Supporting Information for

Theoretical Study on DBU-Catalyzed Insertion of Isatins into Aryl Difluoronitromethyl Ketones: A Case for Predicting Chemoselectivity Using Electrophilic Parr Function

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1. The combined energy profiles of the insertion reactions and the optimized geometries

![Diagram of energy profiles and optimized geometries]

**Figure S1.** The combined energy profiles of the DBU-catalyzed insertion reactions and the optimized geometries. All the energies were calculated at M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM<sub>chloroform</sub>/M06-2X/6-31G(d, p)/IEF-PCM<sub>chloroform</sub> level.
2. Energy scans along with the changes of N1–C6 and N1–C8 distances

We have scanned the two bonds by 70 steps per 0.03 Å with 3.03 Å at the beginning, and the corresponding energy profiles have been shown in Figure S2. As presented in Figure S2, the energies become higher and higher accompanied with the approach of N1 atom to the two carbonyl carbons, indicating the nucleophilic attack by catalyst Cat on the carbonyl carbons in reactant R2 would be very difficult to happen under the experimental condition, thus, these two possible paths would not be necessary to consider in the following processes.

Figure S2. The energy scans along with the changes of N1–C6 (black) and N1–C8 (red) distances computing at M06-2X/6-31G(d, p)/IEF-PCM<sub>chloroform</sub> level.
3. Different conformations of 1 and 2

To confirm the lowest energy conformation was selected in the energy profile, four possible conformations of both transition state 1 and intermediate 2 have been investigated and compared. Based on the dihedral angles $\Phi(O2-C3-C4-N5)$ in transition state 1 ($\Phi=52^\circ$) and intermediate 2 ($\Phi=45^\circ$), we have additionally considered other three structures by rotating $90^\circ$, $180^\circ$, $270^\circ$ of $\Phi$ as the initial structures, and the dihedral angles $\Phi$ change to $155^\circ/154^\circ$, $155^\circ/168^\circ$, and $-43^\circ/-48^\circ$ in 1/2 after the optimization, respectively. The optimized geometries and relative energies were shown and provided in Figure S3. As revealed by these data, the dihedral angles $\Phi(O2-C3-C4-N5)$ are still $52^\circ$ and $45^\circ$ in the most stable transition state 1 and intermediate 2, separately.

![Figure S3](image-url)

**Figure S3.** Four possible conformations and relative Gibbs free energies (kcal/mol) of transition state 1 and intermediate 2 with different $\Phi$ obtained at the M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM$_{\text{chloroform}}$/M06-2X/6-31G(d, p)/IEF-PCM$_{\text{chloroform}}$ level of theory. [a] It should be mentioned that only one transition state 1 can be obtained after the optimization even when we rotated $90^\circ$ or $180^\circ$ of $\Phi$ as the initial structures.


4. Design of DBU catalysts

As summarized in Table S1, the energy barrier via $3^\text{α-methoxy}$ (24.0 kcal/mol) is slightly lower than that via $3^{\text{DBU}}$ (24.9 kcal/mol), while the energy barriers via $3^\text{α-methyl}$ (28.5 kcal/mol), $3^\text{α-fluoro}$ (26.6 kcal/mol), and $3^\text{α-cyano}$ (30.3 kcal/mol) are significantly higher than that via $3^{\text{DBU}}$, indicating that the DBU with α-methoxy group might be the catalyst with higher catalytic efficiency.

Table S1. The Relative Gibbs Free Energies (kcal/mol) of Transition States 3 Catalyzed by the DBU and Its Derivatives (All the Relative Energies Were Calculated At the M06-2X/6-31G(d, p)/IEF-PCM<sub>chloroform</sub> Level of Theory)

| Catalyst       | Structure | 3     |
|----------------|-----------|-------|
| DBU            | ![DBU](image) | 24.9  |
| α-methyl       | ![α-methyl](image) | 28.5  |
| α-fluoro       | ![α-fluoro](image) | 26.6  |
| α-cyano        | ![α-cyano](image) | 30.3  |
| α-methoxy      | ![α-methoxy](image) | 24.0  |
5. Test of DFT methods

To justify the choice of computational method (M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}//M06-2X/6-31G(d, p)/IEF-PCM_{chloroform}), we have additionally computed the energies of the transition state 1 and intermediate 2 at the M06-2X /6-311++G(2df, 2pd)/IEF-PCM_{chloroform}/M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} and ωB97X-D/6-311++G(2df, 2pd)/IEF-PCM_{chloroform} levels. As summarized in Table S2, the energies of transition state 1 and intermediate 2 calculated by the three methods have small differences, indicating the selected method is suitable for the reaction.

Table S2. The Relative Gibbs Free Energies of Transition State 1 and Intermediate 2 Calculated by Three DFT Methods

| Method | M06-2X-D3 | M06-2X | ωB97X-D |
|--------|-----------|--------|---------|
| 1      | 12.5\textsuperscript{a} | 14.0\textsuperscript{b} | 16.5\textsuperscript{c} |
| 2      | 12.2\textsuperscript{a} | 13.7\textsuperscript{b} | 16.0\textsuperscript{c} |

\textsuperscript{a}The energy was calculated at M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}/M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level.

\textsuperscript{b}The energy was calculated at M06-2X/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}/M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level.

\textsuperscript{c}The energy was calculated at ωB97X-D/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}/ωB97X-D/6-31G(d, p)/IEF-PCM_{chloroform} level.
6. The two reaction models (models 1 and 2)

As shown in Scheme S1, we have studied the other reaction (model 2) between N-phenyl isatin R1s and 1-naphthyl (1-Np) difluoronitromethyl ketone R2s catalyzed by DBU Cat to synthesize 3,3-disubstituted oxindole Ps and 2,2-disubstituted oxindole Side-Ps, and the corresponding energy profile has been provided in Table S3. Obviously, the product Ps is also the main product, which is consistent with the experiment. As summarized in Table S3, the relative energies of all the transition states involved in the model 2 are similar to those involved in the model 1 discussed in the manuscript, so it indicates that the C–C bond cleavage step (via 3) is still the rate-determining step and the α carbonyl path is more energetically favorable than the β carbonyl path in model 2, thus leads to the 3,3-disubstituted oxindole Ps is the main product, which is in agreement with the experimental observations.

Scheme S1. DBU-Catalyzed Insertions of N-Methyl/N-Phenyl Isatins into Aryl/1-Naphthyl Difluoronitromethyl Ketones, Respectively, to Synthesize 3,3-Disubstituted and 2,2-Disubstituted Oxindoles in the Reaction Models 1/2

Table S3. The Relative Gibbs Free Energies (kcal/mol) of All Transition States Catalyzed by DBU in Model 2 (All the Energies Were Calculated at M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCMchloroform//M06-2X/6-31G(d, p)/IEF-PCMchloroform Level)

| Transition State | Model 1   | Model 2   |
|------------------|-----------|-----------|
| 1                | 12.7      | 14.4      |
| 3                | 24.4      | 22.1      |
| α-5              | 24.0      | 19.0      |
| β-5              | 20.7      | 14.9      |
| α-7              | 26.6      | 19.4      |
| β-7              | 8.6       | 6.3       |
| α-9              | 19.5      | 15.7      |
| β-9              | 4.4       | 5.6       |
7. The protocol used to generate NCI plot

The protocol for generating NCI plot included three steps:

1. The .fchk formatted file was obtained by theoretical calculation, e.g. \( \alpha-5.fchk \) and \( \beta-5.fchk \);

2. The Multiwfn program was used to open the \( \alpha-5.fchk \) file, and then the instructive number was inputted one-by-one in the operated window based on the prompt: 100 Other founctions; 1 Draw scatter graph between two functions and generate their cube files; 15 Sign(\( \lambda_2 \))*rho, 13 Reduced density gradient (RDG); -10 Set extension distance of grid range for mode 1~4; 0 Input extension distance; 2 Medium quality grid; 3 Output cube files to func1.cub and func2.cub;

3. The two generated func1.cub and func2.cub files were dragged into the VMD program, and then a script of \texttt{template.vmd} was loaded from the option of “Load state” in the prompt column of “File”, and eventually, the generated NCI plot was rendered by the option of “Render” in the prompt column of “File” and form a picture of NCI plot.

The script of \texttt{template.vmd} was shown as follows.

\begin{verbatim}
mol new func1.cub
mol addfile func2.cub
mol delrep 0 top
mol representation CPK 0.8 0.3 18.0 16.0
mol addrep top
mol representation Isosurface 0.50000 1 0 0 1 1
mol color Volume 0
mol addrep top
mol scaleminmax top 1 -0.04 0.02
color scale method BGR
color Display Background white
axes location Off
\end{verbatim}
8. Absolute single-point energies and GFE of all the optimized structures in model 1

Table S4. The Single-Point Energies and Relative Gibbs Free Energies (GFE=E+GFEC) of All Stationary Points Involved in the Reaction Calculated at M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM<sub>chloroform</sub>///M06-2X/6-31G(d, p)/IEF-PCM<sub>chloroform</sub> Level (unit: a.u.)

|     | E          | GEE        |
|-----|------------|------------|
| Cat | −462.0418307 | −461.8286187 |
| R1  | −787.8386246 | −787.7511366 |
| R2  | −552.3500153 | −552.2396383 |
| 0   | −1249.896312 | −1249.574205 |
| 1   | −1249.886641 | −1249.559541 |
| 2   | −1249.888422 | −1249.560031 |
| 3   | −1249.870746 | −1249.540909 |
| 4   | −1249.873439 | −1249.547478 |
| β-5 | −1802.247750 | −1801.786416 |
| α-5 | −1802.239850 | −1801.781077 |
| β-3| −1802.226238 | −1801.766499 |
| β-6 | −1802.275563 | −1801.811740 |
| α-6 | −1802.253068 | −1801.789616 |
| β-7 | −1802.272962 | −1801.805740 |
| α-7 | −1802.242457 | −1801.777016 |
| β-8 | −1802.277117 | −1801.812196 |
| α-8 | −1802.252135 | −1801.786432 |
| β-9 | −1802.276045 | −1801.812332 |
| α-9 | −1802.251122 | −1801.788367 |
| P   | −1340.237279 | −1340.013313 |
| Side-P | −1340.215739 | −1339.992483 |
9. Absolute single-point energies and GFE of all the transition states in model 2

Table S5. The Single-Point Energies and Relative Gibbs Free Energies (GFE=E+GFEC) of All Transition States Involved in the Reaction Calculated at M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM$_{chloroform}$//M06-2X/6-31G(d, p)/IEF-PCM$_{chloroform}$ Level (unit: a.u.)

|     | E              | GEE             |
|-----|----------------|-----------------|
| Cat | −462.0418307   | −461.8286187    |
| R1s | −941.4600625   | −941.3281645    |
| R2s | −744.0708775   | −743.9125275    |
| 2s  | −1403.507954   | −1403.133822    |
| 4s  | −1403.495240   | −1403.121540    |
| β-5s| −2147.599875   | −2147.045515    |
| α-5s| −2147.593185   | −2147.039018    |
| β-7s| −2147.620372   | −2147.059225    |
| α-7s| −2147.597237   | −2147.038318    |
| β-9s| −2147.617824   | −2147.060394    |
| α-9s| −2147.603121   | −2147.044274    |
10. List of all the vibrational frequencies of the optimized structures in model 1

| Cat | 65.2491 | 73.9311 | 146.0818 |
|-----|---------|---------|----------|
|     | 236.5792| 245.0067| 302.9263 |
|     | 348.0997| 363.7800| 401.8991 |
|     | 432.9583| 481.0829| 513.2671 |
|     | 516.5765| 644.5669| 704.4557 |
|     | 706.4889| 816.8174| 849.3719 |
|     | 855.2755| 883.5877| 894.2317 |
|     | 911.7876| 935.3334| 980.4080 |
|     | 1002.5633| 1016.2030| 1032.0766 |
|     | 1094.7413| 1114.5457| 1119.0373 |
|     | 1127.9965| 1148.0064| 1180.9305 |
|     | 1215.4248| 1231.8135| 1245.6513 |
|     | 1259.7823| 1272.0940| 1290.0701 |
|     | 1307.6535| 1323.3714| 1351.4887 |
|     | 1363.1964| 1373.5271| 1376.5636 |
|     | 1389.3230| 1404.1313| 1408.4300 |
|     | 1413.0551| 1472.4535| 1484.0430 |
|     | 1487.0985| 1493.2855| 1494.3453 |
|     | 1503.0840| 1508.5004| 1522.4653 |
|     | 1541.5261| 1733.0894| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |
|     | 1538.6123| 1541.5261| 3026.7361 |

| 0   | 7.9278  | 26.4115 | 36.8551  |
|-----|---------|---------|----------|
|     | 43.1618 | 54.1463 | 68.7128  |
|     | 84.7466 | 94.1543 | 102.5314 |
|     | 109.3300| 117.9806| 142.8679 |
|     | 166.9792| 176.5164| 213.9220 |
|     | 249.4085| 256.9535| 260.0740 |
|     | 304.4777| 308.7623| 314.9629 |
|     | 352.2541| 378.0429| 382.1952 |
|     | 405.3205| 411.6656| 415.3740 |
|     | 438.2248| 442.4175| 489.4656 |
|     | 511.8890| 515.8423| 525.4963 |
|     | 575.2855| 598.4380| 620.7036 |
|     | 631.0050| 646.8783| 698.3713 |
|     | 703.3748| 712.2870| 714.3807 |
|     | 757.1314| 816.8048| 819.1140 |
|     | 848.8699| 849.4321| 856.2128 |
|     | 877.0048| 887.6979| 893.6227 |
|     | 917.4590| 937.8256| 941.8179 |
|     | 971.2183| 985.4955| 1001.8421|
|     | 1008.4592| 1016.3451| 1017.2894|
|     | 1032.4388| 1034.3681| 1038.7234|
|     | 1074.7907| 1097.8434| 1115.6748|
|     | 1119.5169| 1129.0715| 1129.7347|

S12
| S13  | 1146.3617 | 1179.9081 | 1181.7377 |
|------|-----------|-----------|-----------|
| 1216.2711 | 1216.6241 | 1235.6175 |
| 1246.1354 | 1253.6882 | 1308.9286 |
| 1272.9656 | 1348.8483 | 1383.7290 |
| 1325.1506 | 1405.5219 | 1408.5948 |
| 1356.9335 | 1476.2688 | 1483.6277 |
| 1372.5630 | 1491.2265 | 1499.0170 |
| 1502.2669 | 1504.1426 | 1510.3678 |
| 1512.7375 | 1523.3847 | 1541.8506 |
| 1554.2644 | 1676.4420 | 1693.9753 |
| 1721.9302 | 1779.6130 | 1846.3743 |
| 3032.0921 | 3041.5428 | 3047.4532 |
| 3058.5570 | 3062.0315 | 3068.9429 |
| 3072.1592 | 3078.7502 | 3086.2013 |
| 3105.0198 | 3110.4599 | 3114.0191 |
| 3125.6686 | 3127.7856 | 3139.8548 |
| 3178.4747 | 3209.9803 | 3215.7138 |
| 3230.9574 | 3235.7285 | 3243.8886 |

2

|        | 26.7810 | 42.0006 | 54.6717 |
|--------|---------|---------|---------|
| 65.0191 | 73.8447 | 88.3767 |
| 97.9820 | 103.3240 | 125.2958 |
| 150.3308 | 171.4980 | 198.4127 |
| 211.6120 | 235.0382 | 245.2305 |
| 263.0092 | 275.2005 | 303.0855 |
| 313.8329 | 316.4232 | 330.4790 |
| 366.9549 | 379.4593 | 401.8353 |
| 415.4832 | 419.0823 | 446.3320 |
| 452.3088 | 489.5373 | 509.4102 |
| 521.4532 | 527.6520 | 545.7859 |
| 559.5888 | 606.2053 | 628.3661 |
| 642.7264 | 668.8249 | 711.7952 |
| 726.7178 | 729.1547 | 741.0736 |
| 777.8679 | 812.0192 | 828.5420 |
| 848.0968 | 858.1014 | 862.2468 |
| 880.8288 | 884.1852 | 896.2438 |
| 932.6073 | 940.6871 | 950.4839 |
| 969.3062 | 988.9811 | 1001.6542 |
| 1010.0801 | 1019.6447 | 1027.5854 |
| 1032.9016 | 1039.3111 | 1065.9931 |
| 1082.2123 | 1105.0720 | 1111.5972 |
| 1117.7974 | 1127.6132 | 1134.9554 |
| 1138.0793 | 1179.5202 | 1182.2176 |
| 1190.8998 | 1211.0116 | 1227.2758 |
| 1233.5561 | 1250.3630 | 1259.1102 |
| 1266.3694 | 1273.7205 | 1295.2021 |
| 1313.8806 | 1321.0343 | 1328.4475 |
| 1355.7551 | 1354.0404 | 1359.2187 |
| 1364.5239 | 1374.0728 | 1382.6840 |
| 1391.3011 | 1404.0816 | 1407.8412 |
| 1417.6161 | 1435.7571 | 1479.1729 |
| 1485.5890 | 1491.7953 | 1491.9236 |
| 1500.9584 | 1505.0590 | 1509.3223 |
| 1520.0237 | 1523.4563 | 1527.7150 |
| 1542.5328 | 1574.9032 | 1664.9333 |
| 1682.3153 | 1781.8532 | 3051.4016 |
| 3051.4016 | 3093.6580 | 3099.2554 |
| 3099.2554 | 3107.7361 | 3112.3089 |
| 3112.3089 | 3121.8423 | 3125.1037 |
| 3125.1037 | 3144.9799 | 3149.4982 |
| 3149.4982 | 3174.9032 | 3202.7978 |
| 3202.7978 | 3210.6947 | 3218.2452 |
| 3218.2452 | 3221.6215 | 3227.7150 |

| 4 | 23.6187 | 40.0378 | 51.3432 |
| 40.0378 | 55.9637 | 114.3992 |
| 114.3992 | 122.8273 | 145.0355 |
| 145.0355 | 173.9883 | 252.5927 |
| 252.5927 | 251.1542 | 282.2512 |
| 282.2512 | 295.6679 | 312.3089 |
| 312.3089 | 341.1888 | 391.9917 |
| 391.9917 | 410.2081 | 433.3440 |
| 433.3440 | 439.4185 | 469.0336 |
| 469.0336 | 501.6351 | 555.2477 |
| 555.2477 | 573.7224 | 616.0033 |
| 616.0033 | 625.1266 | 675.2462 |
| 675.2462 | 695.9790 | 731.4774 |
| 731.4774 | 767.4762 | 803.1668 |
| 803.1668 | 817.3780 | 857.7655 |
| 857.7655 | 884.7387 | 891.2194 |
| 891.2194 | 903.3884 | 963.9971 |
| 963.9971 | 967.5032 | 1008.2409 |
| 1008.2409 | 1010.8243 | 1029.4387 |
| 1029.4387 | 1034.4556 | 1065.8978 |
| 1065.8978 | 1076.6492 | 1115.9319 |
| 1115.9319 | 1119.5378 | 1136.7731 |
| 1136.7731 | 1155.7457 | 1181.5827 |
| 1181.5827 | 1183.4039 | 1202.2686 |
| 1202.2686 | 1227.2896 | 1269.9268 |
| 1269.9268 | 1272.4927 | 1296.4969 |
| 1296.4969 | 1307.9436 | 1341.1166 |
| 1341.1166 | 1345.2134 | 1362.9569 |
| 1362.9569 | 1368.5295 | 1394.4734 |
| 1394.4734 | 1404.9091 | 1423.4060 |
| 1423.4060 | 1432.6407 | 1470.2256 |
| 1470.2256 | 1475.7539 | 1491.6149 |
| 1491.6149 | 1494.0432 | 1503.8136 |
| 1503.8136 | 1511.6396 | 1537.1502 |
| 1537.1502 | 1548.9042 | 1567.9266 |
| 1567.9266 | 1688.2480 | 1850.8258 |
| 1850.8258 | 3048.2647 | 3086.4793 |
| 3086.4793 | 3088.4575 | 3100.7897 |
| 3100.7897 | 3110.3924 | 3126.3579 |
| 3126.3579 | 3129.5106 | 3154.4133 |
| 3154.4133 | 3166.4818 | 3204.6402 |
| 3204.6402 | 3211.6478 | 3222.9616 |
|         | 3223.7905 | 3228.1790 | 3237.3236 |
|---------|-----------|-----------|-----------|
| \( \beta \) |           |           |           |
|         | 29.7989   | 32.8071   | 38.1322   |
|         | 47.5186   | 50.5484   | 57.3940   |
|         | 60.0558   | 71.5036   | 84.2786   |
|         | 87.3141   | 95.3310   | 104.5122  |
|         | 111.3746  | 121.8970  | 139.6851  |
|         | 149.5665  | 162.9091  | 170.6354  |
|         | 181.2248  | 201.2363  | 204.4657  |
|         | 214.0933  | 238.0569  | 246.2207  |
|         | 262.0835  | 281.0349  | 285.3357  |
|         | 293.7307  | 297.2831  | 299.6288  |
|         | 315.5045  | 317.5762  | 339.2216  |
|         | 343.1613  | 347.5041  | 362.1199  |
|         | 389.6600  | 396.8352  | 403.3062  |
|         | 414.7192  | 433.5331  | 444.6646  |
|         | 447.9472  | 467.9428  | 492.5358  |
|         | 495.6029  | 509.4174  | 525.2021  |
|         | 542.0222  | 548.8775  | 551.8269  |
|         | 577.3038  | 594.6184  | 610.1828  |
|         | 627.5948  | 634.4057  | 665.1470  |
|         | 678.3302  | 693.7763  | 702.1516  |
|         | 709.6977  | 713.6072  | 732.1407  |
|         | 753.6845  | 772.1675  | 773.8558  |
|         | 781.1016  | 797.3691  | 816.1103  |
|         | 842.1361  | 845.1631  | 856.7011  |
|         | 864.4910  | 881.2681  | 883.4766  |
|         | 892.5094  | 895.6880  | 930.7480  |
|         | 946.3516  | 949.7235  | 958.6155  |
|         | 968.3545  | 976.0227  | 981.5721  |
|         | 994.9192  | 999.6619  | 1003.3697 |
|         | 1006.6343 | 1013.5846 | 1022.7312 |
|         | 1030.9728 | 1034.4874 | 1062.8987 |
|         | 1064.0180 | 1076.6418 | 1083.9818 |
|         | 1105.0200 | 1110.7830 | 1113.9439 |
|         | 1121.8629 | 1132.6418 | 1135.1709 |
|         | 1145.6058 | 1156.9786 | 1163.6306 |
|         | 1176.3416 | 1182.6921 | 1191.0582 |
|         | 1194.2487 | 1204.5779 | 1227.0091 |
|         | 1233.6744 | 1262.5822 | 1268.2629 |
|         | 1270.3854 | 1274.9063 | 1288.6536 |
|         | 1303.6320 | 1308.7866 | 1314.5122 |
|         | 1325.2953 | 1333.8607 | 1335.2185 |
|         | 1347.9446 | 1349.5355 | 1360.8460 |
|         | 1362.4866 | 1371.5054 | 1375.0238 |
|         | 1391.5409 | 1396.8314 | 1402.0426 |
|         | 1407.2395 | 1413.8768 | 1427.1418 |
|         | 1428.4055 | 1453.3717 | 1468.1705 |
|         | 1479.2642 | 1482.2315 | 1486.2265 |
|         | 1487.7386 | 1497.8888 | 1499.0055 |
|         | 1502.5875 | 1504.7721 | 1511.6322 |
|         | 1514.6494 | 1518.0738 | 1530.1632 |
|         | 1536.3860 | 1548.8432 | 1554.3690 |
|         | 1677.7566 | 1696.1894 | 1697.7179 |
|         | 1707.2287 | 1708.8268 | 1759.8603 |
| α-6            |
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| 21.1869        |
| 31.4046        |
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| 60.6004        |
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| 84.6767        |
| 92.5390        |
| 97.9898        |
| 99.4880        |
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| 201.5719       |
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| 290.0928       |
| 307.1925       |
| 311.4596       |
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| 413.2765       |
| 420.2575       |
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| 709.0891       |
| 723.4010       |
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| 771.2968       |
| 776.8721       |
| 802.3382       |
| 806.9823       |
| 817.9974       |
| 834.4331       |
| 845.2881       |
| 855.5901       |
| 861.6908       |
| 881.2693       |
| 883.7859       |
| 887.4362       |
| 900.5571       |
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| 929.7409       |
| 960.1474       |
| 969.2473       |
| 971.4816       |
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| 1033.2891      |
| 1039.4800      |
| 1061.0090      |
| 1066.5192      |
| 1077.0212      |
| 1087.6849      |
| 1105.2099      |
| 1120.4794      |
| 1121.9491      |
| 1128.5280      |
| 1130.4144      |
| 1131.2777      |
| 1136.9041      |
| 1146.6851      |
| 1156.2675      |
| 1184.5979      |
| 1185.1376      |
| 1198.4179      |
| 1208.9430      |
| 1216.7203      |
| 1225.3396      |
| 1233.4003      |
| 1239.1579      |
| 1260.8751      |
| 1268.8192      |
| 1274.9665      |
| 1290.8408      |
| 1296.8782      |
| 1305.5324      |
| 1316.8356      |
| 1321.0144      |
| 1323.2054      |
| 1344.7110      |
| 1346.6615      |
| 1351.8817      |
| 1356.2731      |
| 1367.5070      |
| 1368.4678      |
| 1368.6512      |
| 1373.2967      |
| 1390.4345      |
| 1395.1647      |
| Value   | Value   | Value   |
|---------|---------|---------|
| 1402.5798 | 1411.8617 | 1415.5332 |
| 1427.7614 | 1446.5798 | 1471.4395 |
| 1481.9232 | 1492.8102 | 1500.0140 |
| 1505.3198 | 1527.7614 | 1533.9232 |
| 1524.4714 | 1546.5798 | 1548.9054 |
| 1536.0360 | 1552.9195 | 1556.3029 |
| 1584.4942 | 1605.3198 | 1607.0359 |
| 1648.9548 | 1670.2242 | 1680.2374 |
| 1695.3029 | 1700.2242 | 1706.0359 |
| 1762.6486 | 1848.9548 | 1857.7220 |
| 1911.0105 | 1927.8102 | 1931.4476 |
| 1946.5798 | 1955.8102 | 1956.3029 |
| 2000.0140 | 2027.8102 | 2031.4476 |
| 2054.2909 | 2063.9537 | 2068.3015 |
| 2127.5643 | 2127.9630 | 2128.4925 |
| 2240.3959 | 2242.5094 | 2243.2188 |

