

## *Supporting Information*

# **Mechanistic Study of Manganese Porphyrin-Catalyzed C–H Isocyanation Reaction**

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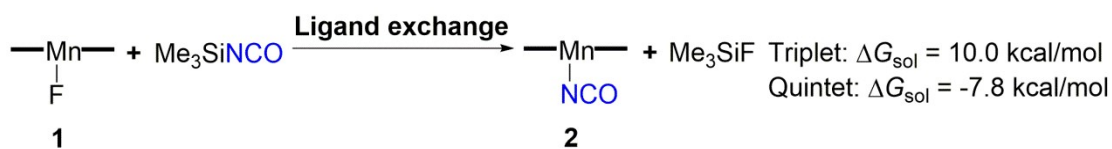
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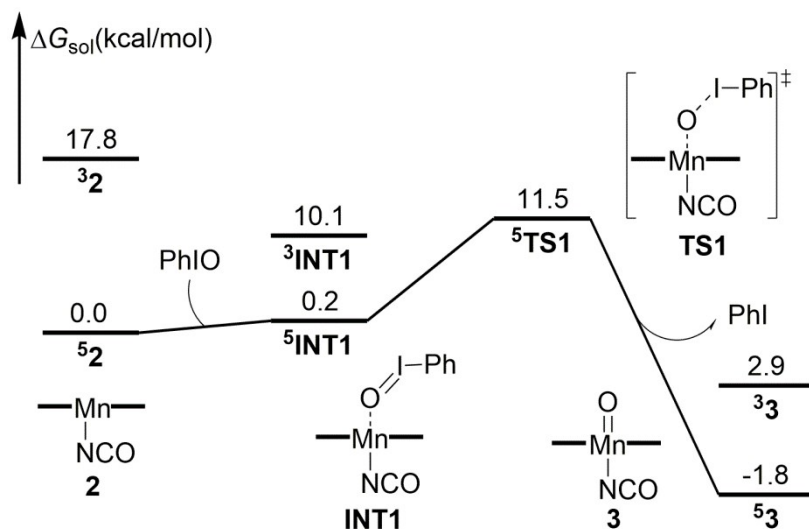
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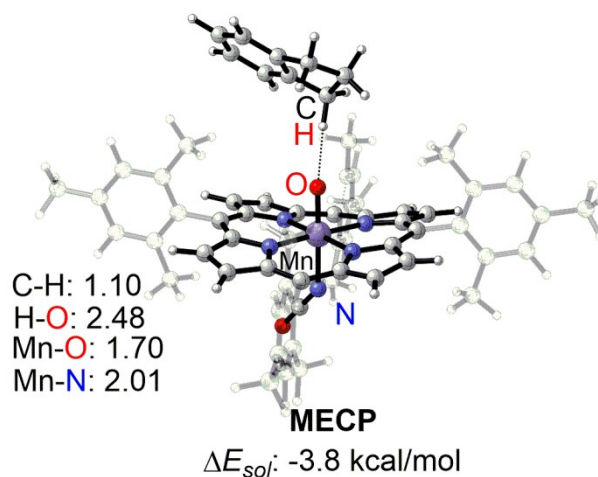
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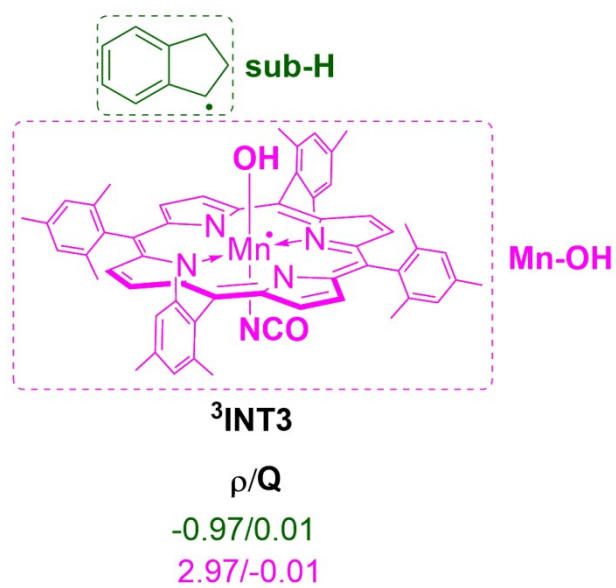
**Fig. S1.** The ligand exchange process of Mn(TMP)F **1** to provide Mn(TMP)NCO **2**.



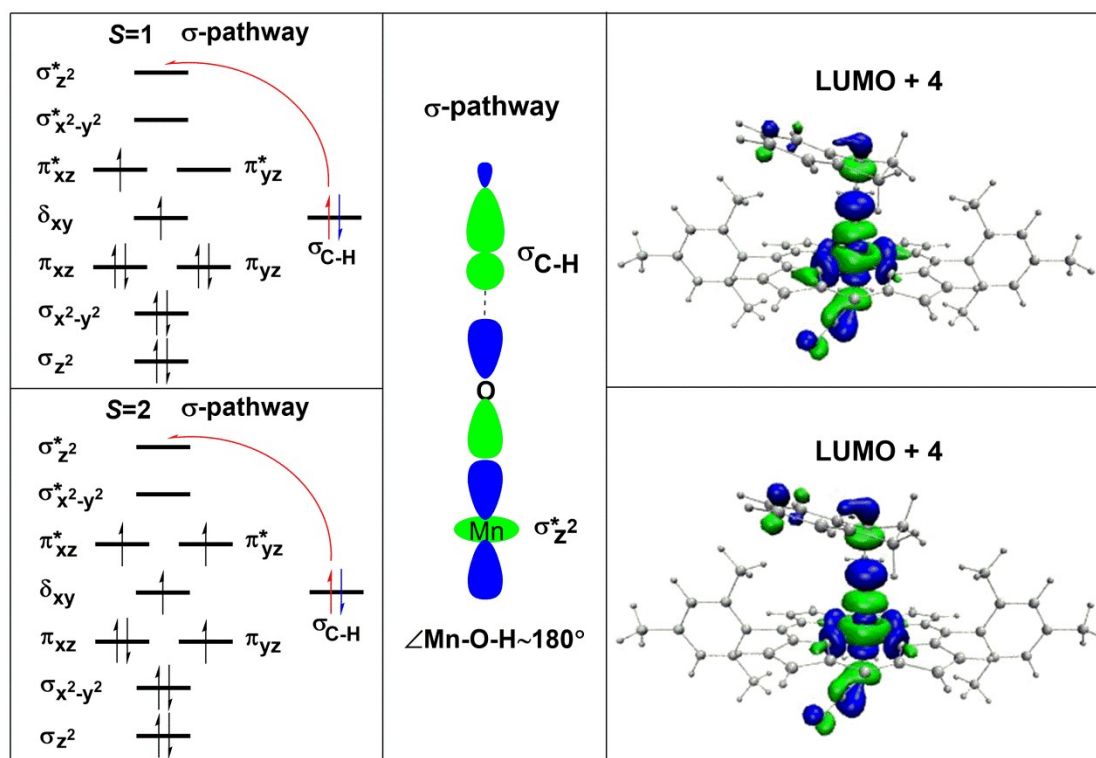
**Fig. S2.** Free energy profiles of the oxidation process with the oxidant iodobenzene (PhIO) oxidizing **2** to the high-valent metal-oxo species O=Mn(TMP)NCO **3**.



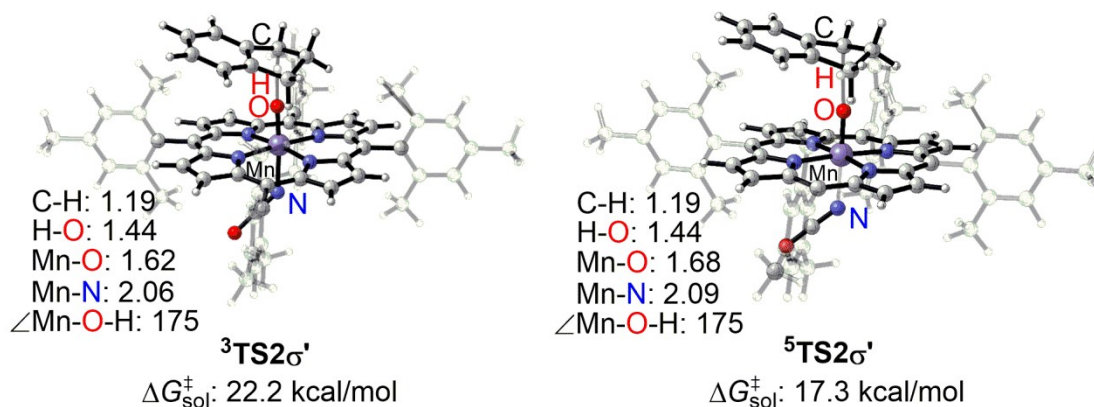
**Fig. S3.** The calculated minimum energy crossing point (MECP) structure. The distances are in Å.



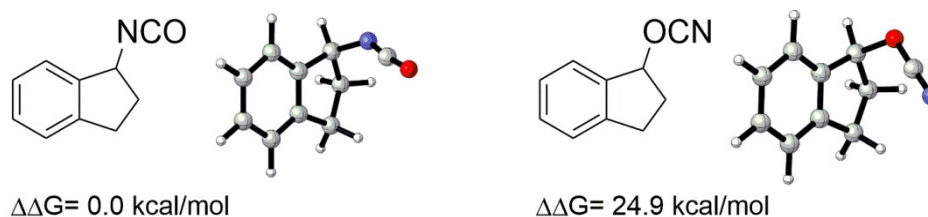
**Fig.S4.** Populations of spin densities ( $\rho$ ) and NPA charges ( $Q$  in e) for the <sup>3</sup>INT3.



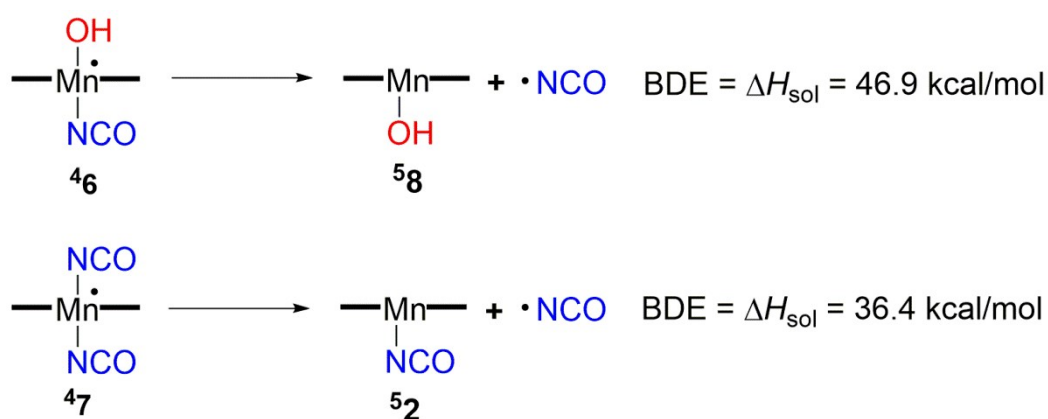
**Fig. S5.** Electron-shift diagrams of the H-abstraction process and the calculated LUMO+4 orbitals for <sup>3</sup>TS2 <sub>$\sigma$</sub>  and <sup>5</sup>TS2 <sub>$\sigma$</sub> .



**Fig. S6.** The calculated H-abstraction transition states through  $\sigma$ -pathway. The TS calculations were conducted by fixing the bonds of C-H and H-O based on the structure of  ${}^3\text{TS}2\pi$  and  ${}^5\text{TS}2\pi$  and freezing the angle of Mn-O-H to 175 degree. The distances are in Å. The angles are in degrees.



**Fig. S7.** The free energy difference between **Pro2** and **Pro3**.



$$H_{\text{sol}} = E_{\text{sol}} + \text{thermal correction to enthalpy}$$

**Fig. S8.** The BDE of Mn-NCO bond in **46** and **47**.

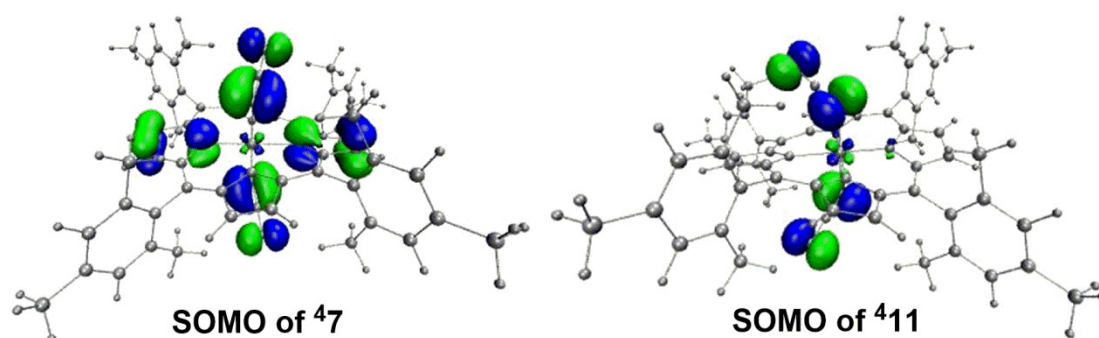


Fig. S9. Representations of the SOMOs in the intermediate <sup>47</sup> and <sup>411</sup>.

Table S1. Electronic Energies, Enthalpies, and Free Energies (in Hartree) of the Structures Calculated at the B3LYP-D3/def2-TZVP (SMD: Ethylethanoate)//B3LYP-D3/6-31G\*-LANL2DZ Level

| Structures                 | ZPVE     | TCE      | TCH      | TCG      | G            | E <sub>sol</sub> | Imaginary Frequency (cm <sup>-1</sup> ) |
|----------------------------|----------|----------|----------|----------|--------------|------------------|---|
| <sup>3</sup> <b>1</b>      | 0.934734 | 0.993121 | 0.994066 | 0.831416 | -2587.522952 | -3636.441772     | —                                       |
| <sup>5</sup> <b>1</b>      | 0.933796 | 0.993379 | 0.994323 | 0.827744 | -2587.535637 | -3636.464380     | —                                       |
| <b>Me<sub>3</sub>SiNCO</b> | 0.125465 | 0.136008 | 0.136952 | 0.088715 | -577.312402  | -577.5700169     | —                                       |
| <b>Me<sub>3</sub>SiF</b>   | 0.114379 | 0.122700 | 0.123644 | 0.082616 | -509.095950  | -509.3220739     | —                                       |
| <sup>3</sup> <b>2</b>      | 0.945968 | 1.007040 | 1.007984 | 0.841515 | -2655.751101 | -3704.704069     | —                                       |
| <sup>5</sup> <b>2</b>      | 0.945047 | 1.006542 | 1.007486 | 0.838006 | -2655.770872 | -3704.728862     | —                                       |
| <b>PhIO</b>                | 0.091972 | 0.099645 | 0.100589 | 0.056761 | -318.040153  | -604.702452      | —                                       |
| <sup>3</sup> <b>INT1</b>   | 1.039618 | 1.109309 | 1.110254 | 0.927858 | -2973.832922 | -4309.448351     | —                                       |
| <sup>5</sup> <b>INT1</b>   | 1.038037 | 1.108598 | 1.109542 | 0.923965 | -2973.837744 | -4309.460246     | —                                       |
| <sup>5</sup> <b>TS1</b>    | 1.037382 | 1.107428 | 1.108372 | 0.923908 | -2973.829967 | -4309.442052     | 380.44 i                                |
| <b>PhI</b>                 | 0.090320 | 0.096209 | 0.097153 | 0.058553 | -242.970939  | -529.548478      | —                                       |
| <sup>1</sup> <b>3</b>      | 0.946157 | 1.008819 | 1.009763 | 0.840897 | -2730.887706 | -3779.880191     | —                                       |
| <sup>3</sup> <b>3</b>      | 0.945959 | 1.008777 | 1.009721 | 0.838482 | -2730.889389 | -3779.880399     | —                                       |
| <sup>5</sup> <b>3</b>      | 0.946902 | 1.009356 | 1.010300 | 0.841352 | -2730.891222 | -3779.890836     | —                                       |
| <b>4</b>                   | 0.165222 | 0.172039 | 0.172983 | 0.134181 | -348.859571  | -349.1367411     | —                                       |
| <sup>3</sup> <b>INT2</b>   | 1.113210 | 1.184639 | 1.185583 | 0.998665 | -3079.747012 | -4129.034895     | —                                       |

|                                    |          |          |          |          |              |              |           |
|------------------------------------|----------|----------|----------|----------|--------------|--------------|-----------|
| <b><sup>5</sup>INT2</b>            | 1.112916 | 1.184322 | 1.185267 | 0.996482 | -3079.751956 | -4129.038073 | —         |
| <b>MECP</b>                        | —        | —        | —        | —        | —            | -4129.033680 | —         |
| <b><sup>1</sup>TS2<sub>π</sub></b> | 1.106400 | 1.177113 | 1.178057 | 0.994218 | -3079.736012 | -4129.006510 | 1508.28 i |
| <b><sup>3</sup>TS2<sub>π</sub></b> | 1.109983 | 1.180348 | 1.181292 | 0.997673 | -3079.746681 | -4129.034788 | 339.51 i  |
| <b><sup>5</sup>TS2<sub>π</sub></b> | 1.109098 | 1.179623 | 1.180567 | 0.995940 | -3079.740762 | -4129.026617 | 567.92 i  |
| <b><sup>3</sup>TS2<sub>σ</sub></b> | 1.109106 | 1.177448 | 1.178392 | 0.999346 | -3079.706215 | -4129.016091 | 556.01 i  |
| <b><sup>5</sup>TS2<sub>σ</sub></b> | 1.108809 | 1.177936 | 1.178880 | 0.995979 | -3079.732149 | -4129.020407 | 264.65 i  |
| <b><sup>3</sup>INT3</b>            | 1.111624 | 1.183116 | 1.184060 | 0.996829 | -3079.772184 | -4129.064535 | —         |
| <b><sup>5</sup>INT3</b>            | 1.111827 | 1.183331 | 1.184275 | 0.996096 | -3079.772673 | -4129.063375 | —         |
| <b><sup>5</sup></b>                | 0.150873 | 0.157884 | 0.158828 | 0.118683 | -348.227530  | -348.4895246 | —         |
| <b><sup>4</sup>6</b>               | 0.958293 | 1.021578 | 1.022522 | 0.851915 | -2731.544879 | -3780.561189 | —         |
| <b><sup>6</sup>6</b>               | 0.955915 | 1.019941 | 1.020885 | 0.848084 | -2731.531369 | -3780.536136 | —         |
| <b>Me<sub>3</sub>SiOH</b>          | 0.125092 | 0.134127 | 0.135071 | 0.092699 | -485.042700  | -485.2747652 | —         |
| <b><sup>4</sup>7</b>               | 0.958150 | 1.022941 | 1.023885 | 0.848446 | -2823.821741 | -3872.865971 | —         |
| <b><sup>3</sup>TS3</b>             | 1.111947 | 1.182557 | 1.183502 | 0.999549 | -3079.764535 | -4129.061115 | 72.65 i   |
| <b><sup>5</sup>TS3</b>             | 1.110468 | 1.181884 | 1.182829 | 0.994447 | -3079.769744 | -4129.060736 | 228.31 i  |
| <b><sup>3</sup>TS4</b>             | 1.111742 | 1.182666 | 1.183610 | 0.998751 | -3079.765373 | -4129.059953 | 51.81 i   |
| <b><sup>5</sup>TS4</b>             | 1.110273 | 1.181669 | 1.182614 | 0.995251 | -3079.764776 | -4129.052607 | 222.26 i  |
| <b><sup>3</sup>TS5</b>             | 1.111926 | 1.184252 | 1.185197 | 0.996290 | -3172.048032 | -4221.375172 | 50.22 i   |
| <b><sup>5</sup>TS5</b>             | 1.110625 | 1.183326 | 1.184270 | 0.994145 | -3172.043996 | -4221.366352 | 171.63 i  |
| <b><sup>3</sup>8</b>               | 0.945289 | 1.005319 | 1.006264 | 0.839375 | -2563.477971 | -3612.397486 | —         |
| <b><sup>5</sup>8</b>               | 0.943341 | 1.004072 | 1.005016 | 0.838801 | -2563.479715 | -3612.406291 | —         |
| <b>Pro1</b>                        | 0.169399 | 0.177390 | 0.178334 | 0.136759 | -424.063895  | -424.3897749 | —         |
| <b>Pro2</b>                        | 0.168879 | 0.178474 | 0.179418 | 0.132191 | -516.338879  | -516.6902832 | —         |
| <b>Pro3</b>                        | 0.168205 | 0.177796 | 0.178740 | 0.132517 | -516.297794  | -516.6509491 | —         |
| <b>•NCO</b>                        | 0.008849 | 0.011963 | 0.012907 | -0.01207 | -168.009269  | -168.0756213 | —         |
| <b><sup>4</sup>9</b>               | 0.460778 | 0.521805 | 0.522749 | 0.357405 | -4244.693454 | —            | —         |
| <b><sup>4</sup>10</b>              | 0.958324 | 1.021455 | 1.022399 | 0.853342 | -2727.650503 | -3776.660049 | —         |
| <b><sup>4</sup>11</b>              | 0.957809 | 1.022444 | 1.023388 | 0.849273 | -2816.037650 | -3865.065029 | —         |

|                  |          |          |          |          |              |              |          |
|------------------|----------|----------|----------|----------|--------------|--------------|----------|
| <sup>3</sup> TS6 | 1.111853 | 1.182422 | 1.183366 | 0.999724 | -3075.869150 | -4125.158704 | 74.39 i  |
| <sup>5</sup> TS6 | 1.110519 | 1.181810 | 1.182754 | 0.995797 | -3075.874899 | -4125.159450 | 237.33 i |
| <sup>3</sup> TS7 | 1.112035 | 1.182754 | 1.183698 | 0.999703 | -3075.869374 | -4125.157284 | 20.45 i  |
| <sup>5</sup> TS7 | 1.110001 | 1.181450 | 1.182394 | 0.995879 | -3075.871681 | -4125.155519 | 287.64 i |
| <sup>3</sup> TS8 | 1.112151 | 1.184137 | 1.185081 | 0.998681 | -3164.256789 | -4213.570559 | 27.45 i  |
| <sup>5</sup> TS8 | 1.109867 | 1.182640 | 1.183584 | 0.993025 | -3164.262576 | -4213.568091 | 89.48 i  |

ZPVE = zero-point vibrational energy; TCE = thermal correction to energy; TCH = thermal correction to enthalpy; TCG = thermal correction to Gibbs free energy; G = Gibbs free energy; E<sub>sol</sub> = Single-point solvation energy.

## Cartesian coordinates of the structures

### Structure: <sup>3</sup>1

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -2.84364900 | -1.08202600 | 0.09671500 |
| C | -4.21971100 | -0.65418000 | 0.10585800 |
| C | -4.21111500 | 0.70743300  | 0.10588800 |
| C | -2.82975200 | 1.11792300  | 0.09664000 |
| N | -2.00164300 | 0.01268000  | 0.10093900 |
| H | -5.06893300 | -1.32279300 | 0.11297800 |
| H | -5.05187500 | 1.38665000  | 0.11302800 |
| C | 1.11816100  | 2.83001200  | 0.09725600 |
| C | 0.70764000  | 4.21136400  | 0.10665100 |
| C | -0.65398300 | 4.21995200  | 0.10634400 |
| C | -1.08176700 | 2.84387700  | 0.09681100 |
| N | 0.01293000  | 2.00188900  | 0.10101400 |
| H | 1.38683100  | 5.05214000  | 0.11416800 |
| H | -1.32260100 | 5.06918800  | 0.11349000 |
| C | 1.08226500  | -2.84391900 | 0.09704400 |
| C | 0.65438700  | -4.21996700 | 0.10638300 |
| C | -0.70723600 | -4.21136000 | 0.10646100 |
| C | -1.11766300 | -2.82998300 | 0.09685600 |
| N | -0.01242700 | -2.00189500 | 0.10095300 |
| H | 1.32297200  | -5.06920700 | 0.11373400 |
| H | -1.38645800 | -5.05213400 | 0.11378400 |
| C | 2.83021000  | -1.11791900 | 0.09795300 |
| C | 4.21158700  | -0.70744300 | 0.10804500 |
| C | 4.22018100  | 0.65417900  | 0.10804700 |
| C | 2.84410400  | 1.08200900  | 0.09812100 |
| N | 2.00210600  | -0.01268900 | 0.10183100 |
| H | 5.05237300  | -1.38664700 | 0.11563000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.06942400  | 1.32278300  | 0.11565200  |
| C  | -2.45188800 | -2.42129900 | 0.08677800  |
| C  | 2.45237900  | 2.42129500  | 0.08785400  |
| C  | -2.42104900 | 2.45213700  | 0.08665400  |
| C  | 2.42154100  | -2.45214700 | 0.08754600  |
| Mn | 0.00031200  | 0.00000000  | -0.19694700 |
| F  | 0.00077300  | 0.00004500  | -1.91958800 |
| C  | -3.51836100 | -3.47397900 | 0.05747800  |
| C  | -3.99239700 | -3.94988200 | -1.18042000 |
| C  | -4.03612600 | -3.98461600 | 1.26316600  |
| C  | -4.98491400 | -4.93515500 | -1.18973400 |
| C  | -5.02782500 | -4.96926800 | 1.21043100  |
| C  | -5.51757100 | -5.45523300 | -0.00594900 |
| H  | -5.35004000 | -5.30602400 | -2.14558100 |
| H  | -5.42641600 | -5.36681700 | 2.14191900  |
| C  | -3.47397500 | 3.51836300  | 0.05717700  |
| C  | -3.94228900 | 3.99966100  | -1.18082800 |
| C  | -3.98525200 | 4.03572200  | 1.26275500  |
| C  | -4.92280100 | 4.99685100  | -1.19034700 |
| C  | -4.96498800 | 5.03229500  | 1.20981500  |
| C  | -5.44887800 | 5.52382400  | -0.00665600 |
| H  | -5.28328500 | 5.37205800  | -2.14626600 |
| H  | -5.35842600 | 5.43513400  | 2.14121900  |
| C  | 3.51862400  | 3.47421300  | 0.05896200  |
| C  | 4.03572300  | 3.98501000  | 1.26468600  |
| C  | 4.00019800  | 3.94297600  | -1.17892700 |
| C  | 5.03243200  | 4.96483400  | 1.21223900  |
| C  | 4.99736100  | 4.92331500  | -1.18794200 |
| C  | 5.52418700  | 5.44902300  | -0.00385700 |
| H  | 5.43501800  | 5.35796900  | 2.14385600  |
| H  | 5.37286100  | 5.28408400  | -2.14366100 |
| C  | 3.47423600  | -3.51860800 | 0.05851900  |
| C  | 3.95041200  | -3.99272500 | -1.17944200 |
| C  | 3.98461200  | -4.03625100 | 1.26416100  |
| C  | 4.93565200  | -4.98502900 | -1.18856400 |
| C  | 4.96940800  | -5.02805800 | 1.21160700  |
| C  | 5.45559400  | -5.51770300 | -0.00452300 |
| H  | 5.30683500  | -5.35014100 | -2.14432300 |
| H  | 5.36668400  | -5.42664300 | 2.14318600  |
| C  | 3.40671100  | -3.43264900 | -2.47372800 |
| H  | 2.32273900  | -3.58091300 | -2.54595000 |
| H  | 3.57745800  | -2.35163700 | -2.54129000 |
| H  | 3.87614100  | -3.90848500 | -3.34019000 |
| C  | 3.47776500  | -3.52281800 | 2.59235800  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.65036500  | -2.44439800 | 2.69196000  |
| H | 2.39665200  | -3.67836100 | 2.69033100  |
| H | 3.97268500  | -4.02681500 | 3.42820600  |
| C | 6.49452900  | -6.61462400 | -0.04009000 |
| H | 6.02209400  | -7.60512800 | -0.08649500 |
| H | 7.14392900  | -6.52422800 | -0.91783700 |
| H | 7.12767000  | -6.59814100 | 0.85372800  |
| C | 3.44907400  | 3.39036300  | -2.47328000 |
| H | 3.60290800  | 2.30678800  | -2.53995300 |
| H | 2.36758900  | 3.55555200  | -2.54651200 |
| H | 3.92658000  | 3.85821200  | -3.33967800 |
| C | 3.52270100  | 3.47758400  | 2.59282000  |
| H | 2.44403800  | 3.64889400  | 2.69184000  |
| H | 3.67952400  | 2.39668200  | 2.69126100  |
| H | 4.02563600  | 3.97348100  | 3.42872800  |
| C | 6.57690300  | 6.53271400  | -0.03919000 |
| H | 6.11696700  | 7.52925600  | -0.08173000 |
| H | 7.21203600  | 6.50580800  | 0.85297500  |
| H | 7.22288700  | 6.43639600  | -0.91881600 |
| C | -3.38922300 | 3.44848200  | -2.47496800 |
| H | -2.30574600 | 3.60304400  | -2.54161500 |
| H | -3.55366000 | 2.36686500  | -2.54787700 |
| H | -3.85732200 | 3.92540200  | -3.34155400 |
| C | -3.47824600 | 3.52281700  | 2.59109400  |
| H | -3.65049900 | 2.44433800  | 2.69054100  |
| H | -2.39721000 | 3.67871600  | 2.68945500  |
| H | -3.97370900 | 4.02651100  | 3.42680400  |
| C | -6.53276200 | 6.57635400  | -0.04146000 |
| H | -6.45517900 | 7.20335000  | -0.93644200 |
| H | -7.53013800 | 6.11636800  | -0.05216000 |
| H | -6.48656300 | 7.23035900  | 0.83626500  |
| C | -3.43229700 | -3.40614200 | -2.47468200 |
| H | -3.57984600 | -2.32205200 | -2.54654100 |
| H | -2.35141500 | -3.57760400 | -2.54257600 |
| H | -3.90865500 | -3.87499300 | -3.34117200 |
| C | -3.52266400 | -3.47787200 | 2.59138800  |
| H | -2.44406100 | -3.64954800 | 2.69053500  |
| H | -3.67911800 | -2.39692800 | 2.68983400  |
| H | -4.02595100 | -3.97355500 | 3.42721400  |
| C | -6.61472400 | -6.49395400 | -0.04040700 |
| H | -7.60626200 | -6.02145000 | -0.04772900 |
| H | -6.54714900 | -7.12001600 | -0.93684100 |
| H | -6.57471900 | -7.15031000 | 0.83587400  |

**Structure: 51**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.82971000 | -1.13582600 | 0.08894400  |
| C  | -4.21208500 | -0.72931300 | 0.11317400  |
| C  | -4.22766200 | 0.63265800  | 0.11543400  |
| C  | -2.85497200 | 1.07076700  | 0.09242500  |
| N  | -2.01608800 | -0.02306300 | 0.08320000  |
| H  | -5.04906000 | -1.41292300 | 0.12964100  |
| H  | -5.07987400 | 1.29708900  | 0.13404000  |
| C  | 1.07064700  | 2.85507000  | 0.09106400  |
| C  | 0.63267500  | 4.22775300  | 0.11789100  |
| C  | -0.72930200 | 4.21214600  | 0.12037900  |
| C  | -1.13587900 | 2.82978100  | 0.09466500  |
| N  | -0.02315300 | 2.01621900  | 0.08407700  |
| H  | 1.29716900  | 5.07995500  | 0.13562800  |
| H  | -1.41284400 | 5.04909400  | 0.14060400  |
| C  | 1.13572000  | -2.82966100 | 0.09256600  |
| C  | 0.72920400  | -4.21205000 | 0.11737700  |
| C  | -0.63276700 | -4.22768300 | 0.11498000  |
| C  | -1.07081100 | -2.85500600 | 0.08946600  |
| N  | 0.02298200  | -2.01611500 | 0.08282600  |
| H  | 1.41278000  | -5.04898800 | 0.13683700  |
| H  | -1.29724700 | -5.07988900 | 0.13218900  |
| C  | 2.85481400  | -1.07064800 | 0.09054500  |
| C  | 4.22752700  | -0.63260100 | 0.11270400  |
| C  | 4.21197700  | 0.72936200  | 0.11083400  |
| C  | 2.82960700  | 1.13595600  | 0.08794800  |
| N  | 2.01594500  | 0.02320500  | 0.08239200  |
| H  | 5.07973200  | -1.29706600 | 0.13039400  |
| H  | 5.04896800  | 1.41293700  | 0.12692400  |
| C  | -2.41274500 | -2.46851800 | 0.07986300  |
| C  | 2.41259700  | 2.46863700  | 0.08019700  |
| C  | -2.46855300 | 2.41275000  | 0.08671100  |
| C  | 2.46838700  | -2.41262200 | 0.08442800  |
| Mn | -0.00015500 | 0.00015900  | -0.23008600 |
| F  | -0.00051300 | 0.00069300  | -2.07012800 |
| C  | 3.54026700  | -3.45967900 | 0.06541400  |
| C  | 4.05916000  | -3.95866100 | 1.27526600  |
| C  | 4.01805900  | -3.94151500 | -1.16922700 |
| C  | 5.05651500  | -4.93832400 | 1.23057700  |
| C  | 5.01579300  | -4.92125800 | -1.17007900 |
| C  | 5.55002400  | -5.42998200 | 0.01824800  |
| H  | 5.45623800  | -5.32710000 | 2.16522000  |
| H  | 5.38402400  | -5.29714100 | -2.12277800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.45977700  | 3.54030000  | 0.05683000  |
| C | 3.92209100  | 4.03175300  | -1.17991300 |
| C | 3.97096500  | 4.05254700  | 1.26442200  |
| C | 4.89711500  | 5.03407500  | -1.18511100 |
| C | 4.94541300  | 5.05480500  | 1.21537000  |
| C | 5.42338900  | 5.55636600  | 0.00087700  |
| H | 5.25337500  | 5.41733400  | -2.13942200 |
| H | 5.33910800  | 5.45380600  | 2.14826000  |
| C | -3.54043300 | 3.45981600  | 0.06843000  |
| C | -4.01889700 | 3.94176500  | -1.16592400 |
| C | -4.05864200 | 3.95869700  | 1.27859900  |
| C | -5.01659000 | 4.92152500  | -1.16614900 |
| C | -5.05601100 | 4.93839500  | 1.23453100  |
| C | -5.55015800 | 5.43016900  | 0.02252700  |
| H | -5.38533300 | 5.29750700  | -2.11861300 |
| H | -5.45523900 | 5.32706700  | 2.16942400  |
| C | -3.45977800 | -3.54032700 | 0.05669500  |
| C | -3.96451500 | -4.05859600 | 1.26446600  |
| C | -3.93577100 | -4.01869100 | -1.17995100 |
| C | -4.94401300 | -5.05587800 | 1.21563400  |
| C | -4.91566500 | -5.01630700 | -1.18493500 |
| C | -5.43003400 | -5.54990200 | 0.00120500  |
| H | -5.33718700 | -5.45517800 | 2.14862100  |
| H | -5.28711800 | -5.38491400 | -2.13921900 |
| C | 3.36792500  | 3.48624000  | -2.47595900 |
| H | 3.52933100  | 2.40462900  | -2.55378900 |
| H | 2.28465400  | 3.64214800  | -2.54242900 |
| H | 3.83663500  | 3.96589600  | -3.34066000 |
| C | 3.46953100  | 3.52936900  | 2.59093200  |
| H | 2.38795500  | 3.67940700  | 2.69286500  |
| H | 3.64700700  | 2.45119900  | 2.68428400  |
| H | 3.96438400  | 4.03074500  | 3.42836800  |
| C | 6.50115700  | 6.61523200  | -0.03183200 |
| H | 7.49891600  | 6.16141900  | -0.10199200 |
| H | 6.38590800  | 7.27852100  | -0.89621100 |
| H | 6.48708300  | 7.23177700  | 0.87349000  |
| C | -6.65273100 | 6.46332000  | -0.00466300 |
| H | -6.55463600 | 7.13259400  | -0.86657100 |
| H | -7.63948600 | 5.98613200  | -0.07540000 |
| H | -6.65214200 | 7.07646100  | 0.90306100  |
| C | -3.45818700 | 3.40969800  | -2.46473500 |
| H | -2.37803800 | 3.58484600  | -2.53343400 |
| H | -3.60073500 | 2.32557300  | -2.54493800 |
| H | -3.93758900 | 3.88304100  | -3.32704800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.54093000 | 3.44488000  | 2.60251100  |
| H | -3.69732600 | 2.36344200  | 2.69611200  |
| H | -2.46198800 | 3.61552000  | 2.69953200  |
| H | -4.04153400 | 3.93620400  | 3.44248300  |
| C | -3.39737700 | -3.45804900 | -2.47618800 |
| H | -3.56993100 | -2.37748300 | -2.54475200 |
| H | -2.31323700 | -3.60282700 | -2.55219800 |
| H | -3.86825300 | -3.93581700 | -3.34075700 |
| C | -3.45704400 | -3.54096800 | 2.59085500  |
| H | -2.37567300 | -3.69521200 | 2.68861700  |
| H | -3.63030800 | -2.46246100 | 2.68813700  |
| H | -3.95070000 | -4.04329200 | 3.42842900  |
| C | -6.46306300 | -6.65246400 | -0.03070400 |
| H | -7.12176400 | -6.56043700 | -0.90134100 |
| H | -5.98530000 | -7.63979900 | -0.08835800 |
| H | -7.08719000 | -6.64529000 | 0.86950800  |
| C | 3.45660800  | -3.40938100 | -2.46768900 |
| H | 2.37649300  | -3.58491600 | -2.53596300 |
| H | 3.59872200  | -2.32518600 | -2.54772100 |
| H | 3.93581500  | -3.88237200 | -3.33030500 |
| C | 3.54219800  | -3.44491600 | 2.59950100  |
| H | 3.69930200  | -2.36359500 | 2.69335200  |
| H | 2.46318600  | -3.61489000 | 2.69683400  |
| H | 4.04279100  | -3.93677400 | 3.43916700  |
| C | 6.65264500  | -6.46306700 | -0.00951400 |
| H | 6.55609800  | -7.13024500 | -0.87320700 |
| H | 7.63953000  | -5.98570900 | -0.07726900 |
| H | 6.65045200  | -7.07840600 | 0.89673100  |

**Structure: Me<sub>3</sub>SiNCO**

|    |            |             |             |
|----|------------|-------------|-------------|
| Si | 0.74473700 | 0.00009400  | 0.00049100  |
| C  | 1.31835500 | 1.62592600  | 0.75400100  |
| H  | 2.41404300 | 1.67801800  | 0.77763700  |
| H  | 0.95419800 | 2.48125100  | 0.17344700  |
| H  | 0.95459700 | 1.73711000  | 1.78185700  |
| C  | 1.31577600 | -0.15835500 | -1.78523300 |
| H  | 0.95187300 | -1.08865100 | -2.23623500 |
| H  | 0.95002300 | 0.67657800  | -2.39382000 |
| H  | 2.41128600 | -0.16250000 | -1.84378500 |
| C  | 1.32013500 | -1.46687500 | 1.02847300  |
| H  | 0.95675200 | -1.39551400 | 2.06000700  |
| H  | 0.95679300 | -2.41154200 | 0.60796300  |
| H  | 2.41587800 | -1.51274200 | 1.06043400  |

|   |             |             |            |
|---|-------------|-------------|------------|
| N | -0.99467800 | -0.00060900 | 0.00217700 |
| C | -2.19269000 | -0.00037000 | 0.00101300 |
| O | -3.37480900 | -0.00012600 | 0.00010800 |

**Structure: Me<sub>3</sub>SiF**

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -0.00016600 | -0.00026800 | 0.03502100  |
| C  | -1.73008200 | -0.45851700 | -0.53329000 |
| H  | -1.78857200 | -0.47512700 | -1.62898000 |
| H  | -2.01944300 | -1.45103100 | -0.16876800 |
| H  | -2.47202900 | 0.26226500  | -0.17049600 |
| C  | 1.26258200  | -1.26895400 | -0.53220800 |
| H  | 2.26640500  | -1.02160100 | -0.16768800 |
| H  | 1.01062100  | -2.27190900 | -0.16858300 |
| H  | 1.30665800  | -1.31232200 | -1.62786000 |
| C  | 0.46829400  | 1.72727800  | -0.53293500 |
| H  | -0.24799200 | 2.47354600  | -0.17004200 |
| H  | 1.46236600  | 2.01036300  | -0.16776700 |
| H  | 0.48584900  | 1.78659100  | -1.62862400 |
| F  | -0.00070000 | 0.00046000  | 1.66656900  |

**Structure: <sup>32</sup>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.15158200  | 2.83977000  | -0.22074300 |
| C | 0.72853000  | 4.21706700  | -0.21585100 |
| C | -0.63282200 | 4.21347400  | -0.24556600 |
| C | -1.04748900 | 2.83414500  | -0.27367600 |
| N | 0.05494700  | 2.00067700  | -0.27110800 |
| H | 1.39986800  | 5.06376200  | -0.19090400 |
| H | -1.30953000 | 5.05622700  | -0.24969600 |
| C | -2.77469900 | -1.10750300 | -0.33769700 |
| C | -4.15268300 | -0.69091800 | -0.35768000 |
| C | -4.15602100 | 0.67061000  | -0.35832100 |
| C | -2.78009400 | 1.09393300  | -0.33847800 |
| N | -1.93948900 | -0.00472600 | -0.34825500 |
| H | -4.99606200 | -1.36663900 | -0.36228300 |
| H | -5.00265300 | 1.34224000  | -0.36346700 |
| C | 2.89687500  | -1.09297400 | -0.17204000 |
| C | 4.27348800  | -0.67048300 | -0.13474400 |
| C | 4.27013400  | 0.69128700  | -0.13424700 |
| C | 2.89145800  | 1.10704400  | -0.17131600 |
| N | 2.05771800  | 0.00497700  | -0.20392900 |
| H | 5.11991200  | -1.34226300 | -0.11342500 |
| H | 5.11329500  | 1.36714700  | -0.11248900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.16548200  | -2.83416500 | -0.22176400 |
| C  | 0.74912900  | -4.21351200 | -0.21670800 |
| C  | -0.61224800 | -4.21655300 | -0.24532800 |
| C  | -1.03361800 | -2.83925600 | -0.27315000 |
| N  | 0.06472200  | -2.00043100 | -0.27138000 |
| H  | 1.42454900  | -5.05697600 | -0.19238000 |
| H  | -1.28491300 | -5.06253700 | -0.24891300 |
| C  | 2.48804500  | 2.44247300  | -0.17025200 |
| C  | -2.37089300 | -2.44176500 | -0.28826500 |
| C  | -2.38278200 | 2.43019700  | -0.28953100 |
| C  | 2.49998200  | -2.43039200 | -0.17163900 |
| Mn | 0.05024500  | 0.00010300  | 0.00572400  |
| C  | 3.54290100  | 3.50413000  | -0.09265700 |
| C  | 4.09827600  | 4.03158800  | -1.27369100 |
| C  | 3.96705400  | 3.97109700  | 1.16681000  |
| C  | 5.07814000  | 5.02481100  | -1.17514600 |
| C  | 4.94898300  | 4.96510600  | 1.22162000  |
| C  | 5.51884600  | 5.50252800  | 0.06286500  |
| H  | 5.50607600  | 5.43574300  | -2.08754400 |
| H  | 5.27556700  | 5.32984700  | 2.19363500  |
| C  | -3.42914400 | -3.49810200 | -0.19825100 |
| C  | -3.99085400 | -4.03969000 | -1.36932000 |
| C  | -3.85259200 | -3.93963900 | 1.07136300  |
| C  | -4.97889100 | -5.02277900 | -1.25262500 |
| C  | -4.84346300 | -4.92389200 | 1.14299700  |
| C  | -5.42101600 | -5.47500600 | -0.00555900 |
| H  | -5.41195500 | -5.44568300 | -2.15711600 |
| H  | -5.17142900 | -5.26969800 | 2.12142100  |
| C  | -3.44639800 | 3.48122200  | -0.20062800 |
| C  | -4.00987700 | 4.01963800  | -1.37232900 |
| C  | -3.87344900 | 3.92062600  | 1.06849700  |
| C  | -5.00331100 | 4.99737700  | -1.25672300 |
| C  | -4.86969200 | 4.89954500  | 1.13904800  |
| C  | -5.44913800 | 5.44732500  | -0.01013100 |
| H  | -5.43780700 | 5.41780000  | -2.16168600 |
| H  | -5.20050100 | 5.24364700  | 2.11711200  |
| C  | 3.56019900  | -3.48676400 | -0.09502800 |
| C  | 4.11762600  | -4.01086300 | -1.27660300 |
| C  | 3.98756900  | -3.95195400 | 1.16399800  |
| C  | 5.10277800  | -4.99891800 | -1.17901800 |
| C  | 4.97475600  | -4.94081400 | 1.21785000  |
| C  | 5.54679800  | -5.47472200 | 0.05856000  |
| H  | 5.53235100  | -5.40722900 | -2.09182400 |
| H  | 5.30386400  | -5.30415600 | 2.18953500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.36468200  | 3.40941600  | 2.43416800  |
| H | 2.28109900  | 3.57446600  | 2.46571800  |
| H | 3.51555100  | 2.32538700  | 2.49924300  |
| H | 3.80717500  | 3.87102100  | 3.32215700  |
| C | 3.63816500  | 3.53351100  | -2.62458500 |
| H | 3.81293700  | 2.45592600  | -2.72986900 |
| H | 2.56148300  | 3.69207100  | -2.75974600 |
| H | 4.16338800  | 4.04539100  | -3.43675700 |
| C | 6.60271200  | 6.55212400  | 0.14916800  |
| H | 7.59523200  | 6.08928100  | 0.23320700  |
| H | 6.61595700  | 7.19074100  | -0.74074300 |
| H | 6.46977000  | 7.19476400  | 1.02642900  |
| C | -3.23722200 | -3.37016400 | 2.32938300  |
| H | -2.16239200 | -3.58537000 | 2.37357600  |
| H | -3.33593800 | -2.27983300 | 2.37794100  |
| H | -3.70406000 | -3.79409500 | 3.22367300  |
| C | -3.52863700 | -3.56715800 | -2.72873800 |
| H | -3.71080400 | -2.49340400 | -2.85810600 |
| H | -2.45023200 | -3.72054300 | -2.85632700 |
| H | -4.04679100 | -4.09992500 | -3.53200300 |
| C | -6.51432800 | -6.51295700 | 0.10088900  |
| H | -7.50191600 | -6.03951200 | 0.18395500  |
| H | -6.53844800 | -7.16360100 | -0.78005900 |
| H | -6.38275500 | -7.14463800 | 0.98629300  |
| C | 3.65421000  | -3.51457600 | -2.62702500 |
| H | 2.57816100  | -3.67796300 | -2.76142200 |
| H | 3.82402100  | -2.43617700 | -2.73216800 |
| H | 4.18116000  | -4.02384400 | -3.43972000 |
| C | 3.38315700  | -3.39376600 | 2.43192600  |
| H | 3.52921700  | -2.30910800 | 2.49759100  |
| H | 2.30033800  | -3.56366700 | 2.46377500  |
| H | 3.82807300  | -3.85389100 | 3.31947200  |
| C | 6.63653400  | -6.51831600 | 0.14366600  |
| H | 6.65117600  | -7.15798100 | -0.74547300 |
| H | 7.62671000  | -6.04994100 | 0.22471300  |
| H | 6.50923100  | -7.16055400 | 1.02205200  |
| C | -3.25643300 | 3.35439200  | 2.32717000  |
| H | -3.34994800 | 2.26360700  | 2.37586300  |
| H | -2.18268200 | 3.57471400  | 2.37225900  |
| H | -3.72608200 | 3.77624100  | 3.22097300  |
| C | -3.54393500 | 3.54926900  | -2.73122300 |
| H | -2.46613400 | 3.70773200  | -2.85766100 |
| H | -3.72089700 | 2.47465400  | -2.86072300 |
| H | -4.06375900 | 4.07952100  | -3.53507400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -6.54845400 | 6.47905200  | 0.09495000  |
| H | -6.57366100 | 7.13104400  | -0.78497400 |
| H | -7.53363400 | 5.99997700  | 0.17429600  |
| H | -6.42300000 | 7.10994200  | 0.98179800  |
| N | -0.08560700 | -0.00024900 | 1.86968200  |
| C | -1.13432700 | -0.00187900 | 2.48309700  |
| O | -2.11772800 | -0.00345400 | 3.14965100  |

