A Single Site mutation (F429H) Converts the Enzyme CYP 2B4 into a Heme Oxygenase: A QM/MM Study

Dandamudi Usharani,[†] Costantino Zazza,[ξ] Wenzhen Lai,[†,‡] Mukesh Chourasia,[†] Lucy Waskell,[§*] Sason Shaik[†*]

[†]Institute of Chemistry and the Lise-Meitner-Minerva Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, 91904 Jerusalem, Israel

[ξ]Centro di Elaborazionedell'Informazione e del Calcolo (CEIC) dellaScuolaNormaleSuperiore di Pisa Palazzo del Castelletto, via del Castelletto, 11, 56126 Pisa, Italy

[§]University of Michigan and VA Medical Research Center, 2215 Fuller Road, Ann Arbor, MI 48105, USA

Supporting Information

Table of Contents:

1. Computational Details:

(a) Setup of the system: Following the QM/MM protocols developed in previous studies,[1] the initial structure of CYP 2B4 is taken from the PDB file 1SUO. We first added the missing hydrogen atoms and determined the protonation states for all acidic, basic and His residues using Propka 2.0[2] and by careful inspection of the environment. All acidic and basic residues were deprotonated. Except His252, all remaining histidines (His226, His285, His335, His354, His269, His397, His412, His429, His231, His284, His319) were singly protonated. Cpd 0 model was built by replacing the inhibitor in 1SUO by O-OH.

After adding the hydrogen atoms, the protein structure was minimized by the adopted Newton Raphson method implemented in CHARMM.[3] Benzphetamine was then docked into the protein. Subsequently, a 16Å solvent layer was added to the substrate-free and the substrate-docked CYP 2B4 wild type (WT) proteins. These solvated enzymes were then relaxed[1] by a series of energy minimizations and molecular dynamics of the inner solvent layer with the CHARMM force field[4] using CHARMM.

(b) Molecular dynamics: Initially we performed a short molecular dynamics (MD) run of 300ps, for the WT protein (with and without substrate) by keeping the coordinates of Cpd 0 and the outer 8Å water layer fixed. To ascertain the substrate conformations, the MD run of the docked substrate 2B4 was extended to 1ns. The single residue replacement of Phe429 to His from these short MD run snapshots did not impart quantitative differences on the O-OH cleavage mechanisms. Hence, we also performed a long time MD simulations, wherein we propagated the trajectory up to 60 ns forboth WT and the F429H mutant (MT) enzyme without substrate. Here we started from the 46ps snapshot, of the short MD, and gradually heated the protein from 50K to 298K in a canonical (i.e. NVT) ensemble applying an integration step of 2 fs. The trajectories were relaxed all degrees of freedom using Gromacs[5] and Gromos96 force field,[6] we then analyzed two classical trajectories in physiological conditions with the aim to characterize local conformational changes occurring in the WT and MT reaction pocket.

Topology of the benzphetamine substrate: As benzphetamine is not among the predefined residues of the CHARMM library we assigned atom types according to CHARMM conventions, which implicitly define most of the force field terms. The missing parameters assigned from corresponding predefined parameters in CHARMM library.

```
!           H6  H5               H11  H12       H14  H15
!           |    |                  \ /          |    |
!           C6--C5    H31   H1     C11-H13      C14--C15
!         //      \\   |     |   /            //      \\
!   H7--C7        C4---C3---C1--N10---C12---C13       C16--H16
!         \  __   /    |     |       /  \     \  __   /
!           C8-- C9   H32   C2-H23 H19  H20   C18--C17
!           |    |         /  \                |    |
!           H8   H9       H21  H22            H18  H17
  27    0
```

RESI RES 0.00000

GROUP	ATOM H6 HP 0.120436	ATOM H20 HA 0.077670
ATOM C1 CT1 0.424968	ATOM C7 CA -0.134031	ATOM C13 CA 0.028623
ATOM H1 HA 0.033312	ATOM H7 HP 0.122021	ATOM C14 CA -0.121855
ATOM C2 CT3 -0.539023	ATOM C8 CA -0.124445	ATOM H14 HP 0.110189
ATOM H21 HA 0.125235	ATOM H8 HP 0.121176	ATOM C15 CA -0.130338
ATOM H22 HA 0.144348	ATOM C9 CA -0.174008	ATOM H15 HP 0.116771
ATOM H23 HA 0.141227	ATOM H9 HP 0.121387	ATOM C16 CA -0.110086
ATOM C3 CT2 -0.345261	ATOM N10 NC2 -0.349897	ATOM H16 HP 0.121427
ATOM H31 HA 0.111527	ATOM C11 CT3 -0.229267	ATOM C17 CA -0.177701
ATOM H32 HA 0.112546	ATOM H11 HA 0.110700	ATOM H17 HP 0.136327
ATOM C4 CA 0.141398	ATOM H12 HA 0.072437	ATOM C18 CA -0.064566
ATOM C5 CA -0.187924	ATOM H13 HA 0.112071	ATOM H18 HP 0.099941
ATOM H5 HP 0.122743	ATOM C12 CT2 -0.160861	
ATOM C6 CA -0.118449	ATOM H19 HA 0.139233	