\[ \beta -8 \]

| Value   | Value   | Value   |
|---------|---------|---------|
| 19.1557 | 28.1484 | 38.4170 |
| 47.1321 | 53.6773 | 56.9671 |
| 62.8996 | 73.8514 | 88.8464 |
| 91.1700 | 98.5478 | 113.5713 |
| 135.6691 | 140.0738 | 152.2519 |
| 163.9537 | 166.0989 | 177.1386 |
| 182.8127 | 198.8826 | 212.7610 |
| 221.9378 | 230.6317 | 244.0585 |
| 262.8171 | 277.0725 | 288.3015 |
| 299.7152 | 309.4753 | 315.1815 |
| 319.3077 | 327.6572 | 340.8789 |
| 358.5581 | 364.8345 | 367.4183 |
| 393.8962 | 403.1582 | 407.5290 |
| 414.6259 | 443.4088 | 457.1236 |
| 470.6222 | 489.6503 | 496.9256 |
| 518.6171 | 522.1194 | 541.6849 |
| 550.6650 | 554.2362 | 565.7607 |
| 593.3942 | 613.9537 | 628.0458 |
| 642.2411 | 670.5990 | 679.0622 |
| 700.2639 | 712.5034 | 721.2282 |
| 726.4060 | 729.6729 | 747.5931 |
| 756.6339 | 760.7190 | 774.9254 |
| 800.3560 | 807.0320 | 822.0378 |
| 847.0946 | 849.7464 | 858.7584 |
| 877.8175 | 879.0225 | 881.6364 |
| 885.6502 | 898.4342 | 933.0500 |
| 941.9190 | 949.5431 | 952.6221 |
| 960.6205 | 984.2814 | 987.4038 |
| 1003.6510 | 1005.7953 | 1007.7708 |
| 1008.2519 | 1020.9569 | 1028.4688 |
| 1031.9397 | 1045.2434 | 1060.9565 |
| 1068.4778 | 1073.2612 | 1102.4807 |
| 1115.7610 | 1119.1864 | 1122.0367 |
| 1131.0703 | 1134.2258 | 1136.5065 |
| 1147.8567 | 1154.0384 | 1158.1405 |
1176.5740 1178.3026 1188.5324
1189.9772 1197.6798 1221.2900
1235.0768 1240.0362 1265.0961
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1301.6691 1302.3351 1321.3674
1324.7768 1327.7354 1335.5642
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1357.7629 1368.2105 1405.3634
1408.9161 1411.5837 1421.6469
1427.8193 1455.3059 1456.2122
1482.2394 1487.1107 1488.6383
1496.6498 1497.8763 1498.7638
1502.2963 1510.5420 1680.6129
1517.3453 1518.9660 1525.8567
1532.1952 1551.7419 1556.6976
1594.8335 1670.9152 1680.6129
1695.9797 1697.0436 1709.5229
1780.0290 1837.6915 3049.6275
3066.2742 3070.7486 3070.9774
3070.9774 3076.7291 3092.6131
3095.3076 3111.8969 3112.5441
3117.6165 3131.1270 3146.0574
3154.5605 3182.1813 3186.9477
3193.9608 3197.3837 3199.4022
3206.1475 3206.6189 3212.7224
3214.8600 3217.5895 3221.8267
3224.6917 3231.7652 3233.5822

α-8

28.4757 33.5203 42.7766
46.4540 51.7864 59.2887
63.8129 71.0131 82.7584
91.6125 109.6018 116.5210
134.5282 140.8739 151.3956
168.3516 171.3432 187.5221
197.3869 199.8008 211.4956
222.2276 247.8396 266.4652
273.6141 275.3535 283.2850
291.2202 297.3683 312.2157
318.4216 325.0382 340.9425
349.8475 363.3793 366.5139
393.7476 405.3596 417.1485
423.4266 430.1920 449.6121
472.9358 502.6473 510.3174
528.1734 534.9726 536.4206
547.3245 553.9624 559.9436
580.4706 602.7768 627.4539
646.5618 663.5045 673.3410
691.1225 704.4100 716.0352
726.6913 728.4932 748.4020
758.9306 769.5849 778.7402
797.6245 806.7559 818.0647
845.8869 850.7026 863.2113
868.8635 879.5157 884.1396
886.9631 897.2467 916.4969
| 931.9112 | 939.5930 | 951.1430 |
| 960.8346 | 979.1379 | 988.0355 |
| 1004.9939 | 1005.4105 | 1008.3115 |
| 1020.5118 | 1027.7503 | 1029.2066 |
| 1035.2110 | 1043.1411 | 1049.8808 |
| 1062.1308 | 1069.4418 | 1103.7023 |
| 1115.7142 | 1181.9666 | 1187.6816 |
| 1201.3738 | 1215.4064 | 1228.7177 |
| 1231.7761 | 1237.2751 | 1246.8036 |
| 1261.7626 | 1269.5693 | 1276.1475 |
| 1290.6553 | 1301.2931 | 1315.9562 |
| 1325.1659 | 1328.9204 | 1331.9647 |
| 1337.3483 | 1343.9063 | 1357.3459 |
| 1358.8631 | 1367.1143 | 1370.6213 |
| 1378.9678 | 1384.8672 | 1398.1127 |
| 1405.8657 | 1411.9825 | 1420.6861 |
| 1421.6360 | 1466.7081 | 1475.7825 |
| 1487.5831 | 1490.3209 | 1495.4092 |
| 1496.9619 | 1498.5717 | 1499.7852 |
| 1504.7917 | 1514.5047 | 1519.3359 |
| 1522.8043 | 1528.0188 | 1533.5310 |
| 1538.0453 | 1549.6782 | 1554.4622 |
| 1593.9689 | 1677.9388 | 1680.0622 |
| 1684.3003 | 1697.4894 | 1710.0912 |
| 1777.1937 | 1885.3684 | 3050.3104 |
| 3056.5513 | 3069.6847 | 3070.4311 |
| 3071.4555 | 3074.2726 | 3098.4345 |
| 3101.3370 | 3112.4815 | 3114.7695 |
| 3120.7891 | 3126.2795 | 3140.2924 |
| 3156.5708 | 3159.5432 | 3173.9361 |
| 3176.2826 | 3182.5271 | 3195.8048 |
| 3206.5742 | 3209.6146 | 3215.3421 |
| 3222.4166 | 3223.3427 | 3226.3210 |
| 3229.0041 | 3236.3706 | 3240.1570 |

**P**

| 26.7012 | 36.7227 | 49.8046 |
| 50.1634 | 62.9779 | 76.0762 |
| 79.1172 | 108.0881 | 115.1358 |
| 128.1922 | 150.5121 | 156.3225 |
| 168.6939 | 201.1083 | 216.0806 |
| 236.1265 | 272.9182 | 278.9795 |
| 295.5295 | 314.9471 | 324.0506 |
| 348.9654 | 361.7140 | 392.6274 |
| 415.0622 | 445.3225 | 449.2601 |
| 475.0313 | 495.4845 | 517.7910 |
| 545.6869 | 552.2425 | 589.7834 |
| 611.9342 | 626.6323 | 682.3768 |
| 697.4735 | 702.6557 | 710.3257 |
| 727.0203 | 733.9065 | 760.4109 |
| 774.0052 | 777.5796 | 820.2741 |
| 826.1864 | 873.4081 | 888.4784 |
| 891.1439 | 893.9154 | 969.2775 |
|      |      |      |
|------|------|------|
| 979.9767 | 994.7344 | 1011.0022 |
| 1013.6973 | 1020.7585 | 1021.6133 |
| 1042.6425 | 1049.4006 | 1063.4550 |
| 1066.5218 | 1114.0034 | 1122.6913 |
| 1135.2938 | 1148.4427 | 1154.6659 |
| 1160.8020 | 1182.8053 | 1183.6185 |
| 1192.4115 | 1200.6850 | 1274.9061 |
| 1306.3384 | 1345.1178 | 1367.8820 |
| 1367.8820 | 1400.6099 | 1430.1194 |
| 1457.6737 | 1495.4703 | 1505.4723 |
| 1511.2792 | 1521.3476 | 1530.9236 |
| 1548.9883 | 1560.1240 | 1678.1869 |
| 1694.3680 | 1860.7454 | 1886.6667 |
| 1789.5086 | 236.2154 | 268.9956 |
| 1817.2475 | 376.5830 | 405.6918 |
| 1839.3172 | 440.8534 | 411.5234 |
| 2019.1213 | 502.2309 | 541.3321 |
| 236.2154 | 584.1872 | 624.2398 |
| 268.9956 | 706.5085 | 735.8149 |
| 3155.2041 | 817.2475 | 867.8753 |
| 108.6089 | 966.7451 | 1014.4208 |
| 1122.6300 | 1019.1213 | 1066.1534 |
| 1209.5808 | 1127.8572 | 1184.7830 |
| 1342.6368 | 1268.0150 | 1313.6109 |
| 1503.8307 | 1367.0415 | 1370.1068 |
| 1672.3781 | 1522.7299 | 1548.4614 |
| 1857.5046 | 1690.6701 | 1799.8477 |
| 3215.8257 | 1857.5046 | 3226.9883 |
| 3232.4658 | 3232.4658 | 3244.6431 |

R1

|      |      |      |
|------|------|------|
| 26.9758 | 45.6970 | 69.9982 |
| 116.0827 | 142.6115 | 191.5694 |
| 236.2154 | 268.9956 | 302.3424 |
| 376.5830 | 405.6918 | 411.5234 |
| 440.8534 | 502.2309 | 541.3321 |
| 584.1872 | 624.2398 | 697.9548 |
| 706.5085 | 727.4708 | 735.8149 |
| 817.2475 | 847.9889 | 867.8753 |
| 939.3172 | 966.7451 | 1014.4208 |
| 1019.1213 | 1041.8956 | 1066.1534 |
| 1122.6300 | 1127.8572 | 1184.7830 |
| 1209.5808 | 1268.0150 | 1313.6109 |
| 1342.6368 | 1367.0415 | 1370.1068 |
| 1503.8307 | 1522.7299 | 1548.4614 |
| 1672.3781 | 1690.6701 | 1799.8477 |
| 1857.5046 | 3215.8257 | 3226.9883 |
| 3232.4658 | 3237.9149 | 3244.6431 |

R2

|      |      |      |
|------|------|------|
| 108.6089 | 121.4239 | 142.5000 |
| 161.8209 | 239.5984 | 280.5989 |
| 294.6160 | 332.0854 | 409.7663 |
| 486.1516 | 490.9875 | 538.3795 |
| 560.0050 | 564.4408 | 697.0349 |
| 721.6259 | 734.3184 | 777.3629 |
| 831.8356 | 882.0294 | 895.7087 |
| 983.4107 | 985.2228 | 1025.2496 |
| 1058.7776 | 1076.7135 | 1128.4095 |
| 1147.2616 | 1150.2523 | 1187.8055 |
| 1230.7745 | 1290.0118 | 1353.0142 |
| 1380.7430 | 1425.3114 | 1456.2188 |
| 1495.9531 | 1514.1632 | 1531.7703 |
| 1554.0943 | 1692.8696 | 1707.1804 |
| 1881.0321 | 1897.3481 | 3074.9360 |
| 3150.7025 | 3192.4164 | 3216.8650 |
|-----------|-----------|-----------|
| 3227.9772 | 3232.0583 | 3242.5227 |

**Side-P**

| 24.5208 | 33.6426 | 41.8183 |
|----------|---------|---------|
| 50.9538 | 62.8538 | 73.5072 |
| 83.0248 | 121.3419 | 125.7500 |
| 144.6681 | 150.1763 | 159.6313 |
| 170.1156 | 194.9402 | 206.4174 |
| 252.6167 | 260.6826 | 280.0129 |
| 289.8397 | 307.9214 | 319.8483 |
| 336.6065 | 358.5026 | 398.7286 |
| 414.0826 | 426.1994 | 449.2135 |
| 463.4726 | 515.7744 | 531.5182 |
| 536.3840 | 555.2472 | 569.4542 |
| 595.8987 | 626.2952 | 663.4650 |
| 689.2104 | 700.5117 | 706.2177 |
| 720.2838 | 729.8880 | 760.7148 |
| 774.4218 | 786.2636 | 820.4409 |
| 824.2345 | 869.9200 | 878.1428 |
| 886.2356 | 891.3328 | 934.9381 |
| 982.9464 | 982.9987 | 1015.1732 |
| 1019.9083 | 1022.7741 | 1028.7672 |
| 1044.9843 | 1055.9717 | 1058.8500 |
| 1066.0537 | 1111.7883 | 1114.7241 |
| 1132.2233 | 1140.2567 | 1146.9067 |
| 1154.6828 | 1180.6523 | 1184.3238 |
| 1201.7637 | 1218.4907 | 1232.9652 |
| 1298.6439 | 1321.0844 | 1330.5594 |
| 1344.0250 | 1346.8306 | 1361.1411 |
| 1367.0333 | 1375.0711 | 1414.7246 |
| 1469.9396 | 1501.1682 | 1505.4779 |
| 1517.0102 | 1521.5717 | 1535.5774 |
| 1543.9552 | 1549.9380 | 1678.1880 |
| 1682.2259 | 1694.9180 | 1704.6157 |
| 1785.5260 | 1866.3223 | 1897.4104 |
| 3070.8554 | 3150.3570 | 3178.6182 |
| 3216.9677 | 3221.5759 | 3221.6782 |
| 3233.4122 | 3233.7708 | 3238.1418 |
| 3246.3107 | 3247.1401 | 3256.7253 |

| 21.3620 | 34.9707 |
|----------|---------|
| 49.9998 | 57.8547 | 67.1950 |
| 77.7109 | 96.3392 | 107.0047 |
| 128.5144 | 158.6257 | 165.3030 |
| 205.7100 | 212.8379 | 238.2077 |
| 259.3479 | 264.1300 | 297.8836 |
| 305.1990 | 307.0848 | 315.7567 |
| 364.8465 | 379.5609 | 397.2894 |
| 413.4245 | 417.2268 | 435.4501 |
| 443.9473 | 483.4628 | 495.7074 |
| 515.4024 | 521.1045 | 528.5846 |
| 551.5956 | 606.9164 | 628.4038 |
| 642.7521 | 648.0610 | 708.4726 |

1
| 720.2585 | 722.3466 | 724.9710 |
| 768.6878 | 802.8694 | 816.0579 |
| 846.3976 | 851.6450 | 857.1718 |
| 880.1372 | 886.3291 | 896.0134 |
| 930.1565 | 941.8083 | 948.1469 |
| 967.6120 | 987.1846 | 1001.6077 |
| 1008.8772 | 1019.8138 | 1023.4623 |
| 1032.7332 | 1036.0534 | 1064.4380 |
| 1076.8293 | 1101.6284 | 1116.6988 |
| 1117.5791 | 1126.1122 | 1132.8131 |
| 1138.1705 | 1221.6349 | 1293.1577 |
| 1235.9314 | 1323.7488 | 1340.1083 |
| 1342.0386 | 1357.2055 | 1360.4095 |
| 1361.9107 | 1375.2393 | 1380.3699 |
| 1391.3682 | 1403.8140 | 1408.4468 |
| 1420.4430 | 1477.4631 | 1482.0356 |
| 1490.8417 | 1492.7188 | 1498.2867 |
| 1500.4800 | 1506.6367 | 1519.3098 |
| 1522.6953 | 1524.2247 | 1546.7766 |
| 1558.1984 | 1600.9440 | 1672.7034 |
| 1684.2945 | 1697.3197 | 1783.0609 |
| 3049.0498 | 3055.9802 | 3061.7893 |
| 3065.2846 | 3077.7988 | 3091.7815 |
| 3094.7726 | 3100.1307 | 3109.5680 |
| 3115.3275 | 3120.6487 | 3140.2507 |
| 3144.4369 | 3158.8165 | 3207.3862 |
| 3208.0945 | 3220.4602 | 3228.8098 |
| 3235.1194 | 3238.2338 | 3241.5575 |

| 3 |
| --- |
| -78.5579 | 38.3437 | 53.4026 |
| 62.8214 | 82.0785 | 89.9790 |
| 110.0060 | 125.0444 | 131.4222 |
| 142.3253 | 160.8004 | 172.4673 |
| 185.5986 | 197.7226 | 244.5157 |
| 259.7994 | 268.1740 | 290.1231 |
| 308.0359 | 319.0427 | 323.6531 |
| 357.3464 | 380.0928 | 390.8359 |
| 418.9347 | 420.1681 | 425.0736 |
| 457.8218 | 462.6695 | 476.3037 |
| 508.1081 | 542.3165 | 569.7331 |
| 571.8060 | 598.0985 | 621.5224 |
| 629.6190 | 633.6921 | 654.7448 |
| 680.7985 | 725.7542 | 731.9648 |
| 768.5507 | 789.3323 | 801.7270 |
| 818.6673 | 849.3077 | 861.5249 |
| 885.4569 | 889.4340 | 895.2551 |
| 906.0229 | 928.1672 | 961.7446 |
| 965.8770 | 973.7023 | 1004.4061 |
| 1010.9655 | 1012.6735 | 1025.2663 |
| 1031.3338 | 1035.0221 | 1062.0259 |
| 1072.1238 | 1103.9389 | 1117.1101 |
| 1119.4720 | 1136.3393 | 1137.9400 |
| \( \beta - 3 \mathbf{N}_2 \) | \(-228.8896\) | \(-32.2835\) | \(52.6608\) | \(78.6334\) | \(104.0619\) | \(134.4862\) | \(155.0351\) | \(190.4689\) | \(228.2300\) | \(264.5378\) | \(295.6140\) | \(313.3546\) | \(350.5013\) | \(413.6113\) | \(444.4785\) | \(486.8988\) | \(536.6007\) | \(560.0964\) | \(603.5875\) | \(633.6650\) | \(708.0947\) | \(726.4233\) | \(768.3771\) | \(814.7988\) | \(860.6368\) | \(883.6306\) | \(906.0285\) | \(965.6906\) | \(990.5888\) | \(1010.3708\) | \(1032.7845\) | \(1066.1900\) | \(1105.1366\) |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|                 | 14.6807   | 33.6517   | 60.9429   | 84.8718   | 111.0399  | 140.7923  | 171.3312  | 193.0854  | 239.4044  | 266.3306  | 302.3813  | 319.0749  | 395.3597  | 426.4085  | 451.3059  | 493.0943  | 544.0472  | 567.9207  | 621.5084  | 680.8683  | 715.5649  | 732.5041  | 774.3374  | 816.4681  | 875.0736  | 887.2213  | 927.1429  | 972.5651  | 1006.7297 | 1022.0150 | 1041.7841 | 1074.5886 | 1117.7327 |
| 1127.9752 | 1129.3930 | 1135.6676 |
| 1147.1928 | 1127.0825 |
| 1151.9963 | 1126.1936 |
| 1174.9785 | 1129.0157 |
| 1179.4915 | 1135.8950 |
| 1182.7057 | 1132.8859 |
| 1191.8955 | 1135.7857 |
| 1198.9349 | 1148.1570 |
| 1203.2944 | 1150.9272 |
| 1227.0825 | 1500.9272 |
| 1231.1872 | 1269.8555 |
| 1240.4235 | 1273.8033 |
| 1262.1936 | 1290.5177 |
| 1269.8555 | 1292.7813 |
| 1273.8033 | 1301.4730 |
| 1290.5177 | 1325.8859 |
| 1301.4730 | 1339.2487 |
| 1325.8859 | 1356.2784 |
| 1348.4159 | 1356.2784 |
| 1364.8154 | 1366.9962 |
| 1366.9962 | 1369.2452 |
| 1369.2452 | 1370.4162 |
| 1370.4162 | 1372.9151 |
| 1372.9151 | 1373.9138 |
| 1373.9138 | 1377.9138 |
| 1377.9138 | 1379.4915 |
| 1379.4915 | 1382.7057 |
| 1382.7057 | 1387.8101 |
| 1387.8101 | 1391.8955 |
| 1391.8955 | 1394.4791 |
| 1394.4791 | 1398.9349 |
| 1398.9349 | 1403.2944 |
| 1403.2944 | 1427.0825 |
| 1427.0825 | 1481.1570 |
| 1481.1570 | 1485.2452 |
| 1485.2452 | 1495.1011 |
| 1495.1011 | 1500.9272 |
| 1500.9272 | 1505.9253 |
| 1505.9253 | 1512.4626 |
| 1512.4626 | 1533.9332 |
| 1533.9332 | 1544.5708 |
| 1544.5708 | 1550.5622 |
| 1550.5622 | 1569.8265 |
| 1569.8265 | 1688.9460 |
| 1688.9460 | 1753.0688 |
| 1753.0688 | 1884.8427 |
| 1884.8427 | 2074.3900 |
| 2074.3900 | 3092.4690 |
| 3092.4690 | 3102.2826 |
| 3102.2826 | 3123.0368 |
| 3123.0368 | 3126.7771 |
| 3126.7771 | 3145.9071 |
| 3145.9071 | 3151.9117 |
| 3151.9117 | 3174.9519 |
| 3174.9519 | 3191.5535 |
| 3191.5535 | 3202.7498 |
| 3202.7498 | 3207.2398 |
| 3207.2398 | 3210.8592 |
| 3210.8592 | 3212.0600 |
| 3212.0600 | 3219.0524 |
| 3219.0524 | 3222.6352 |
| 3222.6352 | 3231.0320 |
| 3231.0320 | 3240.9101 |