**Structure: 52**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.17025200 | -2.84043400 | -0.23124700 |
| C  | -0.74550600 | -4.21586700 | -0.23529000 |
| C  | 0.61646100  | -4.21399100 | -0.26960100 |
| C  | 1.03735400  | -2.83782600 | -0.29348700 |
| N  | -0.06815300 | -2.01048900 | -0.28157200 |
| H  | -1.41828400 | -5.06133200 | -0.21215100 |
| H  | 1.29241300  | -5.05712400 | -0.28058100 |
| C  | 2.77473200  | 1.10302500  | -0.38282900 |
| C  | 4.15057800  | 0.68045400  | -0.41951000 |
| C  | 4.15049000  | -0.68102500 | -0.41947300 |
| C  | 2.77459200  | -1.10341400 | -0.38277900 |
| N  | 1.94540100  | -0.00014300 | -0.38873800 |
| H  | 4.99481400  | 1.35477500  | -0.43129000 |
| H  | 4.99464100  | -1.35545300 | -0.43122200 |
| C  | -2.90550400 | 1.10467100  | -0.16610600 |
| C  | -4.28058600 | 0.68159900  | -0.13438100 |
| C  | -4.28068100 | -0.68103500 | -0.13442300 |
| C  | -2.90565400 | -1.10429400 | -0.16616000 |
| N  | -2.07696800 | 0.00013300  | -0.19106400 |
| H  | -5.12505200 | 1.35577700  | -0.11740500 |
| H  | -5.12524000 | -1.35509700 | -0.11748700 |
| C  | -1.16987200 | 2.84057900  | -0.23121200 |
| C  | -0.74494000 | 4.21595800  | -0.23524700 |
| C  | 0.61702200  | 4.21389900  | -0.26965400 |
| C  | 1.03772900  | 2.83767700  | -0.29358400 |
| N  | -0.06788700 | 2.01049000  | -0.28162500 |
| H  | -1.41760900 | 5.06150800  | -0.21203800 |
| H  | 1.29308600  | 5.05694300  | -0.28065600 |
| C  | -2.50595400 | -2.44134000 | -0.17088300 |
| C  | 2.37458400  | 2.43793400  | -0.31857900 |
| C  | 2.37426400  | -2.43826600 | -0.31845600 |
| C  | -2.50562200 | 2.44166400  | -0.17078800 |
| Mn | -0.05632600 | 0.00000100  | 0.00700600  |
| C  | -3.56261100 | -3.50051800 | -0.08976900 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.12609000 | -4.02548100 | -1.26819400 |
| C | -3.97988100 | -3.96758600 | 1.17225900  |
| C | -5.10762800 | -5.01653500 | -1.16473600 |
| C | -4.96371700 | -4.95949700 | 1.23149800  |
| C | -5.54178900 | -5.49435700 | 0.07558800  |
| H | -5.54204500 | -5.42568100 | -2.07483200 |
| H | -5.28518200 | -5.32469200 | 2.20498800  |
| C | 3.43557300  | 3.48987700  | -0.21675300 |
| C | 3.99255500  | 4.05250800  | -1.38010100 |
| C | 3.86703300  | 3.90255400  | 1.06035600  |
| C | 4.98520500  | 5.02908500  | -1.24927100 |
| C | 4.86240100  | 4.88148800  | 1.14500600  |
| C | 5.43573200  | 5.45359300  | 0.00459600  |
| H | 5.41525800  | 5.46853300  | -2.14727800 |
| H | 5.19748300  | 5.20594000  | 2.12826100  |
| C | 3.43511500  | -3.49034200 | -0.21657200 |
| C | 3.99203200  | -4.05311700 | -1.37990200 |
| C | 3.86652600  | -3.90298800 | 1.06054500  |
| C | 4.98455400  | -5.02979100 | -1.24902100 |
| C | 4.86179700  | -4.88204300 | 1.14524900  |
| C | 5.43505000  | -5.45427700 | 0.00488600  |
| H | 5.41454600  | -5.46935900 | -2.14700100 |
| H | 5.19684800  | -5.20646200 | 2.12852300  |
| C | -3.56213700 | 3.50097400  | -0.08955200 |
| C | -4.12536000 | 4.02635100  | -1.26793600 |
| C | -3.97953700 | 3.96774500  | 1.17252400  |
| C | -5.10675700 | 5.01750900  | -1.16436000 |
| C | -4.96325400 | 4.95979000  | 1.23188100  |
| C | -5.54105600 | 5.49505200  | 0.07604200  |
| H | -5.54097200 | 5.42697800  | -2.07440900 |
| H | -5.28482200 | 5.32475100  | 2.20542400  |
| C | -3.36875600 | -3.40905700 | 2.43679700  |
| H | -2.28522800 | -3.57495000 | 2.46237900  |
| H | -3.51696600 | -2.32495700 | 2.50573500  |
| H | -3.80656600 | -3.87167400 | 3.32648700  |
| C | -3.67337300 | -3.52746000 | -2.62167300 |
| H | -3.84728400 | -2.44961500 | -2.72608200 |
| H | -2.59782400 | -3.68748400 | -2.76391900 |
| H | -4.20427100 | -4.03831400 | -3.43074400 |
| C | -6.62739100 | -6.54162400 | 0.16750900  |
| H | -7.61802300 | -6.07640600 | 0.25998100  |
| H | -6.64876500 | -7.17814800 | -0.72370400 |
| H | -6.48951000 | -7.18641300 | 1.04237800  |
| C | 3.25696400  | 3.30986900  | 2.31009100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.18144500  | 3.52016800  | 2.36086300  |
| H | 3.35647200  | 2.21906300  | 2.34614900  |
| H | 3.72411100  | 3.72265300  | 3.20939800  |
| C | 3.52139100  | 3.60902200  | -2.74634300 |
| H | 3.69315400  | 2.53620400  | -2.89628400 |
| H | 2.44405900  | 3.77465800  | -2.86832800 |
| H | 4.04189400  | 4.15149000  | -3.54153200 |
| C | 6.53390100  | 6.48473800  | 0.12615800  |
| H | 7.51976900  | 6.00546800  | 0.19481200  |
| H | 6.55645200  | 7.15273000  | -0.74175200 |
| H | 6.40944100  | 7.09895500  | 1.02474600  |
| C | -3.67247400 | 3.52864800  | -2.62147400 |
| H | -2.59695900 | 3.68897700  | -2.76366100 |
| H | -3.84609600 | 2.45077400  | -2.72604800 |
| H | -4.20347300 | 4.03949000  | -3.43048500 |
| C | -3.36871400 | 3.40877500  | 2.43701400  |
| H | -3.51737100 | 2.32472400  | 2.50577900  |
| H | -2.28512000 | 3.57422000  | 2.46268900  |
| H | -3.80639300 | 3.87143100  | 3.32674800  |
| C | -6.62655900 | 6.54242100  | 0.16796000  |
| H | -6.64548800 | 7.18125700  | -0.72166300 |
| H | -7.61757400 | 6.07727600  | 0.25665400  |
| H | -6.49069900 | 7.18489500  | 1.04483500  |
| C | 3.25653900  | -3.31017800 | 2.31026100  |
| H | 3.35619900  | -2.21938600 | 2.34629700  |
| H | 2.18099100  | -3.52032900 | 2.36103700  |
| H | 3.72362800  | -3.72300300 | 3.20958000  |
| C | 3.52092400  | -3.60962300 | -2.74615900 |
| H | 2.44355000  | -3.77500800 | -2.86810000 |
| H | 3.69293700  | -2.53685400 | -2.89617900 |
| H | 4.04127500  | -4.15226800 | -3.54132700 |
| C | 6.53314000  | -6.48551000 | 0.12637100  |
| H | 6.55328800  | -7.15572300 | -0.73989600 |
| H | 7.51935900  | -6.00643300 | 0.19126600  |
| H | 6.41070900  | -7.09738400 | 1.02682400  |
| N | 0.17091000  | 0.00009400  | 2.02966300  |
| C | 1.23628600  | 0.00000600  | 2.59835900  |
| O | 2.29335200  | -0.00007900 | 3.16496800  |

**Structure: PhIO**

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -2.86671500 | -1.19051200 | 0.16505300 |
| C | -1.47338100 | -1.21480500 | 0.06200000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.78426000 | -0.01098400 | -0.08586900 |
| C | -1.45286000 | 1.21318900  | -0.10020100 |
| C | -2.84589900 | 1.22571200  | 0.00647300  |
| C | -3.55057000 | 0.02680600  | 0.13680800  |
| H | -3.41369000 | -2.12297700 | 0.27418700  |
| H | -0.93857000 | -2.15883100 | 0.09372200  |
| H | -0.90306900 | 2.14398800  | -0.19771900 |
| H | -3.37739300 | 2.17325200  | -0.00961600 |
| H | -4.63363900 | 0.04155500  | 0.22022400  |
| I | 1.39282400  | -0.04446000 | -0.25001200 |
| O | 2.16110000  | 0.24786700  | 1.47052900  |

**Structure: <sup>3</sup>INT1**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.19780500  | 2.00022100  | -0.61878400 |
| C | 3.63633700  | 1.97486800  | -0.76078300 |
| C | 3.99797700  | 0.66653100  | -0.88722900 |
| C | 2.78410300  | -0.11392700 | -0.81273100 |
| N | 1.70540500  | 0.71769000  | -0.64061300 |
| H | 4.26867500  | 2.85182000  | -0.77189400 |
| H | 4.98792600  | 0.25162300  | -1.01575600 |
| C | -0.51868500 | -2.88061500 | -0.45087800 |
| C | 0.24300000  | -4.08640000 | -0.67007800 |
| C | 1.53855400  | -3.70871700 | -0.85834600 |
| C | 1.58058100  | -2.26988100 | -0.74372600 |
| N | 0.31838800  | -1.78589600 | -0.47556200 |
| H | -0.17715700 | -5.08227200 | -0.69342100 |
| H | 2.39596900  | -4.33347900 | -1.06593700 |
| C | -2.05861700 | 2.58678300  | -0.19013700 |
| C | -2.03557700 | 4.03200800  | -0.17641300 |
| C | -0.73041900 | 4.40861400  | -0.27319800 |
| C | 0.05218000  | 3.19641300  | -0.36145000 |
| N | -0.77798300 | 2.10292700  | -0.30852200 |
| H | -2.91263000 | 4.65898700  | -0.09669500 |
| H | -0.31866000 | 5.40800700  | -0.29043900 |
| C | -3.25298500 | 0.42711200  | -0.03419800 |
| C | -4.46111000 | -0.35464600 | 0.10086300  |
| C | -4.09212700 | -1.66510600 | 0.06326700  |
| C | -2.65698800 | -1.69143800 | -0.10394000 |
| N | -2.16709900 | -0.40738500 | -0.13496500 |
| H | -5.45385800 | 0.06130700  | 0.19963500  |
| H | -4.72045600 | -2.54273700 | 0.12160000  |
| C | 1.44443600  | 3.17245700  | -0.48843200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.90432900 | -2.86056900 | -0.26170700 |
| C  | 2.74585000  | -1.51115300 | -0.89825800 |
| C  | -3.22625700 | 1.82542900  | -0.08258900 |
| O  | -0.08326000 | 0.44882100  | 1.48259100  |
| N  | -0.50680500 | 0.14548000  | -2.36469700 |
| C  | -1.53461400 | -0.10534800 | -2.95010900 |
| O  | -2.52117700 | -0.34711000 | -3.57705200 |
| Mn | -0.24228300 | 0.16570900  | -0.46682300 |
| C  | 2.17352200  | 4.48199900  | -0.49114000 |
| C  | 2.57166500  | 5.06405100  | 0.72764400  |
| C  | 2.45746500  | 5.12447600  | -1.71235700 |
| C  | 3.24992300  | 6.28734900  | 0.70565200  |
| C  | 3.13811000  | 6.34594200  | -1.69140200 |
| C  | 3.53977400  | 6.94541400  | -0.49330000 |
| H  | 3.55864400  | 6.73678600  | 1.64772400  |
| H  | 3.35882900  | 6.84232200  | -2.63459900 |
| C  | 4.01826700  | -2.23100500 | -1.23411000 |
| C  | 4.77390100  | -2.86569500 | -0.22938400 |
| C  | 4.45157000  | -2.26683300 | -2.57611400 |
| C  | 5.95857800  | -3.52113100 | -0.58141400 |
| C  | 5.64073200  | -2.93446800 | -2.88567800 |
| C  | 6.40846600  | -3.56853600 | -1.90388500 |
| H  | 6.54492300  | -4.00454000 | 0.19800200  |
| H  | 5.97499600  | -2.96103900 | -3.92122600 |
| C  | -2.64246900 | -4.16333700 | -0.30229400 |
| C  | -3.09950100 | -4.65770300 | -1.54096900 |
| C  | -2.88882900 | -4.87718600 | 0.88431500  |
| C  | -3.79949600 | -5.86821700 | -1.56336400 |
| C  | -3.59253200 | -6.08434800 | 0.81911600  |
| C  | -4.05448000 | -6.59694000 | -0.39669400 |
| H  | -4.15727500 | -6.25092900 | -2.51739600 |
| H  | -3.78632500 | -6.63491500 | 1.73786800  |
| C  | -4.53866600 | 2.54680500  | -0.05009300 |
| C  | -5.12821800 | 2.89219100  | 1.18007900  |
| C  | -5.17678700 | 2.86586800  | -1.26546800 |
| C  | -6.36053600 | 3.55381100  | 1.17811500  |
| C  | -6.40882500 | 3.52677800  | -1.22282000 |
| C  | -7.01843700 | 3.87522600  | -0.01318000 |
| H  | -6.81644300 | 3.82473700  | 2.12869400  |
| H  | -6.90441500 | 3.77624300  | -2.15919500 |
| C  | 3.65042600  | -1.58829400 | -3.66425900 |
| H  | 2.59120100  | -1.86388200 | -3.61430300 |
| H  | 3.68940300  | -0.49691900 | -3.56315000 |
| H  | 4.03104400  | -1.85125500 | -4.65613700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.31625700  | -2.83829100 | 1.20987800  |
| H | 4.12140900  | -1.81587500 | 1.54444100  |
| H | 3.38112400  | -3.39680800 | 1.33875100  |
| H | 5.06723400  | -3.27721600 | 1.87425200  |
| C | 7.67317100  | -4.31065500 | -2.26957500 |
| H | 8.36456300  | -4.36890800 | -1.42183900 |
| H | 7.45167800  | -5.34018700 | -2.58175800 |
| H | 8.19634700  | -3.82640300 | -3.10170500 |
| C | 2.03253600  | 4.50000000  | -3.02130900 |
| H | 2.50594600  | 3.52172300  | -3.16674400 |
| H | 0.95030500  | 4.32680600  | -3.04428200 |
| H | 2.29692600  | 5.13846700  | -3.86995000 |
| C | 2.27832300  | 4.37291400  | 2.04000400  |
| H | 1.20782000  | 4.16614500  | 2.15208300  |
| H | 2.78966900  | 3.40471800  | 2.10246300  |
| H | 2.60238100  | 4.98111400  | 2.89035300  |
| C | 4.24147200  | 8.28399300  | -0.49548900 |
| H | 4.87639200  | 8.40271600  | -1.38054600 |
| H | 3.51753200  | 9.11001700  | -0.50278500 |
| H | 4.87010900  | 8.41021800  | 0.39273300  |
| C | -4.53284800 | 2.51477700  | -2.58745300 |
| H | -3.58751100 | 3.05601900  | -2.71847500 |
| H | -4.28681800 | 1.44934200  | -2.65841100 |
| H | -5.18815600 | 2.77121800  | -3.42569600 |
| C | -4.43609600 | 2.55138400  | 2.48029500  |
| H | -4.32198100 | 1.46628500  | 2.59406700  |
| H | -3.42634000 | 2.97730100  | 2.51566800  |
| H | -4.99870600 | 2.92746800  | 3.34063200  |
| C | -8.36719100 | 4.55715300  | 0.00504200  |
| H | -8.50021600 | 5.20684900  | -0.86709800 |
| H | -9.18284500 | 3.82157600  | -0.01118800 |
| H | -8.49735300 | 5.16711500  | 0.90574100  |
| C | -2.82639500 | -3.89773700 | -2.81883200 |
| H | -3.18920100 | -2.86494700 | -2.77214000 |
| H | -1.74857900 | -3.83354700 | -3.01268000 |
| H | -3.29639500 | -4.38761200 | -3.67716800 |
| C | -2.40277900 | -4.34213700 | 2.21276400  |
| H | -1.31195300 | -4.22266200 | 2.21174300  |
| H | -2.83444400 | -3.35496100 | 2.42171000  |
| H | -2.67213200 | -5.01187200 | 3.03551400  |
| C | -4.78718300 | -7.91748000 | -0.45655100 |
| H | -5.56904600 | -7.90698500 | -1.22416400 |
| H | -4.10205100 | -8.73953300 | -0.70406000 |
| H | -5.25675800 | -8.16130800 | 0.50254800  |

|   |            |             |            |
|---|------------|-------------|------------|
| C | 4.10729000 | -1.13598200 | 4.45016900 |
| C | 2.77222000 | -1.44462900 | 4.17119400 |
| C | 2.11386700 | -0.65882000 | 3.23351600 |
| C | 2.70145700 | 0.40375800  | 2.56652200 |
| C | 4.04080700 | 0.68550000  | 2.85444100 |
| C | 4.73908700 | -0.07711900 | 3.79296200 |
| H | 4.65012900 | -1.73358600 | 5.17685000 |
| H | 2.28234800 | -2.27486900 | 4.67120600 |
| H | 2.13827300 | 0.97430900  | 1.83633800 |
| H | 4.53040900 | 1.49563700  | 2.32287400 |
| H | 5.77963700 | 0.14722300  | 4.00806000 |
| I | 0.05103200 | -1.06818600 | 2.71041000 |

**Structure: <sup>5</sup>INT1**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.20111800  | 1.97049000  | -0.61714400 |
| C | 3.63120700  | 1.91752600  | -0.79593200 |
| C | 3.96403000  | 0.60776900  | -0.98233400 |
| C | 2.74429800  | -0.15586500 | -0.90064400 |
| N | 1.68543900  | 0.69451400  | -0.67773200 |
| H | 4.28019100  | 2.78213500  | -0.78944500 |
| H | 4.94236600  | 0.17960200  | -1.14893400 |
| C | -0.58100300 | -2.87100800 | -0.41838300 |
| C | 0.16050100  | -4.08878400 | -0.63360200 |
| C | 1.45192000  | -3.73199600 | -0.88463600 |
| C | 1.51775200  | -2.29324400 | -0.80652200 |
| N | 0.27103000  | -1.79208600 | -0.50625000 |
| H | -0.27201400 | -5.07924900 | -0.61354700 |
| H | 2.29417700  | -4.37143800 | -1.10838100 |
| C | -2.04462100 | 2.62327200  | -0.20203200 |
| C | -1.99391500 | 4.06510400  | -0.16377600 |
| C | -0.67966300 | 4.42059700  | -0.21625300 |
| C | 0.08496100  | 3.19986100  | -0.31003700 |
| N | -0.76740300 | 2.12300200  | -0.29363600 |
| H | -2.86250300 | 4.70497600  | -0.09708900 |
| H | -0.25001600 | 5.41234400  | -0.20587000 |
| C | -3.27040800 | 0.48539700  | -0.06292200 |
| C | -4.48329000 | -0.28000800 | 0.10654400  |
| C | -4.12775500 | -1.59414000 | 0.11428100  |
| C | -2.69565800 | -1.64423800 | -0.06811600 |
| N | -2.19869000 | -0.36740500 | -0.15105100 |
| H | -5.46975700 | 0.15117500  | 0.20059800  |
| H | -4.76364900 | -2.46274400 | 0.20943700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.47673500  | 3.15316100  | -0.43684700 |
| C  | -1.96049400 | -2.82703400 | -0.19646900 |
| C  | 2.68553100  | -1.54989200 | -1.00498100 |
| C  | -3.22667900 | 1.88147700  | -0.12395300 |
| O  | -0.13233700 | 0.37846300  | 1.71796700  |
| N  | -0.64989200 | 0.15488500  | -2.60850900 |
| C  | -1.71932700 | -0.15116800 | -3.07359400 |
| O  | -2.79060600 | -0.45653600 | -3.53040200 |
| Mn | -0.27066700 | 0.17379200  | -0.53578800 |
| C  | 2.23027300  | 4.44808400  | -0.41240000 |
| C  | 2.61581300  | 5.01209300  | 0.81901300  |
| C  | 2.54314300  | 5.09781400  | -1.62318500 |
| C  | 3.31529200  | 6.22360700  | 0.81936300  |
| C  | 3.24430400  | 6.30702500  | -1.57864600 |
| C  | 3.63692600  | 6.88747600  | -0.36825000 |
| H  | 3.61500900  | 6.65938400  | 1.77065200  |
| H  | 3.48727600  | 6.80949500  | -2.51301900 |
| C  | 3.93549500  | -2.28272100 | -1.38892300 |
| C  | 4.73061200  | -2.91146000 | -0.41162000 |
| C  | 4.30514800  | -2.33425500 | -2.74903600 |
| C  | 5.89107000  | -3.58287600 | -0.81095800 |
| C  | 5.47191200  | -3.01776500 | -3.10540300 |
| C  | 6.27734100  | -3.64992800 | -2.15278200 |
| H  | 6.50898800  | -4.06289300 | -0.05426100 |
| H  | 5.75840600  | -3.05785600 | -4.15466400 |
| C  | -2.71543000 | -4.11994600 | -0.18033300 |
| C  | -3.21921200 | -4.63660700 | -1.39149400 |
| C  | -2.93175100 | -4.79808100 | 1.03263100  |
| C  | -3.93933100 | -5.83535800 | -1.35772300 |
| C  | -3.65626700 | -5.99422800 | 1.02235900  |
| C  | -4.16706000 | -6.52903100 | -0.16437500 |
| H  | -4.33460400 | -6.23656100 | -2.28899700 |
| H  | -3.82832200 | -6.51789500 | 1.96093400  |
| C  | -4.52888600 | 2.62031100  | -0.11833700 |
| C  | -5.12308500 | 3.00348000  | 1.09830100  |
| C  | -5.15138900 | 2.91459300  | -1.34824200 |
| C  | -6.34745500 | 3.67915800  | 1.06861600  |
| C  | -6.37563600 | 3.59109000  | -1.33179600 |
| C  | -6.99099100 | 3.97734200  | -0.13649600 |
| H  | -6.80841200 | 3.97895600  | 2.00795200  |
| H  | -6.86049300 | 3.82252700  | -2.27830500 |
| C  | 3.46269600  | -1.65286000 | -3.80360700 |
| H  | 2.40445800  | -1.92118100 | -3.71188400 |
| H  | 3.51062300  | -0.56157700 | -3.70455000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.80128000  | -1.91709800 | -4.81015700 |
| C | 4.34091700  | -2.85696100 | 1.04674000  |
| H | 4.18449400  | -1.82646300 | 1.37775700  |
| H | 3.40047100  | -3.39212200 | 1.22682100  |
| H | 5.11198400  | -3.30457500 | 1.68140600  |
| C | 7.51588700  | -4.40963900 | -2.56838100 |
| H | 8.24389400  | -4.46928500 | -1.75205200 |
| H | 7.26854900  | -5.43882000 | -2.86161100 |
| H | 8.00677100  | -3.93841800 | -3.42723000 |
| C | 2.12581300  | 4.49721400  | -2.94588400 |
| H | 2.60241500  | 3.52345800  | -3.11008100 |
| H | 1.04443400  | 4.32095300  | -2.97830800 |
| H | 2.39245300  | 5.15299600  | -3.78035600 |
| C | 2.28485100  | 4.31805400  | 2.12083200  |
| H | 1.20806800  | 4.13765800  | 2.21612000  |
| H | 2.76953200  | 3.33689800  | 2.18540700  |
| H | 2.61106600  | 4.91165700  | 2.98050900  |
| C | 4.36146500  | 8.21354900  | -0.34544800 |
| H | 5.00956500  | 8.33179600  | -1.22088500 |
| H | 3.65159800  | 9.05164700  | -0.35192700 |
| H | 4.98046500  | 8.31832700  | 0.55223200  |
| C | -4.50076100 | 2.52022200  | -2.65441900 |
| H | -3.53578600 | 3.02708400  | -2.78047500 |
| H | -4.28816000 | 1.44641500  | -2.70899700 |
| H | -5.13528200 | 2.78609800  | -3.50557800 |
| C | -4.44643600 | 2.68716200  | 2.41279600  |
| H | -4.33070900 | 1.60480000  | 2.54788900  |
| H | -3.43797100 | 3.11558400  | 2.45444000  |
| H | -5.02061700 | 3.07735700  | 3.25899900  |
| C | -8.33166800 | 4.67512800  | -0.14813900 |
| H | -8.44214200 | 5.31697900  | -1.02920500 |
| H | -9.15525400 | 3.94868300  | -0.17114100 |
| H | -8.47002000 | 5.29590800  | 0.74384800  |
| C | -2.97159500 | -3.91675800 | -2.69741800 |
| H | -3.29974700 | -2.87172600 | -2.67091600 |
| H | -1.89976300 | -3.89027500 | -2.93056300 |
| H | -3.48450700 | -4.41598600 | -3.52520000 |
| C | -2.39134900 | -4.23523000 | 2.32824100  |
| H | -1.29909700 | -4.13727600 | 2.28800300  |
| H | -2.79566400 | -3.23350100 | 2.52240600  |
| H | -2.64584500 | -4.87559000 | 3.17859600  |
| C | -4.92235200 | -7.83815600 | -0.16467000 |
| H | -5.71186500 | -7.84466300 | -0.92428000 |
| H | -4.25336200 | -8.68078700 | -0.38578000 |



|   |             |             |            |
|---|-------------|-------------|------------|
| H | -5.38553900 | -8.03599600 | 0.80807700 |
| C | 4.40609900  | -1.10283300 | 4.24929800 |
| C | 3.05896500  | -1.44742100 | 4.09936200 |
| C | 2.29220800  | -0.68135300 | 3.23045700 |
| C | 2.78464900  | 0.39571500  | 2.51293100 |
| C | 4.13635100  | 0.71708900  | 2.67187000 |
| C | 4.94206600  | -0.02649700 | 3.53731500 |
| H | 5.03305000  | -1.68369900 | 4.91985100 |
| H | 2.64055400  | -2.28848000 | 4.64458500 |
| H | 2.13177800  | 0.94849200  | 1.84437900 |
| H | 4.55188300  | 1.54150500  | 2.10103500 |
| H | 5.99161700  | 0.22749500  | 3.65327100 |
| I | 0.19560800  | -1.11694200 | 2.89064300 |

**Structure: <sup>5</sup>TS1**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.24287600  | 1.92861000  | -0.62245300 |
| C | 3.66941700  | 1.83744200  | -0.81705600 |
| C | 3.96362900  | 0.52071200  | -1.01315300 |
| C | 2.72407100  | -0.21070900 | -0.92231900 |
| N | 1.69226100  | 0.66964900  | -0.68744500 |
| H | 4.34168400  | 2.68406300  | -0.81207000 |
| H | 4.92784200  | 0.06605800  | -1.19109800 |
| C | -0.66046300 | -2.84701800 | -0.44200400 |
| C | 0.04937000  | -4.08335900 | -0.66685300 |
| C | 1.34807000  | -3.75712400 | -0.91898200 |
| C | 1.44749800  | -2.31928200 | -0.83331400 |
| N | 0.21628300  | -1.79224500 | -0.53090500 |
| H | -0.40830700 | -5.06249400 | -0.65020300 |
| H | 2.17457800  | -4.41504200 | -1.14768300 |
| C | -1.98246700 | 2.68058800  | -0.17763000 |
| C | -1.89406700 | 4.11961200  | -0.14079600 |
| C | -0.57131000 | 4.44281800  | -0.19114500 |
| C | 0.16475100  | 3.20577300  | -0.28318000 |
| N | -0.71514000 | 2.14942100  | -0.26380500 |
| H | -2.74693300 | 4.78080200  | -0.07989500 |
| H | -0.11784000 | 5.42391000  | -0.18541400 |
| C | -3.26438900 | 0.57693400  | -0.06644600 |
| C | -4.49602900 | -0.15957800 | 0.09484200  |
| C | -4.17213100 | -1.48169100 | 0.09560200  |
| C | -2.74097400 | -1.56679800 | -0.08330100 |
| N | -2.21563500 | -0.30065400 | -0.16067200 |
| H | -5.47157200 | 0.29541500  | 0.19027300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.82871900 | -2.33528300 | 0.18541000  |
| C  | 1.55268400  | 3.12820600  | -0.42381900 |
| C  | -2.03803000 | -2.76773800 | -0.21562500 |
| C  | 2.63209300  | -1.60156200 | -1.02926200 |
| C  | -3.18376100 | 1.97195300  | -0.11297900 |
| O  | -0.07567100 | 0.25684100  | 1.51690800  |
| N  | -0.59667200 | 0.18371900  | -2.50766200 |
| C  | -1.65707600 | -0.09596900 | -3.01205700 |
| O  | -2.71145800 | -0.37064700 | -3.51738000 |
| Mn | -0.26451900 | 0.19994600  | -0.45983800 |
| C  | 2.33816000  | 4.40410500  | -0.40324500 |
| C  | 2.72397400  | 4.97063800  | 0.82719900  |
| C  | 2.68141000  | 5.03399900  | -1.61647000 |
| C  | 3.45650500  | 6.16238900  | 0.82380700  |
| C  | 3.41415900  | 6.22452100  | -1.57535900 |
| C  | 3.80951200  | 6.80564700  | -0.36629900 |
| H  | 3.75750400  | 6.59910500  | 1.77424200  |
| H  | 3.68021700  | 6.71155900  | -2.51160800 |
| C  | 3.86666200  | -2.36395400 | -1.40635000 |
| C  | 4.64856800  | -2.99579600 | -0.42019100 |
| C  | 4.23538200  | -2.43995100 | -2.76512700 |
| C  | 5.79503700  | -3.69557600 | -0.81080600 |
| C  | 5.38826200  | -3.15120400 | -3.11259900 |
| C  | 6.18025200  | -3.78746100 | -2.15158800 |
| H  | 6.40285400  | -4.17849600 | -0.04783100 |
| H  | 5.67433400  | -3.20997400 | -4.16108800 |
| C  | -2.82706800 | -4.04087100 | -0.20064900 |
| C  | -3.33823300 | -4.54753700 | -1.41294800 |
| C  | -3.06755300 | -4.71049900 | 1.01282900  |
| C  | -4.08965100 | -5.72694600 | -1.38083300 |
| C  | -3.82337700 | -5.88713500 | 1.00062600  |
| C  | -4.34169200 | -6.41166200 | -0.18734000 |
| H  | -4.49038100 | -6.11967300 | -2.31340000 |
| H  | -4.01377900 | -6.40378800 | 1.93951200  |
| C  | -4.46681500 | 2.74404300  | -0.11402400 |
| C  | -5.05497500 | 3.14868300  | 1.09854000  |
| C  | -5.07944500 | 3.04551100  | -1.34717400 |
| C  | -6.26285100 | 3.85319300  | 1.06119700  |
| C  | -6.28720100 | 3.75095500  | -1.33862200 |
| C  | -6.89617900 | 4.15921800  | -0.14735800 |
| H  | -6.71928500 | 4.16904800  | 1.99744500  |
| H  | -6.76402600 | 3.98785600  | -2.28785700 |
| C  | 3.40705500  | -1.75392100 | -3.82774100 |
| H  | 2.34462900  | -2.00553600 | -3.73656800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.47185500  | -0.66277700 | -3.73689700 |
| H | 3.74404800  | -2.03150600 | -4.83123300 |
| C | 4.26164300  | -2.91064900 | 1.03735900  |
| H | 4.17145000  | -1.87064500 | 1.36448500  |
| H | 3.28832700  | -3.38229400 | 1.21836000  |
| H | 5.00185800  | -3.40394600 | 1.67478700  |
| C | 7.40334200  | -4.57761100 | -2.55611900 |
| H | 8.13821000  | -4.62410000 | -1.74505800 |
| H | 7.13812100  | -5.61130800 | -2.81600000 |
| H | 7.89269700  | -4.13926200 | -3.43296800 |
| C | 2.26329800  | 4.43382000  | -2.93924100 |
| H | 2.73719400  | 3.45860200  | -3.10281000 |
| H | 1.18142600  | 4.26135800  | -2.97308000 |
| H | 2.53364300  | 5.08818000  | -3.77363700 |
| C | 2.35118100  | 4.30486300  | 2.13244300  |
| H | 1.26328500  | 4.22853700  | 2.24425100  |
| H | 2.73951100  | 3.28164300  | 2.18787400  |
| H | 2.74399700  | 4.86274800  | 2.98812900  |
| C | 4.56987400  | 8.11154000  | -0.34759500 |
| H | 5.22335200  | 8.20801900  | -1.22165900 |
| H | 3.88301300  | 8.96853800  | -0.35976900 |
| H | 5.18894800  | 8.20358600  | 0.55143000  |
| C | -4.43499900 | 2.62861400  | -2.64954800 |
| H | -3.45918400 | 3.11391000  | -2.77718300 |
| H | -4.24587300 | 1.55012600  | -2.69585200 |
| H | -5.06204600 | 2.90199600  | -3.50382500 |
| C | -4.38980600 | 2.82408700  | 2.41673900  |
| H | -4.28824900 | 1.74048300  | 2.55263900  |
| H | -3.37641600 | 3.24024000  | 2.46398800  |
| H | -4.96346700 | 3.22180100  | 3.25971000  |
| C | -8.22003400 | 4.88816700  | -0.16690100 |
| H | -8.31386500 | 5.52570300  | -1.05300600 |
| H | -9.06025200 | 4.18093100  | -0.18599900 |
| H | -8.34535400 | 5.51870600  | 0.72011000  |
| C | -3.06616600 | -3.83825700 | -2.71982800 |
| H | -3.35983100 | -2.78315100 | -2.69340500 |
| H | -1.99409000 | -3.84821500 | -2.95308600 |
| H | -3.59557600 | -4.32093800 | -3.54704100 |
| C | -2.51668000 | -4.16332600 | 2.31043600  |
| H | -1.42115500 | -4.11428000 | 2.28162400  |
| H | -2.87747900 | -3.14367700 | 2.49550400  |
| H | -2.80740100 | -4.78677300 | 3.16167500  |
| C | -5.13055600 | -7.70079800 | -0.18810300 |
| H | -5.90947900 | -7.69332100 | -0.95852200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.48044400 | -8.56210800 | -0.39295500 |
| H | -5.61187500 | -7.87870100 | 0.77968900  |
| C | 4.39560800  | -1.11775700 | 4.25112700  |
| C | 3.05362000  | -1.48175100 | 4.10360700  |
| C | 2.27193900  | -0.73843200 | 3.22595200  |
| C | 2.75493100  | 0.33864100  | 2.49910700  |
| C | 4.10198500  | 0.68009800  | 2.65627600  |
| C | 4.91861100  | -0.04247100 | 3.52873600  |
| H | 5.02910700  | -1.68418800 | 4.92792300  |
| H | 2.64714700  | -2.32306700 | 4.65631600  |
| H | 2.09627900  | 0.87391200  | 1.82452000  |
| H | 4.50524400  | 1.50508700  | 2.07735500  |
| H | 5.96453600  | 0.22738900  | 3.64236600  |
| I | 0.19433200  | -1.25373800 | 2.92377900  |

**Structure: PhI**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.66254100 | -1.20770400 | 0.00001900  |
| C | -1.26478900 | -1.21636300 | 0.00005100  |
| C | -0.58294700 | 0.00027600  | 0.00075300  |
| C | -1.26514600 | 1.21658900  | 0.00005600  |
| C | -2.66292200 | 1.20746000  | -0.00005100 |
| C | -3.36284500 | -0.00021400 | -0.00016800 |
| H | -3.20045200 | -2.15188300 | -0.00021200 |
| H | -0.72256000 | -2.15552000 | 0.00005600  |
| H | -0.72319000 | 2.15591800  | 0.00014400  |
| H | -3.20113500 | 2.15146900  | -0.00008500 |
| H | -4.44916800 | -0.00033400 | -0.00080100 |
| I | 1.56799300  | 0.00000200  | -0.00005800 |

**Structure: <sup>13</sup>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.91459300  | -1.09937500 | -0.13968300 |
| C | 4.30004400  | -0.68991300 | -0.06833400 |
| C | 4.30309500  | 0.67190900  | -0.06866100 |
| C | 2.91948200  | 1.08751500  | -0.14010300 |
| N | 2.09987200  | -0.00410600 | -0.19028200 |
| H | 5.14139300  | -1.36619800 | -0.01716000 |
| H | 5.14743400  | 1.34447500  | -0.01779500 |
| C | -1.03388900 | 2.84570000  | -0.21751500 |
| C | -0.62029500 | 4.22714600  | -0.12791400 |
| C | 0.74157400  | 4.22731200  | -0.09688300 |
| C | 1.15781800  | 2.84541900  | -0.16155200 |
| N | 0.06288100  | 2.02812600  | -0.23938700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.29566200 | 5.06992200  | -0.09322300 |
| H  | 1.41421200  | 5.07039500  | -0.03033600 |
| C  | -1.04652700 | -2.84004600 | -0.21690100 |
| C  | -0.63903900 | -4.22334200 | -0.12740400 |
| C  | 0.72280700  | -4.22951500 | -0.09633700 |
| C  | 1.14516000  | -2.84946800 | -0.16083300 |
| N  | 0.05385000  | -2.02732500 | -0.23865700 |
| H  | -1.31803200 | -5.06322100 | -0.09281100 |
| H  | 1.39171600  | -5.07556100 | -0.02986000 |
| C  | -2.81046000 | -1.08645300 | -0.34500800 |
| C  | -4.19673400 | -0.67027100 | -0.34840700 |
| C  | -4.19370900 | 0.68982900  | -0.34849400 |
| C  | -2.80554400 | 1.09980500  | -0.34529700 |
| N  | -1.98853300 | 0.00483400  | -0.36759100 |
| H  | -5.04229900 | -1.34268800 | -0.33137900 |
| H  | -5.03635100 | 1.36593200  | -0.33154100 |
| C  | 2.48742300  | -2.43732700 | -0.12568300 |
| C  | -2.37730800 | 2.43347600  | -0.25901000 |
| C  | 2.49824400  | 2.42736100  | -0.12641900 |
| C  | -2.38815100 | -2.42193900 | -0.25840400 |
| O  | 0.11824300  | -0.00004400 | -1.99265200 |
| N  | -0.06849400 | 0.00112900  | 1.68745000  |
| C  | -1.07381300 | 0.00147100  | 2.35221400  |
| O  | -2.06277600 | 0.00196400  | 3.03433200  |
| Mn | 0.07110500  | 0.00035500  | -0.37265300 |
| C  | 3.53741900  | -3.50037000 | -0.03493500 |
| C  | 4.08917600  | -4.03734700 | -1.21361400 |
| C  | 3.96553800  | -3.94619600 | 1.23009600  |
| C  | 5.07228900  | -5.02533600 | -1.10422400 |
| C  | 4.95106200  | -4.93647700 | 1.29275300  |
| C  | 5.51425900  | -5.49020700 | 0.13880400  |
| H  | 5.50397800  | -5.44079400 | -2.01270800 |
| H  | 5.28722900  | -5.28215800 | 2.26826900  |
| C  | 3.55318900  | 3.48551600  | -0.03595900 |
| C  | 4.10598200  | 4.02103500  | -1.21477100 |
| C  | 3.98543800  | 3.92763900  | 1.22901200  |
| C  | 5.09441100  | 5.00379300  | -1.10563900 |
| C  | 4.97609700  | 4.91274300  | 1.29140300  |
| C  | 5.54060000  | 5.46484000  | 0.13726100  |
| H  | 5.52701600  | 5.41798700  | -2.01425800 |
| H  | 5.31550100  | 5.25550900  | 2.26683400  |
| C  | -3.43178200 | 3.48764700  | -0.13734600 |
| C  | -3.83437600 | 3.90509100  | 1.14732600  |
| C  | -4.02009300 | 4.03203400  | -1.29374100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.83714000 | 4.87484800  | 1.24617800  |
| C | -5.01702200 | 5.00143800  | -1.14603500 |
| C | -5.43815000 | 5.43609400  | 0.11460900  |
| H | -5.15821400 | 5.19781800  | 2.23453400  |
| H | -5.47630600 | 5.42458400  | -2.03725500 |
| C | -3.44722800 | -3.47153500 | -0.13726000 |
| C | -4.03262700 | -4.01784700 | -1.29465700 |
| C | -3.84894800 | -3.89118100 | 1.14655300  |
| C | -5.02653300 | -4.99001900 | -1.14822100 |
| C | -4.84911500 | -4.86428000 | 1.24420500  |
| C | -5.45131900 | -5.42265400 | 0.11229300  |
| H | -5.47869100 | -5.41958300 | -2.04006600 |
| H | -5.16446800 | -5.19411800 | 2.23207800  |
| C | 3.39130900  | 3.34390300  | 2.49028400  |
| H | 2.30700400  | 3.50213700  | 2.52961500  |
| H | 3.54905400  | 2.25993000  | 2.53987400  |
| H | 3.83489900  | 3.79508200  | 3.38284000  |
| C | 3.64029600  | 3.53611200  | -2.56845100 |
| H | 3.80934700  | 2.45881200  | -2.68482700 |
| H | 2.56393000  | 3.69949500  | -2.70014200 |
| H | 4.16526400  | 4.05320000  | -3.37723500 |
| C | 6.58577000  | 6.55230600  | 0.22930400  |
| H | 7.29471400  | 6.49970800  | -0.60429200 |
| H | 6.12278800  | 7.54778900  | 0.19970600  |
| H | 7.15383100  | 6.48526500  | 1.16336000  |
| C | 3.37223300  | -3.36130000 | 2.49122000  |
| H | 3.53225500  | -2.27769000 | 2.54109100  |
| H | 2.28756400  | -3.51725000 | 2.53005200  |
| H | 3.81440800  | -3.81365100 | 3.38388400  |
| C | 3.62771500  | -3.54864400 | -2.56738100 |
| H | 2.55065100  | -3.70619900 | -2.70049700 |
| H | 3.80262100  | -2.47215000 | -2.68253300 |
| H | 4.15088200  | -4.06775900 | -3.37603200 |
| C | 6.55340700  | -6.58344200 | 0.23071100  |
| H | 7.11512500  | -6.52579500 | 1.16919600  |
| H | 6.08574700  | -7.57636500 | 0.19064400  |
| H | 7.26852200  | -6.52853500 | -0.59747400 |
| C | -3.20286100 | -3.31646300 | 2.38681100  |
| H | -2.14120000 | -3.58923500 | 2.43737300  |
| H | -3.23847400 | -2.22134800 | 2.40990100  |
| H | -3.68935100 | -3.69174800 | 3.29218300  |
| C | -3.58886800 | -3.56224200 | -2.66602400 |
| H | -3.77623300 | -2.49110400 | -2.80879500 |
| H | -2.51172500 | -3.71300600 | -2.80675700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.11541100 | -4.10774100 | -3.45494700 |
| C | -6.55334500 | -6.44791400 | 0.24691100  |
| H | -6.45516500 | -7.02351300 | 1.17360300  |
| H | -7.54018500 | -5.96617500 | 0.26551400  |
| H | -6.55174100 | -7.15183400 | -0.59258300 |
| C | -3.19208000 | 3.32450600  | 2.38681300  |
| H | -3.23372800 | 2.22955800  | 2.40826000  |
| H | -2.12894600 | 3.59129600  | 2.43794900  |
| H | -3.67661800 | 3.70115400  | 3.29266300  |
| C | -3.58332200 | 3.57136700  | -2.66567200 |
| H | -2.50582300 | 3.71611400  | -2.80983300 |
| H | -3.77689300 | 2.50102500  | -2.80620800 |
| H | -4.10920100 | 4.11847800  | -3.45392300 |
| C | -6.49635100 | 6.50610400  | 0.25258600  |
| H | -7.09734200 | 6.36092100  | 1.15693300  |
| H | -6.04240300 | 7.50390000  | 0.32090100  |
| H | -7.17383300 | 6.51494100  | -0.60808600 |