BOND N10 C1 N10 C11 N10 C12 C1 H1 C1 C2
BOND C1 C3 C2 H21 C2 H22 C2 H23 C3 H31
BOND C3 H32 C3 C4 C4 C9 C5 H5
BOND C5 C6 C6 H6 C7 H7 C7 C8
BOND C8 H8 C9 H9 C11 H11 C11 H12
BOND C11 H13 C12 H19 C12 H20 C12 C13
BOND C13 C18 C14 H14 C14 C15 C15 H15
BOND C16 H16 C16 C17 C17 H17 C18 H18
DOUBLE C4 C5 C6 C7 C8 C9
DOUBLE C13 C14 C15 C16 C17 C18
IMPH C4 C9 C5 C3 C5 C4 C6 H5 C6 C5 C7 H6
IMPH C7 C6 C8 H7 C8 C7 C9 H8 C9 C4 C8 H9
IMPH C13 C18 C14 C12 C14 C13 C15 H14 C15 C14 C16 H15
IMPH C16 C15 C17 H16 C17 C16 C18 H17 C18 C13 C17 H18
IC C11 N10 C1 C2 1.4599 114.1780 -66.7054 110.6907 1.5245
IC C11 N10 C1 H1 1.4599 114.1780 177.9939 105.1699 1.0955
IC C11 N10 C1 C3 1.4599 114.1780 60.4650 114.9139 1.5446
IC C12 N10 C1 H1 1.4644 113.1008 51.6286 105.1699 1.0955
IC C12 N10 C11 H13 1.4644 109.6850 -177.0580 110.2011 1.0911
IC C1 N10 C11 H11 1.4734 114.1780 172.7082 108.5559 1.0941
IC C1 N10 C11 H12 1.4734 114.1780 -67.3615 113.7243 1.1034
IC C1 N10 C12 C13 1.4734 113.1008 -56.2535 111.9207 1.5066
IC C1 N10 C12 H19 1.4734 113.1008 -175.9631 106.6729 1.0991
IC C1 N10 C12 H20 1.4734 113.1008 67.7559 113.0755 1.1065
IC C3 C1 C2 H23 1.5446 111.3326 63.4023 109.9333 1.0934

```
IC N10  C1   C2   H21   1.4734  110.6907  -47.6900  109.7321  1.0931
IC N10  C1   C2   H22   1.4734  110.6907   73.0695  112.0356  1.0946
IC N10  C1   C3   C4    1.4734  114.9139  165.6758  111.3702  1.5056
IC N10  C1   C3   H31   1.4734  114.9139   44.8708  109.5807  1.0981
IC N10  C1   C3   H32   1.4734  114.9139  -72.3088  109.9556  1.0976
IC C1   C3   C4   C5    1.5446  111.3702  107.5672  121.6285  1.3997
IC C1   C3   C4   C9    1.5446  111.3702  -70.3912  119.7435  1.4037
IC C5   C9   *C4  C3    1.3997  118.5974  178.0201  119.7435  1.5056
IC C3   C4   C5   C6    1.5056  121.6285 -178.3023  120.8560  1.3976
IC C3   C4   C5   H5    1.5056  121.6285    2.0696  119.3755  1.0895
IC C6   C4   *C5  H5    1.3976  120.8560 -179.6280  119.3755  1.0895
IC C3   C4   C9   C8    1.5056  119.7435  178.3467  120.6934  1.3953
IC C3   C4   C9   H9    1.5056  119.7435   -2.0891  119.4182  1.0897
IC C8   C4   *C9  H9    1.3953  120.6934  179.5642  119.4182  1.0897
IC C4   C5   C6   C7    1.3997  120.8560    0.2478  120.0493  1.3962
IC C4   C5   C6   H6    1.3997  120.8560 -179.7411  119.7998  1.0872
IC C7   C5   *C6  H6    1.3962  120.0493 -179.9888  119.7998  1.0872
IC C5   C6   C7   C8    1.3976  120.0493   -0.1717  119.5998  1.3969
IC C5   C6   C7   H7    1.3976  120.0493 -179.9595  120.1440  1.0872
IC C8   C6   *C7  H7    1.3969  119.5998 -179.7878  120.1440  1.0872
IC C6   C7   C8   C9    1.3962  119.5998    0.1778  120.2030  1.3953
IC C6   C7   C8   H8    1.3962  119.5998 -179.8605  120.0247  1.0877
IC C9   C7   *C8  H8    1.3953  120.2030  179.9617  120.0247  1.0877