**β-5**

| -54.2421 | 23.1157 | 32.0735 |
| 39.5763 | 44.2192 | 49.9297 |
| 57.6966 | 68.7081 | 73.5050 |
| 75.7439 | 92.3049 | 96.4956 |
| 105.3077 | 116.2639 | 119.6988 |
| 126.8242 | 142.5999 | 148.2470 |
| 159.3728 | 169.5836 | 180.6290 |
| 187.6582 | 203.0498 | 212.6266 |
| 226.4145 | 249.3465 | 257.5570 |
| 264.9104 | 273.6728 | 304.7896 |
| 308.6925 | 311.5874 | 316.1523 |
| 321.2949 | 347.4096 | 361.3156 |
| 388.3862 | 394.4116 | 398.7711 |
| 406.4365 | 415.8670 | 419.4589 |
| 459.9156 | 471.7490 | 504.3866 |
| 505.2147 | 511.5688 | 521.2098 |
| 535.1541 | 548.0594 | 559.9424 |
| 571.5119 | 582.3193 | 604.5238 |
| 613.4133 | 619.5421 | 626.1078 |
| 635.1176 | 678.0220 | 681.3154 |
| 711.8053 | 714.9146 | 728.0349 |
| 729.9796 | 740.4458 | 764.5906 |
| 776.8229 | 782.3098 | 813.4153 |
| 817.4922 | 823.1042 | 857.4818 |
| a-5 | 864.7251 | 873.0479 | 881.2887 |
|-----|----------|----------|----------|
|     | 882.9286 | 888.4189 | 904.8534 |
|     | 905.3278 | 934.8711 | 957.5448 |
|     | 958.8605 | 964.6015 | 984.0362 |
|     | 995.8270 | 1003.8901| 1006.7721|
|     | 1011.4113| 1013.1788| 1027.8684|
|     | 1031.7111| 1043.7111| 1051.5504|
|     | 1061.3564| 1071.4358| 1083.3587|
|     | 1109.3840| 1112.7972| 1123.6421|
|     | 1125.2648| 1136.2181| 1137.6523|
|     | 1145.4723| 1153.5932| 1155.3825|
|     | 1177.3852| 1178.2909| 1192.3334|
|     | 1197.4265| 1206.8602| 1216.6031|
|     | 1227.9665| 1241.8528| 1250.2743|
|     | 1254.3072| 1272.5779| 1279.3598|
|     | 1281.7415| 1304.5258| 1307.2317|
|     | 1331.1615| 1336.2796| 1338.9196|
|     | 1347.2100| 1359.0959| 1361.3333|
|     | 1364.7257| 1375.4501| 1380.2230|
|     | 1398.1127| 1402.3385| 1409.4176|
|     | 1419.7919| 1421.1657| 1427.2440|
|     | 1443.3408| 1452.2575| 1481.8056|
|     | 1487.4841| 1492.0739| 1495.5211|
|     | 1498.7237| 1499.3446| 1500.0748|
|     | 1506.5395| 1513.0014| 1514.7175|
|     | 1528.0800| 1528.9472| 1541.9633|
|     | 1545.0260| 1546.6296| 1677.7154|
|     | 1687.6120| 1688.7587| 1690.3701|
|     | 1695.2024| 1707.6009| 1754.8973|
|     | 1810.9423| 1853.9406| 3044.0767|
|     | 3061.2247| 3082.7846| 3085.8506|
|     | 3090.5852| 3091.7150| 3092.9479|
|     | 3107.2938| 3110.7035| 3134.6982|
|     | 3143.0780| 3144.7902| 3161.5590|
|     | 3169.1133| 3172.9328| 3181.0278|
|     | 3182.5494| 3196.7249| 3201.6487|
|     | 3201.8981| 3208.5078| 3209.0962|
|     | 3216.1580| 3218.1956| 3224.3063|
|     | 3227.9707| 3235.9685| 3236.0565|

\[\alpha = 5.5409 \times 10^{-2}\]
| 500.6131 | 503.4088 | 530.5048 |
| 535.4975 | 546.9709 | 547.7183 |
| 566.5580 | 577.3837 | 599.2338 |
| 610.7459 | 628.1907 | 630.0613 |
| 636.0800 | 672.2705 | 683.3356 |
| 706.8309 | 712.5891 | 727.2367 |
| 731.3304 | 739.2791 | 767.2347 |
| 772.7623 | 779.2221 | 807.2003 |
| 815.6735 | 816.4107 | 848.8063 |
| 861.5837 | 880.1604 | 883.4639 |
| 886.2601 | 888.4093 | 899.6151 |
| 907.2799 | 929.5963 | 959.0172 |
| 911.3956 | 975.5063 | 981.3968 |
| 986.2464 | 1007.5038 | 1009.7039 |
| 1012.8091 | 1018.2693 | 1029.2591 |
| 1030.7680 | 1039.7364 | 1054.5404 |
| 1064.9217 | 1077.0193 | 1085.3673 |
| 1103.6676 | 1117.9032 | 1123.4691 |
| 1125.4977 | 1125.9760 | 1132.7329 |
| 1147.0894 | 1154.2413 | 1155.3886 |
| 1179.2775 | 1186.1113 | 1195.5103 |
| 1200.2102 | 1202.5164 | 1222.5862 |
| 1225.9160 | 1236.2480 | 1240.6132 |
| 1262.8195 | 1270.4916 | 1272.7821 |
| 1277.1602 | 1295.9279 | 1308.4453 |
| 1323.7695 | 1343.5123 | 1347.7546 |
| 1348.2508 | 1356.4444 | 1364.7335 |
| 1367.4480 | 1371.4039 | 1373.9940 |
| 1394.7735 | 1403.8143 | 1409.1755 |
| 1414.0966 | 1415.6634 | 1425.0853 |
| 1438.4503 | 1457.0277 | 1469.2489 |
| 1480.2254 | 1482.7247 | 1486.0449 |
| 1491.8614 | 1496.9545 | 1504.4758 |
| 1505.8646 | 1509.7955 | 1510.8646 |
| 1524.5906 | 1533.0342 | 1536.6116 |
| 1542.0496 | 1551.5867 | 1677.0048 |
| 1678.4422 | 1682.1871 | 1694.4421 |
| 1699.7314 | 1704.1160 | 1771.0267 |
| 1843.0274 | 1847.8148 | 3062.9217 |
| 3065.3821 | 3074.2091 | 3085.9832 |
| 3089.0482 | 3090.3146 | 3097.7115 |
| 3111.0848 | 3125.1571 | 3128.7224 |
| 3132.9779 | 3140.0499 | 3143.7710 |
| 3147.4305 | 3171.0710 | 3185.7770 |
| 3194.3206 | 3208.6196 | 3210.6688 |
| 3214.5301 | 3214.9863 | 3222.3649 |
| 3224.8621 | 3226.7552 | 3230.6302 |
| 3233.7645 | 3236.6069 | 3246.4827 |

\( \beta \cdot 7 \)

| -95.3147 | 34.8509  | 42.9835  |
| 47.2009  | 55.3311  | 58.9295  |
| 61.3400  | 64.1867  | 79.8067  |
| 88.6831  | 96.1125  | 113.3143 |
| 119.1232 | 131.0752 | 144.1793 |
| 155.8198 | 168.4454 | 179.7037 |
| 183.3931 | 189.0961 | 206.6690 |
| 232.6951 | 245.5186 | 258.5948 |
| 263.2627 | 283.7037 | 290.5158 |
| 296.6951 | 307.5016 | 334.8096 |
| 348.6606 | 353.2736 | 370.5870 |
| 393.6452 | 412.8877 | 416.3112 |
| 417.4346 | 446.3112 | 454.6012 |
| 456.8888 | 494.6012 | 509.2149 |
| 504.0782 | 529.6664 | 530.7733 |
| 581.7803 | 613.1472 | 634.8164 |
| 626.9439 | 668.4084 | 677.0020 |
| 714.6076 | 734.2990 | 773.0020 |
| 755.9607 | 773.1850 | 818.2926 |
| 843.0803 | 860.4072 | 886.7774 |
| 874.2330 | 935.2234 | 905.5888 |
| 951.4688 | 960.5880 | 1008.5768 |
| 999.7421 | 1008.5768 | 1027.9523 |
| 1010.6638 | 1027.9523 | 1063.2977 |
| 1034.0583 | 1063.2977 | 1087.2847 |
| 1107.0200 | 1117.8679 | 1141.2302 |
| 1123.4571 | 1163.8159 | 1192.3260 |
| 1147.9193 | 1229.6571 | 1247.3083 |
| 1178.1529 | 1268.4796 | 1278.8506 |
| 1202.1184 | 1288.9838 | 1308.5999 |
| 1239.4686 | 1314.7528 | 1324.0687 |
| 1274.2516 | 1341.4839 | 1348.3977 |
| 1299.1012 | 1361.9246 | 1370.7035 |
| 1319.6581 | 1375.7126 | 1400.6020 |
| 1345.8649 | 1403.2446 | 1410.8437 |
| 1362.0168 | 1427.3083 | 1455.2244 |
| 1394.2540 | 1472.0420 | 1484.8765 |
| 1405.6555 | 1492.0348 | 1499.2093 |
| 1432.6101 | 1501.5569 | 1514.2692 |
| 1478.9420 | 1516.4131 | 1527.9553 |
| 1497.5898 | 1531.6598 | 1552.9942 |
| 1504.0370 | 1556.3605 | 1603.7323 |
| 1523.2763 | 1606.7359 | 1693.7323 |
| 1544.8521 | 1696.7359 | 1708.8732 |
| 1567.1985 | 1765.8106 | 1824.8775 |
| 1679.1625 | 3046.6408 | 3076.1716 |
| 1698.1625 | 3076.1716 | 3082.4737 |
| 1788.5975 | 3096.2222 | 3106.0877 |
| 3063.6174 | 3118.0618 | 3133.5989 |
| 3077.8374 | 3135.4118 | 3177.8567 |
| 3097.8662 | 3181.7583 | 3192.0836 |
| 3131.2044 | 3206.8822 | 3202.8498 |
| 3159.0017 | 3223.1134 | 3220.2972 |
| 3201.2098 | 3232.1842 | 3231.4760 |
| 3216.5992 | 3240.1109 | 3237.3245 |
\begin{table}
\begin{center}
\begin{tabular}{cccc}
\textbf{a-7} & \\
-113.7510 & 27.9102 & 35.4432 & \\
40.1400 & 46.2396 & 54.4698 & \\
57.9094 & 62.4886 & 86.9357 & \\
96.1407 & 99.8101 & 104.2346 & \\
126.1437 & 130.6692 & 145.8436 & \\
155.8662 & 167.9602 & 175.9893 & \\
189.7096 & 201.7052 & 233.5607 & \\
232.5770 & 243.4327 & 253.0118 & \\
268.0015 & 271.1737 & 284.0855 & \\
284.7657 & 297.9183 & 321.5232 & \\
321.5232 & 328.7663 & 335.0666 & \\
343.1396 & 355.0666 & 374.5294 & \\
395.8444 & 403.7575 & 428.6586 & \\
425.2688 & 479.7183 & 497.9546 & \\
450.2719 & 503.7087 & 529.1122 & \\
539.1914 & 546.9692 & 549.6262 & \\
562.8820 & 601.0431 & 613.6141 & \\
629.2275 & 633.2566 & 657.7266 & \\
673.8376 & 690.4626 & 704.4316 & \\
710.4853 & 723.8880 & 730.3781 & \\
759.6466 & 764.3998 & 777.4844 & \\
792.5444 & 800.9025 & 815.0616 & \\
840.2405 & 845.5099 & 858.6839 & \\
866.7103 & 876.4967 & 883.6076 & \\
884.8963 & 897.3474 & 910.3850 & \\
934.3399 & 948.5078 & 961.7550 & \\
963.8601 & 976.1035 & 1001.1667 & \\
1006.0230 & 1009.7661 & 1011.5492 & \\
1012.4261 & 1023.1262 & 1031.2210 & \\
1033.2783 & 1046.3147 & 1053.6981 & \\
1058.1041 & 1075.6753 & 1100.7571 & \\
1103.9243 & 1120.3091 & 1120.9773 & \\
1127.3964 & 1130.1822 & 1132.3231 & \\
1135.4847 & 1147.8172 & 1149.6251 & \\
1177.8449 & 1179.6840 & 1188.5083 & \\
1211.1260 & 1221.8800 & 1228.3711 & \\
1231.3127 & 1245.5330 & 1249.7889 & \\
1261.5531 & 1271.3523 & 1277.8762 & \\
1284.5677 & 1299.3419 & 1311.1224 & \\
1323.5520 & 1326.2455 & 1334.3134 & \\
1335.6740 & 1343.4626 & 1354.7246 & \\
1362.9337 & 1364.0200 & 1365.3622 & \\
1375.3870 & 1388.2840 & 1395.2040 & \\
1400.2129 & 1409.5817 & 1416.5588 & \\
1419.1700 & 1455.1241 & 1469.3512 & \\
1482.0165 & 1490.8357 & 1492.2385 & \\
1494.9244 & 1499.0732 & 1499.7202 & \\
1501.8869 & 1511.5516 & 1517.0858 & \\
1521.4033 & 1523.6015 & 1527.1898 & \\
1544.3057 & 1548.8279 & 1555.7897 & \\
1669.6295 & 1671.9348 & 1674.1765 & \\
1698.6489 & 1704.6468 & 1739.8930 & \\
\end{tabular}
\end{center}
\end{table}
| 1768.6759 | 1869.3219 | 3052.5729 |
| 3065.9929 | 3068.3892 | 3068.7266 |
| 3072.7556 | 3079.2932 | 3091.1696 |
| 3099.2396 | 3117.7385 | 3122.5691 |
| 3126.7107 | 3148.7153 | 3141.1032 |
| 3160.4611 | 3173.5286 | 3127.3839 |
| 3198.6036 | 3206.4508 | 3148.7153 |
| 3201.7405 | 3221.3029 | 3160.4611 |
| 3207.7273 | 3230.7895 | 3198.6036 |
| 3223.4260 | 3240.9055 | 3207.7273 |
| 3231.0002 | 3276.5165 | 3223.4260 |
| β-9       |          |          |
| -186.1153 | 17.0609  | 33.6395  |
| 34.3609   | 43.3915  | 52.8844  |
| 55.9381   | 62.4780  | 74.7970  |
| 84.5368   | 86.5147  | 89.7345  |
| 108.1499  | 126.6439 | 137.1820 |
| 145.4604  | 155.1508 | 159.9983 |
| 170.1594  | 182.3805 | 198.6830 |
| 216.6901  | 222.9377 | 236.3078 |
| 254.3105  | 272.5879 | 286.6323 |
| 293.6092  | 298.9489 | 307.3165 |
| 315.6021  | 323.5338 | 327.4930 |
| 353.7656  | 362.3016 | 364.7307 |
| 393.2431  | 398.6489 | 407.2502 |
| 415.9236  | 435.4365 | 450.4997 |
| 460.7709  | 489.6130 | 496.5872 |
| 516.5593  | 517.4866 | 537.0863 |
| 542.6396  | 548.0054 | 559.3355 |
| 593.1300  | 613.9259 | 627.1890 |
| 634.1612  | 649.3538 | 680.8258 |
| 702.3274  | 709.2665 | 715.6617 |
| 723.0962  | 726.0637 | 735.2632 |
| 753.1477  | 761.2619 | 776.6354 |
| 797.9503  | 807.2051 | 821.0671 |
| 846.4217  | 854.2836 | 858.8454 |
| 877.9552  | 879.2704 | 883.5185 |
| 884.4864  | 894.3150 | 931.0722 |
| 942.3668  | 956.7774 | 959.1496 |
| 979.4544  | 985.7953 | 992.4650 |
| 1004.5085 | 1006.1099 | 1007.3643 |
| 1010.2801 | 1024.5328 | 1027.4158 |
| 1029.8949 | 1041.8731 | 1063.0730 |
| 1069.1129 | 1076.2587 | 1101.7087 |
| 1114.2203 | 1121.1308 | 1121.4388 |
| 1131.5117 | 1135.4562 | 1136.4043 |
| 1146.6257 | 1152.6198 | 1161.2975 |
| 1177.5414 | 1180.4909 | 1189.4696 |
| 1192.6373 | 1197.0673 | 1232.0251 |
| 1238.8335 | 1242.6346 | 1258.2788 |
| 1266.9770 | 1273.6107 | 1282.2867 |
| 1301.7965 | 1303.6539 | 1319.2414 |
| 1324.4194 | 1326.6975 | 1336.6684 |
| 1340.2059 | 1347.0556 | 1353.8304 |
| 1359.8323 | 1367.8441 | 1377.9593 |
| 1387.7955 | 1393.6246 | 1404.3833 |
| 1408.4724 | 1411.2919 | 1416.6473 |
| 1428.3543 | 1456.4741 | 1468.3981 |
| 1478.7588 | 1498.2220 | 1508.1310 |
| 1501.5040 | 1519.9225 | 1527.3465 |
| 1517.0743 | 1557.8756 | 1563.1252 |
| 1545.1003 | 1678.8326 | 1701.6805 |
| 1627.4829 | 1783.1281 | 1844.6989 |
| 1698.2558 | 1944.5039 | 3047.8412 |
| 1783.1281 | 2305.7997 | 3072.1739 |
| 1844.6989 | 3073.1616 | 3087.9241 |
| 1944.5039 | 3106.4237 | 3107.9988 |
| 2305.7997 | 3126.6034 | 3146.3818 |
| 3047.8412 | 3148.8097 | 3181.2897 |
| 3072.1739 | 3188.4002 | 3201.1229 |
| 3087.9241 | 3207.5834 | 3216.2574 |
| 3107.9988 | 3216.6138 | 3224.0664 |
| 3146.3818 | 3225.8303 | 3233.2491 |

\( \alpha - 9 \)

| -137.4207 | 17.2689 | 27.9896 |
| 36.3915 | 45.3172 | 50.1327 |
| 56.8231 | 61.1220 | 65.6029 |
| 74.7169 | 83.1431 | 91.4658 |
| 107.5200 | 125.3019 | 132.8121 |
| 145.0550 | 155.3906 | 170.8343 |
| 184.5382 | 189.9162 | 202.3654 |
| 209.9313 | 241.1376 | 248.3092 |
| 256.3083 | 257.6721 | 279.5483 |
| 291.6062 | 297.3570 | 308.2733 |
| 312.6761 | 317.0339 | 328.0022 |
| 338.9231 | 354.9424 | 364.7970 |
| 392.0677 | 400.9551 | 413.6349 |
| 418.9242 | 431.9533 | 444.5830 |
| 456.3076 | 489.5096 | 506.9998 |
| 522.9791 | 533.2262 | 534.1451 |
| 540.9817 | 548.9781 | 558.4234 |
| 579.0912 | 598.1450 | 626.3656 |
| 639.5547 | 646.3166 | 666.0961 |
| 690.4486 | 704.4377 | 712.2195 |
| 718.3711 | 720.8716 | 733.4579 |
| 752.2736 | 769.1537 | 774.3849 |
| 799.9085 | 807.8780 | 817.1311 |
| 847.5233 | 853.0276 | 857.7470 |
| 871.4989 | 878.8152 | 881.7798 |
| 887.1230 | 899.3410 | 921.2085 |
| 924.8731 | 945.1165 | 958.7298 |
| 975.1262 | 983.7980 | 988.3030 |
| 1001.7866 | 1005.2716 | 1009.8232 |
| 1023.8369 | 1029.0274 | 1030.4715 |
| 1038.6164 | 1042.6871 | 1058.1310 |
| 1061.6328 | 1070.9692 | 1104.3170 |
| 1111.7377 | 1119.1679 | 1119.8291 |
| 1128.4638 | 1132.3812 | 1135.5456 |
| 1142.8768 | 1147.5462 | 1152.4534 |

S30
|    | 1175.3040 | 1180.0555 | 1181.4006 |
|----|-----------|-----------|-----------|
| 1200.9087 | 1224.4371 | 1228.6819 |
| 1231.1848 | 1244.5339 | 1249.8689 |
| 1225.4174 | 1272.9297 | 1275.1781 |
| 1295.1215 | 1304.4617 | 1321.8144 |
| 1322.7863 | 1327.7437 | 1334.3742 |
| 1337.3246 | 1355.3611 | 1360.1434 |
| 1361.6645 | 1368.7096 | 1369.7508 |
| 1379.6165 | 1388.6837 | 1395.9588 |
| 1404.8708 | 1408.6224 | 1420.2943 |
| 1426.2419 | 1458.2132 | 1473.1923 |
| 1480.4470 | 1482.1452 | 1488.0458 |
| 1492.9068 | 1496.3391 | 1498.4153 |
| 1504.3359 | 1512.1284 | 1520.2648 |
| 1520.6427 | 1525.4664 | 1540.0721 |
| 1543.6898 | 1545.2468 | 1557.1101 |
| 1626.9202 | 1680.2478 | 1681.7072 |
| 1696.3698 | 1707.7693 | 1711.2621 |
| 1782.6920 | 1889.9391 | 3047.6471 |
| 3051.0393 | 3055.5159 | 3061.2478 |
| 3064.6732 | 3084.7740 | 3090.4990 |
| 3095.7149 | 3105.2908 | 3108.8841 |
| 3113.0811 | 3118.6201 | 3122.3341 |
| 3135.8959 | 3147.9321 | 3158.3114 |
| 3163.3968 | 3191.1010 | 3195.0791 |
| 3203.2991 | 3205.7466 | 3212.2368 |
| 3214.3047 | 3219.3096 | 3220.3424 |
| 3220.5056 | 3229.3548 | 3229.9597 |
11. List of the Cartesian coordinates of the optimized structures

**R1**

|     |          |          |          |
|-----|----------|----------|----------|
| 0   | 1        | 2        |
| C   | -1.296341| -0.482117|  0.000463|
| F   | -1.195683| -1.244086| -1.085151|
| F   | -1.195228| -1.242020|  1.087402|
| N   | -2.699426|  0.133191|  0.000074|
| O   | -3.173982|  0.365466|  1.086190|
| O   | -3.174049|  0.363915| -1.086335|
| C   | -0.261352|  0.672221| -0.000847|
| O   | -0.689707|  1.802091| -0.001692|
| C   |  1.167206|  0.300211| -0.000505|
| C   |  1.597392| -1.032204| -0.000865|
| C   |  2.100810|  1.344216|  0.000194|
| C   |  2.958953| -1.312019| -0.000439|
| H   |  0.886953| -1.850679| -0.001679|
| C   |  3.457720|  1.056450|  0.000643|
| H   |  1.741760|  2.367877|  0.000428|
| C   |  3.885649| -0.271898|  0.000344|
| H   |  3.296603| -2.342348| -0.000745|
| H   |  4.182812|  1.862908|  0.001255|
| H   |  4.947312| -0.496385|  0.000734|