**Structure: 33**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.14984400  | 2.84590300  | -0.15656800 |
| C | 0.73102100  | 4.22702200  | -0.09014600 |
| C | -0.63085400 | 4.22471000  | -0.12365900 |
| C | -1.04120800 | 2.84258800  | -0.21540600 |
| N | 0.05594100  | 2.02711900  | -0.23590500 |
| H | 1.40211000  | 5.07118300  | -0.02184900 |
| H | -1.30783600 | 5.06620500  | -0.08954100 |
| C | -2.80625700 | -1.09453100 | -0.34926500 |
| C | -4.19334700 | -0.68184700 | -0.34536600 |
| C | -4.19395100 | 0.67813800  | -0.34555100 |
| C | -2.80722800 | 1.09204800  | -0.34953300 |
| N | -1.98665100 | -0.00087300 | -0.37801400 |
| H | -5.03704500 | -1.35640900 | -0.32220800 |
| H | -5.03825000 | 1.35195500  | -0.32258400 |
| C | 2.91984300  | -1.09149300 | -0.14455700 |
| C | 4.30530800  | -0.67901000 | -0.08225000 |
| C | 4.30469200  | 0.68284500  | -0.08212900 |
| C | 2.91886300  | 1.09409500  | -0.14445600 |
| N | 2.10290800  | 0.00092100  | -0.18969000 |
| H | 5.14868900  | -1.35317100 | -0.03663900 |
| H | 5.14745300  | 1.35777000  | -0.03639800 |
| C | 1.15239700  | -2.84488300 | -0.15646500 |
| C | 0.73478300  | -4.22635600 | -0.08974600 |
| C | -0.62709700 | -4.22523200 | -0.12304600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.03866100 | -2.84348200 | -0.21495300 |
| N  | 0.05775500  | -2.02706100 | -0.23574300 |
| H  | 1.40662300  | -5.06991500 | -0.02138700 |
| H  | -1.30334600 | -5.06730800 | -0.08868300 |
| C  | 2.49190600  | 2.43236400  | -0.12507800 |
| C  | -2.38164100 | -2.42887300 | -0.26002000 |
| C  | -2.38381100 | 2.42678600  | -0.26052000 |
| C  | 2.49408600  | -2.43016300 | -0.12517600 |
| O  | 0.14539000  | -0.00013200 | -1.98899500 |
| N  | -0.06049000 | -0.00006400 | 1.68479700  |
| C  | -1.06790500 | -0.00040400 | 2.34617700  |
| O  | -2.06078400 | -0.00075800 | 3.02341800  |
| Mn | 0.06592800  | 0.00003900  | -0.38322500 |
| C  | 3.54319300  | 3.49415000  | -0.03516100 |
| C  | 4.08722600  | 4.03786900  | -1.21428900 |
| C  | 3.98079000  | 3.93130200  | 1.22968700  |
| C  | 5.07254400  | 5.02378900  | -1.10554700 |
| C  | 4.96787200  | 4.92000700  | 1.29163200  |
| C  | 5.52379900  | 5.48021900  | 0.13722800  |
| H  | 5.49851500  | 5.44428500  | -2.01440500 |
| H  | 5.31130000  | 5.25914500  | 2.26692200  |
| C  | -3.43826000 | -3.48046500 | -0.13602300 |
| C  | -4.03150800 | -4.02228700 | -1.29130700 |
| C  | -3.83807700 | -3.89792400 | 1.14941300  |
| C  | -5.03034400 | -4.98917600 | -1.14151000 |
| C  | -4.84331000 | -4.86511800 | 1.25028400  |
| C  | -5.44900400 | -5.42380400 | 0.12012300  |
| H  | -5.49335200 | -5.41041500 | -2.03172600 |
| H  | -5.16245500 | -5.18788300 | 2.23930600  |
| C  | -3.44140500 | 3.47743100  | -0.13675800 |
| C  | -4.03505000 | 4.01854600  | -1.29214600 |
| C  | -3.84185000 | 3.89455200  | 1.14861400  |
| C  | -5.03492900 | 4.98441100  | -1.14255100 |
| C  | -4.84809800 | 4.86068700  | 1.24927900  |
| C  | -5.45422300 | 5.41866700  | 0.11898200  |
| H  | -5.49825700 | 5.40509500  | -2.03286100 |
| H  | -5.16773500 | 5.18317900  | 2.23823200  |
| C  | 3.54635700  | -3.49098000 | -0.03537100 |
| C  | 3.98618800  | -3.92607600 | 1.22944300  |
| C  | 4.08914000  | -4.03577700 | -1.21454700 |
| C  | 4.97421400  | -4.91380400 | 1.29126300  |
| C  | 5.07554600  | -5.02066300 | -1.10592600 |
| C  | 5.52900100  | -5.47503300 | 0.13677200  |
| H  | 5.31935200  | -5.25137200 | 2.26649900  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.50060000  | -5.44194400 | -2.01484500 |
| C | 3.40253500  | -3.33232400 | 2.49092400  |
| H | 3.56692100  | -2.24905600 | 2.53392100  |
| H | 2.31754800  | -3.48384000 | 2.53712700  |
| H | 3.84848100  | -3.78143400 | 3.38335000  |
| C | 3.61487300  | -3.55859600 | -2.56800000 |
| H | 2.53814500  | -3.72510700 | -2.69281400 |
| H | 3.78069800  | -2.48151800 | -2.69071200 |
| H | 4.13642200  | -4.07859700 | -3.37712500 |
| C | 6.57146400  | -6.56510000 | 0.22879500  |
| H | 6.10471900  | -7.55919500 | 0.21652900  |
| H | 7.27042400  | -6.52471600 | -0.61383400 |
| H | 7.15101200  | -6.48928200 | 1.15511100  |
| C | 3.39575100  | 3.33881100  | 2.49111900  |
| H | 2.31086800  | 3.49138000  | 2.53646300  |
| H | 3.55908200  | 2.25542200  | 2.53489400  |
| H | 3.84146600  | 3.78807100  | 3.38358500  |
| C | 3.61534700  | 3.55843600  | -2.56778100 |
| H | 3.78343800  | 2.48156600  | -2.68925700 |
| H | 2.53842800  | 3.72269300  | -2.69390800 |
| H | 4.13674800  | 4.07866000  | -3.37685900 |
| C | 6.56515400  | 6.57135600  | 0.22910900  |
| H | 7.26866700  | 6.52688300  | -0.60953700 |
| H | 6.09795400  | 7.56510400  | 0.20891700  |
| H | 7.13975600  | 6.50079800  | 1.15889900  |
| C | -3.19449500 | 3.31728900  | 2.38702600  |
| H | -3.22959800 | 2.22211000  | 2.40839400  |
| H | -2.13288100 | 3.59032500  | 2.43682700  |
| H | -3.67996700 | 3.69099100  | 3.29359500  |
| C | -3.60057900 | 3.55808900  | -2.66488700 |
| H | -2.52359500 | 3.70419600  | -2.81149000 |
| H | -3.79314000 | 2.48747400  | -2.80474700 |
| H | -4.12892000 | 4.10428400  | -3.45212500 |
| C | -6.51588400 | 6.48508600  | 0.25795400  |
| H | -7.21128500 | 6.47267800  | -0.58835100 |
| H | -7.09688200 | 6.35480300  | 1.17741600  |
| H | -6.06677000 | 7.48668200  | 0.29608900  |
| C | -3.19108800 | -3.32001100 | 2.38771300  |
| H | -2.12937500 | -3.59265700 | 2.43769700  |
| H | -3.22662800 | -2.22484200 | 2.40877000  |
| H | -3.67650000 | -3.69363800 | 3.29434600  |
| C | -3.59762800 | -3.56155200 | -2.66414400 |
| H | -3.79113000 | -2.49111700 | -2.80407100 |
| H | -2.52053700 | -3.70674400 | -2.81087500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.12559800 | -4.10827100 | -3.45126600 |
| C | -6.50950500 | -6.49135900 | 0.25921400  |
| H | -7.08880200 | -6.36327700 | 1.18004900  |
| H | -7.20658000 | -6.47794600 | -0.58570600 |
| H | -6.05950000 | -7.49265900 | 0.29453700  |

**Structure: 53**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.90743900  | -1.09920100 | -0.10601100 |
| C | 4.29059400  | -0.68570500 | -0.04535300 |
| C | 4.29235100  | 0.67570300  | -0.04548500 |
| C | 2.91026900  | 1.09275200  | -0.10620300 |
| N | 2.09150000  | -0.00220700 | -0.14385800 |
| H | 5.13219400  | -1.36209200 | -0.00411100 |
| H | 5.13567900  | 1.34994100  | -0.00436500 |
| C | -1.03421800 | 2.85150900  | -0.22398400 |
| C | -0.62039400 | 4.23438000  | -0.15648400 |
| C | 0.74025900  | 4.23453000  | -0.12031500 |
| C | 1.15696600  | 2.85138400  | -0.16074100 |
| N | 0.06181300  | 2.03381000  | -0.23108700 |
| H | -1.29715000 | 5.07640800  | -0.13700400 |
| H | 1.41432200  | 5.07709200  | -0.06387600 |
| C | -1.04144700 | -2.84790300 | -0.22404300 |
| C | -0.63116700 | -4.23187800 | -0.15681000 |
| C | 0.72947100  | -4.23548400 | -0.12048200 |
| C | 1.14972200  | -2.85340700 | -0.16065200 |
| N | 0.05660000  | -2.03301500 | -0.23098500 |
| H | -1.30999300 | -5.07226000 | -0.13753700 |
| H | 1.40138100  | -5.07976400 | -0.06409400 |
| C | -2.79632900 | -1.09179000 | -0.32585700 |
| C | -4.17987500 | -0.67403400 | -0.32371200 |
| C | -4.17814200 | 0.68557000  | -0.32372400 |
| C | -2.79347300 | 1.09974200  | -0.32595000 |
| N | -1.97491600 | 0.00294900  | -0.34898200 |
| H | -5.02374300 | -1.34818200 | -0.30406000 |
| H | -5.02035900 | 1.36180200  | -0.30402400 |
| C | 2.48828200  | -2.43845700 | -0.10885300 |
| C | -2.37457400 | 2.43587200  | -0.25609000 |
| C | 2.49453200  | 2.43301900  | -0.10913000 |
| C | -2.38083800 | -2.42887900 | -0.25595800 |
| O | 0.16704600  | 0.00024700  | -1.99270200 |
| N | -0.09492500 | 0.00057200  | 1.77305800  |
| C | -1.12696300 | 0.00025300  | 2.39383200  |
| O | -2.14989300 | -0.00006700 | 3.02949200  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Mn | 0.06797000  | 0.00038200  | -0.33620500 |
| C  | 3.54268600  | -3.49766100 | -0.03056200 |
| C  | 4.09672200  | -4.01695600 | -1.21624600 |
| C  | 3.97109200  | -3.95803200 | 1.22904600  |
| C  | 5.08325200  | -5.00273700 | -1.11863700 |
| C  | 4.96008400  | -4.94556900 | 1.27944600  |
| C  | 5.52593700  | -5.48211600 | 0.11869700  |
| H  | 5.51708400  | -5.40486000 | -2.03206000 |
| H  | 5.29662300  | -5.30294800 | 2.25058000  |
| C  | 3.55172700  | 3.48946900  | -0.03125600 |
| C  | 4.10679200  | 4.00711200  | -1.21716600 |
| C  | 3.98189700  | 3.94871900  | 1.22817500  |
| C  | 5.09615300  | 4.99011700  | -1.11998400 |
| C  | 4.97366400  | 4.93346900  | 1.27814600  |
| C  | 5.54065300  | 5.46830400  | 0.11714200  |
| H  | 5.53083100  | 5.39089500  | -2.03359300 |
| H  | 5.31161300  | 5.28992700  | 2.24913200  |
| C  | -3.43332100 | 3.48613700  | -0.14349700 |
| C  | -3.83490000 | 3.91433300  | 1.13788100  |
| C  | -4.02467200 | 4.01683100  | -1.30486000 |
| C  | -4.84122400 | 4.88138900  | 1.22835800  |
| C  | -5.02468100 | 4.98404100  | -1.16500700 |
| C  | -5.44565200 | 5.42926900  | 0.09216900  |
| H  | -5.16197900 | 5.21301500  | 2.21389900  |
| H  | -5.48664700 | 5.39701600  | -2.05959400 |
| C  | -3.44207300 | -3.47667700 | -0.14388700 |
| C  | -4.02990900 | -4.00985600 | -1.30582600 |
| C  | -3.84115400 | -3.90871300 | 1.13703500  |
| C  | -5.02509800 | -4.98226000 | -1.16706600 |
| C  | -4.84242800 | -4.88103800 | 1.22640700  |
| C  | -5.44784200 | -5.42684700 | 0.08967700  |
| H  | -5.47963100 | -5.40200400 | -2.06229100 |
| H  | -5.15614100 | -5.22092800 | 2.21141000  |
| C  | 3.38393900  | 3.38455600  | 2.49651500  |
| H  | 2.30013300  | 3.54713300  | 2.53227300  |
| H  | 3.53757100  | 2.30084900  | 2.56188200  |
| H  | 3.82778000  | 3.84660600  | 3.38333700  |
| C  | 3.64298800  | 3.50283700  | -2.56439800 |
| H  | 3.81410100  | 2.42441600  | -2.66641200 |
| H  | 2.56637000  | 3.66112600  | -2.69939700 |
| H  | 4.16751900  | 4.01013200  | -3.37960400 |
| C  | 6.58668300  | 6.55601300  | 0.19508900  |
| H  | 7.30281200  | 6.48459200  | -0.63095100 |
| H  | 6.12535400  | 7.55114500  | 0.13976100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 7.14641000  | 6.50841000  | 1.13531000  |
| C | 3.37415600  | -3.39223500 | 2.49714100  |
| H | 3.53036800  | -2.30889200 | 2.56240700  |
| H | 2.28995400  | -3.55221200 | 2.53263100  |
| H | 3.81662900  | -3.85524100 | 3.38414800  |
| C | 3.63474000  | -3.51154300 | -2.56367600 |
| H | 2.55772500  | -3.66683700 | -2.69897600 |
| H | 3.80891300  | -2.43361800 | -2.66576400 |
| H | 4.15808500  | -4.02041200 | -3.37866300 |
| C | 6.56873800  | -6.57289800 | 0.19696300  |
| H | 7.12616600  | -6.52895400 | 1.13871700  |
| H | 6.10477400  | -7.56660400 | 0.13816600  |
| H | 7.28719100  | -6.50164800 | -0.62708100 |
| C | -3.19120100 | -3.34757900 | 2.38148900  |
| H | -2.12870900 | -3.61862100 | 2.42396300  |
| H | -3.22924500 | -2.25280000 | 2.41930400  |
| H | -3.67279000 | -3.73584100 | 3.28398600  |
| C | -3.58819200 | -3.54083100 | -2.67330500 |
| H | -3.77678500 | -2.46862600 | -2.80613000 |
| H | -2.51109000 | -3.68849200 | -2.81711000 |
| H | -4.11520800 | -4.07945600 | -3.46658700 |
| C | -6.55083700 | -6.45180400 | 0.21847900  |
| H | -6.41412600 | -7.07864400 | 1.10641600  |
| H | -7.53145500 | -5.96607400 | 0.31166300  |
| H | -6.59439100 | -7.10780900 | -0.65765300 |
| C | -3.18847500 | 3.34832500  | 2.38196300  |
| H | -3.23012100 | 2.25360100  | 2.41777200  |
| H | -2.12514100 | 3.61572300  | 2.42602600  |
| H | -3.66965900 | 3.73656300  | 3.28468500  |
| C | -3.58803500 | 3.54388300  | -2.67262400 |
| H | -2.51062900 | 3.68681900  | -2.81871500 |
| H | -3.78143000 | 2.47230900  | -2.80379100 |
| H | -4.11431100 | 4.08379700  | -3.46552400 |
| C | -6.50721000 | 6.49712300  | 0.22039300  |
| H | -7.09116300 | 6.37345200  | 1.13888900  |
| H | -6.05754900 | 7.49865200  | 0.25316500  |
| H | -7.19989200 | 6.47935800  | -0.62802300 |

**Structure: 4**

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 1.04983700  | 1.40752000  | 0.00521400 |
| C | -0.15000800 | 0.70111500  | 0.05475500 |
| C | -0.15000900 | -0.70111300 | 0.05475400 |
| C | 1.04983500  | -1.40751900 | 0.00521900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.25544900  | -0.69934600 | -0.04912500 |
| C | 2.25544900  | 0.69934400  | -0.04913000 |
| H | 1.05145600  | 2.49519000  | 0.00128900  |
| H | 1.05145200  | -2.49518900 | 0.00130000  |
| H | 3.19761500  | -1.23929000 | -0.09738100 |
| H | 3.19761600  | 1.23928800  | -0.09739100 |
| C | -1.56757400 | -1.22827600 | 0.13445400  |
| C | -1.56757400 | 1.22827500  | 0.13446200  |
| C | -2.41769200 | 0.00000100  | -0.27920000 |
| H | -3.41676400 | 0.00000300  | 0.16776000  |
| H | -2.54200100 | 0.00000300  | -1.36889600 |
| H | -1.80074100 | 1.53439700  | 1.16531500  |
| H | -1.74208700 | 2.10275100  | -0.50284500 |
| H | -1.74207700 | -2.10274000 | -0.50287300 |
| H | -1.80074800 | -1.53442300 | 1.16529700  |

**Structure: <sup>3</sup>INT2**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.15985400 | 2.99700200  | -0.42093900 |
| C | -0.56810100 | 4.31333500  | -0.37990100 |
| C | 0.76649500  | 4.14821700  | -0.15062200 |
| C | 1.01930100  | 2.72755900  | -0.10971000 |
| N | -0.17022800 | 2.06024700  | -0.26480300 |
| H | -1.12378600 | 5.23461400  | -0.48486700 |
| H | 1.53178100  | 4.90513000  | -0.05190600 |
| C | 2.17270800  | -1.30047500 | -1.00818600 |
| C | 3.58734800  | -1.04735500 | -1.11186600 |
| C | 3.80442600  | 0.22271200  | -0.66122500 |
| C | 2.51696200  | 0.78944500  | -0.34414900 |
| N | 1.54990900  | -0.16938300 | -0.53541000 |
| H | 4.31077000  | -1.77160900 | -1.45939000 |
| H | 4.74010600  | 0.75687200  | -0.58114500 |
| C | -3.26667800 | -0.66318400 | 0.33344400  |
| C | -4.58477900 | -0.08204800 | 0.42524000  |
| C | -4.47754700 | 1.22282400  | 0.04046300  |
| C | -3.08158800 | 1.47545600  | -0.22525300 |
| N | -2.37865000 | 0.31053000  | -0.05087800 |
| H | -5.47331200 | -0.62684800 | 0.71199000  |
| H | -5.25589300 | 1.96968900  | -0.02961100 |
| C | -1.76282900 | -2.59103100 | 0.06971700  |
| C | -1.54964300 | -3.99901600 | -0.16289500 |
| C | -0.33278000 | -4.12821300 | -0.76787600 |
| C | 0.24846000  | -2.81105000 | -0.84084300 |
| N | -0.64357800 | -1.90024300 | -0.32786000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.26988100 | -4.77105300 | 0.06879000  |
| H  | 0.15626800  | -5.02916700 | -1.11117100 |
| C  | -2.53421900 | 2.73965400  | -0.47131900 |
| C  | 1.55997100  | -2.53598300 | -1.24205800 |
| C  | 2.29157800  | 2.14594400  | -0.08508700 |
| C  | -2.98563000 | -2.02900100 | 0.45523200  |
| O  | -0.25804500 | 0.09945300  | 1.44810800  |
| N  | -0.65003600 | 0.16439400  | -2.24420600 |
| C  | 0.17578400  | 0.54105400  | -3.04374300 |
| O  | 0.97196600  | 0.88890000  | -3.86183800 |
| Mn | -0.41009700 | 0.07448600  | -0.27299000 |
| C  | -3.46617200 | 3.88596400  | -0.71162500 |
| C  | -3.95048200 | 4.65308300  | 0.36532200  |
| C  | -3.85250500 | 4.18133800  | -2.03377300 |
| C  | -4.82273600 | 5.71350200  | 0.09817700  |
| C  | -4.72580400 | 5.25042900  | -2.25641400 |
| C  | -5.21930600 | 6.02966300  | -1.20509000 |
| H  | -5.20178600 | 6.30607000  | 0.92859700  |
| H  | -5.02856500 | 5.47952900  | -3.27632900 |
| C  | 2.34972600  | -3.60498900 | -1.93172800 |
| C  | 3.08503100  | -4.56023200 | -1.20440300 |
| C  | 2.35018700  | -3.62343000 | -3.34240200 |
| C  | 3.81244600  | -5.52914500 | -1.90377400 |
| C  | 3.09059700  | -4.61041100 | -4.00040100 |
| C  | 3.82560700  | -5.57271200 | -3.30098100 |
| H  | 4.38400300  | -6.26556800 | -1.34225900 |
| H  | 3.09402700  | -4.62594600 | -5.08853600 |
| C  | 3.48098300  | 3.04056600  | 0.06960300  |
| C  | 3.99976900  | 3.27831500  | 1.35628800  |
| C  | 4.06978100  | 3.62788800  | -1.06821500 |
| C  | 5.12292600  | 4.10174000  | 1.48436900  |
| C  | 5.19144800  | 4.44500300  | -0.89299000 |
| C  | 5.73538800  | 4.68876700  | 0.37268300  |
| H  | 5.52817500  | 4.28787300  | 2.47708700  |
| H  | 5.65091000  | 4.90269600  | -1.76701300 |
| C  | -4.08518200 | -2.94863300 | 0.88981900  |
| C  | -4.99864700 | -3.46065600 | -0.05377500 |
| C  | -4.19349200 | -3.29548300 | 2.24999600  |
| C  | -6.01585700 | -4.31258000 | 0.38761900  |
| C  | -5.22681300 | -4.14918800 | 2.64937400  |
| C  | -6.14629100 | -4.66955500 | 1.73389300  |
| H  | -6.72449600 | -4.70675700 | -0.33829700 |
| H  | -5.31480600 | -4.41367800 | 3.70133500  |
| C  | -4.87936600 | -3.09786900 | -1.51650500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.98019100 | -2.01698900 | -1.66901400 |
| H | -3.89780400 | -3.37926900 | -1.91583400 |
| H | -5.64752700 | -3.59991600 | -2.11241300 |
| C | -3.20152500 | -2.76207400 | 3.25810200  |
| H | -2.19281200 | -3.14182300 | 3.05606600  |
| H | -3.13470000 | -1.66866300 | 3.21774500  |
| H | -3.47445800 | -3.05284900 | 4.27717000  |
| C | -7.23552000 | -5.61737300 | 2.17979500  |
| H | -7.49208400 | -5.46752500 | 3.23397200  |
| H | -8.14753500 | -5.48840900 | 1.58646400  |
| H | -6.91970200 | -6.66311600 | 2.06589100  |
| C | -3.33163900 | 3.35343700  | -3.18660200 |
| H | -2.23627500 | 3.37393000  | -3.22970800 |
| H | -3.61323200 | 2.29902000  | -3.08167500 |
| H | -3.71869600 | 3.71828000  | -4.14284600 |
| C | -3.53595700 | 4.33513500  | 1.78398600  |
| H | -3.80456800 | 3.30768800  | 2.05704200  |
| H | -2.44954800 | 4.41848600  | 1.90802000  |
| H | -4.01314100 | 5.01369600  | 2.49758700  |
| C | -6.13497400 | 7.20136800  | -1.47425100 |
| H | -6.79779000 | 7.39743000  | -0.62441300 |
| H | -5.55884100 | 8.11851300  | -1.65653000 |
| H | -6.75804300 | 7.02875100  | -2.35858700 |
| C | 3.48928600  | 3.39656600  | -2.44534600 |
| H | 3.38403800  | 2.33045800  | -2.67447800 |
| H | 2.48285600  | 3.82505600  | -2.52707100 |
| H | 4.11451600  | 3.85316500  | -3.21862200 |
| C | 3.34929900  | 2.65590900  | 2.56896500  |
| H | 2.30516700  | 2.97774900  | 2.66766600  |
| H | 3.33688500  | 1.56375500  | 2.50136900  |
| H | 3.87896900  | 2.92331500  | 3.48714300  |
| C | 6.97150400  | 5.54393700  | 0.53071900  |
| H | 7.02450100  | 6.32023600  | -0.24055500 |
| H | 6.99802000  | 6.03504000  | 1.50957400  |
| H | 7.88398000  | 4.93846800  | 0.44531200  |
| C | 1.57345000  | -2.59257000 | -4.13000800 |
| H | 0.52343300  | -2.55613900 | -3.81735500 |
| H | 1.96975500  | -1.58080400 | -3.98471700 |
| H | 1.60307300  | -2.81309600 | -5.20141800 |
| C | 3.10081600  | -4.53838600 | 0.30622300  |
| H | 3.47776000  | -3.58254100 | 0.68674700  |
| H | 2.09258900  | -4.66497300 | 0.71795400  |
| H | 3.73359500  | -5.33519000 | 0.70853800  |
| C | 4.59107400  | -6.64792100 | -4.03687700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.95068300  | -7.51531200 | -4.24622000 |
| H | 4.96872200  | -6.28424700 | -4.99879500 |
| H | 5.44394700  | -7.00689400 | -3.45066400 |
| C | 4.19025500  | -1.16497400 | 2.65068700  |
| C | 2.90500400  | -1.17855100 | 3.19150400  |
| C | 2.63783400  | -0.52190600 | 4.40372500  |
| C | 3.65906800  | 0.12476700  | 5.09583000  |
| C | 4.95392400  | 0.12016800  | 4.56381300  |
| C | 5.21617900  | -0.51415400 | 3.34511100  |
| H | 4.39298100  | -1.64393700 | 1.69701200  |
| H | 3.45537400  | 0.62797800  | 6.03835900  |
| H | 5.75946600  | 0.61775900  | 5.09790200  |
| H | 6.22310900  | -0.50313800 | 2.93585700  |
| C | 1.16480700  | -0.62275500 | 4.73945100  |
| C | 1.64199500  | -1.79382800 | 2.64212600  |
| C | 0.68241700  | -1.79901700 | 3.85367600  |
| H | -0.36155500 | -1.69572900 | 3.54875300  |
| H | 0.79013400  | -2.74110900 | 4.40624900  |
| H | 1.23299400  | -1.14474900 | 1.85208900  |
| H | 1.78481000  | -2.78135600 | 2.19333600  |
| H | 0.97054000  | -0.77593000 | 5.80734600  |
| H | 0.65473300  | 0.30532000  | 4.44444200  |

**Structure: <sup>5</sup>INT2**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.10551500 | 3.01513300  | -0.42054600 |
| C | -0.51504700 | 4.33485300  | -0.45137300 |
| C | 0.83301600  | 4.16413800  | -0.36944900 |
| C | 1.07197900  | 2.73914300  | -0.32072900 |
| N | -0.11997700 | 2.06878300  | -0.34697400 |
| H | -1.07534200 | 5.25667900  | -0.51413700 |
| H | 1.60950800  | 4.91533500  | -0.35828800 |
| C | 2.27680100  | -1.37636300 | -0.74699900 |
| C | 3.69891300  | -1.14045800 | -0.83490500 |
| C | 3.89279200  | 0.18481200  | -0.59370600 |
| C | 2.58476200  | 0.76762900  | -0.39511300 |
| N | 1.62679500  | -0.20477800 | -0.45531600 |
| H | 4.43443000  | -1.90225900 | -1.04935700 |
| H | 4.81955100  | 0.73938600  | -0.57936900 |
| C | -3.31521400 | -0.66776800 | 0.04365500  |
| C | -4.62918800 | -0.07652600 | 0.15296200  |
| C | -4.47652300 | 1.26129200  | -0.05507100 |
| C | -3.06361500 | 1.49303800  | -0.25352900 |
| N | -2.38700400 | 0.30792700  | -0.20013900 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -5.53806500 | -0.62946900 | 0.34284400  |
| H  | -5.23235600 | 2.03357300  | -0.06052200 |
| C  | -1.80079900 | -2.62592500 | -0.13811200 |
| C  | -1.58418400 | -4.04365100 | -0.30819700 |
| C  | -0.28106200 | -4.19905200 | -0.67798200 |
| C  | 0.30854700  | -2.88150000 | -0.68459500 |
| N  | -0.63398200 | -1.94690300 | -0.35674400 |
| H  | -2.34610700 | -4.80041000 | -0.18734100 |
| H  | 0.25039900  | -5.11056900 | -0.91136800 |
| C  | -2.48549400 | 2.76517800  | -0.40699600 |
| C  | 1.66740600  | -2.62364500 | -0.93652400 |
| C  | 2.34637400  | 2.15000400  | -0.30630500 |
| C  | -3.05455900 | -2.04481500 | 0.11347300  |
| O  | -0.31820400 | 0.07721500  | 1.40917300  |
| N  | -0.44130000 | 0.12155800  | -2.35962200 |
| C  | 0.49922600  | 0.34587800  | -3.07824500 |
| O  | 1.43010400  | 0.55401900  | -3.81164600 |
| Mn | -0.38004900 | 0.06571000  | -0.24986100 |
| C  | -3.40795600 | 3.93762500  | -0.51987000 |
| C  | -3.80906800 | 4.63192600  | 0.63740700  |
| C  | -3.87035500 | 4.32477900  | -1.79233400 |
| C  | -4.67890800 | 5.71786600  | 0.49815900  |
| C  | -4.73745100 | 5.41770500  | -1.88447600 |
| C  | -5.15094500 | 6.12815200  | -0.75289200 |
| H  | -4.99600500 | 6.25537500  | 1.38962200  |
| H  | -5.09942200 | 5.72009900  | -2.86510600 |
| C  | 2.50979600  | -3.73615100 | -1.47692400 |
| C  | 3.16128800  | -4.63797200 | -0.61699400 |
| C  | 2.63391000  | -3.85197300 | -2.87786000 |
| C  | 3.93874200  | -5.65765500 | -1.17651500 |
| C  | 3.41856200  | -4.88845700 | -3.39120000 |
| C  | 4.08121800  | -5.79797000 | -2.55967400 |
| H  | 4.44501800  | -6.35666400 | -0.51389400 |
| H  | 3.51471500  | -4.98700400 | -4.47069900 |
| C  | 3.53733400  | 3.05260100  | -0.28654900 |
| C  | 4.19410100  | 3.29229800  | 0.93581900  |
| C  | 4.00054100  | 3.62436200  | -1.48847800 |
| C  | 5.32132400  | 4.11908500  | 0.93522600  |
| C  | 5.13580100  | 4.44048100  | -1.43869800 |
| C  | 5.80678300  | 4.70212500  | -0.23989100 |
| H  | 5.83372600  | 4.30861100  | 1.87638600  |
| H  | 5.50662100  | 4.87908200  | -2.36302600 |
| C  | -4.19186600 | -2.96056200 | 0.43680100  |
| C  | -5.05489300 | -3.40679000 | -0.58239400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.37260100 | -3.37616100 | 1.77033800  |
| C | -6.10332300 | -4.26728400 | -0.24208400 |
| C | -5.43663800 | -4.23393200 | 2.06527000  |
| C | -6.31410000 | -4.68758100 | 1.07522900  |
| H | -6.76978500 | -4.61978600 | -1.02676300 |
| H | -5.58155500 | -4.55720400 | 3.09417200  |
| C | -4.84286100 | -2.97426300 | -2.01533300 |
| H | -4.94641300 | -1.88805800 | -2.12347800 |
| H | -3.83436500 | -3.22851200 | -2.36284000 |
| H | -5.56471500 | -3.45266700 | -2.68388500 |
| C | -3.42756200 | -2.91087500 | 2.85487100  |
| H | -2.41084500 | -3.28433200 | 2.68310100  |
| H | -3.35381200 | -1.81736000 | 2.88258800  |
| H | -3.75327900 | -3.25728900 | 3.84018400  |
| C | -7.47610100 | -5.58846400 | 1.42352700  |
| H | -7.73014400 | -6.25568300 | 0.59268700  |
| H | -7.25631800 | -6.20632900 | 2.30082400  |
| H | -8.37447900 | -5.00080600 | 1.65538900  |
| C | -3.43807100 | 3.56898600  | -3.02796800 |
| H | -2.34660300 | 3.56374400  | -3.13229300 |
| H | -3.74804700 | 2.51816500  | -2.98134500 |
| H | -3.86566200 | 4.01117300  | -3.93269700 |
| C | -3.31333300 | 4.20482300  | 2.00004200  |
| H | -3.58709400 | 3.16495300  | 2.21525500  |
| H | -2.21975400 | 4.25938400  | 2.06029800  |
| H | -3.73006500 | 4.83742000  | 2.78940000  |
| C | -6.06232400 | 7.32659600  | -0.88147900 |
| H | -6.73303200 | 7.23068500  | -1.74222100 |
| H | -6.67680100 | 7.46204000  | 0.01512900  |
| H | -5.48284000 | 8.24892100  | -1.02174500 |
| C | 3.28924300  | 3.37043400  | -2.79843100 |
| H | 3.08187300  | 2.30841000  | -2.96758600 |
| H | 2.31607400  | 3.87725400  | -2.82087600 |
| H | 3.87827500  | 3.74324400  | -3.64187300 |
| C | 3.69568100  | 2.65985900  | 2.21335100  |
| H | 2.63569300  | 2.88019200  | 2.38682200  |
| H | 3.78504500  | 1.56816600  | 2.19038200  |
| H | 4.26101300  | 3.01317600  | 3.07943100  |
| C | 7.01084300  | 5.61486700  | -0.20953900 |
| H | 6.71299900  | 6.65447900  | -0.01744900 |
| H | 7.71248700  | 5.32734700  | 0.58114500  |
| H | 7.54897200  | 5.60169200  | -1.16349600 |
| C | 1.93643100  | -2.87901600 | -3.80056800 |
| H | 0.86130600  | -2.82724600 | -3.59190700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.31607800  | -1.85699200 | -3.68676000 |
| H | 2.06573300  | -3.17006700 | -4.84729100 |
| C | 3.02152400  | -4.50597200 | 0.88075600  |
| H | 3.29358800  | -3.49967300 | 1.21599500  |
| H | 1.98541200  | -4.66900800 | 1.20137700  |
| H | 3.65646400  | -5.22563300 | 1.40614700  |
| C | 4.94947700  | -6.88605200 | -3.14743100 |
| H | 5.93138000  | -6.49130800 | -3.44054300 |
| H | 5.12198900  | -7.69538700 | -2.43023400 |
| H | 4.49515500  | -7.31914700 | -4.04580400 |
| C | 3.98362700  | -1.30531200 | 3.36473500  |
| C | 2.61497500  | -1.14843800 | 3.57615300  |
| C | 2.14141400  | -0.12257900 | 4.40931100  |
| C | 3.03406000  | 0.73071500  | 5.05429000  |
| C | 4.40993300  | 0.55776400  | 4.86072400  |
| C | 4.88210100  | -0.44890400 | 4.01351400  |
| H | 4.35702500  | -2.09538000 | 2.71723800  |
| H | 2.66784300  | 1.51905900  | 5.70848700  |
| H | 5.11453800  | 1.21188200  | 5.36867500  |
| H | 5.95182800  | -0.57386500 | 3.86461200  |
| C | 0.62871000  | -0.13207400 | 4.44473900  |
| C | 1.45802800  | -1.95182400 | 3.02123400  |
| C | 0.27412700  | -1.55176300 | 3.93675900  |
| H | -0.67750600 | -1.56918800 | 3.40108600  |
| H | 0.21424000  | -2.24373000 | 4.78726100  |
| H | 1.24272600  | -1.64616300 | 1.99150400  |
| H | 1.65022600  | -3.03070500 | 3.02145400  |
| H | 0.21804100  | 0.08857300  | 5.43748700  |
| H | 0.23572100  | 0.61253100  | 3.74077000  |

**Structure: MECP**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.31787800 | 2.96474400  | -0.42394200 |
| C | -0.79420200 | 4.30850500  | -0.45167800 |
| C | 0.56270000  | 4.21157400  | -0.38216200 |
| C | 0.88727700  | 2.80626700  | -0.35909400 |
| N | -0.27439900 | 2.07384300  | -0.37368500 |
| H | -1.40002000 | 5.20182700  | -0.50322800 |
| H | 1.29146800  | 5.00928500  | -0.37498500 |
| C | 2.24099700  | -1.19775900 | -1.14539000 |
| C | 3.64364700  | -0.88522800 | -1.27824900 |
| C | 3.79444600  | 0.42475100  | -0.94101600 |
| C | 2.47845200  | 0.94152700  | -0.65089500 |
| N | 1.55803400  | -0.07129900 | -0.76432100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 4.40505700  | -1.59275200 | -1.57358400 |
| H  | 4.70280000  | 1.00895200  | -0.91370000 |
| C  | -3.25639900 | -0.82949600 | 0.21971500  |
| C  | -4.59290700 | -0.31186900 | 0.39141000  |
| C  | -4.54127700 | 1.02274900  | 0.12611600  |
| C  | -3.16349800 | 1.34497800  | -0.15941000 |
| N  | -2.40925800 | 0.20103900  | -0.10213200 |
| H  | -5.45393000 | -0.90971300 | 0.65387400  |
| H  | -5.34946100 | 1.73980100  | 0.13915000  |
| C  | -1.67026800 | -2.68763900 | -0.12807000 |
| C  | -1.38351100 | -4.08392900 | -0.34941300 |
| C  | -0.13207600 | -4.15660000 | -0.88243000 |
| C  | 0.38535300  | -2.81123900 | -0.93578300 |
| N  | -0.57282600 | -1.93965900 | -0.47768300 |
| H  | -2.07330400 | -4.89125500 | -0.14901900 |
| H  | 0.41164600  | -5.03605300 | -1.19626200 |
| C  | -2.68261900 | 2.64614000  | -0.36872700 |
| C  | 1.69679200  | -2.48079900 | -1.30648600 |
| C  | 2.19305500  | 2.29638100  | -0.42851100 |
| C  | -2.92357500 | -2.19144100 | 0.26140900  |
| O  | -0.13930000 | 0.00403300  | 1.28524000  |
| N  | -0.74421400 | 0.15820900  | -2.37148100 |
| C  | -0.08030000 | 0.36348100  | -3.35706700 |
| O  | 0.53659700  | 0.55173900  | -4.36486700 |
| Mn | -0.42115500 | 0.06601000  | -0.38925100 |
| C  | -3.67949800 | 3.76447900  | -0.48592700 |
| C  | -4.11105800 | 4.46288400  | 0.66161200  |
| C  | -4.18471900 | 4.10811800  | -1.75869700 |
| C  | -5.04297200 | 5.49625200  | 0.51295800  |
| C  | -5.11409500 | 5.14905900  | -1.85759700 |
| C  | -5.55411300 | 5.85867000  | -0.73637500 |
| H  | -5.37777300 | 6.03042600  | 1.40020300  |
| H  | -5.50468600 | 5.40988400  | -2.83945700 |
| C  | 2.57997600  | -3.55580200 | -1.87187900 |
| C  | 3.31620400  | -4.40762400 | -1.02228800 |
| C  | 2.66892400  | -3.69728700 | -3.27449200 |
| C  | 4.12666100  | -5.39537500 | -1.59266100 |
| C  | 3.49212500  | -4.70022600 | -3.79758200 |
| C  | 4.23063600  | -5.55784500 | -2.97693000 |
| H  | 4.69187800  | -6.05281200 | -0.93465600 |
| H  | 3.55568900  | -4.81232800 | -4.87832700 |
| C  | 3.34197700  | 3.26252600  | -0.35989900 |
| C  | 3.89336600  | 3.60019000  | 0.89436600  |
| C  | 3.86574500  | 3.82625600  | -1.54425200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.96327300  | 4.50153500  | 0.93998500  |
| C | 4.93782500  | 4.71999700  | -1.44706300 |
| C | 5.50310600  | 5.06980300  | -0.21708800 |
| H | 5.38497700  | 4.76376500  | 1.90849900  |
| H | 5.33917500  | 5.15533900  | -2.36039200 |
| C | -3.98662100 | -3.17447100 | 0.66619700  |
| C | -4.86329700 | -3.71985500 | -0.29693600 |
| C | -4.10581100 | -3.54464700 | 2.02266500  |
| C | -5.84381300 | -4.62708000 | 0.11903000  |
| C | -5.10355200 | -4.45381000 | 2.39186100  |
| C | -5.98107700 | -5.00955100 | 1.45691700  |
| H | -6.51998400 | -5.04304900 | -0.62558600 |
| H | -5.19595200 | -4.73298500 | 3.43982100  |
| C | -4.76369900 | -3.33996100 | -1.75801500 |
| H | -4.92468400 | -2.26608900 | -1.90886900 |
| H | -3.77451500 | -3.57029500 | -2.17021300 |
| H | -5.50930700 | -3.87901700 | -2.35041500 |
| C | -3.17860200 | -2.97765100 | 3.07507400  |
| H | -2.13353800 | -3.24449700 | 2.87686900  |
| H | -3.22073200 | -1.88268000 | 3.10617500  |
| H | -3.44004400 | -3.35559000 | 4.06830600  |
| C | -7.03180700 | -6.01239500 | 1.87430700  |
| H | -7.30316400 | -5.89266100 | 2.92843200  |
| H | -7.94368700 | -5.91137600 | 1.27553400  |
| H | -6.67236800 | -7.04218700 | 1.74494400  |
| C | -3.74206000 | 3.37372000  | -3.00491600 |
| H | -2.65911500 | 3.44906600  | -3.15712200 |
| H | -3.97304400 | 2.30358100  | -2.94981300 |
| H | -4.23677700 | 3.78140900  | -3.89183400 |
| C | -3.58973000 | 4.11421200  | 2.03863000  |
| H | -3.78492800 | 3.06595500  | 2.29330400  |
| H | -2.50506300 | 4.25913300  | 2.10944800  |
| H | -4.06202000 | 4.73988500  | 2.80218700  |
| C | -6.53525800 | 6.99958400  | -0.87551900 |
| H | -7.13144400 | 7.12939500  | 0.03400100  |
| H | -6.01624100 | 7.94932600  | -1.06281300 |
| H | -7.22286400 | 6.83640400  | -1.71235400 |
| C | 3.28316400  | 3.49946100  | -2.90208500 |
| H | 3.25404600  | 2.42110200  | -3.09236600 |
| H | 2.25121000  | 3.85923000  | -2.99551400 |
| H | 3.87204700  | 3.96562400  | -3.69792200 |
| C | 3.35348000  | 3.00601300  | 2.17627900  |
| H | 2.29287700  | 3.24572700  | 2.31800700  |
| H | 3.43386900  | 1.91301100  | 2.18511000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.90363700  | 3.38367600  | 3.04306900  |
| C | 6.67976100  | 6.01571000  | -0.14539500 |
| H | 6.63141100  | 6.77640000  | -0.93231200 |
| H | 6.72292100  | 6.52911900  | 0.82098100  |
| H | 7.62987800  | 5.47924700  | -0.27203900 |
| C | 1.89268500  | -2.79621300 | -4.20905900 |
| H | 0.81623600  | -2.83127300 | -4.00561400 |
| H | 2.18760900  | -1.74508600 | -4.11448000 |
| H | 2.04816800  | -3.09261700 | -5.25087400 |
| C | 3.24653300  | -4.26943100 | 0.48253700  |
| H | 3.49250200  | -3.25111100 | 0.80517600  |
| H | 2.24153800  | -4.48515500 | 0.86504600  |
| H | 3.94508500  | -4.95679400 | 0.96949200  |
| C | 5.13659500  | -6.61120100 | -3.57099800 |
| H | 5.25482600  | -7.46582600 | -2.89632700 |
| H | 4.74694900  | -6.98235600 | -4.52500800 |
| H | 6.13980600  | -6.20834400 | -3.76518800 |
| C | 4.37499200  | -1.11532300 | 3.49115600  |
| C | 3.06250300  | -1.08777200 | 3.96121700  |
| C | 2.70538800  | -0.23174600 | 5.01503700  |
| C | 3.65756900  | 0.59840600  | 5.60335600  |
| C | 4.97638000  | 0.56551700  | 5.13568000  |
| C | 5.33307400  | -0.28602400 | 4.08583600  |
| H | 4.65752400  | -1.78014500 | 2.67763700  |
| H | 3.38542700  | 1.25868600  | 6.42403500  |
| H | 5.72925800  | 1.19971600  | 5.59706400  |
| H | 6.36185200  | -0.30928600 | 3.73478500  |
| C | 1.22953900  | -0.37534700 | 5.32995000  |
| C | 1.85442900  | -1.86977200 | 3.48797900  |
| C | 0.86464500  | -1.72927700 | 4.67128500  |
| H | -0.18119000 | -1.77842300 | 4.35346900  |
| H | 1.03727100  | -2.54000200 | 5.39056900  |
| H | 1.42985900  | -1.40595600 | 2.58575600  |
| H | 2.08228400  | -2.91425500 | 3.24425600  |
| H | 1.00958300  | -0.34745200 | 6.40368000  |
| H | 0.66074600  | 0.44226900  | 4.86327100  |