IC C4   C9   C8   C7    1.4037  120.6934   -0.2588  120.2030  1.3969
IC N10  C12  C13  C14   1.4644  111.9207  126.8237  121.2254  1.3994
IC N10  C12  C13  C18   1.4644  111.9207  -53.4315  119.7779  1.4022
IC C14  C18  *C13 C12   1.3994  118.9963 -179.7504  119.7779  1.5066
IC C12  C13  C14  C15   1.5066  121.2254  179.5693  120.6655  1.3976
IC C12  C13  C14  H14   1.5066  121.2254   -0.0140  119.5147  1.0897
IC C15  C13  *C14 H14   1.3976  120.6655 -179.5833  119.5147  1.0897
IC C12  C13  C18  C17   1.5066  119.7779 -179.7848  120.4528  1.3940
IC C12  C13  C18  H18   1.5066  119.7779    1.3930  118.7870  1.0877
IC C17  C13  *C18 H18   1.3940  120.4528 -178.8222  118.7870  1.0877
IC C13  C14  C15  C16   1.3994  120.6655    0.2852  119.9409  1.3963
IC C13  C14  C15  H15   1.3994  120.6655 -179.8763  119.9840  1.0876
IC C16  C14  *C15 H15   1.3963  119.9409  179.8385  119.9840  1.0876
IC C14  C15  C16  C17   1.3976  119.9409   -0.1791  119.7274  1.3982
IC C14  C15  C16  H16   1.3976  119.9409  179.8021  120.1125  1.0877
IC C17  C15  *C16 H16   1.3982  119.7274  179.9812  120.1125  1.0877
IC C15  C16  C17  C18   1.3963  119.7274   -0.0311  120.2166  1.3940
IC C15  C16  C17  H17   1.3963  119.7274  179.9840  119.9361  1.0881
IC C18  C16  *C17 H17   1.3940  120.2166 -179.9849  119.9361  1.0881
IC C13  C18  C17  C16   1.4022  120.4528    0.1384  120.2166  1.3982
PATCHING FIRS NONE LAST NONE
!BONDS
CT1  NC2   235.000     1.4540 !  trimethylamine,

!ANGLES
CT1  NC2  CT3    53.000   110.90 ! trimethylamine, admjr.
CT1  NC2  CT2    53.000   110.90 ! trimethylamine, admjr.
CT3  NC2  CT2    53.000   110.90 ! trimethylamine, admjr.
```

```
NC2  CT1  HA     51.50    107.50 ! ALLOW   ALI POL !arg, (DS)
NC2  CT1  CT3    67.70    107.50 ! ALLOW   ALI POL !arg, (DS)
NC2  CT1  CT2    67.70    107.50 ! ALLOW   ALI POL !arg, (DS)
NC2  CT2  CA     67.70    107.50 ! ALLOW   ALI POL !arg, (DS)
!DIHEDRALS
HA   CT1  NC2  CT3     2.2500  2   180.00 ! ALLOW   PEP POL ARO
          ! 9.0->2.25 GUANIDINIUM (KK)
HA   CT1  NC2  CT2     2.2500  2   180.00 !  ALLOW   PEP POL ARO
          ! 9.0->2.25 GUANIDINIUM (KK)
CT3  CT1  NC2  CT3     0.0000  6   180.00 !  ALLOW   ALI POL
          ! methylguanidinium, admjr., 3/26/92
CT3  CT1  NC2  CT2     0.0000  6   180.00 !  ALLOW   ALI POL
          ! methylguanidinium, admjr., 3/26/92
CT2  CT1  NC2  CT3     0.0000  6   180.00 !  ALLOW   ALI POL
          ! methylguanidinium, admjr., 3/26/92
CT2  CT1  NC2  CT2     0.0000  6   180.00 !  ALLOW   ALI POL
          ! methylguanidinium, admjr., 3/26/92
!IMPROPER
CA   CACA   CT2    90.0000        0      0.0000 ! ALLOW HEM
          ! Heme (6-liganded): substituents (KK 05/13/91)
CA   CACA   HP     20.0000        0      0.0000 ! ALLOW HEM
end
```