**R2**

|     |          |          |          |
|-----|----------|----------|----------|
| 0   | 1        | 2        |
| C   | -0.370918| -0.610869|  0.000455|
| C   | -0.536559|  0.783261|  0.000415|
| C   | -1.798753|  1.357286| -0.000041|
| C   | -2.908707|  0.512747| -0.000299|
| C   | -2.732577| -0.872368| -0.000231|
| C   | -1.464070| -1.462180|  0.000104|
| H   | -1.905351|  2.437342| -0.000147|
| H   | -3.909915|  0.927873| -0.000555|
| H   | -3.606034| -1.516508| -0.000472|
| H   | -1.346611| -2.539994| -0.000104|
| C   |  0.808537|  1.376211|  0.000105|
| O   |  1.168909|  2.526564| -0.000115|
| C   |  1.785744|  0.157797|  0.000244|
| O   |  2.993930|  0.200220| -0.000531|
| N   |  0.989426| -0.959502|  0.000794|
| C   |  1.492044| -2.316318| -0.000311|
| H   |  1.155022| -2.851039|  0.891827|
| H   |  1.154552| -2.849928| -0.892957|
| H   |  2.580361| -2.258903| -0.000630|

**Cat**

|     |          |          |          |
|-----|----------|----------|----------|
| 0   | 1        | 2        |
| C   |  2.752920|  0.000106|  0.387085|
| C   |  1.900813| -1.249953|  0.614353|
| C   |  0.889202| -1.548848| -0.506310|
| C   |  1.966392|  1.307736|  0.295490|
| C   | -0.403360| -0.777830| -0.364241|
|     | x           | y           | z           |
|-----|-------------|-------------|-------------|
| C   | 0.90544000  | 1.29064000  | -0.80888700 |
| H   | 3.31799000  | -0.13073200 | -0.54640000 |
| H   | 2.57198500  | -2.10983700 | 0.70906600  |
| H   | 1.35142700  | -1.35917000 | -1.48363400 |
| H   | 1.47067700  | 1.52420800  | 1.25086000  |
| H   | 0.61336300  | 2.31404400  | -1.06248900 |
| C   | -2.69869090  | -0.67483400 | 0.01479900  |
| H   | -3.44123700  | -1.28972100 | 0.53239100  |
| H   | -2.57198500  | -2.10983700 | 0.70906600  |
| H   | -1.35142700  | -1.35917000 | -1.48363400 |
| H   | -1.47067700  | 1.52420800  | 1.25086000  |
| N   | -0.32083200  | 0.59290900  | -0.44434800 |
| N   | -1.47710300  | -1.45210400 | 0.11836000  |
| H   | 1.32630600   | 0.85741600  | -1.72399700 |
| H   | 2.66479900   | 2.13006000  | 0.10365700  |
| H   | 3.49441000   | 0.08064700  | 1.18939400  |
| H   | 1.36102700   | -1.16979700 | 1.56664500  |
| H   | 0.60112800   | -2.60045200 | -0.48349900 |
| H   | -3.11935400  | -0.43534900 | 0.97413400  |
| C   | 0.61336300   | 2.31404400  | -1.06248900 |
| F   | 1.05735100   | 1.51762000  | -0.44312100 |
| F   | -0.10746300  | 2.10865000  | -0.23337000 |
| N   | 2.07909500   | 2.67082600  | -0.61961100 |
| O   | 3.04081300   | 2.43266100  | -1.31843300 |
| O   | 1.85153000   | 3.68613900  | -0.00787000 |
| C   | 1.50263900   | 0.69961500  | 0.79725200  |
| O   | 1.17923300   | 1.16339800  | 1.86580500  |
| C   | 2.37369900   | -0.49039700 | 0.63426200  |
| C   | 2.37003500   | -1.40234500 | 1.69499600  |
| C   | 3.18103800   | -0.71552200 | -0.48413000 |
| C   | 3.15336200   | -2.54499700 | 1.63085000  |
| H   | 1.73713300   | -1.20336900 | 2.54937600  |
| C   | 3.97798600   | -1.85754400 | -0.53396300 |
| H   | 3.20091100   | -0.00761600 | -1.30487800 |
| C   | 3.95941700   | -2.77261800 | 0.51431500  |
| H   | 3.13810000   | -3.25939400 | 2.44709800  |
| H   | 4.61163400   | -2.03176500 | -1.39705700 |
| H   | 4.57426100   | -3.66552900 | 0.46438700  |
| C   | -4.50750200  | 1.26057100  | 0.73724100  |
| C   | -3.01042400  | 1.57317300  | 0.74850600  |
| C   | -2.13086600  | 0.46805800  | 1.35963800  |
| C   | -4.89774000  | 0.04448200  | -0.10234500 |
| C   | -1.77534300  | -0.61545600 | 0.36891200  |
| C   | -4.17959400  | -1.23643000 | 0.33039500  |
| H   | -4.83700000  | 1.09019200  | 1.77166500  |
| H   | -2.85049300  | 2.49178300  | 1.32215700  |
| H   | -2.63156400  | 0.03395900  | 2.23407200  |
| H   | -4.67815000  | 0.22611100  | -1.16264100 |
| H   | -4.71054400  | -2.11288500 | -0.05309300 |
| C   | -0.24165900  | -1.81287100 | -0.92060300 |
|      |       |       |       |
|------|-------|-------|-------|
| H    | 0.75794300 | -1.64071900 | -1.32955300 |
| C    | -2.64380300 | -2.11226700 | -1.39381000 |
| C    | -1.29199300 | -1.82723400 | -2.02612000 |
| H    | -1.30012900 | -0.84312900 | -2.50783600 |
| H    | -1.07394800 | -2.57778100 | -2.79005100 |
| H    | -3.45680500 | -1.84103900 | -2.07926000 |
| N    | -2.80902700 | -1.34510100 | -0.15826000 |
| N    | -0.53337800 | -0.76781500 | 0.04981000 |
| H    | -4.19247600 | -1.32358500 | 1.42261400 |
| H    | -2.66322800 | 1.78083400 | -0.27125800 |
| H    | -1.18474700 | 0.88680100 | 1.70535200 |
| H    | -0.21946500 | -2.79336500 | -0.42051800 |
| H    | -2.74607700 | -3.18342800 | -1.17322500 |
|      |       |       |       |
| 1    |       |       |       |
| C    | 1.51687100 | -1.57471600 | -0.09655600 |
| F    | 0.62657900 | -2.55878200 | -0.17431000 |
| F    | 2.19907800 | -1.68984800 | 1.05342600 |
| N    | 2.55012800 | -1.83934100 | -1.20253700 |
| O    | 3.56414500 | -1.17931900 | -1.11995400 |
| O    | 2.27220100 | -2.64825400 | -2.05445000 |
| C    | 0.90034000 | -0.17753900 | -0.41932000 |
| O    | 0.51170400 | -0.14586500 | -1.60685200 |
| C    | 1.69931100 | 0.98840500 | 0.14755700 |
| C    | 2.22961900 | 1.88886400 | -0.77494300 |
| C    | 1.94002900 | 1.17546200 | 1.51007100 |
| C    | 2.98712700 | 2.97460400 | -0.34217600 |
| H    | 2.03287500 | 1.71757900 | -1.82833100 |
| C    | 2.70115400 | 2.25580900 | 1.94232800 |
| H    | 1.52545500 | 0.48205400 | 2.23525500 |
| C    | 3.22549100 | 3.15854700 | 1.01679800 |
| H    | 3.39391400 | 3.67360500 | -1.06605100 |
| H    | 2.88238000 | 2.39869700 | 3.00289100 |
| H    | 3.81709200 | 4.00289100 | 1.35635400 |
| C    | -3.83842500 | 1.28697400 | -1.94157400 |
| C    | -2.32804200 | 1.05377700 | -1.97435000 |
| C    | -1.60590800 | 1.44894200 | -0.67399700 |
| C    | -4.57998700 | 0.50718700 | -0.85541700 |
| C    | -1.63873700 | 0.35612800 | 0.36451100 |
| C    | -4.06271800 | 0.79393500 | 0.55606600 |
| H    | -4.02503300 | 2.35855000 | -1.78701300 |
| H    | -1.89632300 | 1.64327400 | -2.78820800 |
| H    | -2.07147700 | 2.34042300 | -0.23636300 |
| H    | -4.50656500 | -0.57225300 | -1.04039400 |
| H    | -4.80669500 | 0.49586800 | 1.29900300 |
| C    | -0.65566900 | -1.13677400 | 1.89963600 |
| H    | 0.26395000 | -1.69998700 | 2.03237600 |
| C    | -3.09144000 | -1.18197700 | 1.65664100 |
| C    | -1.85379400 | -2.05637400 | 1.70848400 |
| H    | -1.72393300 | -2.60868300 | 0.77417300 |
| H    | -1.94285500 | -2.77575700 | 2.52531500 |
| H    | -3.92458600 | -1.70730500 | 1.17668700 |
| N    | -2.84346200 | 0.05156000 | 0.89530800 |

S34
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| N       | -0.53839200 | -0.24588000 | 0.74521400 |
| H       | -3.89721900 | 1.86634500  | 0.69768600 |
| H       | -5.64378700 | 0.76440700  | -0.89145400 |
| H       | -4.26463300 | 1.03500800  | -2.91813300 |
| H       | -2.09690000 | 0.00728000  | -2.19827000 |
| H       | -0.57150100 | 1.69768000  | -0.88428500 |
| H       | -0.79705700 | -0.52453400 | 2.80152000  |
| H       | -3.41187300 | -0.90188100 | 2.66695400  |

2

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| O       | -0.57060200 | 0.48057700  | -0.79759200 |
| C       | -1.60603400 | 0.35986000  | 0.32029300 |
| C       | -0.01286900 | 0.80228000  | 0.59074200 |
| H       | -0.06924400 | 2.31848400  | -1.78346200 |
| H       | -1.96489600 | 1.61848400  | -2.83241500 |
| H       | -2.06953700 | 2.32919900  | -0.28045800 |
| H       | -4.49143500 | -0.60157700 | -0.96234500 |
| C       | -0.56019100 | -1.06942000 | 1.90054600 |
| C       | 0.36724100  | -1.61839100 | 2.03143900 |
| C       | -2.99928900 | -1.12935200 | 1.73280300 |
| C       | -1.75972400 | -1.99925100 | 1.79797100 |
| H       | -1.65614600 | -2.60813300 | 0.89674400 |
| H       | -1.82154400 | -2.66504800 | 2.66106600 |
| H       | -3.84305400 | -1.67564600 | 1.29820900 |
| N       | -0.49305400 | -0.25113200 | 0.68632300 |
| H       | -3.84539600 | 1.87725400  | 0.70483300 |
| H       | -5.63759800 | 0.72573700  | -0.80202600 |
| H       | -4.33165500 | 0.96991000  | -2.87930100 |
| H       | -2.12277200 | -0.01546200 | -2.22510700 |
| H       | -0.58059600 | 1.68894700  | -0.97543500 |
| H       | -0.67536700 | -0.40168400 | 2.76465100 |
H  
-3.29566700 -0.79546500 2.73332400

4

H  

0 1
C -0.84006600 2.01386100 0.66435800
F -0.69082900 2.24748300 1.98774600

3

H  

0 1
C -0.92320700 1.76429100 0.79704200
F -0.83141600 1.73560100 2.15977000
F -1.88908200 2.66980700 0.50663500
N 0.32978900 2.24150900 0.79704200
O 0.29874500 2.88192100 -0.78894200
O 1.37711500 1.77307100 0.73361600
C -0.89348800 -0.16244300 -0.69696000
O -0.52594300 0.42374400 -1.69531900
C -2.32672800 -0.57287600 -0.51916500
C -3.31748200 0.36635500 -0.81486500
C -2.68173000 -1.89314600 -0.24069000
C -4.65512100 -0.00625800 -0.78933600
H -3.02165700 1.38346700 -1.04550100
C -4.02425600 -2.26604100 -0.22636500
H -1.91212800 -2.63709100 -0.05735700
C -5.01159500 -1.32241400 -0.49262400
H -5.42338700 0.72941900 -1.00373200
H -4.29472900 -3.29460000 -0.01276300
C -6.05756800 -1.61137000 -0.47610700
H 4.00249600 0.15734400 -1.74981500
C 2.51302000 0.27455400 -2.06949600
C 1.73062000 -1.00279500 -1.70401200
C 4.31139700 -0.15976400 -0.28431000
C 1.34852500 -1.04574900 -0.24711900
C 3.70580000 -1.47961600 0.20753500
H 4.44118100 -0.63193800 -2.37594300
H 2.38665100 0.44599000 -3.14207800
H 2.35109500 -1.88568500 -1.89727000
H 3.94940600 0.64744500 0.36315100
H 4.23843200 -1.83657300 1.09076400
C -0.29593000 -1.18057700 1.54142100
H -1.23254700 -0.66338800 1.75166600
C 2.10619500 -1.35372700 2.08761100
C 0.79278800 -0.72284400 2.49068500
H 0.87230000 0.36119000 2.45120300
H 0.53977500 -1.02766500 3.50848200
H 2.94298500 -0.80340900 2.52535900
N 2.29885000 -1.33254600 0.62698800
N 0.07016700 -0.87994100 0.14534100
H 3.79227700 -2.26592000 -0.54820500
H 5.39635000 -0.22146000 -0.15440000
H 4.50660900 1.08920200 -2.02366600
H 2.06276000 1.12749300 -1.55251800
H 0.83921400 -1.09422100 -2.30891000
H -0.46168100 -2.26004700 1.63314200
H 2.18064600 -2.39812400 2.41125900
|   |         |         |         |         |         |        |
|---|---------|---------|---------|---------|---------|---------|
| F | 37      | -1.72998900 | 2.94573900 | 0.19627900 |         |         |
| N | 37      | 0.41638400 | 2.23596900 | -0.00660100 |         |         |
| O | 37      | 0.41541100 | 2.67345100 | -1.15721800 |         |         |
| O | 37      | 1.44159700 | 1.76486900 | 0.52971300  |         |         |
| C | 37      | -0.90551700 | -0.40496100 | -0.76962100 |         |         |
| O | 37      | -0.52989200 | 0.13613800 | -1.78079100 |         |         |
| C | 37      | -2.34856000 | -0.69882600 | -0.51555400 |         |         |
| C | 37      | -2.77168900 | -1.98046400 | -0.16076200 |         |         |
| C | 37      | -4.63777200 | 0.32281000 | -0.65178400 |         |         |
| C | 37      | -2.92421400 | 1.29776300 | -1.03675100 |         |         |
| C | 37      | -4.13272700 | -2.25412000 | -0.05472200 |         |         |
| H | 37      | -2.04247200 | -2.76698800 | 0.01357600  |         |         |
| C | 37      | -5.06417200 | -1.24716600 | -0.29442300 |         |         |
| H | 37      | -5.36578000 | 0.81564500 | -0.83422100 |         |         |
| H | 37      | -4.46364600 | -3.25196400 | 0.21306500  |         |         |
| C | 37      | -6.12474700 | -1.45861200 | -0.20366800 |         |         |
| C | 37      | 4.01613800  | -0.08034700 | -1.69019100 |         |         |
| C | 37      | 2.53869000  | -0.03758100 | -2.07726700 |         |         |
| C | 37      | 1.76119900  | -1.27029200 | -1.57599100 |         |         |
| C | 37      | 4.27034500  | -0.19067000 | -0.18471700 |         |         |
| C | 37      | 1.32958900  | -1.13427500 | -0.13887600 |         |         |
| C | 37      | 3.67290100  | -1.45026100 | 0.45071300  |         |         |
| H | 37      | 4.49394600  | -0.93561600 | -2.18793100 |         |         |
| H | 37      | 2.45258400  | -0.01460100 | -3.16719800 |         |         |
| H | 37      | 2.39059000  | -2.16362100 | -1.63536700 |         |         |
| H | 37      | 3.86011800  | 0.68443800  | 0.33288600  |         |         |
| H | 37      | 4.17346600  | -1.68033900 | 1.39180600  |         |         |
| C | 37      | -0.39515000 | -1.07111000 | 1.59685800  |         |         |
| H | 37      | -1.33296500 | -0.52867900 | 1.69906700  |         |         |
| C | 37      | 1.99828700  | -1.11051500 | 2.23874900  |         |         |
| C | 37      | 0.65579300  | -0.47228600 | 2.51064800  |         |         |
| H | 37      | 0.71439000  | 0.59888900  | 2.33155300  |         |         |
| H | 37      | 0.37302800  | -0.64954400 | 3.55052000  |         |         |
| H | 37      | 2.80315700  | -0.47789200 | 2.62152700  |         |         |
| N | 37      | 2.24589300  | -1.27988500 | 0.79578700  |         |         |
| N | 37      | 0.02741400  | -0.95336200 | 0.18614500  |         |         |
| H | 37      | 3.79754800  | -2.32498400 | -0.19361900 |         |         |
| H | 37      | 5.34947300  | -0.20667200 | -0.00330900 |         |         |
| H | 37      | 4.51254100  | 0.81864200  | -2.06796400 |         |         |
| H | 37      | 2.05863700  | 0.86806600  | -1.69472200 |         |         |
| H | 37      | 0.88976300  | -1.45305600 | -2.19406100 |         |         |
| H | 37      | -0.56323800 | -2.12954800 | 1.82340900  |         |         |
| H | 37      | 2.09231300  | -2.09936000 | 2.70113300  |         |         |

β-5

|   |         |         |         |         |         |         |
|---|---------|---------|---------|---------|---------|---------|
| 0 | 1       | 2.23019600 | -0.53763000 | 1.59923800 |         |         |
| F | 1       | 3.56613000 | -0.68743200 | 1.55886200 |         |         |
| F | 1       | 1.69680600 | -1.73436800 | 1.93697300 |         |         |
| N | 1       | 1.86674700 | 0.43593400 | 2.61637700 |         |         |
| O | 1       | 0.74142200 | 0.33581500 | 3.10134100 |         |         |
| O | 1       | 2.60991500 | 1.39469600 | 2.77605100 |         |         |
| C | 1       | -2.03948400 | 0.91728000 | -0.86135400 |         |         |
| O | 1       | -1.50735900 | 0.53682200 | -1.87602700 |         |         |
| C | 1       | -2.42509200 | 2.33952400 | -0.64745700 |         |         |

β-5
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -2.2666500| -2.10851400| -0.98119700 |
| F    | -3.10907700| -2.35281100| -2.00434100 |
| F    | -2.66367000| -2.84915000| 0.07771600  |
| N    | -0.92520300| -2.52270400| -1.36780800 |
| O    | -0.14113800| -2.80976100| -0.46588400 |
| O    | -0.59578500| -2.35719600| 0.07771600  |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| C    | 0.77578900 | 2.74068200 | 0.09544900  |
| F    | -3.10907700| -2.35281100| -2.00434100 |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| O    | 0.77578900 | 2.74068200 | 0.09544900  |
| C    | -0.49981000| -2.94770400| 0.62650900  |
| F    | -0.92520300| -2.52270400| -1.36780800 |
| O    | -0.14113800| -2.80976100| -0.46588400 |
| C    | -0.59578500| -2.35719600| 0.07771600  |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| C    | 0.77578900 | 2.74068200 | 0.09544900  |
| F    | -3.10907700| -2.35281100| -2.00434100 |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| O    | 0.77578900 | 2.74068200 | 0.09544900  |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| C    | 0.77578900 | 2.74068200 | 0.09544900  |
| F    | -3.10907700| -2.35281100| -2.00434100 |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| O    | 0.77578900 | 2.74068200 | 0.09544900  |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| C    | 0.77578900 | 2.74068200 | 0.09544900  |
| F    | -3.10907700| -2.35281100| -2.00434100 |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| O    | 0.77578900 | 2.74068200 | 0.09544900  |
| C    | 1.52919500 | 1.55242200 | 0.57169800  |
| O    | 1.42428100 | 1.11236000 | 1.69203700  |
| C    | 0.77578900 | 2.74068200 | 0.09544900  |

S39
| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| H    | -6.03738300 | -0.70975600 | 3.15282200 |
| H    | -3.57647200 | -0.93614400 | 3.33859700 |
| C    | -2.78933200 | 0.28667000 | -0.90939200 |
| O    | -2.85527500 | 0.74036900 | -2.03556700 |
| C    | -1.50890800 | -0.09569300 | -0.16769300 |
| O    | -0.34381000 | 0.03567000 | -0.54909400 |
| N    | -1.87836500 | -0.35132300 | 1.15988800 |
| C    | -0.99517700 | -1.01705400 | 2.09228700 |
| H    | -1.04821000 | -0.53935100 | 3.07450700 |
| H    | 0.01723400 | -0.91759000 | 1.70033500 |
| H    | -1.25441300 | -2.07769900 | 2.17702300 |

