915   | -0.742177  |
| H | 2.301997   | 0.428218   | 1.607258   |
| H | 0.580935   | 0.055720   | 1.632924   |
| H | 0.125940   | 2.216601   | 2.336004   |
| H | 1.822861   | 2.695438   | 2.127019   |
| H | 0.160610   | 3.661995   | 0.297105   |
| H | 2.177537   | -1.792921  | -2.498415  |
| H | 4.655942   | -1.849864  | -2.834812  |
| H | 4.169980   | -4.394541  | -1.532687  |
| H | 5.877035   | -4.190028  | -1.564400  |
| H | 4.073553   | -4.683900  | -3.902899  |
| H | 7.046530   | -5.230557  | -3.138294  |
| H | 6.128477   | -6.037786  | -4.498109  |
| H | 5.963289   | -3.764907  | -5.547320  |
space group P2₁2₁2₁(protomer B), model 2, product (heteroatoms frozen, free hydrogens)

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | 6.656506 | -2.978977 | -4.203724 |
| H    | 6.790309 | -3.428765 | -0.339120 |
| H    | 8.657825 | -2.234643 | 1.280365 |
| H    | 9.410239 | 1.262843 |
| H    | 9.970678 | 5.671771 | 0.030071 |
| H    | 9.781939 | 6.653210 | -0.152453 |
| H    | 9.709547 | 7.112110 | 0.530910 |
| H    | -5.81746 | 6.305212 | -1.469395 |

Zero-point correction= 1.411167 (Hartree/Particle)
Thermal correction to Energy= 1.474791
Thermal correction to Enthalpy= 1.475736
Thermal correction to Gibbs Free Energy= 1.318565
Sum of electronic and zero-point Energies= -4471.790042
Sum of electronic and thermal Energies= -4471.726419
Sum of electronic and thermal Enthalpies= -4471.725474
Sum of electronic and thermal Free Energies= -4471.882645

SOLVENT: -4497.813759

RX2Hisimpl3F SCF Done: -4473.20120991 A.U.
H      1.612643    -1.998184     0.397427  
H      0.128595    -0.417133    -1.798439  
H     -0.538230    -0.633544    -0.194929  
H      2.238774     0.555989    -0.742141  
H      2.302061     0.428235     1.607169  
H      0.581039     0.055699     1.632924  
H      0.125954     2.216591     2.335968  
H      1.822869     2.695449     2.126986  
H      0.160658     3.662015     0.297104  
H      2.176916    -1.795515    -2.497736  
H      4.655349    -1.849132    -2.834951  
H      4.160992    -4.394569    -1.532657  
H      5.877040     -1.900601    -1.564419  
H      4.073535    -4.883853    -3.902941  
H      7.040506    -5.230574    -3.138294  
H      6.128425    -6.037830    -4.498073  
H      5.693254    -3.764699    -5.547315  
H      6.656564    -2.979033    -4.207085  
H      6.790169    -3.428704    -0.338788  
H      8.657888    -2.236847     0.667010  
H      8.864424     0.246970     0.484656  
H      6.339395     2.182378    -1.421058  
H      1.975931    -4.334464    -1.280275  
H      7.269653     3.622361     1.943830  
H      5.863006     4.242171     1.033862  
H      6.654347     5.258205     2.266705  
H      9.610599     4.410120     1.262374  
H      9.770664     5.672211     0.030191  
H      9.192203     6.106751     1.661193  
H      6.150158     6.112429    -0.604841  
H      7.781781     6.653059    -1.052616  
H      7.099847     7.112142     0.530866  
H      5.781785     6.305549    -1.469335  

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