(c) Substrate docking: We used Autodock 4.02[7a] to dock benzphetamine into (a) the WT enzyme (PDB: 1SUO), and (b) the structures of the WT and F429H mutant snapshots from the long MD. Firstly, the substrate and the protein inputs were prepared using ADT tools.[7b] A grid of 70X70X66Å^3 was then defined with the proximal oxygen of Cpd 0 as the grid centre, and 50 docked substrate conformations were searched based on Lamarckian genetic algorithm[8] for all the snapshots. All other docking and grid parameters were maintained at their default settings. The substrate conformation with the lowest docked energy in the cluster was chosen for further QM/MM study. In the case of the long MD run-snapshots of LW2 and LM4, the benzphetamine could not be fitted into pocket because of the hindrance of the Arg98/Phe206 residues.

(d) Snapshots details: From the short MD run, we selected three snapshots labeled as S that signifies short MD: (a) Conf S (without the substrate at 46ps), (b) Conf S1 at 93ps, and (c) Conf S2 at 251ps with the substrate in different orientations. These snapshots were used then for the QM/MM study of the WT enzyme. Subsequently, we replaced the Phe429 residue in these snapshots with His and generated the F429H mutated (MT) snapshots.

In the long MD run (60 ns), we used an essential dynamics analysis, taking into account the Cpd0 complex and its protein host environment (Ala298, Gly299, Thr300, Glu301, Thr302; Pro428, Phe429/His in the F429H mutant, Ser430; Cys436, Leu437, Gly438, Glu439). It is

worth to note that such a technique is largely applied in literature for addressing the mechanical behavior of large and flexible molecular systems in different contexts (see Ref. 6b of the manuscript and the references cited therein). The essential dynamics consists of building the covariance matrix of the atomic positional fluctuations obtained from MD simulations; after its diagonalization, an orthonormal set of eigenvectors then defines a new set of internal (generalized) coordinates along which the fluctuations occur. In particular, the eigenvectors with the largest eigenvalues allow us to define the essential subspace where to search for the relevant conformational transitions. After carrying out essential dynamics analysis, the classical MD trajectories were then projected onto the respective planes defined by the first two essential eigenvectors. In so doing, we find that in the simulated conditions the reactive pocket, modeled in terms of Cpd 0 and its surrounding environment, mainly exhibits either for WT or MT four different conformational basins (see Figure S1). These are labeled as L to signify long MD, W for the WT enzyme and M for the MT, i for the number of the conformational basin.

Looking at the occurrence frequency within the first essential plane we find that the WT enzyme prefers LW3 (most sampled) and LW1 conformations, with the latter resembling the crystallographic structure. Similarly, in the F429H mutant LM3 represents the most recurring conformational rearrangement under physiological condition, and secondly LM1. Interestingly, we have also observed that the less sampled basin, labeled as LM2, spontaneously decays to LM3 and, to a lesser extent, to LM1. This analysis also reveals that LM4 and LW4 conformations always switch to their most sampled (i.e., LM3 and LW3) local counterparts, respectively. We explored without substrate Conf LW1-LW3 for WT, and LM1-LM4 for the MT enzymes and with substrate LW1 and LW3 and LM1-LM3.

(e) The QM region: All the above snapshots were minimized using CHARMM force field in CHARMM before being subjected to subsequent QM/MM study. For the protein delivery pathways Conf S included Cpd 0, the crucial Thr302, Glu301, and three water molecules that may be involved in the proton shuttle. In all other snapshots, we included also the Phe/His429 residues and additional water molecules. For the investigation of electronic structural features of Cpd 0 we considered only the Cpd 0 complex.

(f) The optimized QM/MM region: The MM region that is relaxed during QM/MM geometry optimization comprises of all the residues within 6 Å around Cpd 0 (Arg98, Ile114, Phe115, Trp121, Arg125, Ile179, Leu295, Phe297, Glu301, Thr302, Gln357, Ile363, Val367, Phe429,

Ser430, Arg434, Cys436 (including Cpd 0), Leu437, Glu438, Glu439, Ile441, Ala442, Glu445, and 30 surrounding water molecules). In the substrate containing snapshots, the benzphetamine is also relaxed during optimization.