β-6

| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| C    | 1.99180700 | -0.84416900 | 1.88084400 |
| F    | 1.11004000 | -1.31177800 | 2.77210000 |
| F    | 2.79244800 | 0.02797200 | 2.48973700 |
| N    | 2.87756900 | -2.04748300 | 1.52102100 |
| O    | 4.07121700 | -1.86439300 | 1.42846000 |
| O    | 2.29031700 | -3.08897500 | 1.29653200 |
| C    | 1.02938300 | 1.52329200 | -0.55393000 |
| O    | -0.59569700 | 0.87487300 | -1.48028700 |
| C    | -0.69220800 | 2.95919800 | -0.33989500 |
| C    | -1.67554400 | 3.86961400 | -0.02379900 |
| C    | 0.62060600 | 3.36900700 | -0.58007600 |
| C    | -1.34371900 | 5.24676100 | 0.06253800 |
| H    | -2.70034600 | 3.57510300 | 0.14227000 |
| C    | 0.94861300 | 4.71440100 | -0.48482600 |
| H    | 1.36271700 | 2.61361000 | -0.81227000 |
| C    | -0.03224300 | 5.65415900 | -0.16259600 |
| H    | -2.10921900 | 5.97713900 | 0.30304400 |
| H    | 1.97104400 | 5.03467300 | -0.65732700 |
| H    | 0.22795700 | 6.70532100 | -0.08846500 |
| C    | -3.33984900 | -2.67707900 | -2.03913200 |
| C    | -2.54320400 | -1.39880000 | -2.29736000 |
| C    | -3.15587700 | -0.14594300 | -1.65189100 |
| C    | -3.55195400 | -3.00814200 | -0.56068600 |
| C    | -2.85382200 | -0.01442600 | -0.18072500 |
| C    | -4.31684400 | -1.92085600 | 0.19998700 |
| H    | -4.32256300 | -2.58778600 | -2.52223700 |
| H    | -2.49003000 | -1.22241600 | -3.37576300 |
| H    | -4.24814700 | -0.16193300 | -1.75157100 |
| H    | -2.58800600 | -3.16508700 | -0.06369900 |
| H    | -4.77445500 | -2.33134700 | 1.10115400 |
| C    | -2.12468000 | 1.33359600 | 1.70561400 |
| H    | -1.27632500 | 1.97995700 | 1.91056200 |
| C    | -3.10892500 | -0.90768600 | 2.10283700 |
| C    | -2.00923400 | 0.05236600 | 2.50842900 |
| H    | -1.02492900 | -0.36721800 | 2.30789300 |
| H    | -2.10190100 | 0.27308300 | 3.57452800 |
| H    | -2.80862800 | -1.94251300 | 2.29229800 |
| N    | -3.43721200 | -0.83220000 | 0.66556200 |
| N    | -2.08933600 | 1.00381400 | 0.26961700 |
| H    | -5.12567100 | -1.50237600 | -0.40664600 |
| H    | -4.12544500 | -3.93692200 | -0.48229300 |
| H    | -2.83104300 | -3.51700800 | -2.52392000 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| C | 1.89679900 | 1.12291300 | -1.98224000 |   |   |   |
| H | 0.91824200 | 1.55364900 | -2.17169800 |   |   |   |
| C | 3.28989000 | -0.91180100 | -2.17865000 |   |   |   |
| C | 1.96588200 | -0.27884800 | -2.55640400 |   |   |   |
| H | 1.10542400 | -0.82217800 | -2.16415300 |   |   |   |
| H | 1.88650500 | -0.24059100 | -3.64493900 |   |   |   |
| H | 3.24110700 | -0.24059100 | -2.16415300 |   |   |   |
| C | 1.96658200 | -0.27884800 | -2.17865000 |   |   |   |
| H | 1.10542400 | -0.82217800 | -2.16415300 |   |   |   |
| H | 1.88650500 | -0.24059100 | -3.64493900 |   |   |   |
| H | 3.24110700 | -0.24059100 | -2.16415300 |   |   |   |
| N | 3.68582000 | -0.59220600 | -0.79121400 |   |   |   |
| N | 2.06569400 | 1.04030700 | -0.51699800 |   |   |   |
| H | 5.58141300 | -0.72265700 | 0.12928600 |   |   |   |
| H | 5.16541100 | -3.24467800 | 0.70836900 |   |   |   |
| H | 3.98939000 | -2.75922100 | 2.80686000 |   |   |   |
| H | 2.20320700 | -1.17918900 | 2.10282900 |   |   |   |
| C | 0.13711400 | -2.10264000 | 0.21688000 |   |   |   |
| H | 0.27591400 | -2.84730400 | 1.00416000 |   |   |   |
| H | 0.92934300 | -1.34638100 | 0.28589700 |   |   |   |
| H | 0.21681800 | -2.61322700 | -0.74590200 |   |   |   |

β-7

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| C | 0.18835500 | -0.88236800 | 1.88823200 |   |   |   |
| F | 0.98247900 | -1.31507100 | 2.77684200 |   |   |   |
| F | 2.68084600 | 0.00053200 | 2.48218400 |   |   |   |
| N | 2.76456800 | -2.10813000 | 1.58441800 |   |   |   |
| O | 3.96495900 | -1.95646200 | 1.57905300 |   |   |   |
| O | 2.16382400 | -3.13364200 | 1.32889500 |   |   |   |
| C | -0.80078200 | 1.49545300 | -0.46462400 |   |   |   |
| O | -0.47394900 | 0.83950500 | -1.43789700 |   |   |   |
| C | 2.26723200 | -0.26454300 | -0.30804300 |   |   |   |
| C | -1.34331100 | 3.91130100 | 0.04778900 |   |   |   |
| C | 0.88287000 | 3.30742400 | -0.66376500 |   |   |   |
| C | -0.96977300 | 5.25494300 | 0.07107500 |   |   |   |
| H | -2.36308100 | 3.62979000 | 0.29412100 |   |   |   |
| C | 1.25464400 | -4.64419200 | -0.63614300 |   |   |   |
| H | 1.58316200 | 2.53057700 | -0.95114500 |   |   |   |
| C | 0.32902400 | 5.62157100 | -0.26450100 |   |   |   |
| H | -1.69652400 | 6.01185700 | 0.34795600 |   |   |   |
| H | 2.26723200 | 4.92890500 | -0.90373500 |   |   |   |
| Ch  | α   | β  |
|-----|-----|----|
| H   | 0.62170900 | 6.66655000 | -0.24198900 |
| C   | -3.53966000 | -2.39675500 | -2.08777500 |
| C   | -2.61008900 | -1.20476400 | -2.30818100 |
| C   | -3.09867100 | 0.09404900 | -1.64949800 |
| C   | -3.81051900 | -2.72887000 | -0.61954800 |
| C   | -2.81529000 | 0.17029100 | -0.17031400 |
| C   | -4.47726400 | -1.58298100 | 0.14749900 |
| H   | -4.50014000 | -2.19674200 | -2.58302800 |
| H   | -2.51835800 | -1.01699200 | -3.38216000 |
| H   | -4.18443700 | 0.19575800 | -1.76925100 |
| H   | -2.87540000 | -2.97713000 | -0.10922300 |
| H   | -4.99378800 | -1.96096100 | 1.03117800 |
| C   | -2.02205200 | 1.39775500 | 1.75344800 |
| H   | -1.14893800 | 1.99553200 | 1.99736400 |
| C   | -3.19451600 | -0.75329800 | 2.08614700 |
| C   | -2.02230500 | 0.09757300 | 2.53393700 |
| H   | -1.07851800 | -0.40395800 | 2.33161700 |
| H   | -2.10948500 | 0.29719500 | 3.60456300 |
| H   | -2.98135900 | -1.81546500 | 2.24141900 |
| N   | -3.50228700 | -0.59872500 | 0.65062400 |
| N   | -1.96335200 | 1.08933900 | -0.31739500 |
| H   | -5.22845000 | -1.07632300 | -0.46596400 |
| H   | -4.47221500 | -3.59902200 | -0.56644700 |
| H   | -3.11408000 | -3.27712700 | -2.58082700 |
| H   | -1.60697900 | -1.41271100 | -1.93095900 |
| H   | -2.64078900 | 0.95464400 | 2.12792200 |
| H   | -2.93567700 | 1.97562100 | 1.93993800 |
| H   | -4.11160400 | -0.50257400 | 2.62993400 |
| C   | 2.13387000 | -1.11696000 | -1.40953600 |
| C   | 2.31722800 | -0.13392200 | -0.43334300 |
| C   | 3.40421500 | 0.71782500 | -0.49533900 |
| C   | 4.30104200 | 0.58897200 | -1.56170500 |
| C   | 4.10540300 | -0.39411600 | -2.52851100 |
| C   | 3.01516300 | -1.26938600 | -2.46892800 |
| H   | 3.54654500 | 1.47007300 | 0.27491100 |
| H   | 5.15719500 | 1.97562100 | 1.93993800 |
| H   | 4.81207500 | -0.48864500 | -3.34685800 |
| H   | 2.86797100 | -2.03411300 | -3.22435000 |
| C   | 1.21897900 | -0.26043200 | 0.62064400 |
| O   | 0.57572000 | 0.83191100 | 1.04618500 |
| C   | 0.33825000 | -1.39637700 | -0.02127000 |
| O   | -0.73092400 | -1.81139900 | 0.40592800 |
| N   | 0.97582500 | -1.86063800 | -1.13910800 |
| C   | 0.53507400 | -2.99366100 | -1.91782800 |
| H   | 1.31462100 | -3.76134700 | -1.94154000 |
| H   | 0.29173700 | -2.69508800 | -2.94261200 |
| H   | -0.35603700 | -3.39706400 | -1.43449400 |

\( \alpha = 7.01 \)
H 1.02699100 -1.60629800 0.05667700
H 0.21017300 -2.52516900 -1.24044200

β-8
0 1
C 1.90742900 -0.58132100 1.82965300
F 1.06728100 -0.93900600 2.80137600
F 2.61027800 0.47371200 2.22567200
N 2.90361800 -1.74959300 1.70460900
O 4.08132300 -1.50065400 1.79153200
O 2.39308500 -2.83579500 1.52375300
C -0.42326400 1.30626200 -0.31118500
O -0.26820200 0.68719200 -1.39555600
C -0.97371700 3.50561000 -0.32313800
O -1.10728700 3.55582700 -1.17197100
C 0.70971000 3.50610000 0.40653900
C -0.97371700 4.93354300 -1.29216400
H -1.63114400 5.48697100 -1.95694000
H 1.61206000 5.40622300 0.85585100
H 0.11583300 6.68152400 -0.65643400
C -3.55841100 -2.48098500 -1.91300200
C -2.50751700 -1.39451600 -2.13502200
C -2.89767700 -0.01014800 -1.59875900
C -3.95198200 -2.68607700 -0.45008800
C -2.72243600 0.16419500 -1.09564000
C -4.55919200 -1.43194100 0.18724500
H -4.46203600 -2.22695900 -2.48424000
H -2.32313100 -1.29258400 -3.20913200
H -3.95400600 0.19709100 -1.81580700
H -3.07575600 -2.98195400 0.13969900
H -5.17943800 -1.70067900 1.04482200
C -1.99602500 1.41053700 1.78441300
H -1.13218800 2.01382000 2.05949400
C -3.32750300 -0.61906100 2.15748700
C -2.10230200 0.14682600 2.62264100
H -1.20119700 -0.44446300 2.46231800
H -2.19188800 0.37848000 3.68602600
H -3.22636200 -1.68594400 2.38468700
N -3.54565100 -0.50440900 0.70460300
N -1.86063700 1.03957200 0.37851000
H -5.21235600 -0.91091900 -0.52022500
H -4.68543800 -3.49622700 -0.38432400
H -3.18769600 -3.42712500 -2.32256700
H -1.55805200 -1.67484800 -1.67542500
H -2.29592600 0.74794000 -2.08744000
H -2.89786900 2.02621600 1.89501700
H -4.23461100 -0.25260700 2.65155100
C 2.09795500 -1.33905500 -1.42259900
C 2.24006900 -0.22163300 -0.59557200
C 3.26778100 0.68251400 -0.79732700
C 4.14788300 0.46234500 -1.86346700
C 3.99500400 -0.65316000 -2.68175800
|     | x    | y    | z    |
|-----|------|------|------|
| C   | 2.96465900 | -1.57852600 | -2.47575700 |
| H   | 3.37526100 | 1.54516300  | -0.14744700  |
| H   | 4.95425500 | 1.16260200  | -2.05079800  |
| H   | 4.68922900 | -0.81418700 | -3.50013900  |
| H   | 2.85052500 | -2.44449000 | -3.11882000  |
| C   | 1.20159900 | -0.30006800 | 0.49402000   |
| O   | 0.45336500 | 0.82715100  | 0.79919300   |
| O   | 0.36066000 | -1.53714500 | 0.05407200   |
| O   | -0.65569600 | -1.93265700 | 0.59225500   |
| C   | 3.37526100 | 1.54516300  | -0.14744700  |
| H   | 3.37526100 | 1.54516300  | -0.14744700  |
| H   | 3.37526100 | 1.54516300  | -0.14744700  |
| H   | 3.37526100 | 1.54516300  | -0.14744700  |
| C   | 3.37526100 | 1.54516300  | -0.14744700  |
| H   | 3.37526100 | 1.54516300  | -0.14744700  |
| H   | 3.37526100 | 1.54516300  | -0.14744700  |

α-8

|     | x    | y    | z    |
|-----|------|------|------|
| C   | 2.06223200 | 1.03450900 | 1.70786900 |
| F   | 1.39440300 | 0.88897800 | 2.85058500 |
| F   | 2.40981000 | 2.31085500 | 1.57083200 |
| N   | 3.36867900 | 0.23725600 | 1.86089000 |
| O   | 3.47587700 | -0.50019700 | 2.81312000 |
| C   | -0.85739600 | -1.02991100 | -0.53107400 |
| O   | -1.30861000 | 2.47353800 | -0.77502400 |
| C   | -2.47912100 | 2.68750600 | -1.50458000 |
| C   | -0.53473800 | 3.56368200 | -0.38218800 |
| C   | -2.87977300 | 3.97814000 | -1.83270900 |
| H   | -3.07735100 | 1.83197900 | -1.80844400 |
| C   | -0.93564900 | 4.85774200 | -0.71307400 |
| H   | 0.38338500 | 3.39111700 | 0.16766300 |
| C   | -2.10712100 | 5.06885000 | -1.43411300 |
| H   | -3.79373500 | 4.13564600 | -2.39716700 |
| H   | -0.32873000 | 5.70345600 | -0.40477700 |
| H   | -2.41789400 | 6.07773100 | -1.68688600 |
| C   | -1.99171200 | -4.00109600 | -1.10106700 |
| C   | -1.92618000 | -2.65967800 | -1.52347800 |
| C   | -2.37849100 | -1.48305000 | -1.47088000 |
| C   | -2.58277200 | -4.03443300 | 0.30974700  |
| C   | -2.53010800 | -0.90145000 | -0.08928300 |
| C   | -3.67187700 | -2.98381100 | 0.54415600  |
| H   | -2.78589100 | -4.26781400 | -1.81162400 |
| H   | -1.02402000 | -2.74338310 | -2.55003700 |
| H   | -2.37549000 | -1.80417400 | -1.79757100 |
| H   | -1.79723100 | -3.89434100 | 1.06379600  |
| H   | -4.28488900 | -3.25906900 | 1.40491700  |
| C   | -2.57705200 | 0.93216300 | 1.43694900  |
| H   | -2.02270600 | 1.85809900 | 1.58130000  |
| C   | -3.13268200 | -1.31191700 | 2.28051600  |
| C   | -2.34858300 | -0.04412900 | 2.57742600  |
| H   | -1.27530500 | -0.23466200 | 2.64583900  |
| H   | -2.68253300 | 0.37182900 | 3.55031200  |
| H   | -2.71317400 | -2.16998400 | 2.81841900  |
| N   | -3.13307800 | -1.65049700 | 0.84620700  |
| N   | -2.13278700 | 0.32531500 | 0.18311800  |
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| H    | -4.34648900 | -2.92528100 | -0.31526400 |
| H    | -3.01826100 | -5.02273000 | 0.48917300  |
| H    | -1.22636300 | -4.77970100 | -1.18661800 |
| H    | -0.51758300 | -2.40546200 | -0.91737500 |
| H    | -2.04221900 | -0.68706500 | -2.12630700 |
| H    | -3.64170700 | 1.17971400  | 1.34301000  |
| H    | -4.17684700 | -1.20221500 | 2.59368200  |
| C    | 1.98768400  | -1.44627200 | -0.62456800 |
| C    | 2.41971700  | -0.40319000 | 1.45594300  |
| C    | 3.08533800  | -0.64309300 | 2.64831700  |
| C    | 3.33294400  | -1.96182900 | 3.01778900  |
| C    | 2.89987800  | -3.00308600 | 3.26701000  |
| C    | 2.22478400  | -2.77201800 | -0.99228900 |
| C    | 3.95951000  | 0.19295800  | -3.26701000 |
| C    | 3.85478400  | -2.18559500 | -3.94108100 |
| H    | 3.39595100  | 0.19295800  | -3.26701000 |
| H    | 2.22478400  | -2.77201800 | -0.99228900 |
| H    | 0.81174100  | -1.35387200 | 2.49497400  |

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| Atom | x     | y     | z     |
|------|-------|-------|-------|
| 0    | 1.89043800 | -0.56113100 | 1.84288400 |
| 1    | 1.03018000 | -0.92053500 | 2.79514300 |
| C    | 2.56280900 | 0.51155400  | 0.49988000 |
| F    | 2.90756800 | -1.71316800 | 1.75523700 |
| N    | 4.07559800 | -1.44962800 | 1.90291500 |
| O    | 2.41938400 | -2.80313800 | 1.53925400 |
| C    | -0.32227800 | 1.30975800  | -0.37850700 |
| O    | -0.22693900 | 0.67297200  | -1.43824700 |
| C    | -0.23267400 | 2.82790800  | -0.37746300 |
| C    | -0.94847800 | 3.51963600  | -1.35616700 |
| C    | 0.57108800  | 3.53502500  | 0.51498800 |
| C    | -0.87300000 | 4.90423300  | -1.43517400 |
| H    | -1.55944600 | 2.95854600  | -2.05714600 |
| C    | 0.64912400  | 4.92628300  | 0.43344000 |
| H    | 1.13980300  | 2.99352400  | 1.26343700 |
| C    | -0.07253900 | 5.61242000  | -0.53707700 |
| H    | -1.43183200 | 5.43461200  | -2.19986300 |
| H    | 1.27836600  | 5.47157300  | 1.13001000 |
| H    | 0.01041500  | 6.69428400  | -0.59991500 |
| C    | 3.55936700  | -2.47965100 | -1.91666100 |
| C    | -2.51582400 | -1.38193900 | -2.11774000 |
| C    | -2.92447000 | -0.00206500 | -1.58307200 |
| C    | -3.96189300 | -2.70531500 | -0.45937400 |
| C    | -2.77366200 | 0.17727100  | -0.09105500 |
| C    | -4.58561200 | -1.46279100 | 0.18503200 |
| H    | -4.46093400 | -2.22630900 | -2.49190200 |
| H    | -2.31511500 | -1.27588600 | -3.18887000 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -3.97513000 | 0.20351200 | -1.82758900 |
| H    | -3.08690800 | -2.99877800 | 0.13360200 |
| H    | -5.21021100 | -1.74651400 | 1.03522200 |
| C    | -2.01946600 | 1.38337100 | 1.79897400 |
| H    | -1.14134500 | 1.96815900 | 2.07470700 |
| C    | -3.36800200 | -0.64281300 | 2.16338200 |
| H    | -1.23581300 | -0.50201900 | 2.40979000 |
| H    | -2.18198800 | 1.06181500 | 0.38132100 |
| H    | -3.28182600 | -2.99877800 | 2.39617900 |
| C    | -3.59286700 | -0.52451200 | 0.71468920 |
| H    | -2.12168600 | 0.10005000 | 2.61059800 |
| C    | -4.68666900 | -3.52471700 | -0.40905100 |
| H    | -1.92980200 | 1.06181500 | 0.38132100 |
| H    | -1.82758900 | -1.70396000 | 2.39617900 |
| C    | -5.00124000 | -0.94825300 | -0.52501000 |
| C    | -4.68666900 | -3.52471700 | -0.40905100 |
| C    | -3.17742400 | -3.41755700 | -2.33526600 |
| H    | -2.31902900 | 0.76250900 | -2.05925000 |
| H    | -1.74651400 | 1.96129700 | 0.38132100 |
| C    | -0.29309100 | -3.67710400 | -1.16830000 |
| C    | -0.52451200 | 0.71468920 | -0.40905100 |
| C    | -2.40979000 | -0.52501000 | 2.61059800 |
| C    | -2.33526600 | -2.33526600 | -0.40905100 |
| C    | -3.67710400 | -1.16830000 | -2.05925000 |

α-9

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 2.24798400 | 1.36901400 | 1.45549800 |
| F    | 1.62226500 | 1.41030700 | 2.62840200 |
| F    | 2.61961300 | 2.59861400 | 1.11709100 |
| N    | 3.53852400 | 0.56038900 | 1.67906900 |
| O    | 4.33990400 | 0.62006700 | 0.77207000 |
| O    | 3.63499100 | -0.07458700 | 2.70377100 |
| C    | -0.73351600 | 1.09760800 | -0.61120700 |
| O    | -0.29109700 | 0.47179300 | -1.58637700 |
| C    | -1.49086500 | 2.40110000 | -0.82488700 |
| C    | -2.76262700 | 2.38086900 | -1.39736900 |
| C    | -0.86475100 | 3.62129700 | -0.57556800 |
| C    | -3.41296200 | 3.57161600 | -1.70209800 |
| H    | -3.24140800 | 1.42517600 | -1.59424040 |
| C    | -1.51689200 | 4.81447200 | -0.88302300 |
| H    | 0.13417900 | 3.62737600 | -0.15248300 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -2.79112700| 4.79281900 | -1.44190600|
| H       | -4.40478200| 3.54870300 | -2.14275000|
| H       | -1.02576400| 5.76218300 | -0.68584800|
| H       | -3.29921100| 5.72257200 | -1.67740300|
| C       | -1.91746600| -4.12702100| -0.97032700|
| C       | -1.22226700| -2.80791600| -1.30391100|
| C       | -2.17629800| -1.60520000| -1.36858400|
| C       | -2.68960000| -4.13014500| 0.35005700 |
| C       | -2.45492700| -1.00996300| 0.01023900 |
| C       | -3.77125900| -3.04838900| 0.43906900 |
| H       | -2.62100700| -4.36280600| -1.78027700|
| H       | -0.72086400| -2.90249200| -2.27207100|
| H       | -3.13238600| -1.90491700| -1.81173300|
| H       | -2.00481200| -4.00300100| 1.19904700 |
| H       | -4.49922600| -3.31121200| 1.20896900 |
| C       | -2.37834800| 0.78784400 | 1.56392900 |
| H       | -1.61699900| 1.51602700 | 1.84730700 |
| C       | -3.56431900| -1.29757100| 2.18230000 |
| C       | -2.58579800| -0.24265300| 2.66246400 |
| H       | -1.63187900| -0.71400600| 2.91072500 |
| H       | -2.96997100| 0.23113100 | 3.56841400 |
| H       | -3.52152500| -2.17838800| 2.82984200 |
| N       | -3.24882200| -1.72900700| 0.81640400 |
| N       | -1.95081700| 0.15023000 | 0.32139500 |
| H       | -4.32911400| -2.98296100| -0.50079700|
| H       | -3.17083900| -5.10579300| 0.47515800 |
| H       | -1.17848200| -4.93522500| -0.95579600|
| H       | -0.42939200| -2.58985500| -0.57974400|
| H       | -1.74602000| -0.82665900| -1.98859600|
| H       | -3.31425000| 1.33578700 | 1.37700500 |
| H       | -4.59303100| -0.91730800| 2.20579700 |
| C       | 2.06574200 | -1.42207100| -0.42312400|
| C       | 2.50283700 | -0.54557300| -1.42789700|
| C       | 3.17206200 | -1.00872900| -2.55124000|
| C       | 3.41748300 | -2.37494100| -2.66208000|
| C       | 2.99115700 | -3.24362400| -1.65076900|
| C       | 2.31648700 | -2.79090400| -0.51813300|
| H       | 3.49533300 | -0.30803000| -3.31463700|
| H       | 3.94222700 | -2.76858900| -3.52505200|
| H       | 3.19382400 | -4.30602900| -1.74678700|
| H       | 1.99410700 | -3.47972200| 0.25583200 |
| C       | 2.11756500 | 0.81563900 | -1.03740000|
| O       | 2.32164000 | 1.88022200 | -1.56371000|
| C       | 1.40914400 | 0.66843600 | 0.36744700 |
| O       | 0.18883400 | 1.31541400 | 0.48176100 |
| N       | 1.41008000 | -0.75461300| 0.59285900 |
| C       | 0.85845700 | -1.38714000| 1.76825900 |
| H       | 1.63711500 | -1.88268600| 2.35975600 |
| H       | 0.08887500 | -2.12104700| 1.49726300 |
| H       | 0.39327700 | -0.61419300| 2.37976400 |

**P**

| 0 1   |            |            |            |
|-------|------------|------------|------------|
| C     | 0.98815000 | 1.84876400 | -0.09396300|
| F     | 0.58972300 | 2.68500600 | 0.85802900 |
| F     | 0.58535700 | 2.29458100 | -1.27685600|