**Structure:  ${}^1\text{TS2}_\pi$**

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.02469500 | 3.04884300 | -0.40687100 |
| C | -0.42069800 | 4.36555800 | -0.43253900 |
| C | 0.92552200  | 4.17800400 | -0.35126100 |
| C | 1.14244200  | 2.74691500 | -0.30270400 |
| N | -0.05539500 | 2.09078500 | -0.33498600 |
| H | -0.96817000 | 5.29530300 | -0.49566300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.71037900  | 4.92094800  | -0.34128300 |
| C  | 2.31709700  | -1.39303800 | -0.70071700 |
| C  | 3.73790300  | -1.16440600 | -0.83597500 |
| C  | 3.94234900  | 0.16569500  | -0.61871500 |
| C  | 2.64090800  | 0.75410800  | -0.39254600 |
| N  | 1.67717300  | -0.21407800 | -0.42007900 |
| H  | 4.46723300  | -1.92978100 | -1.06002300 |
| H  | 4.87269600  | 0.71442700  | -0.63625700 |
| C  | -3.29360200 | -0.61162400 | -0.00431600 |
| C  | -4.60769500 | -0.00869900 | 0.06923800  |
| C  | -4.43284400 | 1.32983700  | -0.11475800 |
| C  | -3.00900800 | 1.54438400  | -0.26723100 |
| N  | -2.34646300 | 0.35315800  | -0.20280500 |
| H  | -5.52954300 | -0.55152600 | 0.22363200  |
| H  | -5.18072500 | 2.10989300  | -0.13465000 |
| C  | -1.79303200 | -2.59658400 | -0.14210600 |
| C  | -1.59422500 | -4.02000400 | -0.29741000 |
| C  | -0.27970800 | -4.19830500 | -0.61467000 |
| C  | 0.32985000  | -2.88840500 | -0.60714600 |
| N  | -0.60879900 | -1.93541600 | -0.31561400 |
| H  | -2.37086200 | -4.76594000 | -0.20511700 |
| H  | 0.24154700  | -5.12080600 | -0.82800100 |
| C  | -2.41028300 | 2.81082200  | -0.40221800 |
| C  | 1.69593500  | -2.64522000 | -0.84014600 |
| C  | 2.40856800  | 2.13981800  | -0.29207000 |
| C  | -3.04903400 | -1.99390700 | 0.05901000  |
| O  | -0.28205700 | 0.16091800  | 1.48591000  |
| N  | -0.38876900 | 0.11160200  | -2.29720700 |
| C  | 0.53738800  | 0.31102800  | -3.04195700 |
| O  | 1.44713300  | 0.49207200  | -3.80482500 |
| Mn | -0.33616400 | 0.07390100  | -0.26012400 |
| C  | -3.31808500 | 3.99568300  | -0.51175900 |
| C  | -3.71559000 | 4.68795100  | 0.64779800  |
| C  | -3.77153800 | 4.39733800  | -1.78293900 |
| C  | -4.57122600 | 5.78573600  | 0.51283200  |
| C  | -4.62475700 | 5.50147400  | -1.87153500 |
| C  | -5.03360100 | 6.20995500  | -0.73708600 |
| H  | -4.88497000 | 6.32135400  | 1.40671000  |
| H  | -4.97943800 | 5.81439800  | -2.85160400 |
| C  | 2.54178100  | -3.78147400 | -1.32376900 |
| C  | 3.11349800  | -4.70209700 | -0.42616300 |
| C  | 2.76104800  | -3.89518500 | -2.71371900 |
| C  | 3.90994100  | -5.73244800 | -0.93824000 |
| C  | 3.56240100  | -4.94169100 | -3.17830400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.14534800  | -5.86978100 | -2.30890400 |
| H | 4.35904500  | -6.44268200 | -0.24685000 |
| H | 3.73551400  | -5.03370900 | -4.24874700 |
| C | 3.60695200  | 3.03350900  | -0.25087600 |
| C | 4.14336800  | 3.40175700  | 0.99737600  |
| C | 4.18626300  | 3.48190200  | -1.45403700 |
| C | 5.28395200  | 4.21035200  | 1.02064900  |
| C | 5.32679500  | 4.28846500  | -1.38084700 |
| C | 5.89029300  | 4.66173900  | -0.15612600 |
| H | 5.70874800  | 4.49269900  | 1.98208100  |
| H | 5.78613300  | 4.63284600  | -2.30542100 |
| C | -4.21615600 | -2.89921600 | 0.30105000  |
| C | -5.02861200 | -3.30680600 | -0.77501200 |
| C | -4.48566600 | -3.33689700 | 1.61163300  |
| C | -6.11227100 | -4.15097600 | -0.51399200 |
| C | -5.58205400 | -4.17749500 | 1.82786300  |
| C | -6.40541100 | -4.59752100 | 0.77877100  |
| H | -6.74305800 | -4.46790900 | -1.34225400 |
| H | -5.79722100 | -4.51163900 | 2.84092500  |
| C | -4.73122700 | -2.84322800 | -2.18263200 |
| H | -4.81954500 | -1.75387400 | -2.27047600 |
| H | -3.70618000 | -3.09823700 | -2.47679200 |
| H | -5.41707400 | -3.29975800 | -2.90257500 |
| C | -3.60133900 | -2.90790100 | 2.76016900  |
| H | -2.58557100 | -3.30531500 | 2.64514200  |
| H | -3.50565000 | -1.81664200 | 2.80631400  |
| H | -3.99605200 | -3.25892500 | 3.71845100  |
| C | -7.56343800 | -5.53562900 | 1.02846200  |
| H | -8.38989100 | -5.34677400 | 0.33454300  |
| H | -7.25901900 | -6.58223400 | 0.89356900  |
| H | -7.94756700 | -5.43722000 | 2.04944700  |
| C | -3.34553500 | 3.64312700  | -3.02169400 |
| H | -2.25376100 | 3.62079300  | -3.12025300 |
| H | -3.67311500 | 2.59732800  | -2.98288400 |
| H | -3.76140000 | 4.09822300  | -3.92558800 |
| C | -3.23058700 | 4.24532000  | 2.00932600  |
| H | -3.51796300 | 3.20720000  | 2.21518000  |
| H | -2.13660900 | 4.28567300  | 2.07341000  |
| H | -3.64268800 | 4.87743400  | 2.80167000  |
| C | -5.92950600 | 7.42054100  | -0.86150500 |
| H | -5.33860400 | 8.33622600  | -0.99798000 |
| H | -6.60099700 | 7.33651000  | -1.72296800 |
| H | -6.54292800 | 7.56027500  | 0.03522900  |
| C | 3.57375300  | 3.12073200  | -2.78809600 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.39028000  | 2.04629500  | -2.89184000 |
| H | 2.59666200  | 3.60496600  | -2.91146900 |
| H | 4.21392500  | 3.44214500  | -3.61527200 |
| C | 3.48541400  | 2.94501600  | 2.27917300  |
| H | 2.48850900  | 3.39093100  | 2.38743200  |
| H | 3.34790700  | 1.85951300  | 2.30385800  |
| H | 4.07962700  | 3.22616900  | 3.15365700  |
| C | 7.10611500  | 5.55823600  | -0.10614500 |
| H | 7.70404300  | 5.37451500  | 0.79317100  |
| H | 7.75066900  | 5.40931100  | -0.97931200 |
| H | 6.81560600  | 6.61740900  | -0.09333500 |
| C | 2.13986400  | -2.91082300 | -3.67876600 |
| H | 1.05330900  | -2.85158500 | -3.54375200 |
| H | 2.51675000  | -1.89192600 | -3.53504100 |
| H | 2.33805900  | -3.19964100 | -4.71528400 |
| C | 2.88220900  | -4.58552400 | 1.06333000  |
| H | 3.22791100  | -3.62190200 | 1.45385000  |
| H | 1.81628900  | -4.66201800 | 1.30887400  |
| H | 3.40984700  | -5.37468300 | 1.60746500  |
| C | 4.98350500  | -7.00703900 | -2.84517000 |
| H | 5.65045400  | -7.41286600 | -2.07715900 |
| H | 4.34998900  | -7.83147000 | -3.19880800 |
| H | 5.59811600  | -6.68589500 | -3.69369200 |
| C | 3.50318400  | -0.96984900 | 2.78213200  |
| C | 2.21225700  | -1.03061600 | 3.31884000  |
| C | 1.93436000  | -0.44792100 | 4.57332000  |
| C | 2.94354000  | 0.17647400  | 5.29802100  |
| C | 4.24001400  | 0.21885900  | 4.76745000  |
| C | 4.51562300  | -0.35030400 | 3.51790800  |
| H | 3.71406400  | -1.38540800 | 1.80291600  |
| H | 2.73420700  | 0.62128600  | 6.26815400  |
| H | 5.03745100  | 0.69795500  | 5.32960200  |
| H | 5.52314300  | -0.30292700 | 3.11296300  |
| C | 0.46803300  | -0.61675100 | 4.90937000  |
| C | 0.98154500  | -1.61184700 | 2.75648900  |
| C | 0.00294400  | -1.72397700 | 3.92756300  |
| H | -1.03573800 | -1.60246700 | 3.60885000  |
| H | 0.09990500  | -2.71203500 | 4.40050300  |
| H | 0.45529100  | -0.71574300 | 2.03424400  |
| H | 1.06605000  | -2.45859600 | 2.07533700  |
| H | 0.29120700  | -0.86744000 | 5.96154500  |
| H | -0.07018700 | 0.31778900  | 4.70029100  |

Structure:  ${}^3\text{TS2}_\pi$

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.04761300 | 3.03301200  | -0.41956200 |
| C  | -0.43380000 | 4.34079700  | -0.37956100 |
| C  | 0.90073900  | 4.15132600  | -0.17855200 |
| C  | 1.12648600  | 2.72460700  | -0.14843600 |
| N  | -0.07430300 | 2.07765600  | -0.28736200 |
| H  | -0.97579100 | 5.27168500  | -0.46981400 |
| H  | 1.68157700  | 4.89357300  | -0.09066500 |
| C  | 2.22605100  | -1.35560900 | -0.92352600 |
| C  | 3.63896000  | -1.11514700 | -1.07467200 |
| C  | 3.87036100  | 0.17526000  | -0.69586500 |
| C  | 2.59320900  | 0.76000200  | -0.36945500 |
| N  | 1.61653200  | -0.20004400 | -0.49290200 |
| H  | 4.35105900  | -1.85798600 | -1.40565600 |
| H  | 4.80905300  | 0.70955000  | -0.66750100 |
| C  | -3.25846500 | -0.59516900 | 0.23218700  |
| C  | -4.56665200 | 0.01465000  | 0.29979100  |
| C  | -4.41393800 | 1.32741800  | -0.03290300 |
| C  | -3.00292500 | 1.54908100  | -0.25048700 |
| N  | -2.33294900 | 0.36377200  | -0.08989800 |
| H  | -5.47707700 | -0.51680400 | 0.53887500  |
| H  | -5.16983000 | 2.09703100  | -0.10196600 |
| C  | -1.78654000 | -2.55528800 | 0.02705600  |
| C  | -1.59330100 | -3.97087300 | -0.17427100 |
| C  | -0.34026400 | -4.13735000 | -0.68694900 |
| C  | 0.27285500  | -2.83362000 | -0.74393700 |
| N  | -0.62710100 | -1.89288000 | -0.30102700 |
| H  | -2.34771900 | -4.72175900 | 0.01377800  |
| H  | 0.14820700  | -5.05400300 | -0.98648200 |
| C  | -2.42673300 | 2.80503500  | -0.46604600 |
| C  | 1.60369400  | -2.59521500 | -1.09991300 |
| C  | 2.38864400  | 2.12416500  | -0.13440200 |
| C  | -3.01762100 | -1.96904200 | 0.33970300  |
| O  | -0.23004500 | 0.16406300  | 1.46942800  |
| N  | -0.55513500 | 0.15826700  | -2.24471500 |
| C  | 0.31805800  | 0.44933900  | -3.02849300 |
| O  | 1.16311600  | 0.71478000  | -3.83054900 |
| Mn | -0.35008500 | 0.08552600  | -0.25646400 |
| C  | -3.33468200 | 3.97632700  | -0.67964900 |
| C  | -3.79747900 | 4.72958500  | 0.41640500  |
| C  | -3.72242600 | 4.30874300  | -1.99242100 |
| C  | -4.64784400 | 5.81424500  | 0.17786300  |
| C  | -4.57373200 | 5.40100400  | -2.18671200 |
| C  | -5.04445300 | 6.16750100  | -1.11582400 |
| H  | -5.01010900 | 6.39606500  | 1.02330700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.87745600 | 5.65846200  | -3.19958100 |
| C | 2.40637700  | -3.70908300 | -1.69698900 |
| C | 3.05444400  | -4.65977200 | -0.88520400 |
| C | 2.50340000  | -3.78141800 | -3.10251600 |
| C | 3.79727500  | -5.67530800 | -1.49696500 |
| C | 3.25698000  | -4.81305000 | -3.67120500 |
| C | 3.91416100  | -5.76634200 | -2.88713700 |
| H | 4.29751500  | -6.41219200 | -0.87147000 |
| H | 3.32968300  | -4.87452100 | -4.75530200 |
| C | 3.59035400  | 3.00358000  | 0.01259000  |
| C | 4.07244400  | 3.29603800  | 1.30252100  |
| C | 4.22041400  | 3.53312700  | -1.13156400 |
| C | 5.20796300  | 4.10330700  | 1.42741500  |
| C | 5.35260400  | 4.33610100  | -0.95968700 |
| C | 5.86555200  | 4.62566600  | 0.30943400  |
| H | 5.58530500  | 4.33105000  | 2.42256600  |
| H | 5.84381500  | 4.74865200  | -1.83894000 |
| C | -4.16820800 | -2.87081500 | 0.66951400  |
| C | -5.02988000 | -3.31522700 | -0.35401700 |
| C | -4.38071400 | -3.27029300 | 2.00230700  |
| C | -6.10019200 | -4.15036800 | -0.01879100 |
| C | -5.46437800 | -4.10479300 | 2.29536100  |
| C | -6.33435600 | -4.55675200 | 1.29897400  |
| H | -6.76827200 | -4.49187500 | -0.80715800 |
| H | -5.63229300 | -4.40864600 | 3.32684000  |
| C | -4.80185000 | -2.89763000 | -1.78886700 |
| H | -4.89078600 | -1.81131100 | -1.90690900 |
| H | -3.79347100 | -3.16588100 | -2.12525500 |
| H | -5.52446600 | -3.37371700 | -2.45858900 |
| C | -3.44275200 | -2.81524000 | 3.09628000  |
| H | -2.44309400 | -3.24446000 | 2.95730500  |
| H | -3.31866200 | -1.72614000 | 3.09164100  |
| H | -3.80587000 | -3.11711400 | 4.08359100  |
| C | -7.47975600 | -5.48553600 | 1.62951200  |
| H | -7.81070400 | -5.36275100 | 2.66639900  |
| H | -8.34066600 | -5.30981800 | 0.97503500  |
| H | -7.18526000 | -6.53606700 | 1.50295700  |
| C | -3.22996100 | 3.49244500  | -3.16567300 |
| H | -2.13466100 | 3.47188700  | -3.20669500 |
| H | -3.55205900 | 2.44725200  | -3.08757500 |
| H | -3.60133000 | 3.89568600  | -4.11273600 |
| C | -3.38582400 | 4.36771600  | 1.82525400  |
| H | -3.68984100 | 3.34477600  | 2.07749000  |
| H | -2.29641600 | 4.40824500  | 1.94326900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.83430600 | 5.04758900  | 2.55615900  |
| C | -5.93628000 | 7.36417600  | -1.35373900 |
| H | -6.59057600 | 7.55494200  | -0.49607700 |
| H | -5.34196500 | 8.27301000  | -1.51863000 |
| H | -6.56741600 | 7.22475200  | -2.23826000 |
| C | 3.66603000  | 3.26155700  | -2.51196900 |
| H | 3.57095100  | 2.18968700  | -2.71630100 |
| H | 2.65769000  | 3.67960700  | -2.61946500 |
| H | 4.30056800  | 3.70372900  | -3.28609000 |
| C | 3.35699000  | 2.76947400  | 2.52538900  |
| H | 2.35997000  | 3.21845000  | 2.61843000  |
| H | 3.21029800  | 1.68652000  | 2.47423700  |
| H | 3.91655700  | 2.98965200  | 3.43916000  |
| C | 7.11364900  | 5.46384100  | 0.46439600  |
| H | 7.18634800  | 6.22470900  | -0.32066800 |
| H | 7.13861100  | 5.97297000  | 1.43399000  |
| H | 8.01732300  | 4.84290000  | 0.39852100  |
| C | 1.80051800  | -2.76810500 | -3.97743100 |
| H | 0.73032700  | -2.71512900 | -3.74518600 |
| H | 2.19215700  | -1.75481500 | -3.83181500 |
| H | 1.90803600  | -3.02157800 | -5.03648900 |
| C | 2.95109800  | -4.59601200 | 0.62194200  |
| H | 3.30494000  | -3.63457500 | 1.01026700  |
| H | 1.91288200  | -4.70768000 | 0.95661900  |
| H | 3.54364600  | -5.38639300 | 1.09273100  |
| C | 4.75126100  | -6.85032200 | -3.52594000 |
| H | 4.79639000  | -7.74663400 | -2.89776300 |
| H | 4.35282600  | -7.14060200 | -4.50427600 |
| H | 5.78367600  | -6.51032500 | -3.68375400 |
| C | 3.71925400  | -1.08576400 | 2.57158100  |
| C | 2.45554900  | -1.13642100 | 3.16781100  |
| C | 2.25223500  | -0.60913000 | 4.45924200  |
| C | 3.31212900  | -0.04624900 | 5.16294400  |
| C | 4.58084000  | -0.01093900 | 4.57038800  |
| C | 4.78199500  | -0.52665500 | 3.28371500  |
| H | 3.86985300  | -1.46262500 | 1.56637800  |
| H | 3.16217000  | 0.35585100  | 6.16201500  |
| H | 5.41691800  | 0.42209100  | 5.11329900  |
| H | 5.77014300  | -0.48549300 | 2.83366200  |
| C | 0.80250500  | -0.76585800 | 4.86245100  |
| C | 1.17821900  | -1.66799700 | 2.63545300  |
| C | 0.27084700  | -1.82544300 | 3.86356100  |
| H | -0.78391400 | -1.68761400 | 3.61607300  |
| H | 0.39433700  | -2.83269400 | 4.28475100  |

|   |            |             |            |
|---|------------|-------------|------------|
| H | 0.67142400 | -0.81074400 | 1.99307100 |
| H | 1.23367400 | -2.51218900 | 1.94461800 |
| H | 0.67430100 | -1.05570900 | 5.91145300 |
| H | 0.27085000 | 0.18542600  | 4.72022200 |

**Structure:  ${}^5\text{TS2}_\pi$**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.13971800 | 2.99880700  | -0.45923300 |
| C | -0.55662500 | 4.32062500  | -0.42081600 |
| C | 0.78239200  | 4.16263100  | -0.23035200 |
| C | 1.04489700  | 2.74234500  | -0.20366400 |
| N | -0.14736900 | 2.06234400  | -0.33751600 |
| H | -1.12157200 | 5.23826600  | -0.50547000 |
| H | 1.54509300  | 4.92366800  | -0.14492400 |
| C | 2.27088600  | -1.31576300 | -0.89478900 |
| C | 3.67783500  | -1.03922900 | -1.04976500 |
| C | 3.86902000  | 0.26733500  | -0.70516800 |
| C | 2.57132300  | 0.81498500  | -0.39201900 |
| N | 1.62657900  | -0.16933200 | -0.49219300 |
| H | 4.41286200  | -1.76792600 | -1.36153400 |
| H | 4.79017500  | 0.83169500  | -0.68872600 |
| C | -3.24437700 | -0.68910800 | 0.19412900  |
| C | -4.56633800 | -0.11371000 | 0.27234500  |
| C | -4.45329500 | 1.20415100  | -0.05344100 |
| C | -3.05188900 | 1.46837400  | -0.27874200 |
| N | -2.34185500 | 0.30192800  | -0.13074900 |
| H | -5.46001900 | -0.67091000 | 0.51553400  |
| H | -5.23128100 | 1.95207300  | -0.11417800 |
| C | -1.72045600 | -2.61502800 | 0.00751300  |
| C | -1.48875100 | -4.02893800 | -0.16301900 |
| C | -0.21940000 | -4.16886400 | -0.64437000 |
| C | 0.35276600  | -2.84682900 | -0.71680300 |
| N | -0.58308300 | -1.92560000 | -0.31468600 |
| H | -2.22493600 | -4.79704500 | 0.02755900  |
| H | 0.30327900  | -5.07653600 | -0.91171700 |
| C | -2.51341200 | 2.73900300  | -0.49569700 |
| C | 1.68437100  | -2.57547400 | -1.05348700 |
| C | 2.31984300  | 2.18136800  | -0.18046700 |
| C | -2.97072700 | -2.05197400 | 0.30676700  |
| O | -0.26700000 | 0.14520800  | 1.45627400  |
| N | -0.48688200 | 0.05336300  | -2.29647400 |
| C | 0.38479000  | 0.35075100  | -3.07920400 |
| O | 1.22815500  | 0.62387500  | -3.88037700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Mn | -0.37920900 | 0.08668700  | -0.30595400 |
| C  | -3.45264100 | 3.88961200  | -0.68311100 |
| C  | -3.91792400 | 4.61575500  | 0.43028100  |
| C  | -3.86688300 | 4.23126900  | -1.98525300 |
| C  | -4.79756000 | 5.68256700  | 0.21930100  |
| C  | -4.74704400 | 5.30506800  | -2.15185400 |
| C  | -5.22090300 | 6.04452600  | -1.06346800 |
| H  | -5.16157100 | 6.24336800  | 1.07807300  |
| H  | -5.07123900 | 5.56945300  | -3.15655300 |
| C  | 2.52401400  | -3.67894400 | -1.62008300 |
| C  | 3.20283200  | -4.58445800 | -0.78322200 |
| C  | 2.62027600  | -3.78944500 | -3.02371800 |
| C  | 3.97568200  | -5.59431800 | -1.36766100 |
| C  | 3.40287800  | -4.81395400 | -3.56400400 |
| C  | 4.09122200  | -5.72347200 | -2.75428400 |
| H  | 4.49995900  | -6.29619900 | -0.72209700 |
| H  | 3.47469600  | -4.90507400 | -4.64614500 |
| C  | 3.49404200  | 3.09760500  | -0.03569700 |
| C  | 3.95055900  | 3.42830100  | 1.25470900  |
| C  | 4.13045500  | 3.61406400  | -1.18206300 |
| C  | 5.06792000  | 4.26052800  | 1.37740100  |
| C  | 5.24419700  | 4.44305300  | -1.01183100 |
| C  | 5.72864100  | 4.77555400  | 0.25768900  |
| H  | 5.42956500  | 4.51268600  | 2.37252600  |
| H  | 5.74397200  | 4.84066100  | -1.89309300 |
| C  | -4.09699900 | -2.97892400 | 0.64957200  |
| C  | -4.95083900 | -3.45654300 | -0.36512100 |
| C  | -4.28521900 | -3.37810300 | 1.98628300  |
| C  | -5.99178000 | -4.32316100 | -0.01725100 |
| C  | -5.34011000 | -4.24415400 | 2.29182100  |
| C  | -6.20670400 | -4.72418200 | 1.30542500  |
| H  | -6.64995300 | -4.69593800 | -0.79974500 |
| H  | -5.48637900 | -4.55269000 | 3.32520700  |
| C  | -4.74037600 | -3.04660500 | -1.80488600 |
| H  | -4.86256900 | -1.96458000 | -1.93271100 |
| H  | -3.72567800 | -3.28781000 | -2.14279100 |
| H  | -5.45090000 | -3.55031400 | -2.46726400 |
| C  | -3.34768000 | -2.89484100 | 3.06854100  |
| H  | -2.33842700 | -3.29771600 | 2.92027000  |
| H  | -3.25197200 | -1.80296400 | 3.05873100  |
| H  | -3.69229800 | -3.20254000 | 4.06063800  |
| C  | -7.36136900 | -5.63193500 | 1.66070000  |
| H  | -7.58187600 | -6.33669000 | 0.85131400  |
| H  | -7.15382800 | -6.21031400 | 2.56745300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -8.27632400 | -5.05300500 | 1.84517100  |
| C | -3.37120600 | 3.44488600  | -3.17739500 |
| H | -2.27646800 | 3.45579500  | -3.23591600 |
| H | -3.66421000 | 2.39041800  | -3.10929400 |
| H | -3.76832800 | 3.85063700  | -4.11285000 |
| C | -3.47664700 | 4.24450100  | 1.82766600  |
| H | -3.75047500 | 3.21066400  | 2.06972100  |
| H | -2.38699700 | 4.31116000  | 1.93081200  |
| H | -3.93141600 | 4.90232600  | 2.57465100  |
| C | -6.14467000 | 7.22239200  | -1.27151200 |
| H | -6.78653000 | 7.07913600  | -2.14765500 |
| H | -6.78924000 | 7.38645500  | -0.40110400 |
| H | -5.57481800 | 8.14718600  | -1.43393400 |
| C | 3.60604600  | 3.29634200  | -2.56439800 |
| H | 3.55293700  | 2.21820500  | -2.75027500 |
| H | 2.58500800  | 3.67586500  | -2.69312200 |
| H | 4.23501300  | 3.74698000  | -3.33815700 |
| C | 3.23017400  | 2.91303400  | 2.47933100  |
| H | 2.22735600  | 3.35222100  | 2.55513700  |
| H | 3.09608900  | 1.82794100  | 2.44609500  |
| H | 3.77833200  | 3.15544200  | 3.39420400  |
| C | 6.91465400  | 5.69900600  | 0.41524600  |
| H | 6.59437200  | 6.74857800  | 0.46335300  |
| H | 7.46997700  | 5.48687100  | 1.33550000  |
| H | 7.60832300  | 5.61030200  | -0.42809400 |
| C | 1.89016300  | -2.82061500 | -3.92575600 |
| H | 0.82265100  | -2.77286100 | -3.68099900 |
| H | 2.27090200  | -1.79802200 | -3.82314200 |
| H | 1.98750800  | -3.11183900 | -4.97604700 |
| C | 3.09980100  | -4.48110300 | 0.72145800  |
| H | 3.42416600  | -3.49834100 | 1.08104400  |
| H | 2.06579500  | -4.61590100 | 1.06083400  |
| H | 3.71709600  | -5.23906400 | 1.21323900  |
| C | 4.95601500  | -6.80046400 | -3.36736200 |
| H | 5.93714600  | -6.40138000 | -3.65759300 |
| H | 5.13155500  | -7.62358200 | -2.66660800 |
| H | 4.49705200  | -7.21622000 | -4.27153300 |
| C | 3.77734700  | -0.89197600 | 2.59296500  |
| C | 2.50668500  | -0.99160900 | 3.16996500  |
| C | 2.25921900  | -0.44951100 | 4.44951900  |
| C | 3.28039900  | 0.17370100  | 5.15840100  |
| C | 4.55629200  | 0.25617000  | 4.58511200  |
| C | 4.80164100  | -0.27289800 | 3.31123000  |
| H | 3.96187800  | -1.27878300 | 1.59712600  |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | 3.09630000  | 0.58620500  | 6.14752400 |
| H | 5.36276500  | 0.73698400  | 5.13263300 |
| H | 5.79416200  | -0.19397100 | 2.87596700 |
| C | 0.81189900  | -0.66732900 | 4.83107900 |
| C | 1.26545300  | -1.59155900 | 2.63142600 |
| C | 0.35351200  | -1.77836400 | 3.85271000 |
| H | -0.70405300 | -1.70484400 | 3.58994500 |
| H | 0.52869400  | -2.76701900 | 4.29967200 |
| H | 0.71233000  | -0.76929500 | 1.97460800 |
| H | 1.37033900  | -2.44097900 | 1.95309200 |
| H | 0.67632300  | -0.93073400 | 5.88614100 |
| H | 0.23736600  | 0.25154900  | 4.64678900 |

**Structure: <sup>3</sup>TS2<sub>g</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.59720600  | -2.67359100 | -0.21816800 |
| C | 1.29557200  | -4.07202400 | -0.40175100 |
| C | -0.04074500 | -4.15483200 | -0.66375000 |
| C | -0.55881600 | -2.81054600 | -0.60815200 |
| N | 0.45193500  | -1.92859400 | -0.33365500 |
| H | 2.02292200  | -4.86975100 | -0.35369700 |
| H | -0.63466100 | -5.03428100 | -0.86734600 |
| C | -2.62604500 | 0.96458500  | -0.35854800 |
| C | -3.97035600 | 0.45724300  | -0.53294200 |
| C | -3.86033800 | -0.88674200 | -0.71021900 |
| C | -2.45217400 | -1.20204000 | -0.61847800 |
| N | -1.72798200 | -0.06490300 | -0.38038100 |
| H | -4.86154400 | 1.06756200  | -0.54527100 |
| H | -4.64275200 | -1.60955000 | -0.89116000 |
| C | 3.07057000  | 1.37239900  | -0.15244800 |
| C | 4.47782500  | 1.06408100  | -0.02279300 |
| C | 4.57164200  | -0.29069600 | 0.08626000  |
| C | 3.22321800  | -0.80563300 | 0.00029300  |
| N | 2.33413300  | 0.22375600  | -0.13027700 |
| H | 5.27169000  | 1.79727600  | -0.01426100 |
| H | 5.45858100  | -0.89813100 | 0.19650400  |
| C | 1.19241800  | 3.00011600  | -0.31436000 |
| C | 0.67970100  | 4.35211800  | -0.35164500 |
| C | -0.67822800 | 4.25639500  | -0.32806500 |
| C | -0.99595500 | 2.84564400  | -0.29488600 |
| N | 0.15494700  | 2.10939000  | -0.28635500 |
| H | 1.29223800  | 5.24187000  | -0.38079200 |
| H | -1.41008500 | 5.05128400  | -0.34013000 |
| C | 2.89578900  | -2.17099500 | -0.02669800 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.30446300 | 2.33157000  | -0.31252100 |
| C  | -1.91620200 | -2.48544200 | -0.78726400 |
| C  | 2.55681500  | 2.67683800  | -0.26661900 |
| O  | 0.19948300  | 0.16078800  | 1.44103300  |
| N  | 0.38995600  | 0.17696100  | -2.22843300 |
| C  | -0.52918800 | 0.33029500  | -2.99394300 |
| O  | -1.42837700 | 0.47445200  | -3.77576800 |
| Mn | 0.30017500  | 0.07705300  | -0.17395300 |
| C  | 4.01602700  | -3.15842400 | 0.08255400  |
| C  | 4.33694400  | -3.71173300 | 1.33631200  |
| C  | 4.74049000  | -3.51963500 | -1.07093700 |
| C  | 5.39422000  | -4.62333900 | 1.41741800  |
| C  | 5.78776600  | -4.43696900 | -0.94389500 |
| C  | 6.12993400  | -5.00036200 | 0.28987600  |
| H  | 5.64914800  | -5.04743800 | 2.38655300  |
| H  | 6.35080100  | -4.71766600 | -1.83184600 |
| C  | -3.43698900 | 3.30613500  | -0.37996100 |
| C  | -4.13801300 | 3.64230500  | 0.79416700  |
| C  | -3.79619000 | 3.86116900  | -1.62504400 |
| C  | -5.19770800 | 4.54962500  | 0.70284700  |
| C  | -4.86750000 | 4.75949000  | -1.66710100 |
| C  | -5.58048600 | 5.11495400  | -0.51777500 |
| H  | -5.73778600 | 4.81940100  | 1.60831700  |
| H  | -5.15220000 | 5.19076300  | -2.62475700 |
| C  | -2.84095400 | -3.57168200 | -1.23957200 |
| C  | -3.54670000 | -4.35007900 | -0.30463300 |
| C  | -2.99838500 | -3.78314400 | -2.62482300 |
| C  | -4.41162900 | -5.34343600 | -0.77460400 |
| C  | -3.87341600 | -4.78813900 | -3.04833900 |
| C  | -4.58635200 | -5.57938500 | -2.14156600 |
| H  | -4.96310500 | -5.94439400 | -0.05423900 |
| H  | -4.00324200 | -4.95383600 | -4.11596700 |
| C  | 3.53778200  | 3.80577600  | -0.32279900 |
| C  | 4.01894600  | 4.23823600  | -1.57370900 |
| C  | 3.96397600  | 4.42384100  | 0.86775100  |
| C  | 4.93240700  | 5.29578800  | -1.60971500 |
| C  | 4.87943200  | 5.47786300  | 0.78475600  |
| C  | 5.37678900  | 5.92644700  | -0.44279600 |
| H  | 5.30456800  | 5.63636300  | -2.57395300 |
| H  | 5.20977700  | 5.96090300  | 1.70216900  |
| C  | 3.54877100  | 3.57339600  | -2.84711300 |
| H  | 3.77525800  | 2.50056200  | -2.84356200 |
| H  | 2.46184300  | 3.65982700  | -2.96379100 |
| H  | 4.02290500  | 4.02022500  | -3.72601900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.43535700  | 3.95896200  | 2.20544200  |
| H | 2.34511600  | 4.06497300  | 2.26039300  |
| H | 3.65565300  | 2.89793400  | 2.37342200  |
| H | 3.87506400  | 4.53263000  | 3.02672200  |
| C | 6.38957700  | 7.04599600  | -0.50807200 |
| H | 6.26516000  | 7.64637900  | -1.41594100 |
| H | 6.30651100  | 7.71448800  | 0.35554000  |
| H | 7.41420600  | 6.65075700  | -0.51796700 |
| C | 4.39060600  | -2.92774300 | -2.41715900 |
| H | 3.34077000  | -3.11367800 | -2.67317500 |
| H | 4.52505200  | -1.83959000 | -2.42098900 |
| H | 5.01520500  | -3.35104300 | -3.20937600 |
| C | 3.54955200  | -3.32982900 | 2.56792700  |
| H | 3.52175700  | -2.24258000 | 2.70584700  |
| H | 2.50742400  | -3.66174700 | 2.48836300  |
| H | 3.97819100  | -3.77718900 | 3.46961700  |
| C | 7.24668300  | -6.01269400 | 0.39515800  |
| H | 8.03600400  | -5.81780100 | -0.33910000 |
| H | 7.70074600  | -6.00751000 | 1.39184500  |
| H | 6.87536200  | -7.02970600 | 0.21086900  |
| C | -2.24051100 | -2.94321900 | -3.62750100 |
| H | -2.46088600 | -1.87434000 | -3.52671700 |
| H | -1.15672900 | -3.04653900 | -3.49232600 |
| H | -2.48200000 | -3.24198900 | -4.65194000 |
| C | -3.36999600 | -4.11151000 | 1.17541800  |
| H | -2.34133000 | -4.31974700 | 1.49222000  |
| H | -3.56998900 | -3.06735200 | 1.43890300  |
| H | -4.03969300 | -4.74598300 | 1.76426300  |
| C | -5.50140600 | -6.67915700 | -2.62810200 |
| H | -4.94718000 | -7.61521300 | -2.77946800 |
| H | -6.29947400 | -6.88609100 | -1.90703700 |
| H | -5.96662900 | -6.41959100 | -3.58533400 |
| C | -3.03934000 | 3.50477400  | -2.88468300 |
| H | -2.02431400 | 3.92139800  | -2.86500600 |
| H | -2.92364300 | 2.42296100  | -3.01298400 |
| H | -3.54541900 | 3.90072600  | -3.77034800 |
| C | -3.75697100 | 3.02651000  | 2.11949200  |
| H | -3.95546900 | 1.94915400  | 2.13881500  |
| H | -2.68748100 | 3.14208200  | 2.32956300  |
| H | -4.31585700 | 3.48049800  | 2.94343700  |
| C | -6.75553800 | 6.06182100  | -0.59661500 |
| H | -7.69429800 | 5.51268400  | -0.74990400 |
| H | -6.86627300 | 6.64211700  | 0.32597800  |
| H | -6.65057800 | 6.76477800  | -1.43011100 |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -2.42275000 | 0.84242200  | 4.60389600 |
| C | -1.60730700 | -0.20833200 | 4.18738600 |
| C | -2.17793800 | -1.44849600 | 3.84351400 |
| C | -3.55377700 | -1.64141000 | 3.92213200 |
| C | -4.37222500 | -0.58361200 | 4.34230500 |
| C | -3.80804400 | 0.64896000  | 4.68215000 |
| H | -1.98772400 | 1.80210000  | 4.87467400 |
| H | -3.99275500 | -2.60671400 | 3.68146300 |
| H | -5.44725200 | -0.72753300 | 4.41706200 |
| H | -4.44808400 | 1.46209500  | 5.01627500 |
| C | -1.08615600 | -2.40561300 | 3.40825000 |
| C | -0.12078300 | -0.25291100 | 3.98429700 |
| C | 0.18860800  | -1.76628100 | 4.01305400 |
| H | 1.09097200  | -2.01906400 | 3.44775600 |
| H | 0.32380300  | -2.11925100 | 5.04512900 |
| H | 0.09424400  | 0.11071800  | 2.87298600 |
| H | 0.45938200  | 0.34576800  | 4.69604700 |
| H | -1.25614000 | -3.44139100 | 3.72562700 |
| H | -1.01022000 | -2.40456300 | 2.31121100 |

**Structure: <sup>5</sup>TS2<sub>o</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.41869000  | -2.76719100 | -0.26852700 |
| C | 1.01935600  | -4.14739600 | -0.41319700 |
| C | -0.32419200 | -4.14629600 | -0.63839800 |
| C | -0.75138200 | -2.76769700 | -0.60195300 |
| N | 0.32270900  | -1.95208300 | -0.36911500 |
| H | 1.69518100  | -4.98936100 | -0.36901100 |
| H | -0.98127900 | -4.98688500 | -0.80935100 |
| C | -2.55254500 | 1.15075600  | -0.39312000 |
| C | -3.92424200 | 0.72718700  | -0.55806200 |
| C | -3.90217700 | -0.62330000 | -0.71598800 |
| C | -2.51955900 | -1.03128000 | -0.62761000 |
| N | -1.72220400 | 0.06264800  | -0.41004700 |
| H | -4.77371100 | 1.39414100  | -0.57375200 |
| H | -4.72985100 | -1.29744700 | -0.88188000 |
| C | 3.14812800  | 1.18840800  | -0.22237600 |
| C | 4.53053100  | 0.78196400  | -0.12013300 |
| C | 4.53601100  | -0.57785200 | -0.04818500 |
| C | 3.15831400  | -1.00541000 | -0.12527000 |
| N | 2.33838200  | 0.08617600  | -0.22917400 |
| H | 5.36969000  | 1.46242500  | -0.10020600 |
| H | 5.38167900  | -1.24492700 | 0.03767600  |
| C | 1.38356000  | 2.93225900  | -0.28897600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.95657700  | 4.31258300  | -0.28345700 |
| C  | -0.40445200 | 4.30321400  | -0.27808200 |
| C  | -0.81344800 | 2.91739600  | -0.29219800 |
| N  | 0.29003200  | 2.10761200  | -0.29417200 |
| H  | 1.62588600  | 5.16083500  | -0.27961900 |
| H  | -1.08506100 | 5.14228300  | -0.27338800 |
| C  | 2.74916800  | -2.34675800 | -0.12790200 |
| C  | -2.15004100 | 2.49290500  | -0.33207000 |
| C  | -2.08156300 | -2.35315800 | -0.77139400 |
| C  | 2.72401200  | 2.52508200  | -0.26863100 |
| O  | 0.26694400  | 0.06808200  | 1.43017400  |
| N  | 0.36149200  | 0.13249800  | -2.33392500 |
| C  | -0.58178000 | 0.35620200  | -3.05086600 |
| O  | -1.50784800 | 0.56844200  | -3.78667800 |
| Mn | 0.31073800  | 0.08052800  | -0.24681600 |
| C  | 3.80666700  | -3.40084500 | -0.01989400 |
| C  | 4.11914300  | -3.94480600 | 1.24047500  |
| C  | 4.47943200  | -3.83505900 | -1.17877200 |
| C  | 5.11707300  | -4.92085800 | 1.32151000  |
| C  | 5.46834500  | -4.81540400 | -1.05168000 |
| C  | 5.80117400  | -5.37097700 | 0.18793000  |
| H  | 5.36611600  | -5.33840900 | 2.29505500  |
| H  | 5.99156800  | -5.15278300 | -1.94420000 |
| C  | -3.21627300 | 3.54006900  | -0.39501300 |
| C  | -3.90372300 | 3.90817700  | 0.77768200  |
| C  | -3.52498100 | 4.13585900  | -1.63486000 |
| C  | -4.90095500 | 4.88408400  | 0.69013700  |
| C  | -4.53448500 | 5.10343800  | -1.67348800 |
| C  | -5.23409900 | 5.48937200  | -0.52586300 |
| H  | -5.42988500 | 5.17773800  | 1.59474500  |
| H  | -4.78006400 | 5.56621300  | -2.62723900 |
| C  | -3.08743700 | -3.37899200 | -1.19017100 |
| C  | -3.80172600 | -4.11716500 | -0.22952700 |
| C  | -3.30822600 | -3.57737500 | -2.56863300 |
| C  | -4.74004900 | -5.05743300 | -0.66690800 |
| C  | -4.25565800 | -4.52864200 | -2.95936200 |
| C  | -4.97895900 | -5.27925600 | -2.02658100 |
| H  | -5.29855200 | -5.62701700 | 0.07328900  |
| H  | -4.43388500 | -4.68491200 | -4.02141300 |
| C  | 3.77545400  | 3.59010600  | -0.27203400 |
| C  | 4.26759300  | 4.07394500  | -1.49904900 |
| C  | 4.25491100  | 4.10030700  | 0.94979200  |
| C  | 5.24693700  | 5.07207700  | -1.48076600 |
| C  | 5.23435700  | 5.09758200  | 0.92105500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.74504600  | 5.59407400  | -0.28282300 |
| H | 5.62838500  | 5.45155600  | -2.42659200 |
| H | 5.60560700  | 5.49757600  | 1.86254100  |
| C | 3.73999300  | 3.52817400  | -2.80612300 |
| H | 3.89124200  | 2.44445900  | -2.87638900 |
| H | 2.66067800  | 3.69716400  | -2.90137700 |
| H | 4.23537600  | 3.99846100  | -3.66075800 |
| C | 3.71442100  | 3.58166900  | 2.26276100  |
| H | 2.63090300  | 3.73470600  | 2.33517900  |
| H | 3.88484600  | 2.50318400  | 2.36511400  |
| H | 4.18734400  | 4.08373700  | 3.11204300  |
| C | 6.82787500  | 6.64801200  | -0.28735800 |
| H | 6.78795000  | 7.26129600  | -1.19400700 |
| H | 6.74325900  | 7.31455300  | 0.57790500  |
| H | 7.82484400  | 6.18898900  | -0.24783800 |
| C | 4.13759300  | -3.25305900 | -2.53136700 |
| H | 3.07097100  | -3.36982400 | -2.75678900 |
| H | 4.34838800  | -2.17760100 | -2.56805000 |
| H | 4.71006300  | -3.73916300 | -3.32696300 |
| C | 3.38542900  | -3.48408800 | 2.47852000  |
| H | 3.43288600  | -2.39468100 | 2.59173300  |
| H | 2.32176900  | -3.74589900 | 2.42708700  |
| H | 3.80241100  | -3.94021100 | 3.38131200  |
| C | 6.85158200  | -6.45183200 | 0.29553700  |
| H | 7.61509300  | -6.34909700 | -0.48317800 |
| H | 7.35327400  | -6.42855700 | 1.26896900  |
| H | 6.40423100  | -7.44856700 | 0.18342100  |
| C | -2.53849700 | -2.78221700 | -3.59839600 |
| H | -2.70443500 | -1.70319400 | -3.50151500 |
| H | -1.45760600 | -2.93500600 | -3.49048800 |
| H | -2.82108200 | -3.07702900 | -4.61345000 |
| C | -3.55830600 | -3.88944500 | 1.24271000  |
| H | -2.53207800 | -4.15474300 | 1.52348000  |
| H | -3.69053800 | -2.83616700 | 1.51235500  |
| H | -4.24088800 | -4.48581500 | 1.85619100  |
| C | -5.97289800 | -6.32349500 | -2.47953900 |
| H | -5.47993800 | -7.29054000 | -2.64721300 |
| H | -6.75738600 | -6.48338200 | -1.73198200 |
| H | -6.45374400 | -6.03739400 | -3.42135900 |
| C | -2.77851900 | 3.75144200  | -2.89232900 |
| H | -1.74038600 | 4.10572900  | -2.85629100 |
| H | -2.72742800 | 2.66659400  | -3.03585800 |
| H | -3.25009700 | 4.19079200  | -3.77658400 |
| C | -3.57127100 | 3.25752400  | 2.09954100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.82304200 | 2.19123900  | 2.10266800  |
| H | -2.49962600 | 3.31738000  | 2.32204500  |
| H | -4.11640200 | 3.73036600  | 2.92229800  |
| C | -6.34299900 | 6.51311500  | -0.60221500 |
| H | -7.31378400 | 6.03007400  | -0.77695200 |
| H | -6.42760400 | 7.08389600  | 0.32904400  |
| H | -6.18037900 | 7.22140800  | -1.42179900 |
| C | -2.41630700 | 0.93267500  | 4.50983400  |
| C | -1.60348600 | -0.15253000 | 4.18156900  |
| C | -2.17938800 | -1.41457300 | 3.93347200  |
| C | -3.55528100 | -1.59630500 | 4.02943700  |
| C | -4.36958300 | -0.50457700 | 4.36131300  |
| C | -3.80136700 | 0.75109400  | 4.59905900  |
| H | -1.97800800 | 1.90946200  | 4.70164200  |
| H | -3.99705800 | -2.57621800 | 3.86562100  |
| H | -5.44521000 | -0.63751600 | 4.44613600  |
| H | -4.43957500 | 1.59060100  | 4.86392400  |
| C | -1.09225600 | -2.40415800 | 3.56698000  |
| C | -0.12230900 | -0.21959000 | 3.99018200  |
| C | 0.18791600  | -1.72610200 | 4.11572800  |
| H | 1.08499500  | -2.01310800 | 3.55891000  |
| H | 0.33358600  | -2.00885500 | 5.16804500  |
| H | 0.10449500  | 0.06214600  | 2.85763600  |
| H | 0.46235800  | 0.43249100  | 4.64906900  |
| H | -1.26430200 | -3.41365000 | 3.95905600  |
| H | -1.02151900 | -2.48065800 | 2.47231000  |