(g) QM/MM Methodology and software: All QM/MM calculations were performed using ChemShell[9] interfaced QM part: Turbomole and MM part: DL_POLY(MM part).[10] The electronic embedding scheme[11] was used to account for the polarization effect of the QM part induced by the protein environment and to treat QM/MM boundary, we used hydrogen link atoms and the charge shift model.[12] QM subsystem was computed with the unrestricted B3LYP functional with two basis sets; a split valence LACVP basis set (B1) was used for geometry optimization, while the energy was corrected by use of a larger, triple-zeta valence polarized (TZVP)basis set (B2).

(h) Intrinsic Protein Electric Field Calculation: The intrinsic electric field generated by the MM charges of the protein[13] at any position was computed using the built in feature of ChemShell 3.1. We evaluated the electric field at the location of iron and its surrounding ligand atoms and computed their average in magnitude and direction. The vector is projected on the iron atom. The direction of the electric field defined in the Chemshell is from + to –. This procedure is similar to our earlier published report.[13]

(i) References:

1. Schöneboom, J. C.; Lin, H.; Reuter, N.; Thiel, W.; Cohen, S.; Ogliaro, F.; Shaik, S. *J. Am. Chem. Soc.* **2002**, *124*, 8142. (b) Zheng, J.; Altun, A.; Theil, W.; *J. Comput. Chem.* **2007**, *28*, 2147-2158.
2. Bas D. C.; Rogers D. M.; Jensen J. H. *Proteins* **2008**, 73, 765-83.
3. Brooks, B. R.; Burccoleri, R. E.; Olafson, B. D.; States D. J.; Karplus, M. *J. Comput. Chem.* **1983**, *4*, 187-217.
4. CHARMM force field: MacKerell, A. D., Jr.; Bashford, D.; Bellott, M.;Dunbrack, R. L., Jr.; Evanseck, J. D.; Field, M. J.; Fischer, S.; Gao, J.;Guo, H.; Ha, S.; Joseph-McCarthy, D.; Kuchnir, L.; Kuczera, K.; Lau, F.T. K.; Mattos, C.; Michnick, S.; Ngo, T.; Nguyen, D. T.; Prodhom, B.; Reiher, W. E., III; Roux, B.; Schlenkrich, M.; Smith, J. C.; Stote, R.; Straub,J.; Watanabe, M.; Wiorkiewicz-Kuczera, J.; Yin, D.; Karplus, M. *J. Phys.Chem. B* **1998**, *102*, 3586.
5. (a) Berendsen, et al. *Comp. Phys. Comm.***1995**, *91*, 43-56. (b) van der Spoel, et al. *J. Comput. Chem.* **2005**, *26*, 1701-1718. (c) Hess, et al. *J. Chem. Theory. Comput.* **2008**, *4*, 435-447.

6. van Gunsteren, W. F.; Billeter, S. R.; Eising, A. A.; Hunemberger, P. H.; Kruger, P.; Mark, A. E.; Scott, V. R. P.; Tironi, I. G. Biomolecular Simulation: The GROMOS96 Manual and User Guide; vdfHochschlverlag AG an der ETH Zurich: Zurich, 1996.
7. (a) AUTODOCK, 10550, North Torrey Pines Road, La Jolla, CA 92037-1000, USA. (b) Michel F.;Sanner. *J. Mol. Graphics Mod.* **1999**, *17*, 57-61.
8. (a) Morris, G. H.; Goodshell, D. S.; Halliday, R. S.; Huey, R.; Hart, W. E.; Belew, R. K.; Olson, A. J. *J. Comput. Chem.***1998**, *19*, 1639-1662. (b) Hu, X.; Balaz, S.; Shelver, W. H. *J. Mol. Graph. Model.* **2004**, *22*, 293-307.
9. Full reference of Chemshell :Sherwood, P.; De Vries, A. H.; Guest, M. F.; Schreckenbach, G.; Catlow,C. R. A.; French, S. A.; Sokol, A. A.; Bromley, S. T.; Thiel, W.; Turner, A. J.; Billeter,S.; Terstegen, F.; Thiel, S.; Kendrick, J.; Rogers, S. C.; Casci, J.; Watson, M.; King, F.;Karlsen, E.; Sjøvoll, M.; Fahmi, A.; Schäfer, A.; Lennartz, C. *J. Mol. Struct. (THEOCHEM)* **2003**, *632*, 1-28.
10. Smith, W.; Forester, T. *J. Mol. Graph.* **1996**, *14*, 136-141.
11. Bakowies, D.; Thiel, W. *J. Phys. Chem.* **1996**, *100*, 10580-10594.
12.(a) Sherwood, P.; De Vries, A. H.; Collins, S. J.; Greatbanks, S. P.; Burton,N. A.; Vincent, M. A.; Hillier, I. H. *Faraday Discuss.* **1997**, *106*, 79–92. (b) de Vries, A. H.; Sherwood, P.; Collins, S. J.; Rigby, A. M.; Rigutto, M.; Kramer, G. J. *J. Phys. Chem. B* **1999**, *103*, 6133.
13. Cho, K.-B.; Hirao, H.; Chen, H.; Carvajal, M. A.; Cohen, S.; Derat, E.; Thiel, W.; Shaik, S. *J. Phys. Chem. A* **2008**, *112*, 13128–13138.