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|      |      |      |
|------|------|------|
| H    | 6.94804500 | 0.29361600 | 0.27706600 |
| C    | -1.95417000 | 1.00453600 | 0.70805700 |
| C    | -1.99144600 | 1.23073600 | -0.67626700 |
| C    | -2.82993500 | 2.18689500 | -1.23658400 |
| C    | -3.65737600 | 2.91497900 | -0.38963500 |
| C    | -3.62562200 | 2.67588600 | 0.99013200  |
| C    | -2.78523100 | 1.72390100 | 1.56415600  |
| H    | -2.82969500 | 2.34421400 | -2.31033400 |
| H    | -4.33110600 | 3.66264900 | -0.79138100 |
| H    | -4.27986200 | 3.24967100 | 1.63918000  |
| H    | -2.78521300 | 1.55242100 | 2.63434400  |
| C    | -1.01664500 | 0.34165000 | -1.30398300 |
| O    | -0.66161600 | 0.21179500 | -2.44668500 |
| C    | -0.41197200 | -0.51099200 | -0.12059800 |
| O    | 1.00110100  | -0.52635300 | -0.09849500 |
| N    | -1.03425700 | 0.02320800 | 1.04516400  |
| C    | -0.71592100 | -0.39414700 | 2.39728900  |
| H    | -1.44605200 | -1.11261200 | 2.78521900  |
| H    | -0.68338200 | 0.48169600 | 3.04925700  |
| H    | 0.27308800  | -0.85504200 | 2.39712700  |

|      |      |      |
|------|------|------|
| C    | 0.81344000 | -0.35552900 | 0.63049400 |
| F    | 0.28932200 | -0.81353500 | 0.26583800 |
| F    | 0.69443100 | 0.60720500 | 1.93239100 |
| N    | 1.44841400 | 1.15375300 | -0.18280700 |
| O    | 1.89342400 | 2.26544500 | 0.26382000 |
| O    | 1.59911500 | 0.80569900 | -1.40711200 |
| C    | -1.75349000 | 1.14543600 | -0.83118200 |
| O    | -1.30607100 | 0.51175400 | 1.75202100 |
| C    | -1.63933800 | 2.61832100 | -0.70112600 |
| C    | -0.51465800 | 3.23227800 | -1.26036100 |
| C    | -2.66108300 | 3.38571100 | -0.12974400 |
| C    | -0.40779300 | 4.61842000 | -1.21872700 |
| H    | 0.26963100  | 2.61467600 | -1.68966100 |
| C    | -2.55402200 | 4.77012400 | -0.11337700 |
| H    | -3.54776600 | 2.90532700 | 0.27317200  |
| C    | -1.42288400 | 5.38473100 | -0.65159700 |
| H    | 0.47381700  | 5.09910000 | -1.62857800 |
| H    | -3.34955200 | 5.36965300 | 0.31594700 |
| H    | -1.33528200 | 6.46630300 | -0.62761000 |
| C    | -3.43236500 | -3.56279300 | -1.54269100 |
| C    | -2.77922500 | -2.23877500 | -1.95211700 |
| C    | -3.57352600 | -1.01150100 | -1.46084600 |
| C    | -3.58940300 | -3.75465100 | -0.03386000 |
| C    | -3.20168700 | -0.65059200 | -0.04812500 |
| C    | -4.41109500 | -2.65752800 | 0.64718400 |
| H    | -4.41337600 | -3.63176700 | -2.01308500 |
| H    | -2.72419800 | -2.18635000 | -3.04224100 |
| H    | -4.64175700 | -1.22407300 | -1.47515500 |
| H    | -2.61081000 | -3.81132500 | 0.45846100  |
| H    | -4.77200700 | -2.99526600 | 1.61913900  |
| C    | -2.28563100 | 0.88416000 | 1.62402900  |
| H    | -1.43058400 | 1.55799400 | 1.64789100  |
| C    | -3.22769400 | -1.27803100 | 2.33769100  |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -2.03942200 | -0.35371700 | 2.46682300 |
| H    | -1.13334800 | -0.85843000 | 2.13109300 |
| H    | -1.90211500 | -0.06883200 | 3.51127300 |
| H    | -2.98897900 | -2.27413300 | 2.71788700 |
| N    | -3.61278200 | -1.44316700 | 0.92267000 |
| N    | -2.50267200 | 0.47272200  | 0.21966600 |
| H    | -5.29275200 | -2.39173000 | 0.05851200 |
| H    | -4.09277500 | -4.70836100 | 0.15073800 |
| H    | -3.16792100 | 1.42567900  | 1.97963400 |
| H    | -3.40918300 | 0.15908300  | 2.11078300 |
| H    | -4.10290000 | -0.90539200 | 2.88043100 |
| C    | 3.78636500  | -0.96883000 | -0.56459900 |
| C    | 3.12107900  | -1.86310300 | 0.28639500 |
| C    | 2.65736300  | -3.08811300 | -0.17451100 |
| C    | 2.88438700  | -3.42253000 | -1.50623200 |
| C    | 3.55727500  | -2.52669800 | -2.34541300 |
| C    | 4.01779500  | -1.28984200 | -1.89532900 |
| H    | 2.13493900  | -3.75853200 | 0.50115900 |
| H    | 2.53898000  | -4.37233900 | -1.89883400 |
| H    | 3.72186000  | -2.79768300 | -3.38304000 |
| H    | 4.51613000  | -0.59759100 | -2.56418200 |
| C    | 3.03743000  | -1.22055000 | 1.60168000 |
| O    | 2.54980800  | -1.60428900 | 2.64017300 |
| C    | 3.75228500  | 0.15444400  | 1.42396400 |
| O    | 3.91879300  | 0.99155400  | 2.28024100 |
| N    | 4.16538600  | 0.19500700  | 0.11399000 |
| C    | 4.67621000  | 1.38239900  | -0.54190600 |
| H    | 3.92379700  | 1.74024500  | -1.25270400 |
| H    | 5.62173900  | 1.16418800  | -1.04011500 |
| H    | 4.82517100  | 2.13574500  | 0.22960500 |

2 (Φ=154°)

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -1.54217800 | -1.25304600 | 1.07670500 |
| F    | -2.11129200 | -0.98480500 | 2.24767000 |
| F    | -0.81435300 | -2.36892000 | 1.20664400 |
| N    | -2.74551200 | -1.61798300 | 0.17788400 |
| O    | -2.59379400 | -2.48654800 | -0.66115300 |
| O    | -3.75516800 | -0.97803300 | 0.35692900 |
| C    | -0.65439300 | 0.04399000  | 0.67330300 |
| O    | -0.12284300 | 0.46343200  | 1.75179400 |
| C    | -1.54294200 | 1.02530900  | -0.11133800 |
| C    | -2.05993300 | 2.10779900  | 0.59599900 |
| C    | -1.88088600 | 0.85681500  | -1.45536100 |
| C    | -2.90497300 | 3.01918800  | -0.03248700 |
| H    | -1.77659000 | 2.21334000  | 1.63823700 |
| C    | -2.72939000 | 1.76389000  | -2.08349200 |
| H    | -1.48551500 | 0.01566400  | -2.02044000 |
| C    | -3.24244800 | 2.84756500  | -1.37274600 |
| H    | -3.30278600 | 3.86235700  | 0.52388700 |
| H    | -2.98756400 | 1.62674700  | -3.12887600 |
| H    | -3.90299000 | 3.55530400  | -1.86369000 |
| C    | 4.16412200  | 1.72646000  | 1.07773500 |
| C    | 2.67306800  | 1.63545600  | 1.39904100 |
C  1.77355700  1.56485800  0.15215300
C  4.71330500  0.54426100  0.27883700
C  1.62776900 -0.37466200
C  1.62776900  0.15965000
H  4.34540000  2.64622100  0.50486300
H  2.37820100  2.51964000  1.97110500
H  4.65535300  0.86953100
H  4.60479400 -1.71421300
C  0.39341500 -0.55953200 -2.18415700
C  2.83051900 -1.68986300 -1.19000000
C  1.56357800 -2.59320200 -0.82987600
H  1.52388200  2.80665600  0.24103900
H  1.51957800  3.53913400 -1.37321400
H  0.79064200  1.95976500  0.37909600
H  0.46256600 -1.39404900 -2.24582100

2 (Φ=168°)

C  0.87523500  1.38280900  0.92358800
C  1.58379400  1.60790200  2.03689900
F  1.87201300  1.09818800
F  -0.35518600  1.87201300  1.09818800
N  1.54852100  2.31933100 -0.09964300
O  0.85780700  3.12570200 -0.68777400
O  2.74171000  2.16184300 -0.25112500
C  0.78486900 -0.22404000  0.69161400
O  0.41205200 -0.68455100  1.81660700
C  2.06795800 -0.85491800  0.12474900
C  3.28205400 -0.59016700  0.76869200
C  2.03908700 -1.83188300 -0.86960700
C  4.44355100 -1.25268800  0.39141800
H  3.31582800  0.14046800  1.56848500
C  3.20420200 -2.50398300 -1.24456400
H  1.09902500 -2.09011800 -1.34663200
C  4.40993200 -2.21006700 -0.62225600
C  5.37789000 -1.02681400  0.89559800
H  3.15772500 -3.2612750 -2.02116200
H  5.31721100 -2.72880500 -0.91511800
C  -4.26866600 -0.83828700  1.58203000
C  -2.77517300 -0.85197300  1.91085400
C  -1.93061300 -1.61120300  0.87341000
C  -4.62378900 -0.22550700  0.22556800
C  -1.56141700 -0.73009500 -0.29087800
C  -3.92066400 -0.89673200 -0.95849800
H  -4.63532400 -1.87359300  1.59776100
H  -2.62797600 -1.33123000  2.88262700
H  -2.49067400 -2.46456500  0.47660800
2 (Φ=48°)

| 01 | C     | -1.86299400 | 1.42283500 | -0.25824400 |
|    | F     | -2.28726900 | 1.78026200 | 0.96942000  |
|    | F     | -2.94751800 | 1.20677400 | -0.99562200 |
|    | N     | -1.18481600 | 2.66101800 | -0.85837300 |
|    | O     | -1.55100000 | 3.04117900 | -1.94139900 |
|    | O     | -0.31060200 | 3.15961500 | -0.17453400 |
|    | C     | -0.91488200 | 0.17729100 | -0.43785900 |
|    | O     | -0.52692500 | 0.19022900 | -1.65697700 |
|    | C     | -1.73034500 | -1.03907200 | 0.05311600  |
|    | C     | -2.24252200 | -1.89481000 | -0.91896800 |
|    | C     | -2.01706600 | -1.27407500 | 1.39859100  |
|    | C     | -3.01069700 | -2.99680000 | -0.55123700 |
|    | H     | -2.01307700 | -1.67361200 | -1.95660700 |
|    | C     | -2.79038000 | -2.37169800 | 1.76783700  |
|    | H     | -1.63656000 | -0.60244600 | 2.16354400  |
|    | C     | -3.28501400 | -3.23719800 | 0.79334400  |
|    | H     | -3.39937100 | -3.66594500 | -1.31261900 |
|    | H     | -3.00552600 | -2.55346100 | 2.81623200  |
|    | H     | -3.88435100 | -4.09473100 | 1.08248900  |
|    | C     | 3.77615800  | -1.41549100 | -1.79958700 |
|    | C     | 2.29292500  | -1.08502400 | -1.96143400 |
|    | C     | 1.43385700  | -1.48383600 | -0.74654600 |
|    | C     | 4.45003800  | -0.74007400 | -0.60501700 |
|    | C     | 1.42581400  | -0.41277600 | 0.31607600  |
|    | C     | 3.77134000  | -1.05178500 | 0.73077400  |
|    | H     | 3.88238700  | -2.50306100 | -1.68642900 |
|    | H     | 1.90319300  | -1.61859600 | -2.83264100 |
|    | H     | 1.82545900  | -2.39923900 | -0.28889600 |
|    | H     | 4.46966700  | 0.34895500  | -0.73921900 |
|    | H     | 4.45132300  | -0.83982200 | 1.55857300  |
|    | C     | 0.39991800  | 1.12155200  | 1.81390400  |
|    | H     | -0.45079000 | 1.78782400  | 1.84447700  |
|    | C     | 2.84150600  | 0.91916100  | 1.86320100  |
|    | C     | 1.69972900  | 1.90929300  | 1.82102700  |
|    | H     | 1.74151600  | 2.52122000  | 0.91775400  |
H 1.74776100 2.56990600 2.68920900
H 3.77700200 1.37954300 0.98300900
N 0.34272600 0.29407900 0.60099000
H 3.51705600 -2.11287000 0.80217600
H 5.49158400 -1.07201400 -0.54436800
H 4.31221500 -1.14424100 -2.71468200
H 2.14147300 -0.01985500 -2.16149700
H 0.42058300 -1.68076900 -1.06893700
H 0.35797800 0.46027000 2.69022600
H 2.99984200 0.53786700 2.87836800

1 (Φ=155°)

0 1

C -1.54520200 -1.30603400 1.10113500
F -2.08436900 -1.21285400 2.31560600
F -0.72971800 -2.35966000 1.08810800
N -2.74547000 -1.65391200 0.19830500
O -2.57356000 -2.46457800 -0.69074900
O -3.76814600 -1.05658500 0.43942300
C -0.81701100 0.08141700 0.89764100
O -0.25161600 0.47704300 1.82765200
C -1.63041500 1.04868900 -0.05074200
C -2.02761600 2.23492500 0.56230000
C -2.01016900 0.79307800 -1.37053900
C -2.79427500 3.16466000 -0.13728400
H -1.72132500 2.41192700 1.58808000
C -2.78110800 1.76184900 -2.06593000
C -1.69882300 -0.12576500 -1.86121500
C -3.17328900 2.90621500 -1.45085800
H -3.09699000 4.08852700 0.34536400
H -3.07132100 1.51281300 -3.09158300
H -3.77164400 3.62773500 -1.99795000
C 4.12088800 1.66992400 1.19376300
C 2.62405600 1.53797500 1.47446700
C 1.75147500 1.53733500 0.20654800
C 4.70766200 0.54933500 0.33491600
C 1.62917900 0.16856700 -0.41675600
C 4.01565600 0.39727700 -1.02241700
H 4.29858700 2.62708500 0.68448100
H 2.30582400 2.37683800 2.10031700
H 2.18231300 2.06573900 -0.54689100
H 4.64103800 -0.41002000 0.86472400
H 4.65603200 -0.16037400 -1.71012100
C 0.45247200 -1.66025100 -1.29992200
C -0.49026200 -2.18285100 -1.17243300
C 2.89723900 -1.77545100 -1.29409800
C 1.63874100 -2.55093000 -0.95440700
H 1.59670100 -2.78830800 0.11198700
H 1.61748900 -3.48707900 -1.51647300
H 3.76268100 -2.16436600 -0.74508200
N 2.75585800 -0.35043000 -0.95968000
N 0.48387600 -0.46603500 -0.45623400
H 3.84709400 1.37608700 -1.48177200
H 5.76976600 0.75018700 0.15960700
H 4.66510300 1.71734600 2.14262000

S55
H  2.41080100  0.62967400  2.04748500  2.04748500
H  0.75840600  1.90836500  0.43330700
H  0.75840600  1.90836500  0.43330700
H  0.52183700  1.34604900  -2.35161900
H  3.12168400  -1.85260800  -2.36443700

1 (Φ=155°)

0 1
C  -1.54453900  1.30626300  -1.10088700
F  -2.08289600  1.21366400  -0.8678800
F  -0.72877500  2.35968200  -1.08678800
N  -2.74527600  1.65419700  -0.19878700
O  -2.57963000  2.46467300  0.69051700
O  -3.76790500  1.05711700  -0.44064200
C  -0.81659100  -0.08131400  -0.79633600
O  -0.25105100  -0.47693100  1.82725200
C  -1.63018900  -1.04877600  0.05081000
C  -2.02660400  -2.23522300  -0.56234900
C  -2.01083100  -0.79323600  1.37037300
C  -2.79341000  -3.16516600  0.13680400
H  -1.71959100  -2.41217500  -1.58805200
C  -2.78187500  -1.71722400  2.06536400
H  -1.70011800  0.12572000  1.86123900
C  -3.17333300  -2.90673600  1.45012500
H  -3.09558800  -4.08914300  -0.34597500
H  -3.07277900  -1.51321600  3.09082500
H  -3.77180100  -3.62840300  1.99690000
C  4.12027800  -1.67037000  -1.19341700
C  2.62342300  -1.53842000  -1.47397000
C  1.75116000  -1.53760200  -0.20582500
C  4.70713800  -0.54940600  -0.33509100
C  1.62887700  -0.16863600  0.41696900
C  4.01540300  -0.39687200  1.02234400
H  4.29799300  -2.62731100  -0.68372300
H  2.30499100  -2.37724100  -2.09976700
H  2.18248900  -2.20731000  0.54778300
H  4.64734700  0.40974500  -0.86524700
H  4.65613400  0.16114100  1.70967300
C  0.45203800  1.65994000  1.30041500
H  -0.49098000  2.18212900  1.17357000
C  2.89687400  1.77591400  1.17357000
C  1.63789800  2.55109700  0.95448000
H  1.59528300  2.78888800  -0.1177600
H  1.61662500  3.48702400  1.51691700
H  3.76168300  2.16474200  0.74316700
N  2.75522100  0.35068000  0.95960800
N  0.48347800  0.46582200  0.45654700
H  3.84706400  -1.37552000  1.48211800
H  5.76928700  -0.75011100  -0.15990200
H  4.66441100  -1.71821700  -2.14229700
H  2.41012700  -0.63010300  -2.04693700
H  0.75806400  -1.90897400  -0.43201600
H  0.52228200  1.34554500  2.35198900
H  3.12244000  1.85351200  2.36331000

1 (Φ=-43°)

S56
2,6-lutidine (solvent= dichloromethane)

0 1
C 1.15898000  -0.26177400 0.00019600
C 1.19452700  1.13165900 0.00029300
C -0.00866700  1.83197400 0.00009500
C -1.19913000  1.12083000 0.00019300
C -1.14867900  -0.27764600 0.00022500
N 0.00637700  -0.94993300 0.00004000
H  -0.01417800   2.91756100   0.00015400
H   2.14619600   1.65228200   0.00050100
H  -2.15831300   1.62885200  -0.00039200
C  -2.41775200  -1.08923800  -0.00039800
H  -3.02429300  -0.86327500   0.88161900
H  -3.02551000  -0.86114700  -0.88100700
H  -2.17714800  -2.15252500  -0.00177200
C   2.42074100  -1.08276600  -0.00028600
H   2.44870100  -1.73053800   0.88076800
H   2.44922200  -1.72989800  -0.88066000
H   3.31056400  -0.45093700   0.00074900

DMAP (solvent= dichloromethane)

C   -1.94756300  -1.13043000   0.00002300
C   -0.56399100  -1.19766900   0.00012200
C    0.18541100  0.00000500  -0.00015900
C   -0.56399600   1.19767700  -0.00001100
C   -1.94756800   1.13043200  -0.00009400
N   -2.66488200  -0.00000100  -0.00008900
H   -2.51740900  -2.05790300   0.00008000
H   -0.08240600  -2.16697700   0.00025000
H   -0.08241900  2.16698800  -0.00006800
H   -2.51741900  2.05790000  -0.00018600
C    2.26946200  1.25877400  -0.00000100
H    3.33911800  1.05578200  -0.00030000
H    2.03350200  1.85615800  -0.88861700
H    2.03314000  1.85656900  -0.88813500
C    2.26943700   1.25878200  -0.00020800
H    2.03307600   1.85614900  -0.88852100
H    3.33909700  -1.05580700  -0.00042900
H    2.03349200  -1.85656900   0.88803700
N    1.54789300  -0.00000100   0.00023400

R1 (solvent= dichloromethane)

C   -1.29547800  -0.48371200   0.00003900
F   -1.19629400  -1.24419000  -1.08618400
F   -1.19600100  -1.24365400   1.08659500
N   -2.69839500   0.13322700   0.00058000
O   -3.17317900   0.36663700   1.08597700
O   -3.17358800   0.36581300  -1.08585600
C   -0.26079900   0.67141000  -0.00036500
O   -0.69148200  1.80084500  -0.00077000
C    1.16714800  0.30048700  -0.00014000
C    1.59740900  -1.03214400  -0.00020800
C    2.10083800  1.34478100   0.00012500
C    2.95901500  -1.31177000  -0.00005000
H    0.88758600  -1.85116500  -0.00045900
C    3.45768900   1.05711300   0.00034500
H    1.74245400   2.36868100   0.00017000
C    3.88562600  -0.27141500   0.00027800
H    3.29667500  -2.34205600  -0.00007100
H    4.18275000  1.86353700   0.00057600
H    4.94726500  -0.49585500   0.00044700

S58
$3^{2,6}$-lutidine (solvent= dichloromethane)

0 1
C  -0.79198600  1.88893200  -0.71065200
F  -1.46599500  1.46488600  -1.82802100
F  -0.36711100  3.15602900  -0.97625600
N  -1.73502700  1.94096100  0.37546800
O  -1.53726900  2.75208200  1.28001200
O  -2.56235700  1.02026900  0.46088000
C  0.43917600  -0.07491600  0.86278900
O  0.08011500  0.52293400  1.83488200
C  1.86051000  -0.18393400  0.45130800
C  2.62689500  0.98279800  0.43510800
C  2.44500100  -1.42943300  -0.03971400
C  3.98489700  0.90151400  0.15405800
H  2.14090900  1.93635500  0.61820500
C  3.81022000  -1.50426500  -0.03971400
H  1.84191700  -2.33318800  0.24935900
C  4.57558700  -1.50426500  -0.03971400
H  4.58431400  1.80471300  0.12043100
H  4.27458200  -2.46923700  -0.21119100
H  5.63734100  -1.50426500  -0.03971400
C  -1.49820000  -1.58708100  0.96402300
C  -2.47464900  -2.36546700  0.36206100
C  -2.50589400  -2.52242400  -1.01272900
C  -1.52693600  -1.91143500  -1.77925700
C  -0.53176500  -1.14948400  -1.18869200
C  -0.54017100  -0.99883800  0.17709700
H  -3.28144700  -3.11723200  -1.48248500
H  -3.21649900  -2.83504600  0.99524700
H  -1.51885100  -2.01155400  -2.85721200
C  0.51421500  -0.54410800  -2.08047700
H  1.39071900  -1.19444100  -2.13449200
H  0.08380500  -0.45235700  -3.07684800
H  0.82343600  -0.43972300  -1.73598700
C  -1.52036500  -1.44266900  2.45830100
H  -0.53394700  -1.55614800  2.90774100
H  -1.90106500  -0.45394200  2.71800500
H  -2.18502600  -2.20730900  2.85885300

$3^{\text{DMAP}}$ (solvent= dichloromethane)

0 1
C  -1.10185700  1.64233600  0.99364100
F  -0.20237100  1.51337000  2.01130500
F  -2.25645900  2.11193800  1.53413800
N  -0.60838400  2.55621700  0.02802300
O  -1.42553100  3.18311000  -0.65727200
O  0.60549100  2.50994600  -0.24123800
C  -1.06185800  -0.08180400  -1.13811800
O  -1.25952600  0.69477100  -2.03556500
C  -2.11189500  -0.93744500  -0.52273500
C  -3.34697200  -0.34121400  -0.25208300
C  -1.93395900  -2.3095200  -0.34424200
C  -4.39421200  -1.11703900  0.22278800
H  -3.44761600  0.73055200  -0.39054700
DBU (DFT method=ωB97X-D)