**Structure: <sup>3</sup>INT3**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.11988800 | 3.01643300  | -0.46050900 |
| C | -0.52942900 | 4.33472000  | -0.42358200 |
| C | 0.80552800  | 4.16981500  | -0.20203000 |
| C | 1.05679000  | 2.74758900  | -0.16059900 |
| N | -0.13052900 | 2.07962900  | -0.31596200 |
| H | -1.08683000 | 5.25549000  | -0.52364800 |
| H | 1.57138000  | 4.92646800  | -0.10515700 |
| C | 2.22446200  | -1.30080200 | -0.95324400 |
| C | 3.63533900  | -1.04019200 | -1.07900400 |
| C | 3.84816300  | 0.24289400  | -0.66278000 |
| C | 2.56045500  | 0.80817400  | -0.34753200 |
| N | 1.59678000  | -0.16254500 | -0.49866400 |
| H | 4.36049800  | -1.76713800 | -1.41735900 |
| H | 4.78098200  | 0.78531500  | -0.60679100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.23577600 | -0.64416400 | 0.29396900  |
| C  | -4.55470900 | -0.06218700 | 0.37175000  |
| C  | -4.43994200 | 1.24605100  | 0.00316800  |
| C  | -3.04035100 | 1.49722300  | -0.24324800 |
| N  | -2.33870400 | 0.33188800  | -0.06418500 |
| H  | -5.44825200 | -0.60833300 | 0.63957600  |
| H  | -5.21608300 | 1.99477600  | -0.07102500 |
| C  | -1.73551000 | -2.57983800 | 0.06303400  |
| C  | -1.51691600 | -3.99253300 | -0.13933600 |
| C  | -0.28153000 | -4.13164700 | -0.70159500 |
| C  | 0.29917200  | -2.81327300 | -0.78291700 |
| N  | -0.60663500 | -1.89389100 | -0.31201300 |
| H  | -2.24403000 | -4.76061800 | 0.08394500  |
| H  | 0.21878100  | -5.03798400 | -1.01304600 |
| C  | -2.49458500 | 2.76099200  | -0.49322300 |
| C  | 1.61848200  | -2.54425200 | -1.16387800 |
| C  | 2.32900500  | 2.16863800  | -0.11510600 |
| C  | -2.96588700 | -2.01227600 | 0.41314700  |
| O  | -0.20282200 | 0.11512200  | 1.51015400  |
| N  | -0.57708100 | 0.12767900  | -2.24428200 |
| C  | 0.25593300  | 0.49806600  | -3.03961300 |
| O  | 1.05693200  | 0.83731100  | -3.85584900 |
| Mn | -0.37812700 | 0.09728400  | -0.28071100 |
| C  | -3.42874100 | 3.90856900  | -0.72021600 |
| C  | -3.90192200 | 4.66950900  | 0.36617900  |
| C  | -3.83009600 | 4.21147300  | -2.03605000 |
| C  | -4.77742500 | 5.73105800  | 0.11460700  |
| C  | -4.70636800 | 5.28130800  | -2.24334500 |
| C  | -5.18858800 | 6.05437700  | -1.18234500 |
| H  | -5.14770000 | 6.31867400  | 0.95252200  |
| H  | -5.02075200 | 5.51567700  | -3.25856500 |
| C  | 2.41768700  | -3.62266300 | -1.82918800 |
| C  | 3.13643400  | -4.57653300 | -1.08413100 |
| C  | 2.43379700  | -3.65788100 | -3.24030300 |
| C  | 3.86488400  | -5.55836300 | -1.76548000 |
| C  | 3.17443500  | -4.65649600 | -3.87921300 |
| C  | 3.89909100  | -5.61343600 | -3.16131000 |
| H  | 4.41824100  | -6.29752600 | -1.18953400 |
| H  | 3.18396600  | -4.68849500 | -4.96702700 |
| C  | 3.51197800  | 3.06443600  | 0.07480300  |
| C  | 3.95176500  | 3.34321500  | 1.38286400  |
| C  | 4.16802400  | 3.61924300  | -1.04182900 |
| C  | 5.07004300  | 4.16560400  | 1.55370500  |
| C  | 5.28169400  | 4.43720600  | -0.82456500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.75161800  | 4.71570200  | 0.46350200  |
| H | 5.41469100  | 4.38297000  | 2.56290400  |
| H | 5.79259400  | 4.86998100  | -1.68260200 |
| C | -4.08763000 | -2.92963100 | 0.79512700  |
| C | -4.96579300 | -3.41960900 | -0.19319900 |
| C | -4.25609700 | -3.29737500 | 2.14335300  |
| C | -6.00746000 | -4.26919600 | 0.19173200  |
| C | -5.31256800 | -4.14779800 | 2.48616800  |
| C | -6.19740100 | -4.64570700 | 1.52554000  |
| H | -6.68852900 | -4.64537500 | -0.56928100 |
| H | -5.44670500 | -4.42763000 | 3.52930700  |
| C | -4.78529700 | -3.03374000 | -1.64369300 |
| H | -4.88436800 | -1.95089000 | -1.78326900 |
| H | -3.78638100 | -3.30468900 | -2.00528900 |
| H | -5.52541800 | -3.52894100 | -2.27953300 |
| C | -3.30022500 | -2.79468400 | 3.20051400  |
| H | -2.29999800 | -3.22086600 | 3.05729800  |
| H | -3.18427300 | -1.70586100 | 3.15534000  |
| H | -3.64068600 | -3.06438600 | 4.20510200  |
| C | -7.31267700 | -5.59009100 | 1.91034100  |
| H | -7.60733500 | -5.45918100 | 2.95708100  |
| H | -8.20029500 | -5.43842400 | 1.28612800  |
| H | -7.00413800 | -6.63685200 | 1.78612100  |
| C | -3.32381600 | 3.38899500  | -3.19916100 |
| H | -2.22874700 | 3.40240800  | -3.25072400 |
| H | -3.61261100 | 2.33592700  | -3.09946900 |
| H | -3.71609100 | 3.76330700  | -4.14965200 |
| C | -3.47222200 | 4.34304200  | 1.77828500  |
| H | -3.73986100 | 3.31469900  | 2.04862500  |
| H | -2.38422800 | 4.42187900  | 1.89006400  |
| H | -3.93953400 | 5.01921900  | 2.50074100  |
| C | -6.10811900 | 7.22688900  | -1.43459900 |
| H | -6.76257600 | 7.41650200  | -0.57681900 |
| H | -5.53503900 | 8.14602900  | -1.61658300 |
| H | -6.73995900 | 7.05938600  | -2.31370900 |
| C | 3.66397500  | 3.35239800  | -2.44224800 |
| H | 3.62270300  | 2.28066000  | -2.66571500 |
| H | 2.64211300  | 3.72846200  | -2.57262200 |
| H | 4.30136700  | 3.83398700  | -3.19004200 |
| C | 3.21182900  | 2.77920100  | 2.57368800  |
| H | 2.19103800  | 3.17803400  | 2.62634500  |
| H | 3.12301000  | 1.69009000  | 2.51414700  |
| H | 3.72240900  | 3.01982700  | 3.51037700  |
| C | 6.98068400  | 5.57097000  | 0.66890600  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 7.07190900  | 6.33687100  | -0.10926300 |
| H | 6.96163900  | 6.07535000  | 1.64112500  |
| H | 7.89510600  | 4.96336400  | 0.63464600  |
| C | 1.66669200  | -2.63586300 | -4.04849500 |
| H | 0.61591500  | -2.58609300 | -3.74059800 |
| H | 2.06996800  | -1.62478400 | -3.91894900 |
| H | 1.69933600  | -2.87490900 | -5.11585700 |
| C | 3.12829900  | -4.55121100 | 0.42682600  |
| H | 3.50649600  | -3.59869900 | 0.81427800  |
| H | 2.11432400  | -4.67391100 | 0.82507600  |
| H | 3.75062600  | -5.35092900 | 0.83968800  |
| C | 4.71635900  | -6.66148000 | -3.88051800 |
| H | 4.90873200  | -7.53038400 | -3.24221100 |
| H | 4.20989700  | -7.01132100 | -4.78711900 |
| H | 5.69045400  | -6.25905800 | -4.18929900 |
| C | 3.97348400  | -1.08893900 | 2.59873500  |
| C | 2.69161500  | -1.28085900 | 3.17076400  |
| C | 2.39045400  | -0.69829900 | 4.44078700  |
| C | 3.35158600  | 0.02045600  | 5.13045800  |
| C | 4.62928800  | 0.18173800  | 4.56559900  |
| C | 4.92614100  | -0.36426400 | 3.30590100  |
| H | 4.20094600  | -1.49399600 | 1.61875500  |
| H | 3.12423200  | 0.45997200  | 6.09896600  |
| H | 5.38912100  | 0.74368000  | 5.10158700  |
| H | 5.91292400  | -0.21262700 | 2.87620600  |
| C | 0.94819100  | -0.98119900 | 4.80324900  |
| C | 1.57215000  | -1.99898200 | 2.69921900  |
| C | 0.47143900  | -2.00252300 | 3.72745000  |
| H | -0.49366000 | -1.72461500 | 3.29053200  |
| H | 0.34686800  | -3.00848700 | 4.15938400  |
| H | 0.62223200  | -0.35439900 | 1.74873900  |
| H | 1.52878000  | -2.55423000 | 1.77079900  |
| H | 0.83745500  | -1.35779000 | 5.82645100  |
| H | 0.35685500  | -0.05843200 | 4.73628100  |

**Structure: <sup>5</sup>INT3**

|    |            |             |             |
|----|------------|-------------|-------------|
| Mn | 0.21319000 | 0.16105900  | -0.21469800 |
| C  | 2.42907500 | -1.91124700 | -0.14401200 |
| C  | 2.67181900 | -3.31259200 | -0.38879600 |
| C  | 1.49431700 | -3.85691700 | -0.80700200 |
| C  | 0.50323800 | -2.80874400 | -0.76507900 |
| N  | 1.10013200 | -1.63923100 | -0.36134600 |
| H  | 3.63512000 | -3.79133200 | -0.28374600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.29063800  | -4.87805600 | -1.09638700 |
| C | -0.86131900 | -2.99876700 | -1.00251500 |
| C | -3.24586600 | -2.24229000 | -0.81280900 |
| C | -3.85620300 | -1.08345100 | -0.43097100 |
| C | -2.81808800 | -0.11470100 | -0.18634500 |
| N | -1.59044800 | -0.72195600 | -0.34435800 |
| C | -1.82422900 | -2.01711700 | -0.74985900 |
| H | -3.70130900 | -3.18127900 | -1.09460200 |
| H | -4.91345600 | -0.87327200 | -0.35449900 |
| C | 3.43200500  | -0.97709600 | 0.12867300  |
| N | 2.00607400  | 1.03435500  | -0.08627000 |
| C | 2.26400900  | 2.37847900  | -0.20697100 |
| C | 3.68218900  | 2.60322500  | -0.07574400 |
| C | 4.26079000  | 1.39098600  | 0.15648200  |
| C | 3.21036200  | 0.40303100  | 0.11463900  |
| H | 4.15234200  | 3.57476800  | -0.13358400 |
| H | 5.30612300  | 1.16267700  | 0.30922600  |
| C | 1.31780000  | 3.39696100  | -0.34784900 |
| N | -0.68511600 | 1.96433300  | -0.14675800 |
| C | -2.02906700 | 2.20826900  | -0.01032000 |
| C | -2.25596100 | 3.63454800  | -0.01904500 |
| C | -1.04595200 | 4.23177300  | -0.19967700 |
| C | -0.05920400 | 3.18054500  | -0.26265600 |
| H | -3.22819100 | 4.09701200  | 0.07223000  |
| H | -0.81780800 | 5.28569500  | -0.27037600 |
| C | -3.04744300 | 1.25127200  | 0.00712900  |
| O | 0.17680500  | 0.06450600  | 1.58676100  |
| H | -0.65372100 | -0.35235800 | 1.88320000  |
| C | 0.09199800  | -1.38891300 | 5.14623100  |
| H | 0.38704700  | -0.89943000 | 6.06826200  |
| C | -1.22569200 | -1.47510100 | 4.66054100  |
| C | -2.44294600 | -0.98232300 | 5.19178100  |
| C | -3.61651200 | -1.15096100 | 4.46422200  |
| C | -3.60524400 | -1.78947800 | 3.21314800  |
| C | -2.40492100 | -2.29919800 | 2.68525200  |
| C | -1.23096800 | -2.16458700 | 3.40620400  |
| H | -2.45207800 | -0.46615600 | 6.14817700  |
| H | -4.55336600 | -0.76532700 | 4.85824400  |
| H | -4.52475100 | -1.88639300 | 2.64326600  |
| H | -2.40576200 | -2.78569300 | 1.71713400  |
| N | 0.25172600  | 0.28802400  | -2.18172600 |
| C | -0.34630500 | 1.09347600  | -2.85883500 |
| O | -0.91476200 | 1.87166600  | -3.56150900 |
| C | 1.06015700  | -1.93017200 | 4.13010100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.16212700  | -2.67210200 | 3.09858600  |
| H | 1.57787900  | -1.09887400 | 3.62770800  |
| H | 1.83563800  | -2.57293400 | 4.56594100  |
| H | 0.46823700  | -2.48064800 | 2.06737300  |
| H | 0.20205600  | -3.75869400 | 3.25888600  |
| C | -1.31160600 | -4.30301200 | -1.58795500 |
| C | -1.52092800 | -4.36344300 | -2.98289600 |
| C | -1.50807700 | -5.44615600 | -0.78897100 |
| C | -1.92255500 | -5.57395000 | -3.55415500 |
| C | -1.90729700 | -6.63863800 | -1.40432500 |
| C | -2.12291200 | -6.72299800 | -2.78215700 |
| H | -2.07676700 | -5.62232200 | -4.63040300 |
| H | -2.05276100 | -7.52414000 | -0.78853900 |
| C | -4.46118600 | 1.74044200  | 0.08152800  |
| C | -5.03338200 | 2.04299400  | 1.33231300  |
| C | -5.19511700 | 1.92829700  | -1.10810200 |
| C | -6.35303900 | 2.50351500  | 1.37649700  |
| C | -6.51110400 | 2.39412300  | -1.01682600 |
| C | -7.10850600 | 2.68436800  | 0.21376900  |
| H | -6.79976400 | 2.72987200  | 2.34282700  |
| H | -7.08245500 | 2.53818500  | -1.93190400 |
| C | 1.79954500  | 4.79762700  | -0.56389400 |
| C | 2.05396900  | 5.64169900  | 0.53359400  |
| C | 1.98501900  | 5.25700300  | -1.88306200 |
| C | 2.49402300  | 6.94717600  | 0.29152200  |
| C | 2.42538800  | 6.56974600  | -2.07963600 |
| C | 2.68146900  | 7.43048200  | -1.00729700 |
| H | 2.69433500  | 7.60156800  | 1.13776600  |
| H | 2.57244400  | 6.92854300  | -3.09651400 |
| C | 4.83575200  | -1.47191200 | 0.30791700  |
| C | 5.29323600  | -1.82786000 | 1.59053100  |
| C | 5.69032900  | -1.57633500 | -0.80841800 |
| C | 6.60859600  | -2.27862700 | 1.74022300  |
| C | 6.99805400  | -2.03303300 | -0.61558500 |
| C | 7.47601100  | -2.38982300 | 0.64949500  |
| H | 6.96348700  | -2.54849300 | 2.73302600  |
| H | 7.66030000  | -2.11143500 | -1.47568000 |
| C | -1.31964900 | -5.40334200 | 0.71086900  |
| H | -0.41140700 | -4.86426600 | 0.99595500  |
| H | -2.15775000 | -4.89392500 | 1.20133200  |
| H | -1.26187100 | -6.41363300 | 1.12808000  |
| C | -1.32281300 | -3.13784000 | -3.84693400 |
| H | -2.08910400 | -2.38056400 | -3.63979700 |
| H | -0.35846700 | -2.65455800 | -3.65502900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.37830300 | -3.39247200 | -4.90971500 |
| C | -2.58368200 | -8.01285500 | -3.42034800 |
| H | -2.15695700 | -8.13988700 | -4.42151400 |
| H | -2.30151500 | -8.88293600 | -2.81791000 |
| H | -3.67640600 | -8.03092200 | -3.52931700 |
| C | 4.37037700  | -1.73254600 | 2.78207200  |
| H | 3.95291900  | -0.72453000 | 2.88705700  |
| H | 3.51671100  | -2.41060700 | 2.67158400  |
| H | 4.88930200  | -1.98784700 | 3.71120000  |
| C | 5.20431800  | -1.19906100 | -2.18921600 |
| H | 4.30962300  | -1.76909600 | -2.46557100 |
| H | 4.92629300  | -0.13953200 | -2.23780100 |
| H | 5.97501600  | -1.38412200 | -2.94361000 |
| C | 8.88347500  | -2.91050600 | 0.82742000  |
| H | 9.26941500  | -2.69014800 | 1.82861600  |
| H | 8.92096100  | -4.00033800 | 0.69622300  |
| H | 9.56966500  | -2.47195700 | 0.09464200  |
| C | -4.58187200 | 1.63159900  | -2.45899300 |
| H | -3.57906200 | 2.06126400  | -2.56083400 |
| H | -4.47289400 | 0.55143400  | -2.61764500 |
| H | -5.20621200 | 2.02589600  | -3.26666300 |
| C | -4.22651400 | 1.89455100  | 2.60098400  |
| H | -3.77029900 | 0.90310100  | 2.67836900  |
| H | -3.40561400 | 2.62211100  | 2.63248100  |
| H | -4.84901900 | 2.05095400  | 3.48766400  |
| C | -8.52143400 | 3.21629400  | 0.28263000  |
| H | -9.13213900 | 2.84297200  | -0.54668600 |
| H | -9.01195100 | 2.93293000  | 1.22027300  |
| H | -8.53367000 | 4.31319000  | 0.22735200  |
| C | 1.85194000  | 5.14426600  | 1.94672700  |
| H | 0.80957700  | 4.84927700  | 2.11792100  |
| H | 2.46406300  | 4.25727000  | 2.14833100  |
| H | 2.11309200  | 5.91406800  | 2.67930400  |
| C | 1.72244800  | 4.34437000  | -3.05964200 |
| H | 2.37006900  | 3.45953500  | -3.02537500 |
| H | 0.69204300  | 3.97046700  | -3.06946100 |
| H | 1.90513000  | 4.86066700  | -4.00704300 |
| C | 3.12173800  | 8.85598600  | -1.24803100 |
| H | 3.72364900  | 8.94174700  | -2.15939900 |
| H | 2.25603800  | 9.52143000  | -1.36695900 |
| H | 3.71507900  | 9.24054400  | -0.41135000 |

**Structure: 5**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.47987900 | 1.24833400  | 0.00010400  |
| H | -1.74369400 | 2.30050200  | 0.00016100  |
| C | -0.16749700 | 0.74112200  | 0.00009100  |
| C | 1.08020400  | 1.41296400  | 0.00008400  |
| C | 2.25094800  | 0.66350600  | -0.00002300 |
| C | 2.21010400  | -0.74093600 | -0.00011800 |
| C | 0.97739100  | -1.41779700 | -0.00006800 |
| C | -0.19769100 | -0.68708400 | 0.00007000  |
| H | 1.11534500  | 2.49928000  | 0.00013600  |
| H | 3.21315200  | 1.16951700  | -0.00008400 |
| H | 3.13725600  | -1.30730800 | -0.00025000 |
| H | 0.95287200  | -2.50535700 | -0.00016600 |
| C | -2.48920000 | 0.13177400  | -0.00036500 |
| C | -1.63179300 | -1.17335200 | 0.00027900  |
| H | -3.15325500 | 0.18232700  | 0.87550400  |
| H | -3.15215600 | 0.18219400  | -0.87707400 |
| H | -1.84245600 | -1.79558100 | 0.87907000  |
| H | -1.84258200 | -1.79675200 | -0.87763200 |

**Structure: 46**

|    |             |             |             |
|----|-------------|-------------|-------------|
| Mn | 0.06847200  | 0.01121200  | -0.22336900 |
| C  | 2.97609000  | 0.83640200  | -0.30927800 |
| C  | 3.82784700  | 1.99463000  | -0.18298100 |
| C  | 3.02451500  | 3.05242700  | 0.12435600  |
| C  | 1.66633200  | 2.56500000  | 0.13231200  |
| N  | 1.66975000  | 1.21623200  | -0.12378500 |
| H  | 4.90340500  | 1.97418800  | -0.28830400 |
| H  | 3.30356100  | 4.08109100  | 0.30416900  |
| C  | 0.53615200  | 3.37718700  | 0.25840600  |
| C  | -1.92688900 | 3.76566500  | -0.04172500 |
| C  | -2.98331500 | 2.97603500  | -0.39066200 |
| C  | -2.48777700 | 1.62801300  | -0.50832400 |
| N  | -1.12720400 | 1.62773400  | -0.29119900 |
| C  | -0.76199300 | 2.92037300  | 0.01338300  |
| H  | -1.91650300 | 4.82939500  | 0.14964800  |
| H  | -4.01775100 | 3.25835100  | -0.52603200 |
| C  | 3.44203500  | -0.47242700 | -0.46400800 |
| N  | 1.25494200  | -1.59029200 | -0.16344500 |
| C  | 0.86867100  | -2.88475600 | 0.08460500  |
| C  | 2.03283000  | -3.73581500 | 0.07830700  |
| C  | 3.10490700  | -2.94751100 | -0.21871400 |
| C  | 2.61834900  | -1.59431600 | -0.33617700 |
| H  | 2.00782100  | -4.80227000 | 0.25246600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.14257100  | -3.23314000 | -0.31820700 |
| C | -0.44425300 | -3.34654500 | 0.21066600  |
| N | -1.54707800 | -1.18934900 | -0.26990400 |
| C | -2.84146400 | -0.80733800 | -0.52516000 |
| C | -3.69791800 | -1.96848100 | -0.47040100 |
| C | -2.91380900 | -3.02934000 | -0.13161500 |
| C | -1.56055100 | -2.53965200 | -0.02406200 |
| H | -4.76520600 | -1.94660800 | -0.63811700 |
| H | -3.20218000 | -4.06003300 | 0.01821000  |
| C | -3.30336100 | 0.50358000  | -0.66877100 |
| O | 0.16525600  | -0.01387200 | -2.03042700 |
| H | -0.07158700 | 0.87288600  | -2.35362300 |
| N | -0.04729100 | 0.04313600  | 1.73828900  |
| C | -0.98044000 | -0.32439500 | 2.41572200  |
| O | -1.87232100 | -0.68247300 | 3.12156100  |
| C | 0.72690500  | 4.81721800  | 0.62173300  |
| C | 0.71187400  | 5.18591900  | 1.98117900  |
| C | 0.91892800  | 5.78754200  | -0.38057200 |
| C | 0.89065400  | 6.53202700  | 2.31559800  |
| C | 1.09488200  | 7.12256800  | -0.00305900 |
| C | 1.08099000  | 7.51496800  | 1.33930100  |
| H | 0.88237600  | 6.81921100  | 3.36527000  |
| H | 1.24699300  | 7.87358000  | -0.77591000 |
| C | -4.77427600 | 0.71546300  | -0.85403900 |
| C | -5.31148000 | 0.80543000  | -2.15139200 |
| C | -5.60768100 | 0.82263500  | 0.27814900  |
| C | -6.68825400 | 1.00113100  | -2.30007100 |
| C | -6.97899100 | 1.01714900  | 0.08418100  |
| C | -7.53840500 | 1.10568300  | -1.19489900 |
| H | -7.10608800 | 1.07361700  | -3.30237600 |
| H | -7.62639100 | 1.10338100  | 0.95472200  |
| C | -0.66923400 | -4.78291700 | 0.56677700  |
| C | -0.75768600 | -5.76360100 | -0.43966900 |
| C | -0.79551500 | -5.13375100 | 1.92567500  |
| C | -0.97227800 | -7.09429700 | -0.06642400 |
| C | -1.00952000 | -6.47624500 | 2.25428800  |
| C | -1.10387600 | -7.46960100 | 1.27436800  |
| H | -1.03805500 | -7.85548900 | -0.84150800 |
| H | -1.10405700 | -6.75231100 | 3.30269800  |
| C | 4.90901000  | -0.68712200 | -0.67781300 |
| C | 5.40778500  | -0.77070200 | -1.99206400 |
| C | 5.77575000  | -0.81436400 | 0.42567000  |
| C | 6.77724600  | -0.98080100 | -2.18214000 |
| C | 7.13851200  | -1.02375000 | 0.19130700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 7.65882300  | -1.10726300 | -1.10419400 |
| H | 7.16427000  | -1.04904900 | -3.19703000 |
| H | 7.80961400  | -1.12694500 | 1.04186100  |
| C | 0.93646100  | 5.39086200  | -1.83926600 |
| H | 1.72947600  | 4.66138700  | -2.04355500 |
| H | -0.00968600 | 4.91996600  | -2.13268700 |
| H | 1.09830100  | 6.25937900  | -2.48494100 |
| C | 0.50638700  | 4.14238700  | 3.05541100  |
| H | -0.45753100 | 3.63352100  | 2.93667700  |
| H | 1.27306400  | 3.36058500  | 3.00505200  |
| H | 0.53639500  | 4.59005300  | 4.05345300  |
| C | 1.23886100  | 8.96819500  | 1.72275700  |
| H | 1.69288900  | 9.07483200  | 2.71389800  |
| H | 1.86371100  | 9.50811500  | 1.00288400  |
| H | 0.26562700  | 9.47629000  | 1.75401100  |
| C | 4.47475400  | -0.63957800 | -3.17419900 |
| H | 3.69455800  | -1.40955700 | -3.15400400 |
| H | 3.95488500  | 0.32586400  | -3.16458500 |
| H | 5.01836500  | -0.72639000 | -4.12001300 |
| C | 5.24041600  | -0.73446800 | 1.83710400  |
| H | 4.74649100  | 0.22675700  | 2.02151400  |
| H | 4.48932000  | -1.51165300 | 2.02178200  |
| H | 6.04248500  | -0.85309100 | 2.57195200  |
| C | 9.14013200  | -1.30128200 | -1.33236000 |
| H | 9.33654200  | -1.82146100 | -2.27617100 |
| H | 9.66276700  | -0.33628200 | -1.37737000 |
| H | 9.59848200  | -1.88064300 | -0.52337700 |
| C | -5.02763100 | 0.75268000  | 1.67287000  |
| H | -4.42459600 | -0.14922200 | 1.82443100  |
| H | -4.36003100 | 1.60193200  | 1.86428400  |
| H | -5.81776500 | 0.76764500  | 2.42969500  |
| C | -4.41100700 | 0.69695700  | -3.36088200 |
| H | -3.65252900 | 1.48941900  | -3.36253500 |
| H | -3.86771200 | -0.25549200 | -3.36895700 |
| H | -4.98324400 | 0.77214200  | -4.29064100 |
| C | -9.02843600 | 1.28173900  | -1.37635200 |
| H | -9.46505800 | 1.87076400  | -0.56226500 |
| H | -9.26195400 | 1.78337500  | -2.32172200 |
| H | -9.54259800 | 0.31121700  | -1.38641800 |
| C | -0.62010900 | -5.38270500 | -1.89609900 |
| H | -1.37653700 | -4.64381900 | -2.18612900 |
| H | 0.35602200  | -4.92547300 | -2.09768400 |
| H | -0.72863400 | -6.25614700 | -2.54635400 |
| C | -0.69066600 | -4.08052000 | 3.00534100  |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | 0.28316200  | -3.57667800 | 2.97301100 |
| H | -1.44598000 | -3.29474000 | 2.88956200 |
| H | -0.81052400 | -4.52201900 | 3.99943000 |
| C | -1.37033400 | -8.90814400 | 1.65356800 |
| H | -0.94638400 | -9.14968700 | 2.63439100 |
| H | -2.44880700 | -9.10915100 | 1.70719600 |
| H | -0.94657400 | -9.60241900 | 0.91972300 |

**Structure: 66**

|    |             |             |             |
|----|-------------|-------------|-------------|
| Mn | 0.06242100  | -0.00955200 | -0.40269600 |
| C  | 2.94041800  | -1.17255600 | -0.15275700 |
| C  | 4.34018500  | -0.78286000 | -0.07881900 |
| C  | 4.37433200  | 0.58328900  | -0.08565000 |
| C  | 2.99576300  | 1.03999000  | -0.16473300 |
| N  | 2.18013600  | -0.04796200 | -0.20625300 |
| H  | 5.17471200  | -1.46803000 | -0.02473700 |
| H  | 5.24161400  | 1.22719200  | -0.04008600 |
| C  | 2.56321000  | 2.39348900  | -0.16999300 |
| C  | 0.83041100  | 4.27270400  | -0.11948600 |
| C  | -0.53727800 | 4.30273400  | -0.15715600 |
| C  | -0.98770600 | 2.93272000  | -0.31186500 |
| N  | 0.10536000  | 2.12115500  | -0.38833300 |
| C  | 1.22831300  | 2.88343100  | -0.24740000 |
| H  | 1.50915300  | 5.10531000  | 0.00234700  |
| H  | -1.18548600 | 5.16385500  | -0.07370700 |
| C  | 2.44694800  | -2.50804200 | -0.14562600 |
| N  | 0.00587600  | -2.12683900 | -0.29840600 |
| C  | -1.11977200 | -2.88892300 | -0.26436300 |
| C  | -0.73034200 | -4.28613800 | -0.15994400 |
| C  | 0.63537400  | -4.31728600 | -0.12377200 |
| C  | 1.09302700  | -2.93902100 | -0.20200300 |
| H  | -1.41581700 | -5.12093000 | -0.11524800 |
| H  | 1.27867500  | -5.18227400 | -0.04182000 |
| C  | -2.45384000 | -2.39570200 | -0.27865600 |
| N  | -2.07195100 | 0.04664900  | -0.42914800 |
| C  | -2.83865700 | 1.17173800  | -0.36783100 |
| C  | -4.23620700 | 0.77783600  | -0.29217300 |
| C  | -4.26483800 | -0.58701800 | -0.28407800 |
| C  | -2.88499200 | -1.04147800 | -0.35417400 |
| H  | -5.07217000 | 1.46056000  | -0.23385400 |
| H  | -5.12852800 | -1.23326000 | -0.21606500 |
| C  | -2.34552500 | 2.50129100  | -0.30720900 |
| O  | 0.17701800  | -0.08543400 | -2.21810200 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.20594400  | 0.81522000  | -2.58446900 |
| N | -0.07585500 | 0.03784200  | 1.62559000  |
| C | -1.06248400 | 0.02485100  | 2.31905500  |
| O | -2.02351900 | 0.01602700  | 3.03628900  |
| C | 3.63848800  | 3.42859300  | -0.03436400 |
| C | 4.10788300  | 3.77768000  | 1.24714100  |
| C | 4.17383400  | 4.03517600  | -1.18620800 |
| C | 5.11536600  | 4.74155800  | 1.35168200  |
| C | 5.18346200  | 4.99083200  | -1.03559800 |
| C | 5.66502600  | 5.36023100  | 0.22415600  |
| H | 5.48095800  | 5.01414600  | 2.33977500  |
| H | 5.60457700  | 5.45615500  | -1.92463700 |
| C | -3.37647000 | 3.57407200  | -0.13156200 |
| C | -3.97008200 | 4.17123600  | -1.25838500 |
| C | -3.73872200 | 3.96781100  | 1.17257600  |
| C | -4.93150700 | 5.16771500  | -1.06275900 |
| C | -4.70550600 | 4.96740500  | 1.32017400  |
| C | -5.31486300 | 5.57668000  | 0.21820900  |
| H | -5.39027600 | 5.63515700  | -1.93185800 |
| H | -4.98835800 | 5.27861800  | 2.32387800  |
| C | -3.53832000 | -3.41721500 | -0.12504700 |
| C | -4.18052400 | -3.93642600 | -1.26432200 |
| C | -3.90766400 | -3.83554700 | 1.16937600  |
| C | -5.19745700 | -4.88027800 | -1.08960100 |
| C | -4.93260200 | -4.77857000 | 1.29561000  |
| C | -5.59091200 | -5.30979600 | 0.18159700  |
| H | -5.69312100 | -5.28892200 | -1.96803400 |
| H | -5.22344000 | -5.10625900 | 2.29178000  |
| C | 3.47763500  | -3.59044400 | -0.03638600 |
| C | 3.99532400  | -4.18058700 | -1.20483200 |
| C | 3.90983600  | -4.01127300 | 1.23616500  |
| C | 4.95102100  | -5.19354500 | -1.07789600 |
| C | 4.86582700  | -5.02847400 | 1.31642200  |
| C | 5.40047400  | -5.62975400 | 0.17243800  |
| H | 5.35221200  | -5.65384000 | -1.97871800 |
| H | 5.19872300  | -5.36060600 | 2.29783900  |
| C | 3.67111200  | 3.65151200  | -2.55932200 |
| H | 3.77307300  | 2.57344900  | -2.73348200 |
| H | 2.60667300  | 3.89130800  | -2.67191000 |
| H | 4.22213700  | 4.17726200  | -3.34486100 |
| C | 3.53501400  | 3.11975900  | 2.48165600  |
| H | 2.44458000  | 3.22537200  | 2.52154700  |
| H | 3.74317700  | 2.04320900  | 2.49029300  |
| H | 3.95523600  | 3.55547500  | 3.39304300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 6.73240500  | 6.42035800  | 0.36660500  |
| H | 7.36221000  | 6.23974100  | 1.24450700  |
| H | 7.38115700  | 6.45835700  | -0.51515400 |
| H | 6.28575000  | 7.41655400  | 0.48621300  |
| C | 3.52131300  | -3.72770000 | -2.56674600 |
| H | 2.44336800  | -3.88960300 | -2.68663600 |
| H | 3.69282700  | -2.65425100 | -2.71085900 |
| H | 4.03850100  | -4.26696700 | -3.36609000 |
| C | 3.34210800  | -3.37998800 | 2.48675800  |
| H | 3.53922600  | -2.30168200 | 2.51286000  |
| H | 2.25291300  | -3.49822400 | 2.53286700  |
| H | 3.77275600  | -3.82798500 | 3.38727200  |
| C | 6.45704900  | -6.70422600 | 0.28512100  |
| H | 6.41716800  | -7.39757200 | -0.56203200 |
| H | 7.46453200  | -6.26716700 | 0.30118500  |
| H | 6.34084400  | -7.28589100 | 1.20606700  |
| C | -3.08475200 | 3.33659100  | 2.38061200  |
| H | -3.18539900 | 2.24538600  | 2.38825600  |
| H | -2.00766200 | 3.54477300  | 2.39760700  |
| H | -3.51709800 | 3.72360600  | 3.30822400  |
| C | -3.56927100 | 3.74365300  | -2.65189800 |
| H | -2.49585200 | 3.89511100  | -2.82002200 |
| H | -3.76643300 | 2.67669700  | -2.81202400 |
| H | -4.11519300 | 4.30858500  | -3.41348900 |
| C | -6.37994100 | 6.63154300  | 0.40968700  |
| H | -6.19147700 | 7.23352700  | 1.30544100  |
| H | -6.43411100 | 7.30857000  | -0.44965100 |
| H | -7.37144200 | 6.17439800  | 0.52864100  |
| C | -3.77351900 | -3.48201200 | -2.64752200 |
| H | -3.95149600 | -2.40791100 | -2.78051600 |
| H | -2.70342000 | -3.64546500 | -2.82264700 |
| H | -4.33217100 | -4.01742800 | -3.42120000 |
| C | -3.20492300 | -3.28686000 | 2.39048500  |
| H | -2.14898600 | -3.58479200 | 2.40191100  |
| H | -3.21522500 | -2.19140400 | 2.42234400  |
| H | -3.66864900 | -3.65768900 | 3.30957300  |
| C | -6.71813400 | -6.30208300 | 0.35084500  |
| H | -6.56215900 | -6.94058300 | 1.22730900  |
| H | -7.67856900 | -5.78797600 | 0.49070900  |
| H | -6.81972500 | -6.94881800 | -0.52733100 |

**Structure: Me<sub>3</sub>SiOH**

|    |             |            |            |
|----|-------------|------------|------------|
| Si | -0.00538000 | 0.00000100 | 0.03786700 |
|----|-------------|------------|------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.92283300  | -1.53923800 | -0.53990100 |
| H | 1.00087000  | -1.56102100 | -1.63451700 |
| H | 1.94410900  | -1.57780600 | -0.13994300 |
| H | 0.40543000  | -2.45250400 | -0.22319200 |
| C | 0.92252900  | 1.53946900  | -0.53977700 |
| H | 0.40494500  | 2.45261200  | -0.22300800 |
| H | 1.94379000  | 1.57820500  | -0.13980100 |
| H | 1.00057400  | 1.56134500  | -1.63439100 |
| C | -1.76518200 | -0.00014500 | -0.61726400 |
| H | -2.31073100 | -0.88600600 | -0.27245700 |
| H | -2.31125800 | 0.88496100  | -0.27135200 |
| H | -1.78135400 | 0.00053700  | -1.71394900 |
| O | -0.16977700 | -0.00008800 | 1.71123000  |
| H | 0.65608100  | -0.00014800 | 2.21427700  |

**Structure: 47**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.79897400  | -1.04549900 | -0.40940300 |
| C | 4.17734900  | -0.62509500 | -0.40949000 |
| C | 4.19532400  | 0.69758700  | -0.07829800 |
| C | 2.82558800  | 1.11673800  | 0.07414700  |
| N | 1.99798100  | 0.03763900  | -0.13148700 |
| H | 5.01330900  | -1.28126100 | -0.60547600 |
| H | 5.04813400  | 1.35169500  | 0.03472300  |
| C | -1.08989000 | 2.84807500  | -0.19385300 |
| C | -0.66660700 | 4.22521000  | -0.14023800 |
| C | 0.66791700  | 4.22501000  | 0.14021600  |
| C | 1.09077800  | 2.84774400  | 0.19386800  |
| N | 0.00031800  | 2.03335800  | 0.00001900  |
| H | -1.32822900 | 5.07019200  | -0.26850400 |
| H | 1.32979900  | 5.06979100  | 0.26846200  |
| C | -1.06884700 | -2.78428800 | 0.29206800  |
| C | -0.65435300 | -4.16162300 | 0.19336700  |
| C | 0.65307500  | -4.16182500 | -0.19327800 |
| C | 1.06799200  | -2.78462000 | -0.29198700 |
| N | -0.00030000 | -1.97037600 | 0.00004200  |
| H | -1.30299800 | -5.00657600 | 0.37597300  |
| H | 1.30145900  | -5.00698100 | -0.37587600 |
| C | -2.79929400 | -1.04463500 | 0.40946100  |
| C | -4.17753800 | -0.62380600 | 0.40953500  |
| C | -4.19510300 | 0.69888100  | 0.07833900  |
| C | -2.82523500 | 1.11760700  | -0.07410200 |
| N | -1.99796300 | 0.03825300  | 0.13154600  |
| H | -5.01370200 | -1.27971300 | 0.60551500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -5.04770800 | 1.35325400  | -0.03469400 |
| C  | 2.38199600  | -2.37301200 | -0.52899600 |
| C  | -2.42113700 | 2.43719100  | -0.29271200 |
| C  | 2.42189800  | 2.43645300  | 0.29273000  |
| C  | -2.38272400 | -2.37227800 | 0.52906100  |
| N  | 0.11981800  | 0.02186700  | 1.92525200  |
| C  | 1.10391600  | -0.22814300 | 2.58849800  |
| O  | 2.03921400  | -0.45534500 | 3.28618600  |
| Mn | 0.00000900  | 0.03526500  | 0.00003100  |
| N  | -0.11980100 | 0.02187200  | -1.92519200 |
| C  | -1.10396800 | -0.22788700 | -2.58843100 |
| O  | -2.03933100 | -0.45485300 | -3.28610800 |
| C  | 3.47415000  | 3.46363600  | 0.57282700  |
| C  | 4.09349900  | 4.15734200  | -0.48440700 |
| C  | 3.84337400  | 3.71180200  | 1.90985000  |
| C  | 5.08179000  | 5.10016300  | -0.18290800 |
| C  | 4.83625800  | 4.66235100  | 2.16604500  |
| C  | 5.46486000  | 5.36830400  | 1.13495200  |
| H  | 5.56493000  | 5.63608600  | -0.99757600 |
| H  | 5.12700900  | 4.85489800  | 3.19693900  |
| C  | -3.47306100 | 3.46469800  | -0.57285300 |
| C  | -3.84225000 | 3.71287500  | -1.90988400 |
| C  | -4.09212300 | 4.15871400  | 0.48434300  |
| C  | -4.83480600 | 4.66375100  | -2.16612500 |
| C  | -5.08009200 | 5.10186100  | 0.18279900  |
| C  | -5.46311700 | 5.37002100  | -1.13506900 |
| H  | -5.12552700 | 4.85631300  | -3.19702500 |
| H  | -5.56300800 | 5.63802800  | 0.99743800  |
| C  | 3.41891200  | -3.41759000 | -0.80253200 |
| C  | 4.09142100  | -4.03330800 | 0.27199300  |
| C  | 3.72078600  | -3.76374300 | -2.13300300 |
| C  | 5.06677100  | -4.99482300 | -0.01076500 |
| C  | 4.70225400  | -4.73122600 | -2.37060100 |
| C  | 5.38450800  | -5.35885800 | -1.32358200 |
| H  | 5.59280900  | -5.46977600 | 0.81511500  |
| H  | 4.94086600  | -4.99899800 | -3.39808300 |
| C  | -3.41998200 | -3.41652500 | 0.80255900  |
| C  | -3.72203900 | -3.76256400 | 2.13301800  |
| C  | -4.09265600 | -4.03201700 | -0.27199300 |
| C  | -4.70385800 | -4.72970100 | 2.37057800  |
| C  | -5.06835800 | -4.99318500 | 0.01072600  |
| C  | -5.38628500 | -5.35709900 | 1.32353100  |
| H  | -4.94261400 | -4.99737900 | 3.39805100  |
| H  | -5.59452800 | -5.46795600 | -0.81517400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.70017800  | 3.88300100  | -1.91806200 |
| H | 3.86061600  | 2.83042100  | -2.18037800 |
| H | 2.63580400  | 4.08745500  | -2.08430400 |
| H | 4.27847800  | 4.49976400  | -2.61264100 |
| C | 3.17657100  | 2.96433900  | 3.04239200  |
| H | 2.09325600  | 3.13652600  | 3.04540300  |
| H | 3.31538400  | 1.88035300  | 2.95726900  |
| H | 3.57267000  | 3.28153100  | 4.01186400  |
| C | 6.51136500  | 6.41476700  | 1.44074300  |
| H | 6.04745600  | 7.38966700  | 1.64240800  |
| H | 7.10007400  | 6.14744000  | 2.32526000  |
| H | 7.20181700  | 6.55017200  | 0.60129500  |
| C | 2.99737900  | -3.09567600 | -3.28004700 |
| H | 1.91454500  | -3.25648000 | -3.21530100 |
| H | 3.14936400  | -2.00981700 | -3.26910100 |
| H | 3.34260200  | -3.47988000 | -4.24472100 |
| C | 3.75896400  | -3.66617200 | 1.70068300  |
| H | 3.84636600  | -2.58799500 | 1.87666900  |
| H | 2.72434300  | -3.93538000 | 1.94626400  |
| H | 4.41847400  | -4.18222800 | 2.40486900  |
| C | 6.41955300  | -6.42446700 | -1.60127900 |
| H | 7.20111000  | -6.43438500 | -0.83371700 |
| H | 5.96383000  | -7.42371300 | -1.61404800 |
| H | 6.90034000  | -6.27409100 | -2.57396700 |
| C | -2.99846400 | -3.09472800 | 3.28009100  |
| H | -1.91567700 | -3.25585800 | 3.21537700  |
| H | -3.15012200 | -2.00882300 | 3.26915200  |
| H | -3.34383300 | -3.47883700 | 4.24475100  |
| C | -3.76000600 | -3.66501000 | -1.70067200 |
| H | -3.84694700 | -2.58679700 | -1.87666000 |
| H | -2.72549100 | -3.93465500 | -1.94622700 |
| H | -4.41971200 | -4.18078800 | -2.40487900 |
| C | -6.42172700 | -6.42233200 | 1.60118500  |
| H | -5.96637000 | -7.42174400 | 1.61397000  |
| H | -6.90250000 | -6.27178200 | 2.57385300  |
| H | -7.20325800 | -6.43196100 | 0.83359100  |
| C | -3.17574300 | 2.96508200  | -3.04238300 |
| H | -2.09236300 | 3.13686000  | -3.04541800 |
| H | -3.31496200 | 1.88115400  | -2.95718200 |
| H | -3.57173500 | 3.28235400  | -4.01187200 |
| C | -3.69882400 | 3.88437700  | 1.91800600  |
| H | -3.85945800 | 2.83184400  | 2.18038600  |
| H | -2.63440600 | 4.08863500  | 2.08421000  |
| H | -4.27698500 | 4.50129600  | 2.61256200  |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -6.50925400 | 6.41683200 | -1.44092700 |
| H | -6.04498000 | 7.39146100 | -1.64305000 |
| H | -7.09831600 | 6.14946100 | -2.32519800 |
| H | -7.19942400 | 6.55281600 | -0.60134100 |

**Structure: <sup>3</sup>TS3**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.54697900 | -2.75279100 | -1.23057500 |
| C  | -1.03221600 | -4.09267500 | -0.99810100 |
| C  | -1.96672000 | -3.99946100 | -0.01177300 |
| C  | -2.05094100 | -2.60149100 | 0.34211100  |
| N  | -1.17544800 | -1.86448700 | -0.40089200 |
| H  | -0.69567900 | -4.97437500 | -1.52819100 |
| H  | -2.55954200 | -4.78833300 | 0.43305900  |
| C  | -2.92848800 | 1.44237300  | 1.57487600  |
| C  | -3.99176900 | 1.12671300  | 2.50177700  |
| C  | -4.10608100 | -0.22806200 | 2.51142500  |
| C  | -3.11802600 | -0.73196000 | 1.58382600  |
| N  | -2.41174400 | 0.30180100  | 1.02909100  |
| H  | -4.56270300 | 1.85727300  | 3.06022000  |
| H  | -4.79315000 | -0.84399100 | 3.07731700  |
| C  | 1.28058400  | 1.01115400  | -2.23009800 |
| C  | 2.19497200  | 0.52183100  | -3.23559400 |
| C  | 1.97678000  | -0.81907300 | -3.33648500 |
| C  | 0.93904300  | -1.13735900 | -2.38404400 |
| N  | 0.53528300  | -0.01068300 | -1.72019600 |
| H  | 2.89125200  | 1.13632200  | -3.79169000 |
| H  | 2.45891500  | -1.53450600 | -3.99028300 |
| C  | 0.21323400  | 2.87926300  | -0.98680100 |
| C  | 0.06182200  | 4.28877900  | -0.70288500 |
| C  | -0.97318800 | 4.39933900  | 0.17177500  |
| C  | -1.44206000 | 3.05568300  | 0.42471900  |
| N  | -0.71137600 | 2.14901000  | -0.28831600 |
| H  | 0.67035200  | 5.07426100  | -1.13215600 |
| H  | -1.39155300 | 5.29408900  | 0.61438500  |
| C  | 0.43274100  | -2.41494900 | -2.16077300 |
| C  | -2.48232700 | 2.72943200  | 1.29014900  |
| C  | -2.93971200 | -2.07654200 | 1.28078300  |
| C  | 1.14721200  | 2.35300400  | -1.87053900 |
| H  | -3.57959700 | -2.78499900 | 1.79931500  |
| H  | -2.98206800 | 3.55050400  | 1.79598700  |
| H  | 1.81437800  | 3.05904000  | -2.35677600 |
| H  | 0.84363800  | -3.22182600 | -2.76097900 |
| Fe | -0.90436600 | 0.14918300  | -0.28944700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Cl | -2.46344400 | 0.33493800  | -2.06631400 |
| O  | 0.23224100  | 0.01914400  | 1.01111400  |
| C  | 5.27057400  | 0.48545500  | 0.51445800  |
| C  | 4.15448100  | -0.31696400 | 0.29645900  |
| C  | 3.36811900  | -0.78585100 | 1.37075700  |
| C  | 3.74575900  | -0.40349600 | 2.67415400  |
| C  | 4.86283800  | 0.40023400  | 2.89195900  |
| C  | 5.63286300  | 0.84848900  | 1.81541200  |
| H  | 5.86367400  | 0.82624900  | -0.33071200 |
| H  | 3.87868900  | -0.59458200 | -0.71837600 |
| H  | 3.15913600  | -0.73995800 | 3.52341500  |
| H  | 5.13500400  | 0.67792900  | 3.90719300  |
| H  | 6.50505300  | 1.47347700  | 1.98780100  |
| C  | 2.17869300  | -1.61570300 | 1.10127300  |
| C  | 1.66228500  | -2.55910400 | 2.17335200  |
| H  | 2.21108400  | -2.07477800 | 0.10918700  |
| H  | 1.17731600  | -0.76254500 | 0.94828900  |
| H  | 0.78067300  | -3.09786100 | 1.81282700  |
| H  | 2.42312300  | -3.30159300 | 2.45486400  |
| H  | 1.36816700  | -2.02273800 | 3.08195600  |