3. Proton delivery mechanism of 2B4 wild (WT) and F429H mutant (MT) types in various snapshots of the short and long MD runs

Note the small differences in the $\mathbf{TS_{OO}}$ barriers for heterolytic cleavage between the **WT** and **MT** enzymes in the snapshots of the short MD.

Table S1. Relative energies (kcal/mol) of 2B4 **WT** and **MT** short MD snapshots atUB3LYP/CHARMM level (B1- LACVP, B2-def-TZVP basis set).[a]

Without substrate				
Conf S-WT	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	8.7	11.0	11.4	13.8
TShooh	4.3	4.4	6.2	6.3
Cpd I	-15.2	-12.7	-27.5	-25.0
Fe RS	-0.8	1.2	-5.1	-3.1
Conf S -MT	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	11.7	11.7	10.7	10.6
Cpd I	-11.2	-9.7	-28.1	-26.6
With substrate				
Conf S1-WT	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	13.7	12.2	13.0	11.6
IC1	8.2	5.1	8.4	5.2
Cpd I	-24.2	-19.7	-36.6	-32.0
Conf S1-MT	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	13.9	13.4	13.5	12.9
IC1	8.5	6.4	9.2	7.1
Cpd I	-17.7	-14.4	-30.6	-27.3
Conf S2-WT	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	12.6	12.6	12.6	12.7
Cpd I	-26.0	-24.5	-39.3	-37.9
Conf S2-MT	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	12.1	11.4	13.2	12.5
IC1	2.3	0.9	4.8	3.4
Cpd I	-30.2	-23.3	-40.8	-33.9

[a] RC is Cpd 0. TSoo is the O-OH cleavage TS. TShooh is the TS for uncoupling, Fe RS is the resting state. IC1 is an intermediate along the O-OH cleavage coordinate that is observed in some snapshots and has a tiny barrier to collapse to Cpd I. The same terminology is used in other tables.

Note from **Table S2** that the differences in the TS_{OO} barriers for heterolytic cleavage of the WT enzyme are somewhat lower than those in the MT enzyme, during the snapshots of the long MD in the absence of the substrate. But the differences are not sufficiently consistent to suggest a longer living Cpd 0 in the MT.

Table S2. Relative energies (kcal/mol) of 2B4 **WT** and **MT**long MD snapshots in the absence of substrate at UB3LYP /CHARMM level (B1- LACVP, B2-def-TZVP basis set)

Conf LW1	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	12.3	12.2	13.1	13.0
Cpd I	-35.7	-33.4	-39.3	-37.0
Conf LW2	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	9.7	11.1	9.3	10.7
Cpd I	-31.2	-19.4	-35.5	-23.7
Conf LW3	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	13.4	12.1	13.6	12.3
IC1	0.3	4.7	-2.9	1.4
Cpd I	-9.6	-5.2	-19.8	-15.5
RC1	0.0	0.0	0.0	0.0
TShooh	10.5	12.1	13.4	15.1
Fe RS	7.2	9.6	5.5	8.0
Conf LM1	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	12.6	15.9	11.8	15.1
Cpd I	-26.6	-9.3	-33.4	-16.0
Conf LM2	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	14.5	14.4	16.3	16.3
IC1	12.2	12.4	14.2	14.4
Cpd I	-16.0	-7.1	-27.4	-18.6
Conf LM3	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TShooh	9.1	9.1	12.4	12.3
Fe RS	8.5	9.0	9.6	10.0
Conf LM4	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
RC	0.0	0.0	0.0	0.0
TS_{OO}	17.3	17.3	18.0	18.1
Cpd I	-20.4	-9.2	-24.2	-12.9

Table S3. Mulliken spin density distribution for 2B4 **WT** and **MT** short MD snapshots in the presence and absence of substrate at QM/MM B1 level.