0 1

C 2.76466900 0.00519800 0.38357500
C 1.92688300 -1.25927100 0.58815700
C 0.89700700 -1.53538100 -0.52206100
C 1.96564700 1.30784100 0.32136300
C -0.39611800 -0.76799200 -0.36185900
C 0.90044100 1.31292600 -0.78027300
H 3.32881600 -0.10038100 -0.55345800
H 2.60775900 -2.11526000 0.64324000
H 1.34881300 -1.33738800 -1.50258400
H 1.47355900 1.50197100 1.28276800
H 0.60880400 2.34215800 -1.00647500
C -2.69717500 -0.70740700 0.04548300
C -3.39985500 -1.32843800 0.61083500
C -1.45297700 1.43415600 -0.02692400
C -2.46465500 0.61947800 0.76297900
H -2.07211100 0.41796900 1.76591000
H -3.39316900 1.18609900 0.87482700
H -1.07392100 2.26149800 0.58477200
N -0.32303400 0.60306400 -0.43244600
N -1.46303800 -1.45547600 -0.13636200
H 1.32195100 0.90768600 -1.70792500
H 2.65883400 2.13814100 0.14421100
H 3.50829400 0.07605000 1.18513000
H 1.40603900 -1.21394800 1.55274200
H 0.60980200 -2.58744900 -0.50881800
H -3.16648200 -0.51597800 -0.93184000
H -1.92696700 1.87687600 -0.91432000
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -1.30679700| -0.48462100| 0.00044000 |
| F       | -1.21619600| -1.24916700| -1.08661600|
| F       | -1.21557500| -1.24675900| 1.08909700 |
| N       | -2.70932000| 0.14398000  | 0.00088000 |
| O       | -3.18992000| 0.37604800  | 1.08764100 |
| C       | -1.17525500| 0.28925200  | -0.00057200|
| C       | 1.62137500 | -1.03906700| -0.00057200|
| C       | 2.10487400 | 1.33807000  | 0.00024100 |
| C       | 2.98394300 | -1.30768800| -0.00052200|
| H       | 0.92230300 | -1.86597400| -0.00171000|
| C       | 3.46335000 | 1.06222000  | 0.00074000 |
| C       | 3.90284300 | -0.26136000| 0.00035500 |
| H       | 3.32916900 | -2.33557900| -0.00087600|
| H       | 4.18155800 | 1.87458600  | 0.00143400 |
| H       | 4.96628100 | -0.47684200| 0.00074900 |

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 1.63319000 | -1.55777600| -0.09002700|
| F       | 0.80813000 | -2.59279700| -0.22020900|
| F       | 2.26617700 | -1.65401500| 1.09330100 |
| N       | 2.73935700 | -1.75132600| -1.14535300|
| O       | 3.71630200 | -1.04033800| -1.00750500|
| O       | 2.55561200 | -2.57366000| -2.01512700|
| C       | 0.94052900 | -0.19379100| -0.42997200|
| O       | 0.58653000 | -0.18910300| -1.62846800|
| C       | 1.64371200 | 1.02872000  | 0.15254700 |
| C       | 2.11480500 | 1.96845800  | -0.76197200|
| C       | 1.84285900 | 1.24470100  | 1.51734100 |
| C       | 2.77004300 | 3.11574100  | -0.32390700|
| H       | 1.95061600 | 1.78297300  | -1.81785400|
| C       | 2.50179500 | 2.38703700  | 1.95633900 |
| H       | 1.47586700 | 0.52855200  | 2.24396900 |
| C       | 2.96656800 | 3.32654200  | 1.03707400 |
| H       | 3.12860700 | 3.84221300  | -1.04625500|
| H       | 2.64959700 | 2.54833800  | 3.01948700 |
| H       | 3.47745500 | 4.21931900  | 1.38367400 |
| C       | -3.91615000| 1.19143100  | -1.95107500|
| C       | -2.40728600| 0.95384100  | -2.01848800|
| C       | -1.64334400| 1.34925600  | -0.74202300|
| C       | -4.63364700| 0.42818400  | -0.83726200|
| C       | -1.65506800| 0.27645200  | 0.31723000 |
| C       | -4.07407500| 0.71902900  | 0.55739500 |
| H       | -4.09549100| 2.26558600  | -1.80711600|
| H       | -1.99654500| 1.53983000  | -2.84565800|
| H       | -2.07487000| 2.25840600  | -0.30632000|
| H       | -4.57799300| -0.65283600 | -1.01670800|
| H       | -4.80211800| 0.43279700  | 1.31971600 |
C   -0.64185900  -1.18678600  1.86113700
H    0.27919200  -1.74786600  1.98202600
C    -3.08145100  -1.24432000  1.65758900
C    -1.83954900  -2.11212900  1.70720900
H    -1.72328000  -2.68460000  0.78326200
H    -1.91107400  -2.81664400  2.53867800
H    -3.91851100  -1.78427000  1.20199900
N    -2.85127800  -0.02484900  0.87262000
N    -0.54663000  -0.31418600  0.69402500
H    -3.90083800  -1.79143800  0.68855800
H    -5.69569600  -0.84525300  0.16752200
H    -4.36651800  -2.91402500  -0.84523000
H    -2.18822100  -2.24921100  -0.09363600
H    -0.61431700  -2.76008700  2.76861800
H    -0.76191800  -0.56647200  2.76008700
H    -3.38710300  -0.95064800  2.66861800

2 (DFT method=ωB97X-D)

0 1
C    1.59594800  -1.56773700  -0.08032200
F    0.79238200  -2.62846700  -0.16752200
F    2.32005400  -1.68199400  1.05501200
N    2.62860900  -1.71204400  -1.21081500
O    3.59391300  -0.97662600  -1.13147300
O    2.42163900  -2.54383400  -2.06678100
O    0.82700200  -0.21619700  -0.35238700
O    0.51506600  -0.21389600  -1.59094300
C    1.61427400  1.00021900  0.17934800
C    2.06654900  1.91562600  -0.76664400
C    1.88204700  1.23244300  1.52974600
C    2.76479000  3.05467300  -0.37665700
H    1.85026900  1.70854400  -1.80903900
C    2.58338900  2.36743800  1.92337900
H    1.54834900  0.53085200  2.28676800
C    3.02525700  3.28384000  0.97115200
H    3.10801800  3.76189200  -1.12544400
H    2.78323200  2.53833700  2.97670900
H    3.57013800  4.17045500  1.28014400
C    -3.96759400  1.13891000  -1.92560100
C    -2.46229000  0.90467000  -2.04974800
C    -1.65069800  1.32948000  -0.81312200
C    -4.63271400  0.40322400  -0.76216100
C    -1.61997700  0.28113800  0.26802400
C    -4.01859000  0.73524400  0.59962100
H    -4.14648200  2.21562500  -1.80240700
H    -2.08612000  1.47686200  -2.90229200
H    -2.07203500  2.24146600  -0.37346800
H    -4.58055700  -0.68203500  -0.91353700
H    -4.71285400  0.46707800  1.39831200
C    -0.53435000  -1.08461500  1.87425900
H    -0.39545600  -1.62614200  2.00550900
C    -2.97482800  -1.16481900  1.76173400
C    -1.72863900  -2.02294400  1.83516200
H    -1.64122100  -2.67187500  0.96057700
H    -1.76547000  -2.65274000  2.72638200
H    -3.82326700  -1.73552400  1.37129400

S62
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| N    | -2.77970900 | 0.00008000 | 0.88605000 |
| N    | -0.49544100  | -0.31039900 | 0.63244100 |
| H    | -3.84094700  | 1.81035200  | 0.69557900  |
| H    | -5.69491300  | 0.66709000  | -0.72931400 |
| H    | -4.45723000  | 0.84849900  | -2.86078700 |
| H    | -2.24380800  | -0.14512600 | -2.26749600 |
| H    | -0.63317500  | 1.54318600  | -1.11397100 |
| H    | -0.62859100  | -0.38916900 | 2.71816200  |
| H    | -3.24934800  | -0.79565600 | 2.75605300  |

α-methyl DBU

0 1
C   -3.09552700 -0.09492800  0.17352000
C   -2.21628500 -1.28789800  0.55213300
C   -1.06980800 -1.57827100 -0.43309900
C   -2.36676700  1.24708400  0.11482200
C    0.16292600 -0.73954000 -0.17874100
C   -1.18281400  1.24229100 -0.85638100
H   -3.54143800 -0.29086700 -0.81163200
H   -2.85145100 -2.17780000  0.60999100
H   -1.42432800 -1.44812200 -1.46369100
H   -1.99796500  1.52707700  1.11018400
H   -0.91034700  2.26953300 -1.11576500
C    2.40797700 -0.52285400  0.44081100
C    3.05204500 -1.07234300  1.13824000
C    1.03422300  1.54056000  0.19090200
H    1.52757500  0.58780300  2.05361900
H    2.88264400  1.43303400  1.29040600
H    0.52970800  2.33946000  0.74865200
N    0.02290000  0.62205400 -0.32178100
N    1.23203900 -1.35312200  0.19435500
H   -1.47181500  0.75669600 -1.79615800
H   -3.07505400  2.02387400 -0.19477600
H   -3.92796300 -0.02331300  0.88195500
H   -1.79251900 -1.14114700  1.55381000
H   -0.73966800 -2.61266900 -0.33203400
H    1.56260400  2.01864500 -0.64621600
C    3.19020900 -0.31906600 -0.85917400
H    4.08865300  0.28256300 -0.68702000
H    3.49064000 -1.28519500 -1.27161600
H    2.57156700  0.18475900 -1.60850900

α-fluoro DBU

0 1
C   -3.08891500 -0.08655000  0.20509600
C   -2.20516000 -1.28924400  0.54042000
C   -1.07421100 -1.55204800 -0.47078400
C   -2.36134300  1.25706500  0.17972200
C    0.16214900 -0.72321800 -0.21068300
C   -1.17940000  1.28210600 -0.79133500
H   -3.54399200 -0.25433800 -0.78075300
H   -2.83817400 -2.18115600  0.58032800
H   -1.44090900 -1.38445600 -1.49136800
H   -1.99134900  1.51328200  1.18053000
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -0.896843 | 2.315530  | -1.007752 |
| C    | 2.402964  | -0.569070 | 0.384005  |
| H    | 3.106937  | -1.154726 | 0.983329  |
| C    | 1.128395  | 1.503734  | 0.104521  |
| C    | 2.075217  | 0.764104  | 1.032383  |
| H    | 1.600420  | 0.579591  | 2.000942  |
| H    | 2.983050  | 1.349400  | 1.195350  |
| H    | 0.716067  | 2.389431  | 0.597511  |
| N    | -0.272136 | 0.630104  | -0.020729 |
| H    | 1.467747  | -0.834470 | -1.749997 |
| H    | 3.069672  | 2.040422  | -0.111688 |
| H    | 3.914232  | -0.035755 | 0.923275  |
| H    | 1.768438  | -1.170880 | 1.539645  |
| H    | 0.744852  | -2.589449 | -0.409644 |
| H    | 1.666824  | 1.833361  | -0.818849 |
| H    | 1.230785  | -0.065548 | -0.022681 |
| C    | 2.434686  | -1.270198 | 0.427544  |
| C    | 1.248436  | 1.256236  | -0.859682 |
| H    | 3.182020  | -0.251473 | -1.045571 |
| H    | 3.081053  | -2.153330 | 0.424603  |
| H    | 1.466680  | -1.432403 | -1.512830 |
| H    | 2.242294  | 1.539904  | 1.023498  |
| H    | 0.933267  | 2.279718  | -1.080648 |
| C    | 2.181588  | -0.567838 | 0.712342  |
| H    | 2.814218  | -1.140920 | 1.397503  |
| C    | 0.868367  | 1.509530  | 0.394674  |
| C    | 1.753632  | 0.751735  | 1.367968  |
| H    | 1.193862  | 0.492905  | 2.271202  |
| H    | 2.613472  | 1.360752  | 1.654844  |
| H    | 0.327354  | 2.304557  | 0.920285  |
| N    | -0.108558 | 0.609064  | -0.214761 |
| H    | 1.035355  | -1.390455 | 0.347305  |
| H    | -1.447218 | 0.780149  | -1.826196 |
| H    | -3.183208 | 2.055018  | -0.375062 |
| H    | -4.155588 | 0.010683  | 0.606937  |
| H    | -2.100681 | -1.132195 | 1.463810  |
| H    | -0.901811 | -2.611086 | -0.332159 |
| H    | 1.473846  | 1.984190  | -0.388968 |
| C    | 3.005677  | -0.283060 | -0.486262 |
| N    | 3.627818  | -0.041843 | -1.430672 |

**α-cyano DBU**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| 0    | -3.262785 | -0.065548 | -0.022681 |
| C    | -2.434686 | -1.270198 | 0.427544  |
| C    | -1.210602 | -1.572574 | -0.455180 |
| C    | -2.517102 | 1.268493  | -0.003952 |
| C    | 0.001837  | -0.746820 | -0.093830 |
| C    | -1.248436 | 1.256236  | -0.859682 |
| H    | -3.618202 | -0.251473 | -1.045571 |
| H    | -3.081053 | -2.153330 | 0.424603  |
| H    | -1.466680 | -1.432403 | -1.512830 |
| H    | -2.242294 | 1.539904  | 1.023498  |
| H    | -0.933267 | 2.279718  | -1.080648 |
| C    | 2.181588  | -0.567838 | 0.712342  |
| H    | 2.814218  | -1.140920 | 1.397503  |
| C    | 0.868367  | 1.509530  | 0.394674  |
| C    | 1.753632  | 0.751735  | 1.367968  |
| H    | 1.193862  | 0.492905  | 2.271202  |
| H    | 2.613472  | 1.360752  | 1.654844  |
| H    | 0.327354  | 2.304557  | 0.920285  |
| N    | -0.108558 | 0.609064  | -0.214761 |
| H    | 1.035355  | -1.390455 | 0.347305  |
| H    | -1.447218 | 0.780149  | -1.826196 |
| H    | -3.183208 | 2.055018  | -0.375062 |
| H    | -4.155588 | 0.010683  | 0.606937  |
| H    | -2.100681 | -1.132195 | 1.463810  |
| H    | -0.901811 | -2.611086 | -0.332159 |
| H    | 1.473846  | 1.984190  | -0.388968 |
| C    | 3.005677  | -0.283060 | -0.486262 |
| N    | 3.627818  | -0.041843 | -1.430672 |

**α-methoxy DBU**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| 0    | -3.462964 | -0.023069 | 0.056001  |
| C    | -2.634381 | -1.247271 | 0.449507  |
| C    | -1.449122 | -1.545780 | -0.486077 |
| C    | -2.701415 | 1.301755  | 0.078621  |
0 1
C -0.93328000 1.33972800 1.31984400
F -0.92662200 0.83930800 2.58740300
F -1.92083300 2.26255400 1.28346600
N 0.32672100 2.01306400 1.06517200
O 0.31378300 2.99402300 0.33397700
O 1.36820100 1.42130100 1.39262100
C -0.87445200 0.14777600 -0.69277700
O -0.48983300 1.04932700 -1.42062700
C -2.34051000 -0.20855200 -0.67915000
C -3.21363200 0.87647000 0.82986000
C -2.86523900 -1.50045100 -0.67774400
C -4.58275000 0.67289100 -0.92278800
H -2.79359800 1.87413800 -0.86582900
C -4.24097900 -1.70468200 -0.77994600
H -2.21528000 -2.36208000 -0.62265700
C -5.10379200 -0.62103100 -0.89209000
H -5.24708400 1.52470600 -1.02604400
H -4.63117000 -2.71724000 -0.77956400
H -6.17454300 -0.78121900 -0.96689600
C 3.96635500 1.04541600 -1.63651300
C 2.46671800 1.17279000 -1.89672600
C 1.76184400 -0.19491800 -1.99522600
C 4.31155300 0.29047300 -0.35205000
C 1.39480700 -0.75520100 -0.64535500
C 3.78660400 -1.14790500 -0.32473200
H 4.43710300 0.52841700 -2.48410400
H 2.30632300 1.69742000 -2.84269200
H 2.42722800 -0.92515500 -2.47003700
H 3.90775900 0.82170800 0.51827300
H 4.34382400 -1.74242000 0.40028000
C -0.17437500 -1.77407900 0.89016400
H -1.18107900 -1.53427300 1.23410400
C 2.23182800 -1.65175200 1.50725400
$^{3}$-fluoro

| Atom | x             | y             | z             |
|------|---------------|---------------|---------------|
| C    | 0.81386200    | -1.50803200   | 2.02316900    |
| H    | 0.66562000    | -0.50872400   | 2.41559000    |
| H    | 0.64587300    | -2.23228800   | 2.82437700    |
| N    | 2.37598000    | -1.22880200   | 0.10409800    |
| N    | 0.10826700    | -0.85751500   | -0.23911700   |
| C    | 3.90758900    | -1.63807000   | -0.23911700   |
| H    | 5.39929700    | 0.25108600    | -0.23739700   |
| H    | 4.41190200    | -2.68392800   | 1.56442500    |
| C    | -0.07530200   | -3.23303600   | 0.43154100    |
| H    | 0.95546200    | -3.48924600   | 0.17097900    |
| H    | 0.86697400    | -0.12832200   | -2.60199600   |
| C    | 3.07501300    | 1.61940300    | 1.16944800    |
| F    | 1.82470200    | 1.26249100    | 2.48526200    |
| F    | 1.91255100    | 2.54338100    | 1.09553500    |
| N    | 0.31483500    | 2.22954200    | 0.75327100    |
| O    | 0.26993100    | 3.10791200    | -0.09940800   |
| O    | 1.37064600    | 1.66300900    | 1.09075200    |
| C    | -0.87319900   | 0.11730800    | -0.77317900   |
| O    | -0.48695500   | 0.93482500    | -1.58151900   |
| C    | -2.30969900   | -0.30480300   | -0.70462200   |
| C    | -3.27228400   | 0.69828000    | -0.85306200   |
| C    | -2.69844200   | -1.64421300   | -0.65520300   |
| C    | -4.61795000   | 0.36318300    | -0.91359400   |
| H    | -2.94405300   | 1.73034300    | -0.90232300   |
| C    | -4.05074700   | -1.97467500   | -0.72396800   |
| H    | -1.95420400   | -2.42784800   | -0.56874300   |
| C    | -5.00986200   | -0.97472300   | -0.84638200   |
| H    | -5.36429200   | 1.14387100    | -1.01644700   |
| H    | -4.35063400   | -3.01679000   | -0.68652800   |
| H    | -6.06235800   | -1.23494700   | -0.89485000   |
| C    | 4.05208800    | 0.68649300    | -1.67212000   |
| C    | 2.56472400    | 0.87931200    | -1.96648500   |
| C    | 1.77863600    | -0.44672900   | -1.93181200   |
| C    | 4.35117900    | 0.02532400    | -0.32487800   |
| C    | 1.38710300    | -0.84201900   | -0.53214000   |
| C    | 3.74089900    | -1.37115500   | -0.17332000   |
| H    | 4.49646200    | 0.07131800    | -2.46655700   |
| H    | 2.44814600    | 1.30544900    | -2.96657100   |
| H    | 2.39393700    | -1.25902000   | -2.33265500   |
| H    | 3.98610000    | 0.65251000    | 0.49724600    |
| H    | 4.26035700    | -1.93521400   | 0.60159600    |
| C    | -0.26412300   | -1.39510700   | 1.14838400    |
| H    | -1.23462400   | -1.00717000   | 1.45240600    |
| C    | 2.10755200    | -1.72757600   | 1.65497800    |
| C    | 0.80467600    | -1.18063500   | 2.18925300    |
| H    | 0.88691200    | -0.11519300   | 2.39146200    |
| H    | 0.52397500    | -1.70898600   | 3.10187900    |
| H    | 2.94675500    | -1.34355700   | 2.23823700    |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| N    | 2.32790700 | -1.31750700 | 0.25766800 |
| N    | 0.09648700  | -0.77740600  | -0.11779700 |
| H    | 3.82572500  | -1.95084200  | -1.09653800 |
| H    | 5.43483200  | -0.07070600  | -0.20611400 |
| H    | 4.55563200  | 1.65715600   | -1.71050400 |
| H    | 2.10957400  | 1.58242000   | -1.26224200 |
| H    | 0.88812500  | -0.38358800  | -2.54519000 |
| H    | 2.13579700  | -2.82156700  | 1.68365600  |
| H    | -0.37103900 | -2.76387300  | 0.93146900  |

α-сито
H  -2.12261000  2.73274100  1.73716300
C   0.56002500  2.73561800  0.93931900
N   0.68076800  3.87877100  0.82115400

3α-methoxy

0 1
C  0.77147900  -1.55088200  1.40045600
F  0.75157200  -0.94997000  2.60897000
F  1.68196000  -2.54843100  1.51107700
N  -0.52877600  -2.15013600  1.16759200
O  -0.57388200  -3.19036300  0.52514800
O  -1.52983500  -1.45671000  1.41247800
N  0.68076800  -3.87877100  0.82115400
O  0.68076800  -3.87877100  0.82115400
O  0.68076800  -3.87877100  0.82115400

C  2.24412000  -0.15910200  -0.79440300
C  3.15425600  -1.21552600  -0.69255000
C  2.60999800  -1.11044900
C  4.51303800  -0.97973600  -0.85540900
H  2.77977800  -2.20881600  -0.47414600
C  4.06502400  -1.35168700  -1.27928900
H  1.98881800  1.93181500  -1.23321500
C  4.97242400  -0.30606800  -1.43987000
H  5.21730700  -1.79986900  -0.76138800
H  4.41427400  2.34931400  -1.52604700
H  6.03476700  0.48763200  -1.27216000
C  4.16255900  -0.92469200  -1.51163800
C  -2.69254400  -1.25551200  -1.77004200
C  -1.83505000  0.02023800  -2.00915900
C  -4.40270000  0.01696000  -0.32963700
C  -1.39874700  0.65112900  -0.72084200
C  -3.71516900  1.37819800  -0.47338800
H  -4.58724600  -0.46299900  -2.41368200
H  -2.61836500  -1.88221500  -2.66309700
H  -2.40987200  0.75024700  -2.56483000
H  -0.85782500  -0.44536400  0.63023000
H  -4.19205800  2.11866900  0.16963200
C  0.31231600  1.46551600  0.79143000
C  1.25021000  1.05893000  1.18134900
C  -2.04249300  1.99817400  1.24293400
C  -0.75710500  1.50810700  1.86777600
H  -0.88678800  0.51273900  2.28483300
H  -0.45195400  2.19124400  2.66379700
H  -2.89079000  1.77406300  1.89346000
H  -2.30175900  1.33630900  -0.04553100
N  -0.11335200  0.59152400  -0.30408500
H  -3.78464200  1.75919000  -1.49609100
H  -5.47776700  0.19494700  -0.22757500
H  -4.71749600  -1.85290200  -1.34451700
H  -2.26215100  -1.82660900  -0.94172400
H  -0.95862600  -0.23649900  -2.59905600
H  -2.01945100  3.07683700  1.05655700
O  0.50323200  2.75056900  0.23451700
C  1.41496900  3.54142000  0.97744500
H  1.50408400  4.49453100  0.45625400
H  1.05918900  3.72569300  1.99797300
H  2.39002500  3.05648200  1.02241200
**R1s (Model 2)**

|   | 0 1 | C   | F    | F    | N    | O    |
|---|-----|-----|------|------|------|------|
|   | 1.78551600 | -0.57713000 | 0.05490000 |
|   | 1.17162000 | -0.96225300 | 1.16839900 |
|   | 2.01444200 | -1.62558200 | -0.72742300 |
|   | 3.15315800 | -0.02785700 | 0.49329800 |
|   | 4.13813200 | -0.48957800 | -0.02447100 |
|   | 3.08784000 | 0.84149200 | 1.33423600 |
|   | 1.77776200 | 1.21573800 | -1.44029300 |
|   | -0.34429300 | 0.89443600 | -0.40067100 |
|   | -1.37803300 | -0.07786100 | -0.21214700 |
|   | 0.61118000 | 2.24383200 | -0.27741400 |
|   | -1.20609700 | -1.46765300 | -0.44524000 |
|   | -2.66626000 | 0.39084300 | 0.17451300 |
|   | -1.89153000 | 2.69473300 | 0.10041900 |
|   | 0.19147000 | 2.95506100 | -0.44318000 |
|   | -2.24447000 | -2.34406300 | -0.25354200 |
|   | -0.25673100 | -1.84752500 | -0.16914000 |
|   | -3.71821400 | -0.54211800 | 0.37029700 |
|   | -2.88932100 | 1.78398000 | 0.33559900 |
|   | -2.07431300 | 3.75717900 | 0.21416900 |
|   | -3.51249500 | -1.88194600 | 0.16914000 |
|   | -2.09367000 | -3.40239000 | -0.43825000 |
|   | -4.69220800 | -0.16902100 | 0.67325700 |
|   | -3.87741600 | 2.11727400 | 0.64007500 |
|   | -4.32080700 | -2.58982900 | 0.31718000 |