**Structure: <sup>5</sup>TS3**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.36514800  | -2.93725100 | 0.50014500  |
| C | 2.23475900  | -3.99743000 | 0.02635800  |
| C | 3.15877800  | -3.41040600 | -0.78853600 |
| C | 2.85377300  | -1.99191400 | -0.80990100 |
| N | 1.76817200  | -1.74916400 | -0.02998700 |
| H | 2.14758900  | -5.04378400 | 0.29044000  |
| H | 3.97538500  | -3.88324600 | -1.31938700 |
| C | 2.47855600  | 2.36340400  | -1.07773900 |
| C | 3.61813700  | 2.58830600  | -1.94746900 |
| C | 4.15523700  | 1.36528100  | -2.21660500 |
| C | 3.34680200  | 0.38779900  | -1.51167600 |
| N | 2.34543500  | 1.02772600  | -0.84236700 |
| H | 3.95618400  | 3.55717700  | -2.29246100 |
| H | 5.01973100  | 1.13486100  | -2.82619000 |
| C | -1.46953100 | -0.11124400 | 2.27375900  |
| C | -2.20191000 | -1.07127000 | 3.07469900  |
| C | -1.64636600 | -2.29401800 | 2.82819100  |
| C | -0.57509900 | -2.08083900 | 1.87659300  |
| N | -0.50845700 | -0.75587400 | 1.55573500  |
| H | -3.01719700 | -0.83138700 | 3.74547000  |
| H | -1.91983200 | -3.25031300 | 3.25584400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.96910300 | 2.27129800  | 1.59188600  |
| C  | -1.21955600 | 3.70044600  | 1.63618600  |
| C  | -0.27707700 | 4.28750700  | 0.84470600  |
| C  | 0.54918800  | 3.21674700  | 0.31634900  |
| N  | 0.10245400  | 2.02405700  | 0.78854600  |
| H  | -2.00972000 | 4.17965700  | 2.20014100  |
| H  | -0.14404600 | 5.34140300  | 0.63561500  |
| C  | 0.27941400  | -3.07926600 | 1.37719300  |
| C  | 1.64721900  | 3.36295600  | -0.54767700 |
| C  | 3.56928600  | -0.99742200 | -1.49975500 |
| C  | -1.69010900 | 1.27918200  | 2.26869000  |
| H  | 4.41869000  | -1.34293300 | -2.08398200 |
| H  | 1.89077700  | 4.38187100  | -0.83845600 |
| H  | -2.51218700 | 1.62712200  | 2.88917400  |
| H  | 0.08326200  | -4.08800100 | 1.73256800  |
| Fe | 0.88217200  | 0.13880300  | 0.29257600  |
| Cl | 2.29174200  | 0.34069000  | 2.18501400  |
| O  | -0.11174500 | 0.03035000  | -1.12723800 |
| C  | -5.29190900 | -0.01599700 | -0.40584200 |
| C  | -4.11219100 | -0.75509300 | -0.41638800 |
| C  | -3.28198900 | -0.79293700 | -1.55712700 |
| C  | -3.68276000 | -0.04596700 | -2.68437700 |
| C  | -4.86210100 | 0.69500500  | -2.67239100 |
| C  | -5.67456800 | 0.71409600  | -1.53505800 |
| H  | -5.91887700 | -0.01268600 | 0.48250400  |
| H  | -3.82168800 | -1.32302900 | 0.46426400  |
| H  | -3.06282800 | -0.04515600 | -3.57561000 |
| H  | -5.15025200 | 1.26054000  | -3.55495400 |
| H  | -6.59574400 | 1.29065200  | -1.52924700 |
| C  | -2.03069100 | -1.57154900 | -1.52923200 |
| C  | -1.47793000 | -2.15904100 | -2.81526600 |
| H  | -1.99800500 | -2.27501000 | -0.69244800 |
| H  | -1.06798500 | -0.72475900 | -1.17726600 |
| H  | -0.53260400 | -2.67461900 | -2.61989000 |
| H  | -2.17811700 | -2.88353400 | -3.25596100 |
| H  | -1.27834400 | -1.38775500 | -3.56627400 |

**Structure: <sup>3</sup>TS4**

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -2.21877400 | 2.60474600 | -0.88804600 |
| C | 3.37027600  | 0.58835100 | -0.40888600 |
| C | 4.32285100  | 1.66124100 | -0.22560400 |
| C | 3.60731700  | 2.81903500 | -0.16800000 |
| C | 2.21349000  | 2.45921500 | -0.31906300 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 2.09897900  | 1.10452600  | -0.48604300 |
| H  | 5.39216400  | 1.52668700  | -0.14087600 |
| H  | 3.97224300  | 3.82717300  | -0.02923500 |
| C  | -2.05330800 | 1.90996000  | -0.71753900 |
| C  | -2.42164700 | 3.30836700  | -0.67345500 |
| C  | -1.27257500 | 4.01223600  | -0.45898300 |
| C  | -0.19552800 | 3.04679700  | -0.39423900 |
| N  | -0.70351800 | 1.77709200  | -0.52982900 |
| H  | -3.42803200 | 3.68483600  | -0.79595400 |
| H  | -1.14601600 | 5.08310200  | -0.37835500 |
| C  | 0.92205200  | -2.96562500 | -0.60259500 |
| C  | 2.00259700  | -3.93219400 | -0.57709300 |
| C  | 3.16235800  | -3.22362700 | -0.53977900 |
| C  | 2.79521900  | -1.82102000 | -0.54094800 |
| N  | 1.43593000  | -1.69504000 | -0.59595300 |
| H  | 1.87068700  | -5.00494800 | -0.58142900 |
| H  | 4.17683500  | -3.59491400 | -0.50429200 |
| C  | -1.48933100 | -2.37965200 | -0.68078100 |
| C  | -2.88280000 | -2.74606100 | -0.80271100 |
| C  | -3.58821100 | -1.58390300 | -0.91814600 |
| C  | -2.63260300 | -0.50193100 | -0.83023900 |
| N  | -1.36740400 | -1.01409700 | -0.67578100 |
| H  | -3.25492600 | -3.76092500 | -0.81897600 |
| H  | -4.65386300 | -1.45734100 | -1.04940300 |
| C  | 3.71630000  | -0.76771800 | -0.44029900 |
| C  | -2.97483800 | 0.85802300  | -0.88304900 |
| C  | 1.15646100  | 3.38447800  | -0.27313500 |
| C  | -0.43494700 | -3.30700600 | -0.61098100 |
| O  | 0.36860500  | 0.08934100  | -2.42937500 |
| N  | 0.43005800  | -0.08383300 | 1.45328100  |
| C  | 0.84569800  | -0.94115900 | 2.19239900  |
| O  | 1.24151900  | -1.77789900 | 2.95417200  |
| Mn | 0.37464900  | 0.03989500  | -0.61954600 |
| C  | -3.39438600 | -2.23692900 | 3.18914400  |
| C  | -2.59072300 | -1.34293200 | 2.50265100  |
| C  | -2.56477000 | 0.00193500  | 2.94616900  |
| C  | -3.32202300 | 0.42839500  | 4.07738600  |
| C  | -4.11441100 | -0.48427700 | 4.75716700  |
| C  | -4.14496400 | -1.81123700 | 4.30369800  |
| H  | -3.44383600 | -3.27384600 | 2.87237100  |
| H  | -1.98082700 | -1.63732100 | 1.65917800  |
| H  | -4.70564200 | -0.18555200 | 5.61818400  |
| H  | -4.76419400 | -2.53398300 | 4.82841300  |
| C  | -1.91403400 | 1.09987300  | 2.37603200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.13488200  | 0.62107000  | -2.70235000 |
| H | -1.33214900 | 1.08053500  | 1.47080400  |
| C | -2.13762300 | 2.32703800  | 3.18479400  |
| C | -3.13088300 | 1.90775200  | 4.30264800  |
| H | -2.75056900 | 2.12040800  | 5.30858600  |
| H | -4.08369000 | 2.44318100  | 4.20694200  |
| H | -1.17467300 | 2.68240700  | 3.57976400  |
| H | -2.50273700 | 3.13979300  | 2.54011000  |
| C | 5.15960100  | -1.12790700 | -0.26215500 |
| C | 5.99771500  | -1.28214200 | -1.38161600 |
| C | 5.65891000  | -1.32672500 | 1.04081900  |
| C | 7.33640400  | -1.63401500 | -1.18052000 |
| C | 7.00365400  | -1.67803700 | 1.19757000  |
| C | 7.85821200  | -1.83378700 | 0.10136500  |
| H | 7.98564500  | -1.75763700 | -2.04543800 |
| H | 7.39262700  | -1.83606100 | 2.20179000  |
| C | 1.50444600  | 4.83219700  | -0.09757200 |
| C | 1.83335200  | 5.61867300  | -1.21813400 |
| C | 1.50967800  | 5.39853900  | 1.19221500  |
| C | 2.16276600  | 6.96521000  | -1.02832100 |
| C | 1.84713000  | 6.74690200  | 1.34094300  |
| C | 2.17424400  | 7.54822000  | 0.24202600  |
| H | 2.41912900  | 7.57220600  | -1.89454100 |
| H | 1.85853900  | 7.18205300  | 2.33878100  |
| C | -4.37341400 | 1.21756800  | -1.29496700 |
| C | -5.44283400 | 1.26047600  | -0.38043300 |
| C | -4.60157500 | 1.50505800  | -2.65958000 |
| C | -6.72366200 | 1.58634300  | -0.84147100 |
| C | -5.89666500 | 1.82356800  | -3.07836100 |
| C | -6.97192700 | 1.87236700  | -2.18586500 |
| H | -7.54742800 | 1.61482200  | -0.13053500 |
| H | -6.07105600 | 2.03437500  | -4.13188900 |
| C | -0.78333100 | -4.76349200 | -0.54408800 |
| C | -0.80182000 | -5.41514100 | 0.70596400  |
| C | -1.06821800 | -5.47731100 | -1.72492600 |
| C | -1.12131400 | -6.77650100 | 0.75109100  |
| C | -1.38373800 | -6.83689400 | -1.63374300 |
| C | -1.42002800 | -7.50348500 | -0.40512600 |
| H | -1.13255400 | -7.28223600 | 1.71493400  |
| H | -1.59836300 | -7.39039200 | -2.54609900 |
| C | -5.22697200 | 0.95744700  | 1.08219200  |
| H | -4.90454200 | -0.07852000 | 1.23768000  |
| H | -4.43848000 | 1.58909200  | 1.50415800  |
| H | -6.14167700 | 1.11905300  | 1.66132100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.46527900 | 1.47473500  | -3.65687100 |
| H | -2.77135900 | 2.30707500  | -3.48702500 |
| H | -2.86947900 | 0.56005100  | -3.56839300 |
| H | -3.84063600 | 1.54979000  | -4.68226900 |
| C | -8.35584700 | 2.25012600  | -2.66095200 |
| H | -9.13148300 | 1.86029500  | -1.99287400 |
| H | -8.47688900 | 3.34109500  | -2.70108800 |
| H | -8.55180300 | 1.86641100  | -3.66844300 |
| C | 1.14842700  | 4.55815300  | 2.39587100  |
| H | 0.09743300  | 4.24758000  | 2.34770000  |
| H | 1.74392200  | 3.63898400  | 2.43693200  |
| H | 1.29918500  | 5.11244200  | 3.32775700  |
| C | 1.83705000  | 5.01310900  | -2.60297900 |
| H | 2.58509600  | 4.21497600  | -2.68160200 |
| H | 0.86756200  | 4.55920200  | -2.83995600 |
| H | 2.05973900  | 5.76590300  | -3.36551900 |
| C | 2.50502900  | 9.01151300  | 0.42529400  |
| H | 1.59229700  | 9.61980000  | 0.48359900  |
| H | 3.06669700  | 9.18260600  | 1.35066000  |
| H | 3.10098500  | 9.39676400  | -0.40892500 |
| C | 5.45245200  | -1.07637900 | -2.77627400 |
| H | 4.62697000  | -1.76753100 | -2.98490200 |
| H | 5.05059600  | -0.06318900 | -2.89781500 |
| H | 6.22754900  | -1.23006400 | -3.53358000 |
| C | 4.75848700  | -1.15601200 | 2.24349100  |
| H | 4.37512500  | -0.12999300 | 2.30366900  |
| H | 3.87843500  | -1.80754500 | 2.19784700  |
| H | 5.29570600  | -1.37290400 | 3.17210400  |
| C | 9.31584500  | -2.18136300 | 0.29891400  |
| H | 9.71535400  | -2.73872700 | -0.55554200 |
| H | 9.92745600  | -1.27579800 | 0.41126900  |
| H | 9.46577700  | -2.78736300 | 1.19929500  |
| C | -1.01949700 | -4.78752000 | -3.06921800 |
| H | -1.78916100 | -4.01061500 | -3.14732200 |
| H | -0.05707900 | -4.28559200 | -3.22179100 |
| H | -1.17023900 | -5.50084200 | -3.88549700 |
| C | -0.48025900 | -4.66345100 | 1.97767000  |
| H | 0.51352000  | -4.20465000 | 1.95166900  |
| H | -1.18125700 | -3.83799600 | 2.14225400  |
| H | -0.52829700 | -5.32388600 | 2.84927400  |
| C | -1.79462600 | -8.96569900 | -0.32766700 |
| H | -1.34105300 | -9.45103400 | 0.54347600  |
| H | -2.88244200 | -9.09236700 | -0.24149000 |
| H | -1.47571000 | -9.51005100 | -1.22346900 |

**Structure: <sup>5</sup>TS4**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.13983500 | 1.05888400  | -0.61211300 |
| C  | -4.50228000 | 0.58159400  | -0.49279400 |
| C  | -4.44265900 | -0.77428600 | -0.37910900 |
| C  | -3.04344800 | -1.14661800 | -0.43650900 |
| N  | -2.28797600 | -0.01359800 | -0.58626600 |
| H  | -5.37635000 | 1.21737000  | -0.48611300 |
| H  | -5.25893900 | -1.47288500 | -0.26070300 |
| C  | 0.97067300  | -2.77596900 | -0.76020300 |
| C  | 0.59367200  | -4.17229300 | -0.70458300 |
| C  | -0.75419000 | -4.21452900 | -0.49343300 |
| C  | -1.22044600 | -2.84488900 | -0.44826100 |
| N  | -0.14952700 | -2.00388700 | -0.59168800 |
| H  | 1.28141700  | -4.99991000 | -0.81038200 |
| H  | -1.39054700 | -5.08364900 | -0.39988000 |
| C  | 0.76135100  | 2.97126400  | -0.71709200 |
| C  | 0.28312600  | 4.33453500  | -0.64467500 |
| C  | -1.08027900 | 4.28476500  | -0.65629000 |
| C  | -1.45627000 | 2.89020800  | -0.73304100 |
| N  | -0.31770300 | 2.12758400  | -0.80878700 |
| H  | 0.92051000  | 5.20560000  | -0.58310800 |
| H  | -1.78072600 | 5.10663300  | -0.60443800 |
| C  | 2.57876900  | 1.26758100  | -0.73417100 |
| C  | 3.97123500  | 0.89342000  | -0.86397000 |
| C  | 4.01386800  | -0.46640400 | -0.97761300 |
| C  | 2.65152800  | -0.94565300 | -0.88491400 |
| N  | 1.81413200  | 0.13008200  | -0.72404500 |
| H  | 4.79569900  | 1.59230000  | -0.88466800 |
| H  | 4.87998300  | -1.10167500 | -1.10078500 |
| C  | -2.77484400 | 2.41368300  | -0.66963700 |
| C  | 2.28336400  | -2.30151300 | -0.92054700 |
| C  | -2.56853700 | -2.46387100 | -0.34214900 |
| C  | 2.11211000  | 2.59330200  | -0.68449300 |
| O  | -0.27779500 | -0.06808700 | -2.51273400 |
| N  | -0.21667100 | 0.26852500  | 1.29656700  |
| C  | -1.14112700 | 0.26997700  | 2.07169200  |
| O  | -2.00856000 | 0.23809700  | 2.89689300  |
| Mn | -0.23566300 | 0.06909700  | -0.71146300 |
| C  | 4.03103600  | 0.72416800  | 3.46450800  |
| C  | 3.22775200  | -0.06573500 | 2.65542600  |
| C  | 2.12702700  | -0.73379300 | 3.24440700  |
| C  | 1.83783900  | -0.57269000 | 4.63176000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.64877700  | 0.22507100  | 5.42348200  |
| C | 3.74875600  | 0.86952600  | 4.83581300  |
| H | 4.87885100  | 1.24853400  | 3.03286000  |
| H | 3.42588600  | -0.16452000 | 1.59532400  |
| H | 2.43854600  | 0.35729600  | 6.48167900  |
| H | 4.39024900  | 1.49731300  | 5.44831700  |
| C | 1.18449800  | -1.59420300 | 2.66193500  |
| H | -0.25693000 | 0.83849100  | -2.86599800 |
| H | 1.17857000  | -1.90159000 | 1.62761700  |
| C | 0.58878800  | -1.34143400 | 4.99104100  |
| C | 0.23143000  | -2.11260200 | 3.68933800  |
| H | -0.22112600 | -0.65124600 | 5.25745600  |
| H | 0.74079600  | -2.00517100 | 5.84996400  |
| H | -0.81159400 | -1.96023300 | 3.39000900  |
| H | 0.35625300  | -3.20105700 | 3.80370800  |
| C | 3.36174300  | -3.30859100 | -1.19677400 |
| C | 3.70855200  | -3.57880800 | -2.53694400 |
| C | 4.02354900  | -3.97388500 | -0.14677000 |
| C | 4.71552700  | -4.51210400 | -2.80147800 |
| C | 5.02508800  | -4.90101200 | -0.45472700 |
| C | 5.38437400  | -5.18603400 | -1.77502000 |
| H | 4.98406100  | -4.71769900 | -3.83600600 |
| H | 5.53841300  | -5.41112800 | 0.35822500  |
| C | -3.58304800 | -3.54730500 | -0.13037100 |
| C | -3.89621300 | -3.95534300 | 1.18042700  |
| C | -4.22512900 | -4.14046100 | -1.23474800 |
| C | -4.85751100 | -4.95434700 | 1.36591600  |
| C | -5.17832200 | -5.13790800 | -1.00639400 |
| C | -5.50790400 | -5.55907100 | 0.28603400  |
| H | -5.10484100 | -5.26658200 | 2.37886800  |
| H | -5.67780400 | -5.59485400 | -1.85869900 |
| C | -3.87455700 | 3.42593600  | -0.55374800 |
| C | -4.51067800 | 3.91527900  | -1.70941600 |
| C | -4.27373600 | 3.86646200  | 0.72453200  |
| C | -5.54630200 | 4.84522300  | -1.56981600 |
| C | -5.31310100 | 4.79724800  | 0.81978300  |
| C | -5.96051800 | 5.29929900  | -0.31404200 |
| H | -6.04247400 | 5.22101200  | -2.46270400 |
| H | -5.62679700 | 5.13679000  | 1.80518600  |
| C | 3.13422300  | 3.68658000  | -0.58570300 |
| C | 3.44519900  | 4.23265200  | 0.67575100  |
| C | 3.76938600  | 4.17086900  | -1.74643800 |
| C | 4.40881800  | 5.24387000  | 0.75498800  |
| C | 4.72614700  | 5.18337100  | -1.62314100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.06485800  | 5.72832900  | -0.38053200 |
| H | 4.64896000  | 5.66653400  | 1.72893900  |
| H | 5.21495600  | 5.55904700  | -2.52013200 |
| C | 3.66604300  | -3.69291800 | 1.29404200  |
| H | 3.80949900  | -2.63617400 | 1.54474800  |
| H | 2.61329800  | -3.92451800 | 1.49375200  |
| H | 4.27926000  | -4.28773000 | 1.97809000  |
| C | 3.00907400  | -2.86342100 | -3.67010000 |
| H | 1.92154400  | -2.98341100 | -3.60816800 |
| H | 3.20138100  | -1.78441700 | -3.63614700 |
| H | 3.34384100  | -3.24016900 | -4.64158700 |
| C | 6.44593700  | -6.21555000 | -2.08637600 |
| H | 6.00133000  | -7.20820700 | -2.23925600 |
| H | 6.99486900  | -5.96264600 | -3.00026600 |
| H | 7.17012800  | -6.30580500 | -1.26941500 |
| C | -3.58546400 | 3.34706200  | 1.96634200  |
| H | -3.62690600 | 2.25429200  | 2.03434600  |
| H | -2.52132200 | 3.61331700  | 1.96577600  |
| H | -4.03846800 | 3.76299200  | 2.87165000  |
| C | -7.06052900 | 6.32753000  | -0.18387400 |
| H | -7.75276600 | 6.28567300  | -1.03189200 |
| H | -7.63971900 | 6.18077000  | 0.73455000  |
| H | -6.64906100 | 7.34538600  | -0.14880200 |
| C | -4.08546100 | 3.43305900  | -3.07753100 |
| H | -3.02301500 | 3.63763600  | -3.25678500 |
| H | -4.21651400 | 2.34844200  | -3.17442200 |
| H | -4.66496900 | 3.91903600  | -3.86859800 |
| C | 3.41588600  | 3.61208200  | -3.10614700 |
| H | 3.69245300  | 2.55414000  | -3.18820800 |
| H | 2.33596400  | 3.66903100  | -3.28727200 |
| H | 3.92627800  | 4.15981900  | -3.90439200 |
| C | 2.72377800  | 3.76320200  | 1.91840900  |
| H | 1.68707100  | 4.12284000  | 1.92677400  |
| H | 2.67123500  | 2.67207600  | 1.97305200  |
| H | 3.21572200  | 4.12950700  | 2.82520700  |
| C | 6.12734700  | 6.79704700  | -0.26646100 |
| H | 7.12338700  | 6.35280700  | -0.13561600 |
| H | 6.16676500  | 7.42180800  | -1.16560500 |
| H | 5.94797800  | 7.45128400  | 0.59369200  |
| C | -3.18961400 | -3.33760100 | 2.36553700  |
| H | -2.12657900 | -3.60938700 | 2.36155900  |
| H | -3.23324300 | -2.24236600 | 2.34907800  |
| H | -3.62185700 | -3.68411300 | 3.30961800  |
| C | -3.89050500 | -3.69877700 | -2.64093400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.12435900 | -2.63779800 | -2.78909300 |
| H | -2.81984200 | -3.81245700 | -2.84773400 |
| H | -4.44775100 | -4.27936500 | -3.38262400 |
| C | -6.51962700 | -6.66000100 | 0.50682500  |
| H | -7.29390300 | -6.65484200 | -0.26827500 |
| H | -6.04115400 | -7.64842800 | 0.48103100  |
| H | -7.01295700 | -6.56294200 | 1.48009100  |

**Structure: <sup>3</sup>TS5**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.61055100  | 0.62309900  | -0.76570900 |
| C | 3.52364800  | 1.73508500  | -0.89661600 |
| C | 2.77653900  | 2.87381300  | -0.80903000 |
| C | 1.39964600  | 2.46072600  | -0.65949900 |
| N | 1.32775100  | 1.09189700  | -0.60917200 |
| H | 4.59169500  | 1.64074200  | -1.03490200 |
| H | 3.10959500  | 3.90084400  | -0.86334500 |
| C | -2.85830400 | 1.74126800  | -0.46720100 |
| C | -3.27792400 | 3.12519800  | -0.52488500 |
| C | -2.14611200 | 3.87702900  | -0.59923600 |
| C | -1.02997200 | 2.95584600  | -0.59144700 |
| N | -1.49489100 | 1.66555200  | -0.52890900 |
| H | -4.30574700 | 3.45817900  | -0.49809400 |
| H | -2.05631400 | 4.95288600  | -0.64918100 |
| C | 0.31404500  | -2.99563800 | -0.18858400 |
| C | 1.42094700  | -3.92106000 | -0.26720600 |
| C | 2.54043100  | -3.18190000 | -0.51579500 |
| C | 2.12602300  | -1.80010800 | -0.57160300 |
| N | 0.77504800  | -1.70785300 | -0.34589800 |
| H | 1.33219800  | -4.99458300 | -0.17719900 |
| H | 3.55478700  | -3.52636300 | -0.66207200 |
| C | -2.11053000 | -2.49392300 | -0.07124600 |
| C | -3.49116200 | -2.90796100 | 0.07334400  |
| C | -4.25044300 | -1.78145600 | -0.00758400 |
| C | -3.33754100 | -0.67485200 | -0.20191200 |
| N | -2.04724600 | -1.13927900 | -0.24018800 |
| H | -3.81527600 | -3.92931900 | 0.21584000  |
| H | -5.32538600 | -1.68751200 | 0.05657300  |
| C | 3.00307600  | -0.72258200 | -0.78979000 |
| C | -3.73882300 | 0.66037800  | -0.30612700 |
| C | 0.31167400  | 3.34966000  | -0.61921900 |
| C | -1.02209100 | -3.38140500 | -0.04729600 |
| N | -0.36424000 | 0.19866000  | 1.53992900  |
| C | -0.84541200 | 1.04521200  | 2.25293300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.29478200 | 1.86542400  | 2.99793300  |
| Mn | -0.37496200 | -0.02068800 | -0.45599600 |
| C  | 3.34117800  | 2.48485300  | 3.29057000  |
| C  | 2.61104800  | 1.54037400  | 2.59057100  |
| C  | 2.57997900  | 0.21658600  | 3.09568700  |
| C  | 3.25740800  | -0.13659000 | 4.30075300  |
| C  | 3.97769800  | 0.82639800  | 4.99167000  |
| C  | 4.01530000  | 2.13070500  | 4.47750100  |
| H  | 3.38962800  | 3.50758500  | 2.93030000  |
| H  | 2.05773100  | 1.78326100  | 1.69339600  |
| H  | 4.50623100  | 0.58357200  | 5.90915000  |
| H  | 4.57693400  | 2.89270900  | 5.01126500  |
| C  | 1.98789600  | -0.92053300 | 2.54055900  |
| H  | 1.47249600  | -0.96099400 | 1.59693100  |
| N  | -0.45657400 | -0.20815700 | -2.37631500 |
| C  | -0.15629500 | -1.16447400 | -3.04855500 |
| O  | 0.13628100  | -2.08425500 | -3.75437100 |
| C  | 3.06727400  | -1.60474400 | 4.59216700  |
| C  | 2.17278900  | -2.10165000 | 3.42368600  |
| H  | 4.03013500  | -2.13010600 | 4.60883500  |
| H  | 2.60533800  | -1.76524000 | 5.57336700  |
| H  | 2.60509000  | -2.93608300 | 2.85301100  |
| H  | 1.18924200  | -2.46284300 | 3.75875000  |
| C  | 4.40638000  | -1.04249300 | -1.21402600 |
| C  | 5.46986000  | -1.10205700 | -0.29475800 |
| C  | 4.63823700  | -1.29218900 | -2.58522300 |
| C  | 6.75440600  | -1.41064600 | -0.75718400 |
| C  | 5.93662500  | -1.59778100 | -3.00373200 |
| C  | 7.00878600  | -1.66026300 | -2.10780400 |
| H  | 7.57453400  | -1.45750800 | -0.04311000 |
| H  | 6.11538000  | -1.78995100 | -4.05995600 |
| C  | -1.31406800 | -4.84632800 | 0.06656500  |
| C  | -1.25645100 | -5.48309100 | 1.32020500  |
| C  | -1.64204800 | -5.57767200 | -1.09326600 |
| C  | -1.52978700 | -6.85244400 | 1.39902500  |
| C  | -1.90598000 | -6.94571000 | -0.97072300 |
| C  | -1.85273300 | -7.60160700 | 0.26354500  |
| H  | -1.49230500 | -7.34454700 | 2.36923600  |
| H  | -2.16137700 | -7.51348200 | -1.86348300 |
| C  | -5.19715500 | 0.97049800  | -0.16318800 |
| C  | -6.01858900 | 1.05295200  | -1.30252000 |
| C  | -5.73045100 | 1.18196200  | 1.12422200  |
| C  | -7.37560100 | 1.34935600  | -1.13543200 |
| C  | -7.09189900 | 1.47650100  | 1.24616200  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -7.92962600 | 1.56798000  | 0.12947500  |
| H | -8.01415400 | 1.40955600  | -2.01473500 |
| H | -7.50877200 | 1.63760300  | 2.23868300  |
| C | 0.60504900  | 4.81916500  | -0.60673200 |
| C | 0.84404300  | 5.50343300  | -1.81462400 |
| C | 0.63004900  | 5.50820800  | 0.62258200  |
| C | 1.11653500  | 6.87454300  | -1.77130300 |
| C | 0.90528800  | 6.87981700  | 0.61986100  |
| C | 1.14977700  | 7.58094400  | -0.56488000 |
| H | 1.30214600  | 7.40438300  | -2.70377400 |
| H | 0.92737800  | 7.41389500  | 1.56807600  |
| C | -0.90030900 | -4.69659300 | 2.56184900  |
| H | 0.13276100  | -4.33026500 | 2.50858800  |
| H | -1.54145900 | -3.81427800 | 2.67255300  |
| H | -0.99793100 | -5.31039500 | 3.46299200  |
| C | -1.72582700 | -4.89319900 | -2.43866300 |
| H | -2.57042000 | -4.19348800 | -2.46875700 |
| H | -0.83161700 | -4.30055800 | -2.66051400 |
| H | -1.86383800 | -5.62218300 | -3.24320500 |
| C | -2.11074100 | -9.08763500 | 0.36068400  |
| H | -1.19508000 | -9.66195100 | 0.16503700  |
| H | -2.46574800 | -9.37008300 | 1.35780500  |
| H | -2.85871900 | -9.41354300 | -0.37061100 |
| C | -5.43988800 | 0.82062000  | -2.67932700 |
| H | -4.65247400 | 1.54922200  | -2.90664500 |
| H | -4.97612900 | -0.17020500 | -2.75307000 |
| H | -6.21049600 | 0.89740600  | -3.45263600 |
| C | -4.84951900 | 1.07508600  | 2.34863000  |
| H | -4.45300500 | 0.05809800  | 2.45871400  |
| H | -3.97919600 | 1.73862100  | 2.29001600  |
| H | -5.40644600 | 1.32186800  | 3.25793200  |
| C | -9.39036000 | 1.92256100  | 0.28720100  |
| H | -9.98912800 | 1.54204800  | -0.54743800 |
| H | -9.80441000 | 1.51434000  | 1.21601000  |
| H | -9.53170300 | 3.01133200  | 0.32067000  |
| C | 0.36928700  | 4.78143800  | 1.92235700  |
| H | -0.61305900 | 4.29745000  | 1.93742100  |
| H | 1.09720400  | 3.97883600  | 2.08511200  |
| H | 0.42515900  | 5.46509200  | 2.77533000  |
| C | 0.80136200  | 4.76766500  | -3.13444500 |
| H | 1.58922000  | 4.00744600  | -3.19328900 |
| H | -0.15023000 | 4.23859800  | -3.26165800 |
| H | 0.92775900  | 5.45588500  | -3.97582200 |
| C | 1.40937600  | 9.06968300  | -0.54685000 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 0.47551600 | 9.63527400  | -0.66686600 |
| H | 1.86226000 | 9.38756300  | 0.39869300  |
| H | 2.07725400 | 9.37071100  | -1.36157000 |
| C | 3.50807800 | -1.22290500 | -3.58675200 |
| H | 2.72471000 | -1.96091500 | -3.38216700 |
| H | 3.01586200 | -0.24348600 | -3.56137800 |
| H | 3.87396500 | -1.39315800 | -4.60386900 |
| C | 5.23744100 | -0.84643700 | 1.17518400  |
| H | 4.81504600 | 0.14906700  | 1.34884800  |
| H | 4.52295600 | -1.56691700 | 1.59090900  |
| H | 6.16899600 | -0.92613600 | 1.74443900  |
| C | 8.40692900 | -1.96093400 | -2.59611800 |
| H | 8.88876600 | -1.05865600 | -2.99606100 |
| H | 9.04266200 | -2.34057300 | -1.78896000 |
| H | 8.39879700 | -2.70533300 | -3.40024200 |

**Structure: <sup>5</sup>TS5**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.82824700 | -2.77667400 | -0.73371800 |
| C | -0.41483600 | -4.15041600 | -0.87448300 |
| C | 0.93889200  | -4.14894200 | -1.04233300 |
| C | 1.37785700  | -2.77830500 | -0.95093300 |
| N | 0.28008500  | -1.96626500 | -0.79155400 |
| H | -1.09039300 | -4.99408100 | -0.86451800 |
| H | 1.59971300  | -4.99296200 | -1.17959100 |
| C | 3.05439100  | 1.02887900  | 0.13566400  |
| C | 4.42647700  | 0.59082100  | 0.22354800  |
| C | 4.46687000  | -0.69879300 | -0.21778800 |
| C | 3.11262500  | -1.08267700 | -0.53558100 |
| N | 2.28202800  | -0.00982900 | -0.32399600 |
| H | 5.24400800  | 1.21270000  | 0.55985200  |
| H | 5.32164000  | -1.35504700 | -0.30100800 |
| C | -2.46861700 | 1.17527900  | -1.07350500 |
| C | -3.84785800 | 0.77312000  | -1.20185200 |
| C | -3.90000000 | -0.56799300 | -0.95247700 |
| C | -2.54420600 | -1.01503700 | -0.74635500 |
| N | -1.70007700 | 0.06615500  | -0.81100500 |
| H | -4.66217000 | 1.45091100  | -1.41746200 |
| H | -4.76449300 | -1.21661100 | -0.93637800 |
| C | -0.74627500 | 2.87727100  | -0.66128300 |
| C | -0.32907500 | 4.23337000  | -0.40538500 |
| C | 0.93498400  | 4.17565700  | 0.10441900  |
| C | 1.32814300  | 2.78769200  | 0.10934100  |
| N | 0.27869600  | 2.02168300  | -0.33541400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.94493600 | 5.10419700  | -0.58064600 |
| H  | 1.57224800  | 4.99185000  | 0.41391900  |
| C  | -2.15797600 | -2.35519800 | -0.63692100 |
| C  | 2.62204900  | 2.33486200  | 0.38665300  |
| C  | 2.71626700  | -2.38007600 | -0.87650400 |
| C  | -2.02793100 | 2.50310600  | -1.07956700 |
| N  | 0.09258300  | -0.19347700 | 1.40659400  |
| C  | 0.36221400  | -1.21088000 | 2.01111700  |
| O  | 0.61201600  | -2.18761700 | 2.65126100  |
| Mn | 0.29508200  | 0.02476600  | -0.59336900 |
| C  | -4.23144600 | 0.27269200  | 2.45979900  |
| C  | -2.91929900 | 0.71581700  | 2.55642200  |
| C  | -2.14100000 | 0.29068400  | 3.65930200  |
| C  | -2.69131600 | -0.59804400 | 4.62851300  |
| C  | -4.00612900 | -1.02332000 | 4.52076800  |
| C  | -4.77793700 | -0.58192200 | 3.43490400  |
| H  | -4.83403900 | 0.56562700  | 1.60615300  |
| H  | -2.47594700 | 1.33981500  | 1.78895000  |
| H  | -4.43407000 | -1.69946100 | 5.25692200  |
| H  | -5.80528300 | -0.92058000 | 3.33366900  |
| C  | -0.80247600 | 0.57892200  | 3.98386400  |
| H  | -0.17579600 | 1.28758700  | 3.45971300  |
| N  | 0.55807100  | 0.26808100  | -2.55557200 |
| C  | 0.96397200  | 1.29314100  | -3.05791600 |
| O  | 1.35086100  | 2.29203800  | -3.58441600 |
| C  | -1.65082300 | -0.93453200 | 5.67212400  |
| C  | -0.35867500 | -0.22518200 | 5.16700600  |
| H  | -1.51445600 | -2.01735100 | 5.77162200  |
| H  | -1.94886400 | -0.56149100 | 6.66067600  |
| H  | 0.39505000  | -0.96278600 | 4.84905700  |
| H  | 0.12120800  | 0.39273300  | 5.93790100  |
| C  | 3.77348400  | -3.42749400 | -1.03825800 |
| C  | 4.28393800  | -3.70763700 | -2.31984600 |
| C  | 4.23461300  | -4.13436400 | 0.09024000  |
| C  | 5.26025400  | -4.69985700 | -2.45363300 |
| C  | 5.21102000  | -5.11986500 | -0.08905500 |
| C  | 5.73780300  | -5.41494900 | -1.35063200 |
| H  | 5.65478200  | -4.92121700 | -3.44350700 |
| H  | 5.56703900  | -5.67202700 | 0.77864600  |
| C  | 3.62094300  | 3.33234800  | 0.88245800  |
| C  | 4.44534000  | 4.01614500  | -0.03265700 |
| C  | 3.71048500  | 3.59147500  | 2.26336000  |
| C  | 5.35801800  | 4.95490200  | 0.46025500  |
| C  | 4.63879200  | 4.53507400  | 2.71376900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.47293900  | 5.22482400  | 1.82776800  |
| H | 5.99323700  | 5.49052000  | -0.24263800 |
| H | 4.71036300  | 4.73879400  | 3.78054300  |
| C | -3.21605000 | -3.39353300 | -0.43361100 |
| C | -3.49060300 | -3.81805700 | 0.88256900  |
| C | -3.91148500 | -3.94420500 | -1.52650900 |
| C | -4.48465300 | -4.78085400 | 1.08187700  |
| C | -4.89682900 | -4.90672500 | -1.28122800 |
| C | -5.20237100 | -5.33227700 | 0.01530700  |
| H | -4.70089600 | -5.11104900 | 2.09623800  |
| H | -5.43490700 | -5.33685300 | -2.12379800 |
| C | -2.97219800 | 3.57480400  | -1.53044100 |
| C | -3.80487800 | 4.24683900  | -0.61567300 |
| C | -2.99616900 | 3.91108800  | -2.90035100 |
| C | -4.65923300 | 5.24896100  | -1.08893700 |
| C | -3.86642600 | 4.91748000  | -3.32997800 |
| C | -4.70749000 | 5.59583000  | -2.44195200 |
| H | -5.30021600 | 5.77189800  | -0.38171800 |
| H | -3.88430800 | 5.18120700  | -4.38569800 |
| C | 3.77635300  | -2.95233000 | -3.52701400 |
| H | 2.69992600  | -3.10589300 | -3.66920800 |
| H | 3.92011600  | -1.87149300 | -3.41133400 |
| H | 4.29048300  | -3.27049600 | -4.43914400 |
| C | 3.69121900  | -3.82789600 | 1.46771800  |
| H | 3.96641300  | -2.81402700 | 1.78382200  |
| H | 2.59692800  | -3.86932100 | 1.49699900  |
| H | 4.08178500  | -4.53040500 | 2.21044100  |
| C | 6.81631100  | -6.46093700 | -1.51447800 |
| H | 7.81614100  | -6.01386700 | -1.43140400 |
| H | 6.74277400  | -7.23748200 | -0.74533400 |
| H | 6.75891000  | -6.94686900 | -2.49465800 |
| C | -3.58993000 | -3.51242600 | -2.93939200 |
| H | -3.81635800 | -2.45101400 | -3.09549800 |
| H | -2.52313500 | -3.63854500 | -3.15860900 |
| H | -4.16104300 | -4.09268900 | -3.67057100 |
| C | -2.71474000 | -3.25221800 | 2.04966100  |
| H | -1.65544700 | -3.53176500 | 2.00701900  |
| H | -2.74618700 | -2.15844800 | 2.05784100  |
| H | -3.12127300 | -3.60484700 | 3.00191700  |
| C | -6.29593000 | -6.34610800 | 0.26121700  |
| H | -6.07312100 | -6.97374400 | 1.13119500  |
| H | -7.25732000 | -5.85157100 | 0.45548400  |
| H | -6.43731400 | -7.00285100 | -0.60398700 |
| C | -3.78684100 | 3.89376700  | 0.85360300  |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -4.18667800 | 2.88828500 | 1.02791100  |
| H | -2.76792100 | 3.90077500 | 1.25647100  |
| H | -4.38890200 | 4.59671200 | 1.43756300  |
| C | -2.09136900 | 3.20466200 | -3.88425100 |
| H | -1.03166600 | 3.36353200 | -3.65267800 |
| H | -2.25084900 | 2.12000200 | -3.86537300 |
| H | -2.27020000 | 3.55678900 | -4.90482400 |
| C | -5.66041200 | 6.65804800 | -2.93936000 |
| H | -6.59801300 | 6.21145100 | -3.29687200 |
| H | -5.91924100 | 7.36930600 | -2.14758700 |
| H | -5.23126300 | 7.22135300 | -3.77536500 |
| C | 4.35286200  | 3.73360000 | -1.51547900 |
| H | 4.73413800  | 2.73141000 | -1.74829400 |
| H | 3.31872300  | 3.75924200 | -1.87623000 |
| H | 4.93702500  | 4.45748700 | -2.09188700 |
| C | 2.80514900  | 2.87017400 | 3.23724800  |
| H | 1.75416600  | 3.13790400 | 3.06954700  |
| H | 2.87159900  | 1.78246900 | 3.11633200  |
| H | 3.05804100  | 3.11858500 | 4.27268400  |
| C | 6.49157700  | 6.21800000 | 2.33781300  |
| H | 7.45139300  | 5.72695200 | 2.54761900  |
| H | 6.68483200  | 7.00769600 | 1.60360000  |
| H | 6.15956700  | 6.69243700 | 3.26775600  |

**Structure: 38**

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 1.09696200  | -2.83980400 | 0.06999100 |
| C | 0.67354200  | -4.21631900 | 0.07205800 |
| C | -0.68959700 | -4.21372300 | 0.07221300 |
| C | -1.10778900 | -2.83560300 | 0.07030500 |
| N | -0.00381400 | -2.00259100 | 0.06808200 |
| H | 1.34464500  | -5.06369100 | 0.08028300 |
| H | -1.36388000 | -5.05856800 | 0.08061600 |
| C | -2.83722600 | 1.10681100  | 0.11352200 |
| C | -4.21892500 | 0.69144000  | 0.13168700 |
| C | -4.22288900 | -0.66976400 | 0.13124000 |
| C | -2.84343100 | -1.09223700 | 0.11258000 |
| N | -2.00704100 | 0.00545300  | 0.11633300 |
| H | -5.06221600 | 1.36755600  | 0.14258800 |
| H | -5.06997400 | -1.34116900 | 0.14156500 |
| C | 2.84149800  | 1.09595800  | 0.11370900 |
| C | 4.22160800  | 0.67531000  | 0.13139900 |
| C | 4.22035200  | -0.68589300 | 0.13037700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.83927000  | -1.10308400 | 0.11199700  |
| N  | 2.00710700  | -0.00219100 | 0.11638200  |
| H  | 5.06744900  | 1.34823100  | 0.14228700  |
| H  | 5.06489000  | -1.36050900 | 0.14019600  |
| C  | 1.10552200  | 2.83841400  | 0.08131900  |
| C  | 0.68898300  | 4.21887100  | 0.07764800  |
| C  | -0.67281300 | 4.22147500  | 0.07741300  |
| C  | -1.09460700 | 2.84262100  | 0.08099100  |
| N  | 0.00386100  | 2.00738300  | 0.08765000  |
| H  | 1.36396800  | 5.06314100  | 0.07909600  |
| H  | -1.34460200 | 5.06829000  | 0.07862700  |
| C  | 2.43509200  | -2.43895400 | 0.08236000  |
| C  | -2.43239600 | 2.44291200  | 0.08701600  |
| C  | -2.44435900 | -2.42966200 | 0.08313000  |
| C  | 2.44176300  | 2.43361600  | 0.08751700  |
| Mn | 0.00004400  | 0.00616100  | -0.18337900 |
| C  | 3.49282100  | -3.50089800 | 0.05911000  |
| C  | 3.99827000  | -4.01675700 | 1.26795800  |
| C  | 3.97256400  | -3.98038600 | -1.17493800 |
| C  | 4.98283900  | -5.00881400 | 1.22142600  |
| C  | 4.95776900  | -4.97296500 | -1.17878600 |
| C  | 5.47797900  | -5.49775000 | 0.00836400  |
| H  | 5.37158300  | -5.41016200 | 2.15545200  |
| H  | 5.32709300  | -5.34568800 | -2.13230900 |
| C  | -3.49032000 | 3.50436600  | 0.05626400  |
| C  | -3.98608300 | 4.03923800  | 1.26077100  |
| C  | -3.97880400 | 3.96393700  | -1.18210500 |
| C  | -4.97032300 | 5.03118200  | 1.20650000  |
| C  | -4.96313200 | 4.95754900  | -1.19311900 |
| C  | -5.47381200 | 5.50151700  | -0.01050700 |
| H  | -5.35178000 | 5.44734200  | 2.13707600  |
| H  | -5.33902900 | 5.31604100  | -2.14953500 |
| C  | -3.50629400 | -3.48741800 | 0.06063500  |
| C  | -4.01069600 | -4.00348300 | 1.26988900  |
| C  | -3.99123500 | -3.96259200 | -1.17298700 |
| C  | -4.99931800 | -4.99146600 | 1.22410200  |
| C  | -4.98044400 | -4.95125200 | -1.17610000 |
| C  | -5.49963200 | -5.47614000 | 0.01139600  |
| H  | -5.38729600 | -5.39294600 | 2.15839700  |
| H  | -5.35378500 | -5.32064700 | -2.12934500 |
| C  | 3.50384700  | 3.49091600  | 0.05706800  |
| C  | 4.00187500  | 4.02329400  | 1.26175200  |
| C  | 3.99409600  | 3.94898300  | -1.18115400 |
| C  | 4.99007900  | 5.01129700  | 1.20779600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.98240700  | 4.93864700  | -1.19185300 |
| C | 5.49538600  | 5.48006100  | -0.00907000 |
| H | 5.37330200  | 5.42553200  | 2.13850700  |
| H | 5.35970000  | 5.29596600  | -2.14815700 |
| C | 3.42506100  | -3.43265400 | -2.47305900 |
| H | 2.34618000  | -3.61341200 | -2.55382800 |
| H | 3.56767500  | -2.34735800 | -2.53713200 |
| H | 3.91350800  | -3.89419100 | -3.33672900 |
| C | 3.47922500  | -3.50708500 | 2.59281200  |
| H | 3.64725800  | -2.42826300 | 2.69472500  |
| H | 2.39785000  | -3.66632300 | 2.68183600  |
| H | 3.96940600  | -4.01043600 | 3.43184500  |
| C | 6.56749600  | -6.54467600 | -0.01825800 |
| H | 7.56260200  | -6.07996700 | -0.00260600 |
| H | 6.50689300  | -7.21007300 | 0.85002400  |
| H | 6.51102600  | -7.16057600 | -0.92244100 |
| C | -3.44326400 | 3.39324900  | -2.47511600 |
| H | -2.36014700 | 3.54214900  | -2.55683200 |
| H | -3.61179500 | 2.31122700  | -2.53056500 |
| H | -3.92058100 | 3.85977400  | -3.34242200 |
| C | -3.45668800 | 3.55013600  | 2.58936000  |
| H | -3.61136600 | 2.47052800  | 2.70362700  |
| H | -2.37698800 | 3.72324900  | 2.67324100  |
| H | -3.95001800 | 4.05677400  | 3.42459600  |
| C | -6.56229900 | 6.54934200  | -0.04542900 |
| H | -7.55785500 | 6.08670800  | -0.00878400 |
| H | -6.49075200 | 7.23206300  | 0.80851300  |
| H | -6.51547300 | 7.14682600  | -0.96241800 |
| C | 3.47081100  | 3.53559400  | 2.59019000  |
| H | 2.39155600  | 3.71153300  | 2.67379700  |
| H | 3.62263100  | 2.45557100  | 2.70446200  |
| H | 3.96528800  | 4.04087500  | 3.42557000  |
| C | 3.45632000  | 3.38081800  | -2.47434900 |
| H | 3.62098100  | 2.29822100  | -2.53030700 |
| H | 2.37373700  | 3.53361700  | -2.55586200 |
| H | 3.93520900  | 3.84600500  | -3.34150700 |
| C | 6.58823700  | 6.52334600  | -0.04360700 |
| H | 6.51889600  | 7.20671000  | 0.81000600  |
| H | 7.58182500  | 6.05657600  | -0.00598100 |
| H | 6.54462100  | 7.12064500  | -0.96087200 |
| C | -3.44530300 | -3.41428100 | -2.47152100 |
| H | -3.58700300 | -2.32877700 | -2.53435700 |
| H | -2.36674400 | -3.59598100 | -2.55425300 |
| H | -3.93567700 | -3.87449800 | -3.33480200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.48629500 | -3.49814500 | 2.59429200  |
| H | -2.40555000 | -3.66290000 | 2.68085900  |
| H | -3.64871500 | -2.41862200 | 2.69788400  |
| H | -3.97724400 | -4.00008900 | 3.43371900  |
| C | -6.59356300 | -6.51848300 | -0.01391600 |
| H | -6.52673300 | -7.19229800 | 0.84742700  |
| H | -7.58655900 | -6.05001700 | 0.01661500  |
| H | -6.54890800 | -7.12603700 | -0.92435100 |
| O | 0.00030900  | 0.00399000  | -1.96142700 |
| H | -0.00427900 | -0.92395100 | -2.25499800 |