Without substrate	Conf S-WT					Conf S-MT		
Spin	RC	TS_{OO}	TShooh	Cpd I	Fe RS	RC	TS_{OO}	Cpd I
Fe	1.07	1.54	1.10	1.42	1.20	1.08	1.48	1.41
Op	0.05	0.10	0.03	0.73	0.01	0.05	0.15	0.74
OH	0.00	-0.42	0.00	0.01	0.00	0.00	-0.42	0.01
SH	-0.04	-0.10	-0.05	-0.25	-0.11	-0.04	-0.09	-0.23
Por	-0.08	-0.12	-0.08	-0.91	-0.10	-0.08	-0.11	-0.93
Glu301	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Thr302	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
rest	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00

With substrate	Conf S1-WT				Conf S2-WT		
Spin	RC	TS_{OO}	IC1	Cpd I	RC	TS_{OO}	Cpd I
Fe	1.00	1.28	1.35	1.26	1.01	1.27	1.23
Op	0.09	0.39	0.77	0.86	0.08	0.40	0.89
OH	0.00	-0.52	-0.77	0.00	0.00	-0.52	0.00
SH	-0.02	-0.06	-0.10	-0.22	-0.03	-0.06	-0.24
Por	-0.07	-0.09	-0.26	-0.90	-0.07	-0.08	-0.88
Glu301	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Thr302	0.00	0.00	0.01	0.00	0.00	-0.01	0.00
Phe429	0.00	0.00	0.00	0.00	0.00	0.00	0.00
rest	0.00	0.00	0.00	0.00	0.00	0.00	0.00

With substrate	Conf S1-MT				Conf S2-MT			
Spin	RC	TS_{OO}	IC1	Cpd I	RC	TS_{OO}	IC1	Cpd I
Fe	1.01	1.34	1.38	1.25	1.01	1.19	1.43	1.19
Op	0.09	0.42	0.74	0.87	0.09	0.42	0.68	0.93
OH	0.00	-0.61	-0.86	0.00	0.00	-0.47	-0.99	0.00
SH	-0.03	-0.07	-0.08	-0.22	-0.03	-0.05	-0.04	-0.23
Por	-0.07	-0.09	-0.19	-0.90	-0.07	-0.08	-0.09	-0.88
Glu301	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Thr302	0.00	0.00	0.01	0.00	0.00	-0.01	0.01	0.00
His429	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
rest	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S4. Mulliken spin density distribution for 2B4 **WT** long MD snapshots in the absence of substrate at QM/MM B1 level.

Without substrate	Conf LW1			Conf LW2		
Spin	RC	TS_{OO}	Cpd I	RC	TS_{OO}	Cpd I
Fe	1.19	1.63	1.54	1.07	1.56	1.53
Op	0.02	0.00	0.62	0.01	-0.08	0.61
OH	0.00	-0.41	0.00	0.00	-0.36	0.00
SH	-0.13	-0.11	-0.26	-0.01	-0.03	-0.33
Por	-0.07	-0.12	-0.91	-0.06	-0.09	-0.82
Glu301	0.00	0.00	0.00	0.00	0.00	0.00
Thr302	0.00	0.00	0.00	0.00	0.00	0.00
Phe429	0.00	0.00	0.00	0.00	0.00	0.00
rest	0.00	0.01	0.01	0.00	0.00	0.01

Without substrate	Conf LW3						
Spin	RC	TS_{OO}	IC1	Cpd I	RC1	TShooh	Fe RS
Fe	1.03	1.35	1.21	1.37	1.05	1.11	1.14
Op	0.01	0.13	0.85	0.73	0.01	-0.01	-0.01
OH	0.00	-0.39	0.03	0.01	0.00	0.00	0.00
SH	0.02	-0.01	-0.18	-0.18	0.01	-0.03	-0.05
Por	-0.06	-0.09	-0.90	-0.92	-0.07	-0.08	-0.09
Glu301	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Thr302	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Phe429	0.00	0.00	0.00	0.00	0.00	0.00	0.00
rest	0.00	0.01	0.00	0.00	0.00	0.00	0.00

Table S5. Mulliken spin density distribution for 2B4 **MT** long MD snapshots in the absence of substrate at QM/MM B1 level.