**R2s (Model 2)**

|   | 0 1 | C   | F    | F    | N    | O    |
|---|-----|-----|------|------|------|------|
|   | -0.95715200 | -0.50678000 | -0.07458200 |
|   | -2.18094900 | 0.17000300 | 0.03387600 |
|   | -3.39100000 | -0.50695500 | -0.02502800 |
|   | -3.36705300 | -1.88892800 | -0.19789900 |
|   | -2.14423200 | -2.55299100 | -0.31857800 |
|   | -0.92009600 | -1.88009300 | -0.26294500 |
|   | -4.32330800 | 0.04232800 | 0.05830700 |
|   | -4.29292400 | -2.45022800 | -0.24575800 |
|   | -2.13802000 | -3.62830600 | -0.46497800 |
|   | 0.01643100 | -2.41392000 | -0.37124000 |
|   | -1.88368800 | 1.60040400 | 0.16403100 |
|   | -2.61115400 | 2.55455900 | 0.27881400 |
|   | -0.32872200 | 1.69885100 | 0.11902400 |
|   | 0.32868100 | 2.70762700 | 0.18917900 |
|   | 0.12890600 | 0.39850400 | -0.00833900 |
|   | 1.50416900 | 0.03513700 | -0.00084000 |
|   | 1.95218800 | -0.96256400 | 0.86546600 |
|   | 2.39492000 | 0.69723800 | -0.84411100 |
|   | 3.29824800 | -1.31386000 | 0.86762500 |
|   | 1.25141100 | -1.44703000 | 1.53818100 |
|   | 3.84215900 | 0.35052500 | -0.81974000 |
|   | 2.02978000 | 1.47627700 | -1.50360400 |
|   | 4.19517000 | -0.65836500 | 0.02744300 |
|   | 3.64696900 | -2.09251900 | 1.53770200 |
H  4.43792100  0.86701500  -1.47252900
H  5.24540000  -0.93012300  0.03589100

1s (Model 2)

0 1
C  -0.79548800  2.11521900  0.37591900
F  0.22082300  2.84258100  0.83152600
F  -1.65020900  1.88049100  1.38157700
N  -1.56197600  3.02706500  -0.59849500
O  -2.67363400  2.64434100  -0.89537800
O  -1.00335400  4.02216200  -0.99312100
C  -0.31237700  0.89663000  -0.46869500
O  0.36147200  1.31702300  -1.43809900
C  4.07537800  -1.25572000  -2.15391400
C  2.69724400  -0.59519000  -2.18081700
C  1.69474800  -1.18738000  -1.73068000
C  4.80886900  -1.13265000  -0.81910500
C  1.81492600  -0.58106800  2.12939100
C  3.40240600  0.01857400  2.00797600
C  2.40012500  1.11728100  2.29922100
H  2.50789000  1.94754200  1.59621500
H  2.54912500  1.49825200  3.31166300
H  4.38977200  0.43291000  1.77534800
N  2.97560400  -0.79099400  0.85815300
N  0.82669300  0.10309300  0.73330600
H  3.56310000  -2.66217800  0.09151000
H  5.76284200  -1.66683800  -0.87928900
H  4.69734000  -0.82745600  -2.94668300
H  2.77391100  0.48237200  -2.00546500
H  0.68165900  -1.04462900  -1.52930600
H  0.92496000  -0.38358900  2.76637900
H  3.51400900  -0.64462100  2.87379000
C  -1.40679400  -0.15479800  -0.75380500
C  -2.08053100  -1.01133000  0.18050800
C  -1.72588800  -0.24042900  -2.09205100
C  -1.87496400  -0.99645800  1.58793700
C  -3.02459900  -1.95842600  -0.32769000
C  -2.67747400  -1.15982000  -2.58305600
C  -1.20106400  0.41699600  -2.77643000
C  -2.53014300  -1.86604500  2.42266600
H  -1.21008900  -0.26798900  2.01967300
C  -3.68485700  -2.84911800  0.56071100
C  -3.30719800  -2.01067200  -1.71710500
H  -2.89560400  -1.18888000  -3.64550700
C  -3.44320000  -2.81431200  1.90808200
H  -2.34915900  -1.81908200  3.49193400
H  -4.39323700  -3.55952600  0.14339100
H  -4.03339900  -2.73570100  -2.07427500
### 3s (Model 2)

| Atom | x    | y    | z    |
|------|------|------|------|
| C    | 0.42161200 | 2.46815300 | 0.25357300 |
| F    | 0.50886000 | 2.70292300 | 1.59505200 |
| F    | -0.02250400 | 3.62485100 | -0.30604900 |
| N    | 1.76299000 | 2.23210700 | -0.25807300 |
| O    | 1.99320300 | 2.54716000 | -1.41810900 |
| O    | 2.52105200 | 1.52485000 | 0.42074000 |
| C    | -0.44868400 | 0.46413600 | -0.70079100 |
| C    | 4.23816400 | -1.36783700 | -1.53942900 |
| C    | 2.91257900 | -0.74699200 | -1.97821100 |
| C    | 1.68956000 | -1.48132100 | -1.39821600 |
| C    | 4.42508500 | -1.45812700 | -0.02378400 |
| C    | 1.36036700 | -1.07030700 | 0.01640600 |
| C    | 3.35962300 | -2.30559200 | 0.67928900 |
| H    | 4.31365400 | -2.38095400 | -1.95818000 |
| H    | 2.83856600 | -0.79458300 | -3.06827900 |
| H    | 1.87811100 | -2.56027400 | -1.37498500 |
| H    | 4.41858600 | -0.45602200 | 0.42168700 |
| H    | 3.72764800 | -2.65989200 | 1.64283400 |
| C    | -0.18212300 | -0.23363500 | 1.70068500 |
| H    | -0.83811800 | 0.63252700 | 1.76429000 |
| C    | 1.98505200 | -1.20140600 | 2.40861000 |
| C    | 1.00662400 | -0.06846400 | 2.62781900 |
| H    | 1.48586900 | 0.88600600 | 2.41990800 |
| H    | 0.66034000 | -0.07849400 | 3.66536300 |
| H    | 2.97676200 | -0.92344500 | 2.77570400 |
| N    | 2.13591100 | -1.53864900 | 0.98309800 |
| N    | 0.26846100 | -0.34157100 | 0.30334900 |
| H    | 3.10774500 | -3.19593800 | 0.09564900 |
| H    | 5.40148300 | -1.90514200 | 0.18805400 |
| H    | 5.06470100 | -0.79182900 | -1.96693000 |
| H    | 2.86144400 | 0.30926100 | -1.70008600 |
| H    | 0.82192100 | -1.31562100 | -2.02507500 |
| H    | 0.31616000 | -1.13283000 | 1.94193600 |
| H    | 1.67553700 | -2.11575400 | 2.92725200 |
| C    | -1.90366600 | 0.59469300 | -0.40034600 |
| C    | -2.72912300 | -0.59488100 | -0.31870000 |
| C    | -2.52764900 | 1.82867100 | -0.32178600 |
| C    | -2.20850800 | -1.90929800 | -0.48967500 |
| C    | -4.12786800 | -0.45779300 | -0.07732700 |
| C    | -3.91890300 | 1.95317500 | -0.10098400 |
| H    | -1.92305600 | 2.72058900 | -0.42004000 |
| H    | -3.01840700 | -3.01223800 | -0.38956000 |
| H    | -1.15811400 | -2.04617400 | -0.71918500 |
| C    | -4.93792300 | -1.61993000 | 0.02682900 |
| C    | -4.69849700 | 0.83688000 | 0.03645400 |
| H    | -4.35765100 | 2.94277400 | -0.03046500 |
| H    | -4.39928700 | -2.87119800 | -0.11831300 |
| H    | -2.59687300 | -4.00245200 | -0.52923200 |
| H    | -6.00042000 | -1.49249700 | 0.21684000 |
| H    | -5.76570600 | 0.92165800 | 0.22102500 |
| H    | -5.02734600 | -3.75245200 | -0.04061200 |
**β-5s (Model 2)**

| 0   | 1     | 2     | 3     |
|-----|-------|-------|-------|
| C   | -2.01492700 | -1.02345900 | 1.77077000 |
| F   | -3.34274800  | -1.22751000  | 1.87421900  |
| F   | -1.78081600  | 0.26652400   | 2.12258800  |
| N   | -1.31013600  | -1.90097300  | 2.68906000  |
| O   | -0.19375200  | -1.51632300  | 3.06036500  |
| O   | -1.76665800  | -3.02363700  | 2.85791000  |
| C   | 2.37230000   | 0.81363900   | -1.08738400 |
| O   | 1.83717500   | 1.39089500   | -2.00442400 |
| C   | -1.16980100  | 4.13685900   | -0.22224000 |
| C   | -0.06131500  | 3.54680200   | -1.08771700 |
| C   | 1.26239400   | 3.40263900   | 1.05093700  |
| C   | -1.43550500  | 3.33547300   | 2.04930900  |
| C   | 1.33438700   | 2.20399000   | 0.59883000  |
| C   | -0.27437600  | 3.32136300   | 2.04930900  |
| H   | -0.90964600  | 5.16865400   | 0.05323100  |
| H   | 0.12715300   | 4.20001100   | -1.08771700 |
| H   | 1.41043000   | 4.28010500   | 0.32478700  |
| H   | -1.69042000  | 2.29904800   | 0.80378900  |
| H   | -0.65459200  | 3.07302700   | 3.04806000  |
| C   | 2.10934800   | -0.02392800  | 1.23055300  |
| H   | 1.19126300   | -0.60492800  | 1.08931800  |
| C   | 1.00322100   | 1.37404700   | 2.90362600  |
| C   | 2.18336600   | 0.51748300   | 2.63753700  |
| H   | 2.23010300   | -0.31360200  | 3.34470700  |
| H   | 3.14550100   | 1.08949900   | 2.75311400  |
| H   | 0.12347100   | 0.74685000   | 3.05105000  |
| N   | 0.74462100   | 2.28390600   | 1.77011900  |
| N   | 2.08163000   | 1.11260000   | 0.27694900  |
| H   | 0.21033600   | 4.30235200   | 2.12505700  |
| H   | -2.29470100  | 3.77025100   | 1.57188200  |
| H   | -2.09438400  | 4.18611400   | -0.80581100 |
| H   | -0.35491300  | 2.56747000   | -1.47004000 |
| H   | 2.10059100   | 3.35820800   | -1.00494200 |
| H   | 2.96145200   | -0.65136100  | 0.98608800  |
| H   | 1.14478300   | 2.01606200   | 3.77798900  |
| C   | -3.18652700  | -1.78673700  | -0.93923900 |
| C   | -2.27600300  | -2.69155000  | -0.37971100 |
| C   | -2.60554300  | -4.02563500  | -0.21758200 |
| C   | -3.87311700  | -4.44941100  | -0.62139500 |
| C   | -4.77587600  | -3.53842400  | -1.17350400 |
| C   | -4.45033000  | -2.18972900  | -1.34345900 |
| H   | -1.88611900  | -4.70825900  | 0.22312800  |
| H   | -4.16210600  | -5.48823800  | -0.50461500 |
| H   | -5.75729400  | -3.88286800  | -1.48397000 |
| H   | -5.15614200  | -1.48734500  | -1.77362300 |
| C   | -1.03450100  | -1.94788000  | -0.05095100 |
| O   | 0.06987300   | -2.38916100  | 0.25624400  |
| C   | -1.30926900  | -0.51692900  | -0.51961600 |
| O   | -0.55647200  | 0.44099100   | -0.47541400 |
| N   | -2.60813800  | -0.50436300  | -1.02063500 |
| C   | 3.33104100   | -0.30650400  | -1.34570100 |
| C   | 4.65392200   | -0.35970700  | -0.80493700 |
| C   | 2.88346500   | -1.27807400  | -2.21037800 |
\alpha-5s (Model 2)

[Table with atomic coordinates and bond lengths]

- C 5.18594500  0.63082800  0.06499500
- C 5.47927400 -1.46146100 -1.17024200
- C 3.70672200 -2.37147300 -2.55858900
- H 1.87818400 -1.20118900 -2.61179400
- C 6.46364200  0.52020000  0.55399800
- H 4.57528000  1.48532300  0.34013800
- C 6.79726800 -1.54333400 -0.64903600
- C 4.97484800 -2.45849100 -2.04779100
- H 3.32633400 -3.13584500 -3.22680200
- C 7.28061000 -0.57867200  0.19652400
- H 6.85447700  1.28394500  1.21840200
- H 7.41530200 -2.38960000 -0.93480000
- H 5.61829100 -3.29457300 -2.30656300
- H 8.28747700 -0.65187000  0.59209900
- C -3.31005000  0.69770700 -1.30279100
- C -2.88139200  1.51786200 -2.34445200
- C -4.40360300  1.05819500 -0.51488800
- C -3.56234500  2.70369500 -2.60638000
- H -2.02518300  1.21701600 -2.93918400
- C -5.08449700  2.24046100 -0.78987700
- H -4.69483000  0.41324600  0.30883200
- C -4.66646400  3.06334000 -1.83480100
- H -3.23194200  3.34468200 -3.41758800
- H -5.93861500  2.52231800 -0.18297800
- H -5.19927300  3.98461100 -2.04650600
β-7s (Model 2)

0 1

C  -1.11452200  -2.16793700  2.00831400
F  -1.08270000  -1.38218600  3.08802800
F  -0.42943600  -3.27771900  2.26142000
α-7s (Model 2)

0 1
C  2.65392100 -1.77143500 -1.37558400
C  2.65841200 -1.15425400 -2.55276000
F  2.27811200 -3.04134000 -1.56767200
N  4.11369900 -1.83480800 -0.91113600
O  4.29554100 -2.48007900  0.10115200
O  4.95350100 -1.23895800 -1.54777800
C  6.67072500  1.15400700 -1.03752800
C  5.59281000  3.02888800 -0.90792300
C  7.43256200 -2.83495200 -1.06769500
H  7.63848600  1.62657200 -1.16890300
H  1.86128500 -2.57886200 -0.45122500
C  5.51060400 -0.70865700 -0.70865700
H  3.41443600  2.00833600 -0.61049700
C  6.55680600 -0.21037300 -1.03614400
C  5.19895900 -2.25693500 -0.91945100
C  5.29544500 -0.84307300 -0.86997800
H  3.90335000 -3.95380500 -0.84983000
C  6.67072500  1.15400700 -1.03752800
H  5.59281000  3.02888800 -0.90792300
H  7.43256200 -2.83495200 -1.06769500
H  6.10698300 -2.83495200 -1.06769500

S77
β-9s (Model 2)

0 1
C  -0.10389500  -1.86568000  1.85083600
C  -0.21907700  -1.05328500  2.89959700
C  1.00044600  -2.59147600  1.97841300
N  -1.28682500  -2.84805700  1.95273800
O  -1.04245900  -4.02803700  1.89803900
O  -2.37539500  -2.32461300  2.07070800
C  1.31968800  0.43233100  -0.59920000
O  0.40865300  0.44366600  -1.44367200
C  -2.37469300  3.93098100  -1.31902800
C  -1.37354000  2.86166700  -1.75327800

S78
C  0.08529800  3.18094500  -1.40379500
C  -2.36031100  4.24402500  0.17788400
C  0.46893400  2.90456400  0.02959200
C  -1.00442300  4.76564600  0.66777800
H  -2.16386700  4.85878800  -1.86870300
H  -1.43869400  2.73620900  -2.83868200
H  0.30016700  3.35013300  0.76138100
H  -2.61821000  3.35013300  0.76138100
H  -1.12912000  5.33641900  1.59075900
C  1.91479000  1.97815600  1.64987200
H  2.49286300  1.06688500  1.78923400
C  0.04566100  3.38791500  2.41832500
C  0.80095400  2.09643600  2.67929700
H  0.13332100  1.24349600  2.56310400
H  1.19752100  2.10435000  3.69761100
H  -0.97592700  3.31913500  2.80867100
N  -0.05186200  3.69774200  0.98313700
N  1.35218100  1.97485700  0.30612600
H  -0.56802600  5.45221000  -0.06556900
H  -3.12058300  5.00293000  0.39061200
H  -3.38451900  3.62343200  -1.31528200
H  -1.60904800  1.88854700  -1.31528200
H  0.30518620  3.69774200  0.98313700
H  -1.61921200  -1.95990600  -1.10964100
C  -0.32650700  -2.11438300  -0.60758900
O  0.52878600  -3.08215300  -0.39061200
C  0.06875800  -3.91134800  -1.09603200
C  -3.38451900  -3.62343200  -1.31528200
H  -2.08624000  -2.76988100  -2.13405400
H  1.53254900  -3.17969600  -0.69372600
H  -0.71721200  -4.67892300  -2.52932900
H  -1.56522500  -4.39760200  -3.42641600
H  -3.08027800  -2.64241200  -2.54666500
C  -0.12117100  -1.11909100  0.50421500
O  1.08540400  -0.42490700  0.54324700
C  -1.40867300  -0.24494100  0.41340900
O  -1.63698100  0.75258100  1.05855300
N  -2.26457800  -0.87287500  -0.47627800
C  -3.66421800  -0.62142800  -0.51164100
C  -4.55274900  -1.69686800  -0.43708700
C  -4.14753800  0.68490200  -0.57148600
C  -5.92298100  -1.46093300  -0.45777200
H  -4.16714600  -2.70691400  -0.34457300
C  -5.52104700  0.90968200  -0.57520700
H  -3.45215200  1.51267500  -0.60571100
C  -6.41261000  -0.15836000  -0.52885300
H  -6.60886900  -2.29979100  -0.40293000
H  -5.89146200  1.92895500  -0.62073300
H  -7.48220500  0.02243000  -0.54026200
C  2.77765300  0.31821700  -1.07630900
C  3.90767500  -0.20945000  -0.35657400
C  2.96189600  0.80340600  -2.35242300
C  3.85676400  -0.84972900  0.92027000
C  5.19470700  -0.12383100  -0.98142500
C  4.23085800  0.86906100  -2.96256000
α-9s (Model 2)

01

C -2.31626400 1.47753600 -1.43608800
F -1.81731700 1.05440800 -2.59448000
F -2.16901800 2.79544900 -1.35526200
N -3.82778600 1.21356800 -1.47871300
O -4.43392200 1.63360500 -0.51626000
O -4.28272700 0.63071600 -2.43408700
C 0.55821900 0.52534800 0.56774000
O 0.07589900 -0.17853900 1.47243200
C 3.27773000 -3.77264800 2.14929600
C 2.22427200 -2.66564800 2.16694400
C 2.72060900 -1.31135700 1.62518500
C 3.81562700 -4.10837200 0.75892500
C 2.58350000 -1.22177800 0.12539000
C 4.40485400 -2.89573500 0.03561000
H 4.12049900 -3.46365000 2.78244900
H 1.88584500 -2.51329000 3.19593300
H 3.77130700 -1.15526300 1.89278700
H 3.02092900 -4.53211500 0.13070400
H 5.05962600 -3.22014200 -0.77635900
C 1.67780900 -0.35122200 -1.89511300
H 0.70703800 0.03868700 -2.19132300
C 3.21574800 -2.27185200 -2.02866600
C 1.88118500 -1.73211700 -2.48998600
H 1.07320900 -2.38156700 -2.14904800
H 1.84947100 -1.68815300 -3.58116800
H 3.27848600 -3.35182300 -2.20134600
N 3.38859800 -2.04221600 -0.59093300
N 1.72245300 -0.40812200 -0.43154900
H 5.02753600 -2.30476400 0.71390600
H 4.59399000 -4.87326300 0.84937000
H 2.86174300 -4.67740000 2.60456100
H 1.34214300 -2.97166000 1.59305900
H 2.14792900 -0.51280400 2.07547200
H 2.45374200 0.33899100 -2.25073500
H 4.04608800 -1.79844200 -2.56705000
C -2.93919000 -0.77803600 1.04020500
C -2.92006400 0.37939100 1.82294700
C -3.55789600 0.44179600 3.05668200
C -4.23481600 -0.68467400 3.50642700
C -4.25284800 -1.84482600 2.71975800
C -3.61395800 -1.91440200 1.48526900
H -3.51734100 1.35643500 3.63962100
H  -4.74964000  -0.67161600  4.46033900
H  -4.78452100  -2.72001400  3.08068300
H  -3.63589900  -2.82125000  0.89156100
C  -2.12071400  1.38319200  1.12415500
O  -1.79728200  2.49953700  1.44210400
C  -1.69427300  0.72768700  -0.24282600
O  -0.34702100  0.84502700  -0.51849600
N  -2.27325500  -0.61366600  -0.18267600
C  -1.69651200  -1.74736700  -0.83771400
C  -0.94381700  -2.65903800  -0.09188300
C  -1.97049100  -1.99713500  -2.18187500
C  -0.51277400  -3.84420900  -0.67928700
H  -0.71946600  -2.41350500  0.94111200
C  -1.50980300  -3.17405400  -2.77139900
H  -2.57125100  -1.29051600  -2.74511300
C  -0.80171600  -4.10802900  -2.01895200
H  0.05117200  -4.56252000  -0.09101100
H  -1.73261800  -3.37226600  -3.81475000
H  -0.46885200  -5.03465000  -2.47565600
C  1.37084700  1.77275500  0.95306900
C  1.89505500  2.75753900  0.04722800
C  1.59960000  1.91201000  2.30190100
C  1.61787800  2.80478600  -1.34931400
C  2.73254800  3.78572500  0.58164800
C  2.40144400  2.95027400  2.82626200
H  1.14375400  1.18815900  2.96886400
C  2.17905000  3.76267700  -2.15893600
H  0.91978000  2.09999900  -1.77489500
C  3.30230500  4.75666400  -0.28441900
C  2.97905700  3.85390300  1.97872000
H  2.56117200  3.01516900  3.89762800
C  3.04368000  4.74463900  -1.62954600
H  1.93580000  3.77387500  -3.21738600
H  3.94369800  5.51926600  0.14927300
H  3.61755900  4.64800500  2.35609900
H  3.48079200  5.49312500  -2.28248400