**Structure: 58**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.96441700  | 0.64733100  | -0.02927900 |
| C | 4.25225700  | 0.00792800  | -0.09433700 |
| C | 4.03585100  | -1.33827600 | -0.08851900 |
| C | 2.61253700  | -1.54130700 | -0.02044800 |
| N | 1.97096800  | -0.31542100 | -0.00722200 |
| H | 5.19476800  | 0.53632500  | -0.11968100 |
| H | 4.76517600  | -2.13569400 | -0.10923700 |
| C | -1.53984100 | -2.64533200 | 0.19214100  |
| C | -1.34413000 | -4.07167300 | 0.30897500  |
| C | 0.00059000  | -4.28807100 | 0.31091500  |
| C | 0.63352900  | -2.99488900 | 0.19337300  |
| N | -0.32266200 | -2.00950700 | 0.15149600  |
| H | -2.14338200 | -4.79663700 | 0.37325800  |
| H | 0.53172000  | -5.22722100 | 0.37704900  |
| C | -0.63369300 | 2.99377300  | 0.19360100  |
| C | -0.00156100 | 4.28760700  | 0.30737800  |
| C | 1.34349400  | 4.07345700  | 0.29854800  |
| C | 1.54018100  | 2.64738700  | 0.17997200  |
| N | 0.32394500  | 2.00970300  | 0.14521200  |
| H | -0.53384600 | 5.22587300  | 0.37646900  |
| H | 2.14190200  | 4.79967300  | 0.35934900  |
| C | -2.61464200 | 1.53944300  | 0.00486100  |
| C | -4.03953500 | 1.33836700  | -0.06608100 |
| C | -4.25558700 | -0.00687200 | -0.07073300 |
| C | -2.96545600 | -0.64448900 | -0.00145800 |
| N | -1.97547500 | 0.31649100  | 0.03006500  |
| H | -4.76796800 | 2.13629900  | -0.09396600 |
| H | -5.19731800 | -0.53620800 | -0.10218000 |
| C | 2.78951900  | 2.03153300  | 0.06533100  |
| C | -2.78943800 | -2.02912100 | 0.08424700  |
| C | 2.01315000  | -2.80057700 | 0.08226500  |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.01397700 | 2.79909100  | 0.09427500  |
| Mn | -0.00355000 | -0.00010000 | -0.25798800 |
| C  | 4.00892000  | 2.90275500  | 0.04935900  |
| C  | 4.69376900  | 3.17745200  | 1.24887900  |
| C  | 4.45800400  | 3.44976500  | -1.16850400 |
| C  | 5.82582300  | 3.99776900  | 1.20912300  |
| C  | 5.59467800  | 4.26447200  | -1.16543700 |
| C  | 6.29416700  | 4.54791800  | 0.01186100  |
| H  | 6.35313300  | 4.21403100  | 2.13634500  |
| H  | 5.94146300  | 4.68899000  | -2.10569500 |
| C  | -4.00773400 | -2.90127300 | 0.05538200  |
| C  | -4.70789600 | -3.17548900 | 1.24591700  |
| C  | -4.44092700 | -3.44685300 | -1.16920800 |
| C  | -5.84065200 | -3.99407800 | 1.19138300  |
| C  | -5.57925900 | -4.25926500 | -1.18038900 |
| C  | -6.29449700 | -4.54207700 | -0.01237900 |
| H  | -6.38028500 | -4.20990400 | 2.11160900  |
| H  | -5.91508300 | -4.68217500 | -2.12536300 |
| C  | 2.89902800  | -4.00963400 | 0.07642100  |
| C  | 3.46116200  | -4.47689300 | 1.28002200  |
| C  | 3.16411100  | -4.67236500 | -1.13801100 |
| C  | 4.28418800  | -5.60737900 | 1.24846500  |
| C  | 3.99290800  | -5.79859700 | -1.12676200 |
| C  | 4.55989300  | -6.28368400 | 0.05606400  |
| H  | 4.72044900  | -5.96813200 | 2.17803700  |
| H  | 4.20180400  | -6.30873400 | -2.06520700 |
| C  | -2.89891400 | 4.00855200  | 0.07911400  |
| C  | -3.47007200 | 4.48014800  | 1.27661300  |
| C  | -3.15558400 | 4.66487800  | -1.14088200 |
| C  | -4.29436900 | 5.60937400  | 1.23427500  |
| C  | -3.98663600 | 5.78959400  | -1.13989500 |
| C  | -4.56281400 | 6.27923500  | 0.03664500  |
| H  | -4.73776700 | 5.97371300  | 2.15907800  |
| H  | -4.19039600 | 6.29464500  | -2.08223000 |
| C  | 3.71813600  | 3.16403000  | -2.45533400 |
| H  | 3.65233000  | 2.08590700  | -2.64428900 |
| H  | 2.68771100  | 3.53661900  | -2.41197600 |
| H  | 4.21499700  | 3.63148600  | -3.31096300 |
| C  | 4.20961700  | 2.59671400  | 2.55785200  |
| H  | 3.16914500  | 2.87959400  | 2.75665800  |
| H  | 4.23881800  | 1.50051600  | 2.53935100  |
| H  | 4.82406800  | 2.94003100  | 3.39579000  |
| C  | 7.53957800  | 5.40354700  | -0.01344300 |
| H  | 7.67902800  | 5.93810800  | 0.93254300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 8.43663300  | 4.79106800  | -0.17652100 |
| H | 7.50163600  | 6.14424000  | -0.81969300 |
| C | -3.68136700 | -3.16523100 | -2.44535100 |
| H | -3.56981100 | -2.08843300 | -2.61618900 |
| H | -2.66572000 | -3.57664300 | -2.40003900 |
| H | -4.18781700 | -3.60140100 | -3.31190400 |
| C | -4.24027500 | -2.59520100 | 2.56118500  |
| H | -3.19925400 | -2.86979700 | 2.76864700  |
| H | -4.27879900 | -1.49918800 | 2.54620200  |
| H | -4.85936000 | -2.94644600 | 3.39243400  |
| C | -7.54148200 | -5.39478400 | -0.05517000 |
| H | -7.48774200 | -6.14508700 | -0.85165900 |
| H | -7.70357100 | -5.91773600 | 0.89368600  |
| H | -8.43287800 | -4.78200100 | -0.24585300 |
| C | -3.20141800 | 3.77184600  | 2.58479100  |
| H | -3.58392900 | 2.74408900  | 2.56446100  |
| H | -2.12562700 | 3.70243600  | 2.78476800  |
| H | -3.67269400 | 4.29419200  | 3.42304200  |
| C | -2.54201000 | 4.15999300  | -2.42669100 |
| H | -1.44745300 | 4.21753000  | -2.39140000 |
| H | -2.78959800 | 3.10682700  | -2.60243300 |
| H | -2.88713600 | 4.74333100  | -3.28591300 |
| C | -5.42971100 | 7.51701200  | 0.01727400  |
| H | -6.15851000 | 7.51011000  | 0.83506700  |
| H | -4.82342800 | 8.42611900  | 0.12870800  |
| H | -5.97896400 | 7.60769700  | -0.92634300 |
| C | 2.56323900  | -4.17072200 | -2.43111900 |
| H | 1.46757900  | -4.19396700 | -2.39436300 |
| H | 2.84687200  | -3.12904100 | -2.62295000 |
| H | 2.88989900  | -4.77646200 | -3.28192700 |
| C | 3.18333100  | -3.76281900 | 2.58304200  |
| H | 3.55913800  | -2.73271400 | 2.55798300  |
| H | 2.10637100  | -3.69929400 | 2.77847500  |
| H | 3.65477600  | -4.27731200 | 3.42600600  |
| C | 5.42428400  | -7.52328800 | 0.04910800  |
| H | 6.15406100  | -7.50887400 | 0.86592800  |
| H | 4.81621300  | -8.42975400 | 0.17150200  |
| H | 5.97215800  | -7.62551900 | -0.89409100 |
| O | -0.07394700 | 0.00466300  | -2.15048100 |
| H | 0.77807400  | -0.11314600 | -2.59903600 |

**Structure: Prol**

|   |            |            |            |
|---|------------|------------|------------|
| C | 1.55860300 | 1.29102200 | 0.24287000 |
|---|------------|------------|------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.24506500  | 0.86399300  | 0.05706800  |
| C | -0.02545500 | -0.48161900 | -0.21690700 |
| C | 1.00096500  | -1.41834400 | -0.29735400 |
| C | 2.31984000  | -0.99069700 | -0.11631300 |
| C | 2.59464500  | 0.35549600  | 0.15103700  |
| H | 1.77841900  | 2.33543800  | 0.45138300  |
| H | 0.77967100  | -2.46329900 | -0.49915200 |
| H | 3.13613800  | -1.70486800 | -0.18515000 |
| H | 3.62421200  | 0.67762800  | 0.28519300  |
| C | -1.51511800 | -0.70814300 | -0.33808200 |
| C | -1.04093600 | 1.66036700  | 0.11927100  |
| C | -2.05235900 | 0.72337400  | -0.58442300 |
| H | -3.08087500 | 0.84093200  | -0.22521400 |
| H | -2.04892500 | 0.92445900  | -1.66300000 |
| H | -1.32868200 | 1.83079700  | 1.16514500  |
| H | -0.96615900 | 2.64246300  | -0.36095500 |
| H | -1.77116800 | -1.39061000 | -1.16337200 |
| O | -1.96415900 | -1.25788100 | 0.90768900  |
| H | -2.92086500 | -1.40258900 | 0.83060600  |

## Structure: Pro2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.01033900 | 0.61403200  | -1.01456800 |
| C | -0.78552700 | 0.82987600  | -0.38544700 |
| C | -0.37911600 | -0.00615300 | 0.66194000  |
| C | -1.17533400 | -1.06437200 | 1.09205500  |
| C | -2.40600300 | -1.27651200 | 0.46362900  |
| C | -2.81870100 | -0.44235700 | -0.58196200 |
| H | -2.33716100 | 1.25902400  | -1.82650700 |
| H | -0.84685700 | -1.71196800 | 1.90106900  |
| H | -3.04703400 | -2.09095600 | 0.78976900  |
| H | -3.77910800 | -0.61548700 | -1.06026300 |
| C | 1.00166200  | 0.39545500  | 1.14967300  |
| C | 0.26817200  | 1.87991400  | -0.66898600 |
| C | 1.13958300  | 1.84358300  | 0.60996200  |
| H | 2.18409600  | 2.12034700  | 0.44584900  |
| H | 0.71808500  | 2.52699900  | 1.35641300  |
| H | 0.85472400  | 1.60426600  | -1.55667200 |
| H | -0.15269600 | 2.87257700  | -0.86219800 |
| H | 1.09866900  | 0.35734400  | 2.23777600  |
| N | 2.04585000  | -0.48385700 | 0.61995600  |
| C | 2.24769000  | -1.05299200 | -0.42887600 |
| O | 2.56172600  | -1.65724900 | -1.39368000 |

**Structure: Pro3**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.89919500  | 1.05933700  | 0.69621800  |
| C | 0.65082000  | 0.92054500  | 0.09056800  |
| C | 0.35093300  | -0.24320000 | -0.62763100 |
| C | 1.27196700  | -1.28396700 | -0.74634300 |
| C | 2.52116900  | -1.14134400 | -0.14082800 |
| C | 2.82955000  | 0.02384000  | 0.57414800  |
| H | 2.14608200  | 1.95728000  | 1.25653200  |
| H | 1.02034100  | -2.18666900 | -1.29689200 |
| H | 3.25822900  | -1.93501200 | -0.22330600 |
| H | 3.80661000  | 0.12308400  | 1.03951800  |
| C | -1.05255700 | -0.18463200 | -1.15504200 |
| C | -0.52293000 | 1.87502400  | 0.09663200  |
| C | -1.46054000 | 1.29162400  | -0.99343200 |
| H | -2.52477000 | 1.39109400  | -0.76275700 |
| H | -1.28134300 | 1.79538600  | -1.94999200 |
| H | -1.00795700 | 1.87091100  | 1.07967400  |
| H | -0.23041300 | 2.90821000  | -0.12023600 |
| H | -1.18433900 | -0.57519600 | -2.16434900 |
| C | -2.04039700 | -0.89584700 | 0.88144500  |
| O | -1.96101400 | -1.10484200 | -0.39114800 |
| N | -2.14251300 | -0.71980400 | 2.03094000  |

**Structure: •NCO**

|   |             |             |            |
|---|-------------|-------------|------------|
| N | 0.36883900  | 1.20497000  | 0.00000000 |
| C | 0.00000000  | 0.04429300  | 0.00000000 |
| O | -0.32273500 | -1.08756900 | 0.00000000 |

**Structure: 49**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.59162700  | 2.50981000  | -0.46642200 |
| C | 1.47239800  | 3.94719200  | -0.42779800 |
| C | 0.20152900  | 4.23334800  | -0.03522700 |
| C | -0.48923500 | 2.97580800  | 0.11834100  |
| N | 0.37823700  | 1.94930300  | -0.14962400 |
| H | 2.26635500  | 4.64399400  | -0.65236000 |
| H | -0.24514400 | 5.20693600  | 0.10534800  |
| C | -3.03825800 | -0.45774600 | -0.26444500 |
| C | -4.29036800 | 0.22164100  | -0.04016000 |
| C | -3.99502100 | 1.50534600  | 0.30262500  |
| C | -2.56214800 | 1.64563300  | 0.23315800  |
| N | -2.00761800 | 0.43428900  | -0.10921800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -5.26477100 | -0.24180300 | -0.09347400 |
| H  | -4.68548900 | 2.29290800  | 0.56558300  |
| C  | 2.47122900  | -1.66904000 | 0.05642900  |
| C  | 3.90480400  | -1.55563300 | -0.05889900 |
| C  | 4.17650100  | -0.27258500 | -0.42088800 |
| C  | 2.91649700  | 0.42777000  | -0.48150300 |
| N  | 1.90024500  | -0.44992600 | -0.19890400 |
| H  | 4.60386600  | -2.36580700 | 0.08896000  |
| H  | 5.14340800  | 0.17525100  | -0.59820700 |
| C  | 0.39910400  | -3.00245700 | 0.11625600  |
| C  | -0.30881300 | -4.26078400 | 0.05255200  |
| C  | -1.59590600 | -3.97816200 | -0.27766000 |
| C  | -1.71141200 | -2.53875800 | -0.34318000 |
| N  | -0.48069600 | -1.97834200 | -0.11905300 |
| H  | 0.13417100  | -5.23304300 | 0.20728600  |
| H  | -2.40495400 | -4.67626300 | -0.43302500 |
| C  | 2.78347200  | 1.80709500  | -0.67047900 |
| C  | -2.91560800 | -1.83862800 | -0.46289100 |
| C  | -1.85988200 | 2.84636600  | 0.37382700  |
| C  | 1.78150000  | -2.86725200 | 0.27489400  |
| O  | -0.05812000 | -0.03091000 | -1.95619100 |
| N  | -0.02627900 | -0.00873800 | 1.78438600  |
| C  | 0.84345000  | -0.20485700 | 2.60462300  |
| O  | 1.65572600  | -0.39763800 | 3.44912300  |
| Mn | -0.05091100 | -0.01419800 | -0.14846300 |
| H  | -0.69931900 | 0.62330000  | -2.28425000 |
| C  | -2.61135900 | 4.08025900  | 0.73429000  |
| C  | -3.55367500 | 4.65443100  | -0.12496900 |
| C  | -2.37278500 | 4.72935100  | 1.95106000  |
| C  | -4.24659600 | 5.81450400  | 0.21198900  |
| C  | -3.04811700 | 5.89493400  | 2.30632300  |
| C  | -3.98971000 | 6.43673300  | 1.43274400  |
| C  | 4.01392400  | 2.57508100  | -1.01258400 |
| C  | 4.60859900  | 2.44581100  | -2.27181900 |
| C  | 4.63468900  | 3.42484900  | -0.09161900 |
| C  | 5.77005900  | 3.13694100  | -2.60951300 |
| C  | 5.79291400  | 4.13078100  | -0.40891800 |
| C  | 6.36171400  | 3.98328500  | -1.67312600 |
| C  | 2.58883400  | -4.06438300 | 0.64008400  |
| C  | 2.78631100  | -5.13488200 | -0.23647900 |
| C  | 3.20468100  | -4.13479700 | 1.89523800  |
| C  | 3.55225600  | -6.24268300 | 0.11874300  |
| C  | 3.98120900  | -5.22964400 | 2.26875900  |
| C  | 4.15265700  | -6.28667600 | 1.37609200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.16965000 | -2.60363300 | -0.71330700 |
| C | -4.85947300 | -2.45844200 | -1.92154000 |
| C | -4.72410000 | -3.45997100 | 0.24318400  |
| C | -6.04597300 | -3.14160900 | -2.17784500 |
| C | -5.90572600 | -4.15890300 | 0.00709100  |
| C | -6.56864000 | -3.99610500 | -1.20838400 |
| F | 2.22435200  | -5.11536400 | -1.45330300 |
| F | 3.72131400  | -7.25558000 | -0.73771600 |
| F | 4.89150900  | -7.34140200 | 1.72525800  |
| F | 4.55861900  | -5.27501000 | 3.47263200  |
| F | 3.05670200  | -3.13119000 | 2.76461100  |
| F | -3.81138000 | 4.08492700  | -1.31125000 |
| F | -1.47132200 | 4.23289600  | 2.80503500  |
| F | -5.14419900 | 6.33878800  | -0.62860300 |
| F | -2.80268000 | 6.49310600  | 3.47542800  |
| F | -4.64383100 | 7.55113200  | 1.76387800  |
| F | 6.31651500  | 2.99754500  | -3.82122000 |
| F | 7.47256000  | 4.65225200  | -1.98669600 |
| F | 4.06152200  | 1.63707700  | -3.18699700 |
| F | 4.11236300  | 3.57878300  | 1.13158000  |
| F | 6.36470600  | 4.93846200  | 0.48935900  |
| F | -7.70307900 | -4.65742500 | -1.44346900 |
| F | -4.38116400 | -1.64063400 | -2.86767700 |
| F | -4.11450400 | -3.62704500 | 1.42398200  |
| F | -6.68234800 | -2.98624400 | -3.34269700 |
| F | -6.41103500 | -4.97332500 | 0.93867300  |

**Structure: <sup>41</sup>0**

|    |             |             |             |
|----|-------------|-------------|-------------|
| Mn | 0.06256800  | -0.00165000 | -0.21044400 |
| C  | 2.96216800  | 0.82920800  | -0.34424000 |
| C  | 3.81358000  | 1.98547300  | -0.20178900 |
| C  | 3.01466900  | 3.03203100  | 0.15491000  |
| C  | 1.65743700  | 2.54345500  | 0.17241500  |
| N  | 1.65866200  | 1.20202000  | -0.12515700 |
| H  | 4.88713600  | 1.97119900  | -0.32720200 |
| H  | 3.29707900  | 4.05468400  | 0.36186100  |
| C  | 0.52561600  | 3.34877600  | 0.33381200  |
| C  | -1.93564900 | 3.74404200  | 0.00624500  |
| C  | -2.98366600 | 2.95947600  | -0.37936400 |
| C  | -2.48952300 | 1.60987400  | -0.48493700 |
| N  | -1.13761600 | 1.60402600  | -0.22341700 |
| C  | -0.77398700 | 2.89526700  | 0.08653200  |
| H  | -1.92764600 | 4.80707700  | 0.20197500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.01288100 | 3.24554000  | -0.54398100 |
| C | 3.42688100  | -0.47745900 | -0.52909900 |
| N | 1.25547600  | -1.59835400 | -0.15870300 |
| C | 0.87922000  | -2.88745900 | 0.12466800  |
| C | 2.04406200  | -3.73863000 | 0.09168200  |
| C | 3.10327400  | -2.95528300 | -0.25970000 |
| C | 2.61107400  | -1.60291100 | -0.37769400 |
| H | 2.02710000  | -4.80184800 | 0.28581800  |
| H | 4.13699900  | -3.24199300 | -0.39225600 |
| C | -0.43085900 | -3.34244300 | 0.29975800  |
| N | -1.54188500 | -1.19422100 | -0.20533200 |
| C | -2.83539100 | -0.82307500 | -0.48621100 |
| C | -3.68729500 | -1.98502100 | -0.41035400 |
| C | -2.90319900 | -3.03423900 | -0.03338400 |
| C | -1.55192100 | -2.53944800 | 0.06848100  |
| H | -4.75304100 | -1.97158000 | -0.58892100 |
| H | -3.19073500 | -4.06132600 | 0.14112400  |
| C | -3.29754300 | 0.48312300  | -0.66983900 |
| O | 0.11921900  | -0.01920300 | -2.02483200 |
| H | 0.02591400  | 0.89614400  | -2.34067000 |
| N | 0.02429900  | 0.02678300  | 1.77384300  |
| C | 0.71539600  | 4.77946000  | 0.73183200  |
| C | 0.66416900  | 5.11674800  | 2.09864400  |
| C | 0.94129400  | 5.77122400  | -0.24210100 |
| C | 0.84858300  | 6.45239300  | 2.46969100  |
| C | 1.11998300  | 7.09508900  | 0.17170700  |
| C | 1.07568800  | 7.45563400  | 1.52235200  |
| H | 0.81520700  | 6.71508700  | 3.52527200  |
| H | 1.29828900  | 7.86285300  | -0.57876300 |
| C | -4.75364700 | 0.68793600  | -0.95350000 |
| C | -5.19859400 | 0.72411900  | -2.28833600 |
| C | -5.66462200 | 0.84164600  | 0.11131900  |
| C | -6.56120900 | 0.91284000  | -2.54134100 |
| C | -7.01824800 | 1.02826500  | -0.18661200 |
| C | -7.48655800 | 1.06383400  | -1.50433100 |
| H | -6.90703100 | 0.94274200  | -3.57280300 |
| H | -7.72479400 | 1.14991000  | 0.63225900  |
| C | -0.65239700 | -4.76676300 | 0.70154300  |
| C | -0.73141800 | -5.78427400 | -0.26832400 |
| C | -0.79069800 | -5.06722800 | 2.07123700  |
| C | -0.94328000 | -7.10098400 | 0.15338900  |
| C | -1.00130800 | -6.39707500 | 2.44914700  |
| C | -1.08282600 | -7.42682400 | 1.50625500  |
| H | -1.00217800 | -7.89061200 | -0.59330000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.10421300 | -6.63391600 | 3.50633000  |
| C | 4.88685900  | -0.68381000 | -0.79242000 |
| C | 5.34451000  | -0.72683000 | -2.12325700 |
| C | 5.78856400  | -0.83950200 | 0.27926800  |
| C | 6.70806400  | -0.92673500 | -2.36241700 |
| C | 7.14356200  | -1.03747300 | -0.00384400 |
| C | 7.62326600  | -1.08197400 | -1.31707700 |
| H | 7.06290500  | -0.96337700 | -3.39058100 |
| H | 7.84150800  | -1.16216300 | 0.82192700  |
| C | 0.98866300  | 5.40994500  | -1.70934700 |
| H | 1.79494500  | 4.69655300  | -1.91829000 |
| H | 0.05389700  | 4.93346300  | -2.02897400 |
| H | 1.14878700  | 6.29591000  | -2.33130500 |
| C | 0.40591700  | 4.05270000  | 3.14125300  |
| H | -0.59436200 | 3.61835000  | 3.02282900  |
| H | 1.11394400  | 3.22095700  | 3.05216000  |
| H | 0.48011100  | 4.46317100  | 4.15287800  |
| C | 1.23920800  | 8.89748000  | 1.94459400  |
| H | 1.67140600  | 8.97533200  | 2.94810500  |
| H | 1.88577700  | 9.44805900  | 1.25252700  |
| H | 0.27060700  | 9.41483100  | 1.96619200  |
| C | 4.37506000  | -0.56141100 | -3.27134600 |
| H | 3.58450200  | -1.32018900 | -3.23940700 |
| H | 3.87036300  | 0.41121000  | -3.22693000 |
| H | 4.88610100  | -0.63754800 | -4.23604300 |
| C | 5.29877300  | -0.79930500 | 1.70887700  |
| H | 4.80037700  | 0.15135000  | 1.93203400  |
| H | 4.56336400  | -1.58981300 | 1.89998800  |
| H | 6.12598500  | -0.92521000 | 2.41405200  |
| C | 9.09734700  | -1.26542500 | -1.59509600 |
| H | 9.26819700  | -1.70806400 | -2.58228000 |
| H | 9.62663200  | -0.30328400 | -1.57248600 |
| H | 9.56934900  | -1.91172600 | -0.84674700 |
| C | -5.18567700 | 0.82033600  | 1.54470000  |
| H | -4.61212700 | -0.08485500 | 1.77060900  |
| H | -4.51444200 | 1.66251800  | 1.75155700  |
| H | -6.02656600 | 0.87826100  | 2.24252900  |
| C | -4.21630100 | 0.56699500  | -3.42680000 |
| H | -3.45167700 | 1.35300600  | -3.40168300 |
| H | -3.68165000 | -0.38817200 | -3.36408100 |
| H | -4.72135800 | 0.61389100  | -4.39647200 |
| C | -8.95976900 | 1.23369100  | -1.79543000 |
| H | -9.43943900 | 1.89403700  | -1.06434000 |
| H | -9.12688900 | 1.65345900  | -2.79319800 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -9.48455600 | 0.26972500  | -1.75420700 |
| C | -0.59128600 | -5.45752200 | -1.73767500 |
| H | -1.33504500 | -4.71523700 | -2.05084800 |
| H | 0.39240100  | -5.02639500 | -1.95904500 |
| H | -0.71839600 | -6.35131700 | -2.35612100 |
| C | -0.70844600 | -3.97123500 | 3.11006500  |
| H | 0.24643800  | -3.43549000 | 3.04851300  |
| H | -1.49339600 | -3.21826700 | 2.96892700  |
| H | -0.80688800 | -4.37764600 | 4.12127000  |
| C | -1.34651500 | -8.85154400 | 1.93604000  |
| H | -0.93468000 | -9.05374300 | 2.93081500  |
| H | -2.42450800 | -9.05682700 | 1.98259000  |
| H | -0.90906300 | -9.57029500 | 1.23450700  |
| N | -1.03242300 | -0.11335700 | 2.35454900  |
| N | -2.01109400 | -0.24956000 | 2.95203400  |

**Structure: 411**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.31522300  | 2.73569200  | 0.19152400  |
| C | 0.98846900  | 4.13135100  | 0.03958100  |
| C | -0.31483100 | 4.19890900  | -0.35910300 |
| C | -0.82107900 | 2.85018200  | -0.38927300 |
| N | 0.19571200  | 1.98099400  | -0.06597200 |
| H | 1.68859900  | 4.94076100  | 0.19118700  |
| H | -0.90625200 | 5.07593300  | -0.58089700 |
| C | -2.79051300 | -0.89587100 | 0.31250200  |
| C | -4.13778800 | -0.39792800 | 0.20819400  |
| C | -4.05844400 | 0.89725600  | -0.21435700 |
| C | -2.66066600 | 1.22690000  | -0.31853700 |
| N | -1.91139100 | 0.11587500  | -0.00226500 |
| H | -5.02155800 | -0.98786400 | 0.40532400  |
| H | -4.86334800 | 1.59048600  | -0.41316900 |
| C | 2.80902200  | -1.25138800 | -0.26708400 |
| C | 4.20984700  | -0.91671100 | -0.18667600 |
| C | 4.28945600  | 0.39353700  | 0.18520500  |
| C | 2.93993000  | 0.89691000  | 0.26034200  |
| N | 2.06319800  | -0.12722800 | -0.00564700 |
| H | 5.01483000  | -1.61737200 | -0.35851600 |
| H | 5.17322700  | 0.99089900  | 0.35987300  |
| C | 0.97239000  | -2.87888200 | -0.19969700 |
| C | 0.47758500  | -4.22441200 | -0.04763800 |
| C | -0.82434100 | -4.13251900 | 0.35031500  |
| C | -1.16261600 | -2.73193700 | 0.37984400  |
| N | -0.04706700 | -1.99354100 | 0.05687300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.07388900  | -5.11349300 | -0.19702400 |
| H  | -1.51775600 | -4.93125600 | 0.57276700  |
| C  | 2.60362500  | 2.24391900  | 0.42471500  |
| C  | -2.45408100 | -2.23019000 | 0.56104800  |
| C  | -2.16414300 | 2.50950400  | -0.56992300 |
| C  | 2.31178200  | -2.54779200 | -0.42987200 |
| N  | 0.08046100  | 0.05013300  | 1.95523200  |
| Mn | 0.07700300  | -0.00658300 | -0.00433600 |
| N  | 0.07443200  | -0.06732900 | -1.96377500 |
| C  | -3.13386300 | 3.58320600  | -0.95124300 |
| C  | -3.44683300 | 3.76627100  | -2.31230200 |
| C  | -3.72705000 | 4.39011300  | 0.03933300  |
| C  | -4.35388600 | 4.77022700  | -2.66424300 |
| C  | -4.63110400 | 5.38132400  | -0.35742600 |
| C  | -4.95796100 | 5.58587100  | -1.70175400 |
| H  | -4.59456900 | 4.91862100  | -3.71516800 |
| H  | -5.09089700 | 6.00899200  | 0.40349000  |
| C  | -3.54928900 | -3.17631000 | 0.94066400  |
| C  | -4.22748800 | -3.91360000 | -0.04973900 |
| C  | -3.89330100 | -3.31010600 | 2.29995800  |
| C  | -5.24629600 | -4.78695500 | 0.34573000  |
| C  | -4.91665600 | -4.19581500 | 2.65069800  |
| C  | -5.60602000 | -4.94084300 | 1.68841300  |
| H  | -5.77229400 | -5.36051900 | -0.41503000 |
| H  | -5.18167400 | -4.30621800 | 3.70044100  |
| C  | 3.68224700  | 3.21711100  | 0.78465200  |
| C  | 3.87646900  | 3.53923900  | 2.14242300  |
| C  | 4.47772500  | 3.81097200  | -0.21432800 |
| C  | 4.88058300  | 4.45154200  | 2.48056100  |
| C  | 5.46998200  | 4.71982600  | 0.16772200  |
| C  | 5.69014400  | 5.04892400  | 1.50905100  |
| H  | 5.03251700  | 4.70336700  | 3.52832400  |
| H  | 6.08425600  | 5.18342600  | -0.60177600 |
| C  | 3.26502900  | -3.64713300 | -0.78072000 |
| C  | 3.97298000  | -4.33229400 | 0.22565100  |
| C  | 3.43087100  | -3.99274400 | -2.13637900 |
| C  | 4.85209800  | -5.35442900 | -0.14700100 |
| C  | 4.32009400  | -5.02042400 | -2.46515300 |
| C  | 5.04295100  | -5.70967900 | -1.48613000 |
| H  | 5.39856400  | -5.88801100 | 0.62826500  |
| H  | 4.44958000  | -5.29054900 | -3.51138700 |
| C  | -2.81326500 | 2.88927900  | -3.36886400 |
| H  | -1.71870100 | 2.92708500  | -3.31724600 |
| H  | -3.09337400 | 1.83730000  | -3.23426400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.11962900 | 3.19543900  | -4.37373100 |
| C | -3.38824100 | 4.19179200  | 1.49905100  |
| H | -3.54191200 | 3.15317700  | 1.81222100  |
| H | -2.33372500 | 4.41504900  | 1.69934500  |
| H | -3.99894000 | 4.83738400  | 2.13751200  |
| C | -5.96242200 | 6.64122700  | -2.10328100 |
| H | -6.97802300 | 6.22485900  | -2.14247700 |
| H | -5.97924800 | 7.47242900  | -1.39002400 |
| H | -5.74092000 | 7.04929600  | -3.09555500 |
| C | 4.25796500  | 3.47756700  | -1.67242100 |
| H | 4.44580400  | 2.41562300  | -1.87101500 |
| H | 3.22196300  | 3.67316000  | -1.97332900 |
| H | 4.91829200  | 4.06579100  | -2.31684600 |
| C | 3.00479000  | 2.91708300  | 3.21014000  |
| H | 1.95407300  | 3.20658600  | 3.08574400  |
| H | 3.03136900  | 1.82216100  | 3.16155600  |
| H | 3.32444300  | 3.22397500  | 4.21061600  |
| C | 6.79277100  | 6.00494900  | 1.90122800  |
| H | 6.54290900  | 6.55281300  | 2.81635500  |
| H | 7.73187000  | 5.46758000  | 2.09007900  |
| H | 6.99077200  | 6.73675400  | 1.11046200  |
| C | 3.77703800  | -3.97660600 | 1.68184700  |
| H | 4.05247200  | -2.93379900 | 1.87843300  |
| H | 2.72667500  | -4.08380800 | 1.97811300  |
| H | 4.38188500  | -4.61717900 | 2.33080500  |
| C | 2.64835400  | -3.27326900 | -3.21184400 |
| H | 1.57080500  | -3.44817700 | -3.10305400 |
| H | 2.79223200  | -2.18805200 | -3.15527400 |
| H | 2.94660400  | -3.60826800 | -4.20992300 |
| C | 6.02442400  | -6.79340300 | -1.86820200 |
| H | 7.02189900  | -6.37392800 | -2.05636300 |
| H | 6.13018200  | -7.53880000 | -1.07248400 |
| H | 5.71356500  | -7.31272400 | -2.78129800 |
| C | -3.85655700 | -3.76959800 | -1.50807000 |
| H | -3.86355400 | -2.72155300 | -1.82679600 |
| H | -2.84180600 | -4.13788000 | -1.70040100 |
| H | -4.54643100 | -4.32846200 | -2.14773600 |
| C | -3.17027300 | -2.50504400 | 3.35627900  |
| H | -2.08499400 | -2.64808000 | 3.29714300  |
| H | -3.34826300 | -1.43019600 | 3.22761800  |
| H | -3.49952600 | -2.78430400 | 4.36175800  |
| C | -6.73328700 | -5.86499900 | 2.08729100  |
| H | -7.69396800 | -5.33275600 | 2.10070000  |
| H | -6.83504400 | -6.70085400 | 1.38656800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.57780100 | -6.27873000 | 3.08967200  |
| N | -0.60974400 | 0.88787200  | 2.50512100  |
| N | -1.24609000 | 1.66516400  | 3.07059000  |
| N | -0.76992600 | -0.74892800 | -2.51419200 |
| N | -1.55194300 | -1.37898100 | -3.08021300 |

**Structure: <sup>3</sup>TS6**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.36492000 | -2.21268200 | 0.06608100  |
| C  | -3.77874000 | -2.48641000 | 0.21618000  |
| C  | -4.41949300 | -1.28501900 | 0.18954100  |
| C  | -3.40087500 | -0.26912300 | 0.03271100  |
| N  | -2.16170700 | -0.86054800 | -0.02499400 |
| H  | -4.20759000 | -3.47408000 | 0.31273300  |
| H  | -5.47966400 | -1.08669300 | 0.26434700  |
| C  | -0.73460400 | 3.11351800  | -0.28612900 |
| C  | -1.74957900 | 4.14728700  | -0.25183800 |
| C  | -2.95285400 | 3.51549500  | -0.18139700 |
| C  | -2.67747400 | 2.09280800  | -0.15989000 |
| N  | -1.32902600 | 1.87939600  | -0.22982000 |
| H  | -1.54925900 | 5.20908300  | -0.28820400 |
| H  | -3.94096500 | 3.95252900  | -0.14448600 |
| C  | 1.89752700  | -1.93846400 | -0.62108100 |
| C  | 2.16552700  | -3.35808400 | -0.64361800 |
| C  | 0.98235800  | -3.98804900 | -0.39178200 |
| C  | -0.01863800 | -2.95688500 | -0.22978700 |
| N  | 0.56893400  | -1.71880800 | -0.35617600 |
| H  | 3.13309900  | -3.79908300 | -0.83922300 |
| H  | 0.78450300  | -5.05000700 | -0.34830700 |
| C  | 2.63598500  | 0.42812700  | -0.69253300 |
| C  | 3.65837900  | 1.44499100  | -0.80655600 |
| C  | 3.03598000  | 2.64991300  | -0.66371800 |
| C  | 1.62609200  | 2.37600200  | -0.48823300 |
| N  | 1.41478800  | 1.02142900  | -0.47993100 |
| H  | 4.70759100  | 1.24715600  | -0.97703000 |
| H  | 3.47340400  | 3.63806200  | -0.69420400 |
| C  | -1.37879600 | -3.20861800 | -0.02015300 |
| C  | 0.63821300  | 3.36898400  | -0.38161400 |
| C  | -3.66568300 | 1.10265100  | -0.04663500 |
| C  | 2.88051500  | -0.94775300 | -0.79529200 |
| O  | -0.18571000 | 0.18717700  | 1.61381800  |
| N  | -0.61172400 | 0.05555000  | -2.23958500 |
| Mn | -0.38164500 | 0.08744800  | -0.26696000 |
| C  | 3.45721100  | 1.99602000  | 3.30359300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.59284600  | 1.14090900  | 2.64059000  |
| C | 2.51563000  | -0.19916700 | 3.09311500  |
| C | 3.26554000  | -0.65504600 | 4.21711400  |
| C | 4.11796200  | 0.22027600  | 4.87376700  |
| C | 4.20968600  | 1.53861100  | 4.40431900  |
| H | 3.55343600  | 3.02735200  | 2.97952000  |
| H | 1.96123000  | 1.45547800  | 1.82084300  |
| H | 4.70850600  | -0.10066000 | 5.72717200  |
| H | 4.87846200  | 2.23152900  | 4.90842100  |
| C | 1.81200400  | -1.27054500 | 2.53424500  |
| H | -1.07714700 | 0.05251300  | 1.97469000  |
| H | 1.26047500  | -1.23811300 | 1.60999900  |
| C | 1.96137200  | -2.49132100 | 3.36943900  |
| C | 2.99694000  | -2.11828800 | 4.46438800  |
| H | 2.63015500  | -2.30006100 | 5.48128900  |
| H | 3.91489900  | -2.70814300 | 4.35083700  |
| H | 0.98193700  | -2.77053600 | 3.78517500  |
| H | 2.25831700  | -3.34207800 | 2.74064700  |
| C | -5.09761800 | 1.54295600  | -0.00067400 |
| C | -5.68151900 | 1.91885700  | 1.22444500  |
| C | -5.85347300 | 1.57419400  | -1.18878700 |
| C | -7.01927000 | 2.32553700  | 1.24146000  |
| C | -7.18854900 | 1.98748100  | -1.12931900 |
| C | -7.78856500 | 2.37014500  | 0.07434300  |
| H | -7.47207300 | 2.61229000  | 2.18893300  |
| H | -7.77401200 | 2.01011400  | -2.04657500 |
| C | -1.82107700 | -4.63969800 | 0.04683400  |
| C | -1.73790300 | -5.34889400 | 1.25943100  |
| C | -2.30709700 | -5.27286800 | -1.11604100 |
| C | -2.14305600 | -6.68718700 | 1.29656900  |
| C | -2.69975000 | -6.61309100 | -1.03680900 |
| C | -2.62880000 | -7.33649500 | 0.15810000  |
| H | -2.07739700 | -7.23453800 | 2.23526300  |
| H | -3.06903600 | -7.10572100 | -1.93441500 |
| C | 4.24312600  | -1.39115900 | -1.24194900 |
| C | 5.28376400  | -1.63101900 | -0.32623800 |
| C | 4.46339600  | -1.56285800 | -2.62663600 |
| C | 6.53219400  | -2.04616600 | -0.80430100 |
| C | 5.72479300  | -1.97958300 | -3.06167600 |
| C | 6.77124500  | -2.23082400 | -2.16802500 |
| H | 7.33583500  | -2.22815800 | -0.09303800 |
| H | 5.89597900  | -2.10682600 | -4.12899500 |
| C | 1.08439700  | 4.80025000  | -0.40842600 |
| C | 1.22795600  | 5.51234400  | 0.79822800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.36291000  | 5.42747400  | -1.64014600 |
| C | 1.66308800  | 6.84139800  | 0.75543600  |
| C | 1.79347700  | 6.75776900  | -1.63923300 |
| C | 1.95005100  | 7.48228000  | -0.45303100 |
| H | 1.77843300  | 7.38931900  | 1.68896800  |
| H | 2.01005500  | 7.24153100  | -2.58996200 |
| C | 5.06407600  | -1.44577200 | 1.15618100  |
| H | 4.73722100  | -0.42677000 | 1.38907000  |
| H | 4.27889300  | -2.11873100 | 1.52181700  |
| H | 5.97795700  | -1.65099900 | 1.72289800  |
| C | 3.36212100  | -1.28196700 | -3.62270400 |
| H | 2.47679400  | -1.90397100 | -3.44966400 |
| H | 3.02111600  | -0.24224400 | -3.54871400 |
| H | 3.70483400  | -1.45569700 | -4.64736700 |
| C | 8.11444400  | -2.70900400 | -2.66904800 |
| H | 8.90237700  | -2.54962200 | -1.92510600 |
| H | 8.09168600  | -3.78262300 | -2.89922200 |
| H | 8.40641500  | -2.18927800 | -3.58878900 |
| C | -1.19840500 | -4.67842300 | 2.50281300  |
| H | -0.13585800 | -4.43389300 | 2.38190300  |
| H | -1.71917000 | -3.73488600 | 2.70504200  |
| H | -1.30175100 | -5.32483400 | 3.38037100  |
| C | -2.41279900 | -4.51606800 | -2.41969500 |
| H | -3.18853600 | -3.74230000 | -2.35935200 |
| H | -1.48362600 | -3.99530200 | -2.67457400 |
| H | -2.67066000 | -5.18775000 | -3.24452200 |
| C | -3.09229900 | -8.77375100 | 0.21952600  |
| H | -4.18046100 | -8.83355100 | 0.35669100  |
| H | -2.85390000 | -9.31160500 | -0.70501900 |
| H | -2.62844500 | -9.31133200 | 1.05369700  |
| C | -4.87235000 | 1.87768900  | 2.50077200  |
| H | -4.46020000 | 0.87623100  | 2.67451200  |
| H | -4.01929400 | 2.56515700  | 2.45048700  |
| H | -5.48221200 | 2.15212900  | 3.36723900  |
| C | -5.23218000 | 1.15633600  | -2.50171900 |
| H | -4.31145500 | 1.71549500  | -2.70372500 |
| H | -4.95113900 | 0.09636300  | -2.48625100 |
| H | -5.92297400 | 1.31446400  | -3.33571400 |
| C | -9.22244700 | 2.84664800  | 0.10969100  |
| H | -9.28137000 | 3.93520600  | -0.02519300 |
| H | -9.81796800 | 2.38832500  | -0.68745400 |
| H | -9.70017400 | 2.61239500  | 1.06752700  |
| C | 0.90010000  | 4.85907500  | 2.12178900  |
| H | -0.17527200 | 4.66070200  | 2.20715500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.39696900  | 3.88885500  | 2.22817900  |
| H | 1.19641500  | 5.49460100  | 2.96260600  |
| C | 1.19970900  | 4.67389100  | -2.94040600 |
| H | 1.92434100  | 3.85477200  | -3.01953400 |
| H | 0.20671400  | 4.21589800  | -3.01175600 |
| H | 1.33791500  | 5.33570400  | -3.80101400 |
| C | 2.38572800  | 8.92915500  | -0.48338400 |
| H | 3.10882700  | 9.11392000  | -1.28579800 |
| H | 1.53077300  | 9.59598100  | -0.65881600 |
| H | 2.84560300  | 9.23117600  | 0.46385600  |
| N | -0.40070000 | -0.93919300 | -2.89177200 |
| N | -0.20598600 | -1.86505500 | -3.56194900 |

**Structure: <sup>5</sup>TS6**

|    |             |             |             |
|----|-------------|-------------|-------------|
| Mn | 0.22571400  | 0.04210300  | -0.32803000 |
| C  | 0.22611900  | -3.00730100 | -0.24601600 |
| C  | -0.65611000 | -4.14133500 | -0.38337600 |
| C  | -1.88665400 | -3.65511900 | -0.70944000 |
| C  | -1.77793700 | -2.21665400 | -0.74465700 |
| N  | -0.48576600 | -1.84981900 | -0.45481500 |
| H  | -0.34972000 | -5.17070800 | -0.26189500 |
| H  | -2.79892800 | -4.20253800 | -0.89991800 |
| C  | -2.85224100 | -1.35773600 | -0.99282000 |
| C  | -3.90020200 | 0.92159900  | -0.99067200 |
| C  | -3.45325500 | 2.17896600  | -0.71073600 |
| C  | -2.04138700 | 2.07856300  | -0.44125800 |
| N  | -1.65591100 | 0.75862000  | -0.52194700 |
| C  | -2.77529000 | 0.03058100  | -0.86085300 |
| H  | -4.90054900 | 0.60550200  | -1.25040900 |
| H  | -4.00946700 | 3.10566600  | -0.70634200 |
| C  | 1.60422500  | -3.10906600 | -0.03350000 |
| N  | 2.09475500  | -0.68061500 | -0.09857300 |
| C  | 3.25565000  | 0.05433400  | -0.15345000 |
| C  | 4.38905000  | -0.83416400 | -0.06784400 |
| C  | 3.89809700  | -2.10001300 | 0.04447300  |
| C  | 2.45885300  | -2.00312900 | -0.00017500 |
| H  | 5.42014000  | -0.51048600 | -0.08605700 |
| H  | 4.44422500  | -3.02915800 | 0.12598200  |
| C  | 3.35646200  | 1.44532700  | -0.23517700 |
| N  | 0.93140200  | 1.93192600  | -0.25266300 |
| C  | 0.18583000  | 3.08123700  | -0.14095600 |
| C  | 1.07106100  | 4.21483400  | -0.02570400 |
| C  | 2.34435800  | 3.73731100  | -0.09921200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.25265500  | 2.30223700  | -0.21988300 |
| H | 0.74039900  | 5.23894300  | 0.07292900  |
| H | 3.27373200  | 4.28755000  | -0.06104500 |
| C | -1.20573700 | 3.17521500  | -0.21358500 |
| O | 0.00928400  | 0.05731900  | 1.52000800  |
| H | -0.92540400 | 0.27932500  | 1.67104400  |
| C | 0.00823800  | -0.09881200 | 3.96009500  |
| H | 0.67953700  | 0.74669200  | 4.04119200  |
| C | -1.39707500 | -0.03906500 | 4.10471200  |
| C | -2.25133700 | 1.06251000  | 4.34124000  |
| C | -3.62354200 | 0.84408500  | 4.42148500  |
| C | -4.15624100 | -0.44727000 | 4.27641500  |
| C | -3.31352300 | -1.54591100 | 4.03149800  |
| C | -1.94750200 | -1.34386700 | 3.93224500  |
| H | -1.83856200 | 2.06000000  | 4.46228100  |
| H | -4.29150400 | 1.68157200  | 4.60552000  |
| H | -5.22960900 | -0.59816400 | 4.34960300  |
| H | -3.73666400 | -2.53953900 | 3.90791400  |
| N | 0.44895100  | 0.05499600  | -2.33735200 |
| C | 0.46485500  | -1.52424400 | 3.86038800  |
| C | -0.84412000 | -2.31797600 | 3.58145200  |
| H | 1.21200900  | -1.65343100 | 3.07463600  |
| H | 0.92287300  | -1.84859100 | 4.80942300  |
| H | -0.90266100 | -2.56568400 | 2.51323400  |
| H | -0.90812200 | -3.25855100 | 4.13976200  |
| C | -4.16297000 | -1.95861600 | -1.40004800 |
| C | -4.41269000 | -2.20157900 | -2.76512000 |
| C | -5.12951100 | -2.28056100 | -0.42846200 |
| C | -5.63826900 | -2.76341800 | -3.13608200 |
| C | -6.34185200 | -2.84263600 | -0.84154800 |
| C | -6.61656900 | -3.08775100 | -2.19050100 |
| H | -5.83302700 | -2.95397400 | -4.18975000 |
| H | -7.08820300 | -3.09687000 | -0.09123700 |
| C | -1.83387400 | 4.53027600  | -0.10872800 |
| C | -2.30338600 | 4.98170000  | 1.13952100  |
| C | -1.95937000 | 5.33628300  | -1.25744000 |
| C | -2.88938000 | 6.24838100  | 1.22290600  |
| C | -2.55132600 | 6.59734300  | -1.12952400 |
| C | -3.01782500 | 7.07262500  | 0.10030600  |
| H | -3.25392300 | 6.59977100  | 2.18638700  |
| H | -2.65370100 | 7.22239500  | -2.01452500 |
| C | 4.71973100  | 2.05782300  | -0.32881900 |
| C | 5.43977300  | 2.37219500  | 0.83924100  |
| C | 5.26219200  | 2.32668000  | -1.60113200 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 6.70404900  | 2.95705000  | 0.71592400  |
| C | 6.53033800  | 2.91165800  | -1.67927900 |
| C | 7.26714200  | 3.23184800  | -0.53450800 |
| H | 7.26075300  | 3.20601900  | 1.61742100  |
| H | 6.95228600  | 3.12338900  | -2.65986100 |
| C | 2.21544400  | -4.47867800 | 0.01530700  |
| C | 2.48249900  | -5.10380800 | 1.24790000  |
| C | 2.53543500  | -5.12926500 | -1.19486000 |
| C | 3.06046000  | -6.37757400 | 1.25255600  |
| C | 3.11308700  | -6.40172700 | -1.14596500 |
| C | 3.37948300  | -7.04509700 | 0.06666400  |
| H | 3.26749000  | -6.85871200 | 2.20657200  |
| H | 3.36474600  | -6.90137600 | -2.07945800 |
| C | -4.85298000 | -2.02777400 | 1.03427100  |
| H | -3.92919000 | -2.52140900 | 1.35533900  |
| H | -4.71523200 | -0.96056400 | 1.24287800  |
| H | -5.67089600 | -2.39142800 | 1.66434300  |
| C | -3.36967400 | -1.86568300 | -3.80644500 |
| H | -3.09025300 | -0.80644800 | -3.76514500 |
| H | -2.44602700 | -2.43320300 | -3.64177800 |
| H | -3.73167400 | -2.08597400 | -4.81534300 |
| C | -7.94648400 | -3.66307400 | -2.61967300 |
| H | -7.84425500 | -4.28609200 | -3.51506800 |
| H | -8.39366100 | -4.27541000 | -1.82907200 |
| H | -8.66294500 | -2.86580700 | -2.85931000 |
| C | 2.15679300  | -4.40716100 | 2.54756200  |
| H | 2.72974000  | -3.47857700 | 2.65339900  |
| H | 1.09846900  | -4.12941600 | 2.59371600  |
| H | 2.38125600  | -5.04443400 | 3.40854000  |
| C | 2.26757100  | -4.46122000 | -2.52427600 |
| H | 1.19464400  | -4.29587100 | -2.67811800 |
| H | 2.74433600  | -3.47576200 | -2.57831100 |
| H | 2.64074000  | -5.06949400 | -3.35383900 |
| C | 3.97203200  | -8.43498000 | 0.09308900  |
| H | 4.55629400  | -8.60561100 | 1.00389300  |
| H | 3.18509500  | -9.20063700 | 0.06280600  |
| H | 4.62656200  | -8.60891800 | -0.76801200 |
| C | -1.48522400 | 4.83627700  | -2.60260800 |
| H | -0.42687000 | 4.55436900  | -2.58624800 |
| H | -2.03289600 | 3.93505300  | -2.90347800 |
| H | -1.62715900 | 5.59470600  | -3.37855600 |
| C | -2.18111400 | 4.10371400  | 2.36422100  |
| H | -2.75057900 | 3.17356200  | 2.25034600  |
| H | -1.13943900 | 3.80837300  | 2.53955200  |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -2.54671200 | 4.61725300 | 3.25936400  |
| C | -3.62108200 | 8.45326900 | 0.21887900  |
| H | -4.36654600 | 8.49865800 | 1.02045800  |
| H | -2.85126100 | 9.20248000 | 0.44800600  |
| H | -4.10599500 | 8.76123800 | -0.71386900 |
| C | 4.84922600  | 2.08938000 | 2.20185600  |
| H | 3.89249300  | 2.60880100 | 2.33448900  |
| H | 4.64516000  | 1.01968900 | 2.33155700  |
| H | 5.52535000  | 2.40757600 | 3.00142800  |
| C | 4.49008400  | 1.98082800 | -2.85405900 |
| H | 4.28146800  | 0.90492600 | -2.90293000 |
| H | 3.51626500  | 2.48279900 | -2.88971800 |
| H | 5.04982800  | 2.25915800 | -3.75219000 |
| C | 8.64920300  | 3.83307400 | -0.64632300 |
| H | 9.41861300  | 3.05024400 | -0.68718700 |
| H | 8.75197000  | 4.43668200 | -1.55467800 |
| H | 8.88097600  | 4.47111600 | 0.21358900  |
| N | 0.62977500  | 1.09291900 | -2.93453100 |
| N | 0.80700500  | 2.06605300 | -3.53590500 |

**Structure: <sup>3</sup>TS7**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.36396200  | 0.69681200  | -0.38482600 |
| C | 4.27481900  | 1.80941300  | -0.22957700 |
| C | 3.51292900  | 2.93638000  | -0.15779200 |
| C | 2.13285400  | 2.51931300  | -0.28503300 |
| N | 2.07036400  | 1.15951900  | -0.44148700 |
| H | 5.35026900  | 1.71996000  | -0.16641300 |
| H | 3.83810000  | 3.95925100  | -0.02782900 |
| C | -2.09863300 | 1.80047900  | -0.74141700 |
| C | -2.52323400 | 3.18273600  | -0.71144700 |
| C | -1.40884000 | 3.93224400  | -0.46891200 |
| C | -0.29573800 | 3.01093300  | -0.38216000 |
| N | -0.74943200 | 1.72145500  | -0.52765600 |
| H | -3.54081600 | 3.51837300  | -0.85852900 |
| H | -1.32699800 | 5.00715500  | -0.38424800 |
| C | 1.04657700  | -2.94946700 | -0.45438600 |
| C | 2.16215200  | -3.87268400 | -0.40757300 |
| C | 3.29461900  | -3.12027400 | -0.40452400 |
| C | 2.87524500  | -1.73371300 | -0.44421900 |
| N | 1.51103500  | -1.65929300 | -0.48562700 |
| H | 2.07053800  | -4.94921000 | -0.37819800 |
| H | 4.32241000  | -3.45257600 | -0.36814600 |
| C | -1.38223000 | -2.45983100 | -0.58611400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.75830300 | -2.88010700 | -0.72852700 |
| C  | -3.50019800 | -1.74926300 | -0.90472500 |
| C  | -2.58665200 | -0.63123100 | -0.82701400 |
| N  | -1.30785600 | -1.09210100 | -0.62367500 |
| H  | -3.09448500 | -3.90749300 | -0.71868200 |
| H  | -4.56585300 | -1.66554300 | -1.06570600 |
| C  | 3.76095200  | -0.64526600 | -0.39965000 |
| C  | -2.97411600 | 0.71254800  | -0.92502800 |
| C  | 1.03996000  | 3.40166600  | -0.24121400 |
| C  | -0.29531400 | -3.34414300 | -0.46912100 |
| O  | 0.40454000  | 0.03912900  | -2.39259000 |
| N  | 0.39763400  | -0.00246900 | 1.51467600  |
| Mn | 0.38862600  | 0.02688000  | -0.58118600 |
| C  | -3.34699000 | -2.22878900 | 3.09618800  |
| C  | -2.52930200 | -1.28122000 | 2.50380000  |
| C  | -2.67066700 | 0.06926000  | 2.91127900  |
| C  | -3.60571300 | 0.44255100  | 3.92454200  |
| C  | -4.40459800 | -0.52339000 | 4.51508800  |
| C  | -4.27080500 | -1.85467400 | 4.09208700  |
| H  | -3.27534700 | -3.26878200 | 2.79441000  |
| H  | -1.79582000 | -1.53500900 | 1.75009000  |
| H  | -5.12751800 | -0.26267500 | 5.28309900  |
| H  | -4.89591300 | -2.61906000 | 4.54590500  |
| C  | -2.04839200 | 1.21211900  | 2.40268300  |
| H  | 1.11892600  | 0.63744700  | -2.66847500 |
| H  | -1.33587100 | 1.22502000  | 1.59357900  |
| C  | -2.48458300 | 2.42789900  | 3.14316400  |
| C  | -3.57324500 | 1.93593800  | 4.13617500  |
| H  | -3.34345300 | 2.19519500  | 5.17636900  |
| H  | -4.54908300 | 2.38283600  | 3.90926800  |
| H  | -1.62171900 | 2.88358500  | 3.65124400  |
| H  | -2.83836500 | 3.19173500  | 2.43588500  |
| C  | 5.22507600  | -0.94671600 | -0.29249300 |
| C  | 5.98352200  | -1.17050900 | -1.45727100 |
| C  | 5.82720300  | -1.02051800 | 0.97954900  |
| C  | 7.34480500  | -1.46521200 | -1.33179200 |
| C  | 7.19169700  | -1.31848100 | 1.05986700  |
| C  | 7.96749200  | -1.54113900 | -0.08200000 |
| H  | 7.93193200  | -1.64128800 | -2.23129500 |
| H  | 7.65895800  | -1.38152000 | 2.04088700  |
| C  | 1.32665100  | 4.85968500  | -0.04410300 |
| C  | 1.61009700  | 5.68110800  | -1.15185600 |
| C  | 1.31957200  | 5.39915300  | 1.25706700  |
| C  | 1.88328700  | 7.03633600  | -0.93773000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.59983500  | 6.75790900  | 1.42979400  |
| C | 1.88170800  | 7.59394500  | 0.34432800  |
| H | 2.10555500  | 7.67086300  | -1.79360300 |
| H | 1.60130100  | 7.17343900  | 2.43596800  |
| C | -4.36444800 | 1.01056000  | -1.40712700 |
| C | -5.47793200 | 1.02555900  | -0.54599800 |
| C | -4.53614200 | 1.26105700  | -2.78707500 |
| C | -6.74767200 | 1.28096500  | -1.07609600 |
| C | -5.82210400 | 1.51114300  | -3.27510700 |
| C | -6.94150200 | 1.52694100  | -2.43751100 |
| H | -7.60608000 | 1.28631700  | -0.40685600 |
| H | -5.95320900 | 1.69271300  | -4.34030000 |
| C | -0.59225600 | -4.81048900 | -0.37644700 |
| C | -0.61853000 | -5.43471000 | 0.88718100  |
| C | -0.82723500 | -5.55854400 | -1.54686300 |
| C | -0.89875100 | -6.80333100 | 0.95669400  |
| C | -1.10345900 | -6.92497400 | -1.43161300 |
| C | -1.14918800 | -7.56458500 | -0.18918000 |
| H | -0.91702800 | -7.28750500 | 1.93141300  |
| H | -1.28017900 | -7.50466400 | -2.33571700 |
| C | -5.31441400 | 0.78555500  | 0.93517300  |
| H | -4.83272500 | -0.17544900 | 1.14130600  |
| H | -4.67911900 | 1.55721100  | 1.38465300  |
| H | -6.28021600 | 0.80107800  | 1.45011900  |
| C | -3.35115800 | 1.26996800  | -3.72694600 |
| H | -2.73320800 | 2.16237400  | -3.56726300 |
| H | -2.69113700 | 0.41137100  | -3.56540000 |
| H | -3.67888000 | 1.26851000  | -4.77132500 |
| C | -8.31608000 | 1.82911200  | -2.98779000 |
| H | -9.10514000 | 1.42009900  | -2.34750900 |
| H | -8.48362900 | 2.91211900  | -3.06189500 |
| H | -8.44567100 | 1.41320400  | -3.99327100 |
| C | 1.00843400  | 4.51805100  | 2.44541800  |
| H | -0.01829300 | 4.13656700  | 2.38608400  |
| H | 1.66301700  | 3.63946500  | 2.47683800  |
| H | 1.11727500  | 5.06605500  | 3.38673600  |
| C | 1.62542700  | 5.10238100  | -2.54802900 |
| H | 2.39727000  | 4.32929300  | -2.64536600 |
| H | 0.66893900  | 4.62340100  | -2.78887300 |
| H | 1.82044500  | 5.87595200  | -3.29719700 |
| C | 2.14947200  | 9.06677900  | 0.55241400  |
| H | 1.21229900  | 9.63877600  | 0.58551100  |
| H | 2.67368700  | 9.24962800  | 1.49712200  |
| H | 2.75657200  | 9.48355800  | -0.25842000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.33148900  | -1.09937900 | -2.81918500 |
| H | 4.53867100  | -1.85045900 | -2.91943200 |
| H | 4.85901400  | -0.12300800 | -2.98129400 |
| H | 6.06112200  | -1.26341900 | -3.61829500 |
| C | 5.01712700  | -0.77555600 | 2.23203000  |
| H | 4.66326200  | 0.26222600  | 2.27313700  |
| H | 4.12214000  | -1.40602900 | 2.27474600  |
| H | 5.61347100  | -0.96506700 | 3.13005400  |
| C | 9.44727200  | -1.82774000 | 0.03014900  |
| H | 9.79964100  | -2.45196000 | -0.79845800 |
| H | 10.03290500 | -0.89860300 | 0.00928500  |
| H | 9.68701500  | -2.34127800 | 0.96773700  |
| C | -0.76761100 | -4.89774400 | -2.90515000 |
| H | -1.55587100 | -4.14406400 | -3.01762300 |
| H | 0.18450700  | -4.37376600 | -3.04831000 |
| H | -0.88102000 | -5.63288500 | -3.70797500 |
| C | -0.33851700 | -4.64579100 | 2.14573200  |
| H | 0.66088700  | -4.19776900 | 2.13795800  |
| H | -1.03542400 | -3.80840600 | 2.25830200  |
| H | -0.42224500 | -5.27768100 | 3.03554800  |
| C | -1.48252200 | -9.03506400 | -0.08506100 |
| H | -0.99667900 | -9.49652900 | 0.78176300  |
| H | -2.56423700 | -9.18928900 | 0.02836100  |
| H | -1.16917300 | -9.58241500 | -0.98082100 |
| N | 0.95263600  | -0.82456300 | 2.19991200  |
| N | 1.46495200  | -1.59943200 | 2.89548600  |

**Structure: <sup>5</sup>TS7**

|    |             |             |             |
|----|-------------|-------------|-------------|
| Mn | 0.29899900  | 0.06322600  | -0.84816800 |
| C  | -2.65979000 | 0.59140300  | -1.23941400 |
| C  | -3.93479800 | -0.08399400 | -1.26855600 |
| C  | -3.70669900 | -1.38715000 | -0.92897400 |
| C  | -2.28154800 | -1.54194000 | -0.76378500 |
| N  | -1.67382700 | -0.32461300 | -0.95488000 |
| H  | -4.87915500 | 0.40150600  | -1.47213900 |
| H  | -4.42605400 | -2.18581700 | -0.81555600 |
| C  | -1.62473000 | -2.76106500 | -0.54858200 |
| C  | 0.44322500  | -4.18569300 | -0.69275400 |
| C  | 1.76519200  | -3.92784900 | -0.91060700 |
| C  | 1.91717500  | -2.49338900 | -0.95070200 |
| N  | 0.68097000  | -1.90657900 | -0.81817600 |
| C  | -0.23786100 | -2.91394600 | -0.65374500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.04726500 | -5.14314700 | -0.58548300 |
| H | 2.58135000  | -4.63067100 | -1.00227800 |
| C | -2.49800000 | 1.98078100  | -1.31556300 |
| N | -0.12176800 | 2.02261200  | -0.64183100 |
| C | 0.74198200  | 3.00008300  | -0.22052700 |
| C | 0.06758000  | 4.27695800  | -0.25547200 |
| C | -1.18165600 | 4.05542400  | -0.75690400 |
| C | -1.30763800 | 2.63138300  | -0.96744900 |
| H | 0.51894200  | 5.21498900  | 0.03620400  |
| H | -1.96790000 | 4.77385100  | -0.94182700 |
| C | 2.09720000  | 2.82501300  | 0.08382500  |
| N | 2.23960800  | 0.43763900  | -0.54502500 |
| C | 3.27167100  | -0.45177000 | -0.72254600 |
| C | 4.52267100  | 0.21684700  | -0.45645500 |
| C | 4.22293600  | 1.48793800  | -0.06476400 |
| C | 2.78877400  | 1.62989100  | -0.14196600 |
| H | 5.49314600  | -0.25375900 | -0.52542600 |
| H | 4.89919600  | 2.27614200  | 0.23486600  |
| C | 3.14610200  | -1.82422900 | -0.96594400 |
| O | 0.46181500  | 0.21697700  | -2.70363400 |
| H | -0.08069800 | -0.46500100 | -3.13415100 |
| N | 0.08396800  | -0.06376300 | 1.31355400  |
| C | -2.44352800 | -3.95560400 | -0.17185900 |
| C | -2.49334800 | -4.32179500 | 1.18999100  |
| C | -3.14963400 | -4.69726500 | -1.13854200 |
| C | -3.29718300 | -5.40283800 | 1.56482800  |
| C | -3.93652800 | -5.77541700 | -0.71943600 |
| C | -4.03440900 | -6.13466900 | 0.62848800  |
| H | -3.34416000 | -5.68266100 | 2.61563900  |
| H | -4.48151900 | -6.35162800 | -1.46480900 |
| C | 4.39777000  | -2.63396300 | -1.10993600 |
| C | 4.96192800  | -2.81357700 | -2.38731300 |
| C | 5.00179000  | -3.20523500 | 0.02820400  |
| C | 6.13346400  | -3.56767200 | -2.50783000 |
| C | 6.17304700  | -3.95187100 | -0.13749000 |
| C | 6.75570300  | -4.14144100 | -1.39470900 |
| H | 6.57003400  | -3.70997300 | -3.49460700 |
| H | 6.64192300  | -4.39603000 | 0.73856800  |
| C | 2.85891100  | 3.98464700  | 0.64580900  |
| C | 3.49406600  | 4.90992900  | -0.20382500 |
| C | 2.94007500  | 4.12368300  | 2.04575200  |
| C | 4.20438400  | 5.97129400  | 0.36730100  |
| C | 3.66036500  | 5.19850400  | 2.57544800  |
| C | 4.29686800  | 6.13397700  | 1.75311500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.69987900  | 6.68639500  | -0.28665300 |
| H | 3.72796900  | 5.30680300  | 3.65632800  |
| C | -3.67037700 | 2.81410000  | -1.73577000 |
| C | -3.87451300 | 3.03505800  | -3.11339200 |
| C | -4.54405900 | 3.38107600  | -0.78724300 |
| C | -4.95359200 | 3.82538700  | -3.51969600 |
| C | -5.61032600 | 4.16781700  | -1.23716100 |
| C | -5.83410300 | 4.39950900  | -2.59737900 |
| H | -5.10703500 | 4.00130600  | -4.58272200 |
| H | -6.28199200 | 4.61168500  | -0.50474100 |
| C | -3.04328900 | -4.35297900 | -2.60757900 |
| H | -3.51039500 | -3.38710400 | -2.83320900 |
| H | -1.99474800 | -4.27463800 | -2.91820000 |
| H | -3.52726300 | -5.11430400 | -3.22712800 |
| C | -1.66353400 | -3.58986400 | 2.22080100  |
| H | -0.60281800 | -3.85401900 | 2.12180100  |
| H | -1.72902500 | -2.50447600 | 2.10486800  |
| H | -1.98415700 | -3.84087000 | 3.23524800  |
| C | -4.92618100 | -7.27396100 | 1.06508200  |
| H | -5.93069800 | -6.91262800 | 1.32400500  |
| H | -5.04403400 | -8.01986200 | 0.27148300  |
| H | -4.52602500 | -7.78035100 | 1.95037700  |
| C | -2.94165400 | 2.42339600  | -4.13410100 |
| H | -1.89474200 | 2.66922000  | -3.92321500 |
| H | -3.00805300 | 1.32846800  | -4.12192800 |
| H | -3.18154400 | 2.76679500  | -5.14514500 |
| C | -4.35486700 | 3.13684200  | 0.69261300  |
| H | -4.60447900 | 2.10315600  | 0.95911800  |
| H | -3.31712000 | 3.30056300  | 1.00200700  |
| H | -4.99619900 | 3.79546200  | 1.28646200  |
| C | -7.01122000 | 5.22652100  | -3.06017100 |
| H | -7.29328900 | 5.97688300  | -2.31358200 |
| H | -6.79202600 | 5.74697400  | -3.99891200 |
| H | -7.89257300 | 4.59523600  | -3.23658300 |
| C | 4.38787800  | -3.02714800 | 1.39782100  |
| H | 4.20775900  | -1.97247100 | 1.63141800  |
| H | 3.41133500  | -3.52231400 | 1.46114600  |
| H | 5.03165400  | -3.44752400 | 2.17662900  |
| C | 4.30663200  | -2.20261100 | -3.60486600 |
| H | 3.28021500  | -2.56816700 | -3.72922000 |
| H | 4.23598700  | -1.11220100 | -3.51481300 |
| H | 4.86604100  | -2.43619300 | -4.51605400 |
| C | 8.04200800  | -4.92110300 | -1.54197000 |
| H | 8.11394900  | -5.39582300 | -2.52666100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 8.91623300  | -4.26521300 | -1.43220400 |
| H | 8.12676300  | -5.70416900 | -0.78040900 |
| C | 3.41522100  | 4.75148600  | -1.70503900 |
| H | 3.83146100  | 3.78872100  | -2.02454200 |
| H | 2.37564300  | 4.77195400  | -2.05268100 |
| H | 3.96330400  | 5.54824200  | -2.21727200 |
| C | 2.26187700  | 3.12326900  | 2.95452600  |
| H | 1.18652500  | 3.06840300  | 2.74745300  |
| H | 2.65531200  | 2.10977900  | 2.80968600  |
| H | 2.39272900  | 3.39210800  | 4.00742200  |
| C | 5.04123100  | 7.30688800  | 2.34829200  |
| H | 4.36846000  | 8.15923900  | 2.51375700  |
| H | 5.48460800  | 7.05129000  | 3.31699900  |
| H | 5.84450700  | 7.65061000  | 1.68750900  |
| N | 1.04938800  | -0.38999500 | 1.96337900  |
| N | 1.95168800  | -0.66674200 | 2.64026100  |
| C | -1.25673900 | 1.10840500  | 3.15411700  |
| H | -1.14844300 | 1.83832200  | 2.36320000  |
| C | -2.30694400 | 0.16945700  | 3.24726800  |
| C | -3.30131500 | -0.16733000 | 2.30354200  |
| C | -4.22924600 | -1.14830900 | 2.62847200  |
| C | -4.18042000 | -1.79725600 | 3.87407100  |
| C | -3.18388000 | -1.47897500 | 4.81106700  |
| C | -2.24748000 | -0.50500200 | 4.49793600  |
| H | -3.30876500 | 0.31066000  | 1.33272900  |
| H | -4.98637000 | -1.43028900 | 1.90252500  |
| H | -4.91148700 | -2.56657800 | 4.10684500  |
| H | -3.14734700 | -1.99716900 | 5.76648300  |
| C | -0.41390000 | 1.08240500  | 4.39260200  |
| C | -1.08023100 | 0.01133300  | 5.30969300  |
| H | 0.62981900  | 0.81836300  | 4.16125000  |
| H | -0.36661500 | 2.07290500  | 4.86733800  |
| H | -0.38146600 | -0.79521500 | 5.56045500  |
| H | -1.41400900 | 0.44508800  | 6.26072800  |

**Structure: <sup>3</sup>TS8**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.58806300 | -0.65526400 | -0.71749300 |
| C | -3.50190900 | -1.76911700 | -0.82368500 |
| C | -2.75993300 | -2.90513000 | -0.68284900 |
| C | -1.38475600 | -2.48996700 | -0.52769000 |
| N | -1.30906600 | -1.11977200 | -0.51982900 |
| H | -4.56696900 | -1.67862300 | -0.98470700 |
| H | -3.09473300 | -3.93269900 | -0.70733900 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.87174800  | -1.76275600 | -0.36595900 |
| C  | 3.29063300  | -3.14667000 | -0.37262400 |
| C  | 2.15799700  | -3.90081200 | -0.41041800 |
| C  | 1.04285500  | -2.98085900 | -0.42990200 |
| N  | 1.50597300  | -1.68777600 | -0.41382600 |
| H  | 4.31859000  | -3.47876300 | -0.34170600 |
| H  | 2.06799000  | -4.97779000 | -0.42006800 |
| C  | -0.28501200 | 2.98065700  | -0.25874300 |
| C  | -1.39338800 | 3.90074300  | -0.35853500 |
| C  | -2.50956400 | 3.15387900  | -0.60271200 |
| C  | -2.09225200 | 1.77270700  | -0.62474900 |
| N  | -0.74127000 | 1.68811400  | -0.39927000 |
| H  | -1.30789600 | 4.97586500  | -0.28534000 |
| H  | -3.52375000 | 3.49283100  | -0.76308500 |
| C  | 2.13755100  | 2.48565700  | -0.12914500 |
| C  | 3.51867400  | 2.89939600  | 0.00800100  |
| C  | 4.27674000  | 1.77133200  | -0.05990200 |
| C  | 3.36191400  | 0.66244600  | -0.22711200 |
| N  | 2.07107000  | 1.12791300  | -0.27843400 |
| H  | 3.84454400  | 3.92201300  | 0.13629200  |
| H  | 5.35166100  | 1.67741600  | 0.00398500  |
| C  | -2.97225500 | 0.68959300  | -0.81169700 |
| C  | 3.75748400  | -0.67738000 | -0.27380800 |
| C  | -0.29864300 | -3.37784400 | -0.45813700 |
| C  | 1.04838000  | 3.37251500  | -0.10666800 |
| N  | 0.38975000  | -0.06128400 | 1.60198900  |
| Mn | 0.39536800  | -0.00067300 | -0.42754700 |
| C  | -3.36207600 | -2.33559900 | 3.26776800  |
| C  | -2.56910300 | -1.39216500 | 2.63667500  |
| C  | -2.70946300 | -0.03586800 | 3.02682100  |
| C  | -3.62290900 | 0.34866500  | 4.05603600  |
| C  | -4.39999100 | -0.61277100 | 4.68165000  |
| C  | -4.26423200 | -1.95041900 | 4.27938600  |
| H  | -3.28703300 | -3.38109700 | 2.98635100  |
| H  | -1.85717300 | -1.65684100 | 1.86599600  |
| H  | -5.10612900 | -0.34475100 | 5.46259000  |
| H  | -4.87073500 | -2.71171800 | 4.76264000  |
| C  | -2.10004900 | 1.10136300  | 2.49262800  |
| H  | -1.40317600 | 1.10106400  | 1.67038900  |
| N  | 0.47011900  | 0.05662800  | -2.37164900 |
| C  | -3.59200400 | 1.84537500  | 4.24343300  |
| C  | -2.51704200 | 2.32489200  | 3.22958200  |
| H  | -4.57189400 | 2.28524600  | 4.02013400  |
| H  | -3.35146400 | 2.12226600  | 5.27649800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.87361600 | 3.08994200  | 2.52531300  |
| H | -1.64151300 | 2.77391700  | 3.72201700  |
| C | -4.35575000 | 0.99535800  | -1.30770900 |
| C | -5.47320500 | 1.04157900  | -0.45425600 |
| C | -4.51156800 | 1.23165500  | -2.69308900 |
| C | -6.73321000 | 1.32469900  | -0.99469400 |
| C | -5.78734400 | 1.51219100  | -3.18976100 |
| C | -6.91180900 | 1.56183200  | -2.35926600 |
| H | -7.59478900 | 1.36093200  | -0.33062400 |
| H | -5.90663300 | 1.69258000  | -4.25642400 |
| C | 1.33392300  | 4.83315600  | 0.06849500  |
| C | 1.22095100  | 5.41418200  | 1.34663600  |
| C | 1.71644200  | 5.61552100  | -1.03957600 |
| C | 1.49156300  | 6.77746300  | 1.49934300  |
| C | 1.97489600  | 6.97642400  | -0.84340400 |
| C | 1.86600200  | 7.57673200  | 0.41475600  |
| H | 1.41096400  | 7.22476600  | 2.48844400  |
| H | 2.27087000  | 7.58240500  | -1.69764100 |
| C | 5.21846200  | -0.98430400 | -0.14979200 |
| C | 6.01361800  | -1.10770900 | -1.30408700 |
| C | 5.78132800  | -1.14981800 | 1.13161900  |
| C | 7.37409500  | -1.39931800 | -1.15766700 |
| C | 7.14512300  | -1.44107000 | 1.23269200  |
| C | 7.95699700  | -1.57332200 | 0.10109400  |
| H | 7.99217400  | -1.49161300 | -2.04870800 |
| H | 7.58457000  | -1.56664200 | 2.22056200  |
| C | -0.59295600 | -4.84764800 | -0.44788100 |
| C | -0.80045300 | -5.53007400 | -1.66309400 |
| C | -0.65370100 | -5.53834000 | 0.77845600  |
| C | -1.07530600 | -6.90083800 | -1.62897800 |
| C | -0.93067700 | -6.90961300 | 0.76690100  |
| C | -1.14267600 | -7.60903200 | -0.42491800 |
| H | -1.23682600 | -7.42884900 | -2.56694500 |
| H | -0.98014400 | -7.44419900 | 1.71375300  |
| C | 0.80674100  | 4.57607700  | 2.53545000  |
| H | -0.23583700 | 4.24918300  | 2.43555100  |
| H | 1.41264100  | 3.66637200  | 2.61668600  |
| H | 0.89922100  | 5.13926400  | 3.46957800  |
| C | 1.86251200  | 4.99505900  | -2.40938300 |
| H | 2.71689800  | 4.30756800  | -2.43916700 |
| H | 0.98626000  | 4.40114100  | -2.68826800 |
| H | 2.02004900  | 5.76158200  | -3.17456400 |
| C | 2.11928000  | 9.05603400  | 0.59217200  |
| H | 1.20050200  | 9.63667400  | 0.43305400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.47719500  | 9.28437000  | 1.60215000  |
| H | 2.86301200  | 9.42454400  | -0.12282000 |
| C | 5.40391500  | -0.92447600 | -2.67495000 |
| H | 4.60958400  | -1.65830500 | -2.85702700 |
| H | 4.94147800  | 0.06464700  | -2.77516100 |
| H | 6.15632800  | -1.03260600 | -3.46224700 |
| C | 4.92901900  | -0.99887400 | 2.37117100  |
| H | 4.52684500  | 0.01880100  | 2.44934800  |
| H | 4.06335400  | -1.67117300 | 2.35862200  |
| H | 5.50875600  | -1.20495900 | 3.27628800  |
| C | 9.42092700  | -1.92316500 | 0.23829900  |
| H | 9.99862500  | -1.58394000 | -0.62831400 |
| H | 9.85881500  | -1.47219400 | 1.13589300  |
| H | 9.56195400  | -3.00939600 | 0.32006500  |
| C | -0.42049600 | -4.81335700 | 2.08344900  |
| H | 0.58176500  | -4.37474600 | 2.13585300  |
| H | -1.11465200 | -3.97483200 | 2.20613800  |
| H | -0.54456700 | -5.48546300 | 2.93835800  |
| C | -0.72438000 | -4.79259300 | -2.98038900 |
| H | -1.50771900 | -4.02910400 | -3.05573200 |
| H | 0.23199700  | -4.26730300 | -3.08547000 |
| H | -0.83451700 | -5.47916100 | -3.82537300 |
| C | -1.40508100 | -9.09731300 | -0.41643400 |
| H | -0.47002900 | -9.66402000 | -0.52077700 |
| H | -1.87626000 | -9.41732200 | 0.51935200  |
| H | -2.05795700 | -9.39459200 | -1.24460600 |
| C | -3.32465400 | 1.17216700  | -3.62810200 |
| H | -2.58832800 | 1.95429300  | -3.41057700 |
| H | -2.79233500 | 0.21834400  | -3.53466100 |
| H | -3.63964300 | 1.28707700  | -4.66965300 |
| C | -5.32545400 | 0.80497600  | 1.02915400  |
| H | -4.85880000 | -0.16250300 | 1.24058500  |
| H | -4.68459100 | 1.56906700  | 1.48360200  |
| H | -6.29550500 | 0.83399800  | 1.53549500  |
| C | -8.28242200 | 1.83677100  | -2.93299800 |
| H | -8.69889900 | 0.93916600  | -3.40926900 |
| H | -8.98777800 | 2.15421600  | -2.15765300 |
| H | -8.24580600 | 2.61967200  | -3.69914200 |
| N | 0.83357800  | -0.96630500 | 2.26759300  |
| N | 1.23654700  | -1.80969200 | 2.95186400  |
| N | 0.33251000  | 1.09821400  | -2.97420300 |
| N | 0.19806500  | 2.05898200  | -3.60370700 |

**Structure: <sup>5</sup>TS8**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.76528600 | -2.82195600 | -0.60890900 |
| C  | -0.31769800 | -4.18593800 | -0.73041100 |
| C  | 1.02947600  | -4.15141200 | -0.94910200 |
| C  | 1.43478900  | -2.76955200 | -0.89403300 |
| N  | 0.31944700  | -1.98358600 | -0.71292200 |
| H  | -0.96889700 | -5.04721700 | -0.68031300 |
| H  | 1.70771300  | -4.98030800 | -1.09432900 |
| C  | 2.98799500  | 1.07045200  | 0.21755500  |
| C  | 4.36754900  | 0.66676000  | 0.32953500  |
| C  | 4.45540400  | -0.60959200 | -0.14521500 |
| C  | 3.12059900  | -1.02698700 | -0.49525200 |
| N  | 2.25352800  | 0.01760700  | -0.27754600 |
| H  | 5.16013100  | 1.30221000  | 0.69855900  |
| H  | 5.33084100  | -1.23845400 | -0.22478900 |
| C  | -2.47647800 | 1.05398400  | -1.19676000 |
| C  | -3.84592400 | 0.61772000  | -1.32439800 |
| C  | -3.88112900 | -0.70118400 | -0.97404200 |
| C  | -2.52162200 | -1.10867800 | -0.71376800 |
| N  | -1.69566100 | -0.01996800 | -0.84331400 |
| H  | -4.66732500 | 1.26264600  | -1.60377500 |
| H  | -4.73567000 | -1.36118100 | -0.92493100 |
| C  | -0.79974000 | 2.80310200  | -0.80347900 |
| C  | -0.43069100 | 4.17309600  | -0.55315100 |
| C  | 0.79898500  | 4.15745600  | 0.04036400  |
| C  | 1.22623400  | 2.78228500  | 0.09818800  |
| N  | 0.22575900  | 1.98069200  | -0.40024100 |
| H  | -1.05603200 | 5.02442000  | -0.78274000 |
| H  | 1.39418900  | 4.99570500  | 0.37406100  |
| C  | -2.10556100 | -2.43018900 | -0.51947500 |
| C  | 2.51263900  | 2.36441200  | 0.45557000  |
| C  | 2.76227800  | -2.33123500 | -0.85367200 |
| C  | -2.05497200 | 2.38630100  | -1.26220300 |
| N  | 0.02619700  | -0.14698700 | 1.39866900  |
| Mn | 0.28306000  | -0.00477500 | -0.57693500 |
| C  | -4.32097600 | 0.19043900  | 2.40568200  |
| C  | -3.04727100 | 0.74354400  | 2.46695200  |
| C  | -2.24229200 | 0.47752200  | 3.60024000  |
| C  | -2.73273500 | -0.36793100 | 4.63928900  |
| C  | -4.00643200 | -0.90739100 | 4.56391700  |
| C  | -4.80644400 | -0.62342100 | 3.44416400  |
| H  | -4.93925000 | 0.36906100  | 1.53108600  |
| H  | -2.65429700 | 1.33985700  | 1.65109600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.38378100 | -1.55146800 | 5.35508800  |
| H | -5.80214900 | -1.05187800 | 3.37050600  |
| C | -0.93440200 | 0.90012300  | 3.90430700  |
| H | -0.34213700 | 1.57242400  | 3.29832000  |
| N | 0.56727800  | 0.16861500  | -2.54018600 |
| C | -1.68349900 | -0.51327700 | 5.72049700  |
| C | -0.43038500 | 0.20929500  | 5.13728700  |
| H | -1.48367100 | -1.56318100 | 5.96303200  |
| H | -2.01542100 | -0.03285800 | 6.65067300  |
| H | 0.34919300  | -0.52136400 | 4.86260500  |
| H | 0.03740500  | 0.89736000  | 5.85426900  |
| C | 3.85082100  | -3.33263400 | -1.08170100 |
| C | 4.34876800  | -3.51689500 | -2.38604400 |
| C | 4.36134500  | -4.08253600 | -0.00391300 |
| C | 5.35824900  | -4.46163800 | -2.59381000 |
| C | 5.37069100  | -5.01759800 | -0.25693000 |
| C | 5.88309000  | -5.22013400 | -1.54234100 |
| H | 5.74262500  | -4.60984300 | -3.60115800 |
| H | 5.76540400  | -5.60259300 | 0.57152400  |
| C | 3.45677800  | 3.38132200  | 1.01619700  |
| C | 4.32625000  | 4.08778900  | 0.16143800  |
| C | 3.45278500  | 3.63108400  | 2.40202100  |
| C | 5.19013000  | 5.03612800  | 0.71933600  |
| C | 4.33479300  | 4.58553000  | 2.91798900  |
| C | 5.21328000  | 5.29566600  | 2.09350200  |
| H | 5.85984200  | 5.58784000  | 0.06247400  |
| H | 4.33372200  | 4.78104800  | 3.98864400  |
| C | -3.13617400 | -3.48084000 | -0.25243100 |
| C | -3.38479300 | -3.84082200 | 1.08822400  |
| C | -3.83044200 | -4.10446900 | -1.30610900 |
| C | -4.35676500 | -4.81060900 | 1.35073600  |
| C | -4.79285500 | -5.07195000 | -0.99721200 |
| C | -5.07575100 | -5.43191000 | 0.32401900  |
| H | -4.55450800 | -5.08987500 | 2.38388600  |
| H | -5.33070100 | -5.55835100 | -1.80871000 |
| C | -2.99407600 | 3.41831000  | -1.80425300 |
| C | -3.92547000 | 4.07005400  | -0.97416300 |
| C | -2.91035900 | 3.73602700  | -3.17604800 |
| C | -4.77456700 | 5.02948300  | -1.53720400 |
| C | -3.77871400 | 4.69961600  | -3.69678900 |
| C | -4.72033300 | 5.35420600  | -2.89559800 |
| H | -5.49276300 | 5.53739100  | -0.89644900 |
| H | -3.71589400 | 4.94805400  | -4.75450900 |
| C | 3.79802900  | -2.70543800 | -3.53682700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.71738500  | -2.85248600 | -3.65010700 |
| H | 3.94703800  | -1.63131500 | -3.37283900 |
| H | 4.28151400  | -2.97651200 | -4.48030600 |
| C | 3.83361400  | -3.87560400 | 1.39750900  |
| H | 4.01848000  | -2.85206300 | 1.74466700  |
| H | 2.74927000  | -4.02275100 | 1.45056200  |
| H | 4.30772500  | -4.56415400 | 2.10356300  |
| C | 6.99669100  | -6.21263000 | -1.78517700 |
| H | 7.97988400  | -5.72854500 | -1.71194100 |
| H | 6.97842900  | -7.02456600 | -1.05015400 |
| H | 6.92794800  | -6.65689300 | -2.78426100 |
| C | -3.52963800 | -3.74816100 | -2.74454000 |
| H | -3.76949200 | -2.69986900 | -2.95789700 |
| H | -2.46390000 | -3.87578200 | -2.96893300 |
| H | -4.10185800 | -4.37474400 | -3.43547400 |
| C | -2.60261300 | -3.20294400 | 2.21327800  |
| H | -1.54108100 | -3.47613000 | 2.16868900  |
| H | -2.64861100 | -2.11082300 | 2.16591300  |
| H | -2.99149400 | -3.50943000 | 3.18815700  |
| C | -6.14634500 | -6.45112000 | 0.63854500  |
| H | -5.88558700 | -7.04844500 | 1.51938200  |
| H | -7.10661900 | -5.96226900 | 0.85148000  |
| H | -6.30877400 | -7.13641000 | -0.20036700 |
| C | -4.01112500 | 3.74517400  | 0.49925700  |
| H | -4.39168900 | 2.73092500  | 0.66644100  |
| H | -3.02656000 | 3.79236800  | 0.97803100  |
| H | -4.67650000 | 4.44014900  | 1.02037500  |
| C | -1.89160700 | 3.05528000  | -4.06268300 |
| H | -0.86587300 | 3.28786100  | -3.75099500 |
| H | -1.98677400 | 1.96395000  | -4.01887900 |
| H | -2.00612100 | 3.36709300  | -5.10527500 |
| C | -5.66860400 | 6.36924500  | -3.49068300 |
| H | -6.55133800 | 5.87897500  | -3.92275600 |
| H | -6.02579100 | 7.07716400  | -2.73511400 |
| H | -5.19107100 | 6.94150700  | -4.29378200 |
| C | 4.32653400  | 3.82535400  | -1.32727700 |
| H | 4.69319100  | 2.81658900  | -1.55237700 |
| H | 3.31865300  | 3.88337200  | -1.75205400 |
| H | 4.96434200  | 4.54167300  | -1.85397900 |
| C | 2.49365500  | 2.89617100  | 3.31172300  |
| H | 1.45724900  | 3.19636500  | 3.11229600  |
| H | 2.53910000  | 1.81209000  | 3.15704500  |
| H | 2.70734000  | 3.10337500  | 4.36482900  |
| C | 6.18131000  | 6.29981600  | 2.67525500  |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 7.13387800 | 5.82185200  | 2.94078100  |
| H | 6.40730800 | 7.09935000  | 1.96134300  |
| H | 5.78388400 | 6.76009300  | 3.58644700  |
| N | 0.49475400 | -1.08546500 | 2.00830400  |
| N | 0.91440700 | -1.95615300 | 2.64196800  |
| N | 1.20584400 | 1.11729600  | -2.94797000 |
| N | 1.79951900 | 2.01108300  | -3.37606200 |