Without substrate		Conf LM1		Conf LM2			
Spin	RC	TS_{OO}	Cpd I	RC	TS_{OO}	IC1	Cpd I
Fe	1.12	1.67	1.45	1.12	1.81	1.79	1.54
Op	0.03	0.27	0.69	0.03	0.26	0.35	0.60
OH	0.00	-0.61	0.00	0.00	-0.83	-0.98	0.01
SH	-0.08	-0.15	-0.18	-0.08	-0.11	-0.04	-0.21
Por	-0.07	-0.19	-0.96	-0.07	-0.15	-0.13	-0.93
Glu301	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Thr302	0.00	-0.01	0.00	0.00	0.01	0.00	-0.01
His429	0.00	0.00	0.00	0.00	0.00	0.00	0.00
rest	0.00	0.02	0.01	0.00	0.02	0.02	0.01
Without substrate		Conf LM3		Conf LM4			
Spin	RC	TShooh	Fe RS	RC	TS_{OO}	Cpd I	
Fe	1.07	1.08	1.09	1.11	1.25	1.37	
Op	-0.02	-0.01	-0.01	0.02	0.28	0.75	
OH	0.01	0.00	0.00	-0.01	-0.39	0.01	
SH	-0.01	-0.02	-0.02	-0.05	-0.06	-0.30	
Por	-0.06	-0.06	-0.06	-0.07	-0.08	-0.82	
Glu301	0.00	0.00	0.00	0.00	0.00	0.00	
Thr302	0.00	0.00	0.00	0.00	0.00	0.00	
His429	0.00	0.00	0.00	0.00	0.00	-0.01	
rest	0.00	0.00	0.00	0.00	0.00	0.00	

Table S6. Mulliken spin density distribution for 2B4 **WT** and **MT** long MD snapshots in the presence of substrate at QM/MM B1 level.

With substrate	Conf LW1			Conf LW3			
Spin	RC	TS_{OO}	Cpd I	RC	TS_{OO}	IC1	Cpd I
Fe	1.11	1.53	1.46	1.01	1.48	1.58	1.47
Op	0.04	0.04	0.69	0.04	0.25	0.46	0.65
OH	0.00	-0.39	0.01	0.00	-0.61	-0.87	0.01
SH	-0.08	-0.08	-0.30	0.02	-0.03	-0.04	-0.17
Por	-0.06	-0.11	-0.84	0.07	-0.10	-0.15	-0.95
Glu301	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Thr302	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
Phe429	0.00	0.00	0.00	0.00	0.00	0.00	0.00
rest	0.00	0.01	0.00	0.00	0.01	0.01	0.00
With substrate	Conf LM2			Conf LM1			
Spin	RC	TS_{OO}	Cpd I	RC	TS_{OO}	I_H	Heme-OH
Fe	1.05	1.54	1.35	1.07	1.58	1.53	1.56
Op	0.07	0.24	0.77	0.05	0.35	0.59	0.57
OH	-0.01	-0.51	0.01	-0.01	-0.61	-0.52	-0.02
SH	-0.06	-0.08	-0.27	-0.06	-0.09	-0.07	-0.07
Por	-0.06	-0.18	-0.85	-0.06	-0.23	-0.54	-1.04
Glu301	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Thr302	0.00	-0.01	-0.01	0.00	-0.01	0.01	0.00
His429	0.00	0.00	0.00	0.00	0.00	0.00	0.00
rest	0.00	0.00	0.00	0.00	0.01	0.01	0.00
With substrate	Conf LM3						
Spin	RC	TS_{OO}	I_H	Heme-OH			
Fe	1.10	1.50	1.58	1.51			
Op	0.05	0.46	0.54	0.62			
OH	0.00	-0.77	-0.99	-0.02			
SH	-0.08	-0.07	-0.05	-0.09			
Por	-0.06	-013	-0.14	-1.04			
Glu301	0.00	0.00	0.00	0.00			
Thr302	0.00	0.01	0.01	0.00			
His 429	0.00	0.00	0.00	0.00			
rest	0.00	0.01	0.01	0.01			

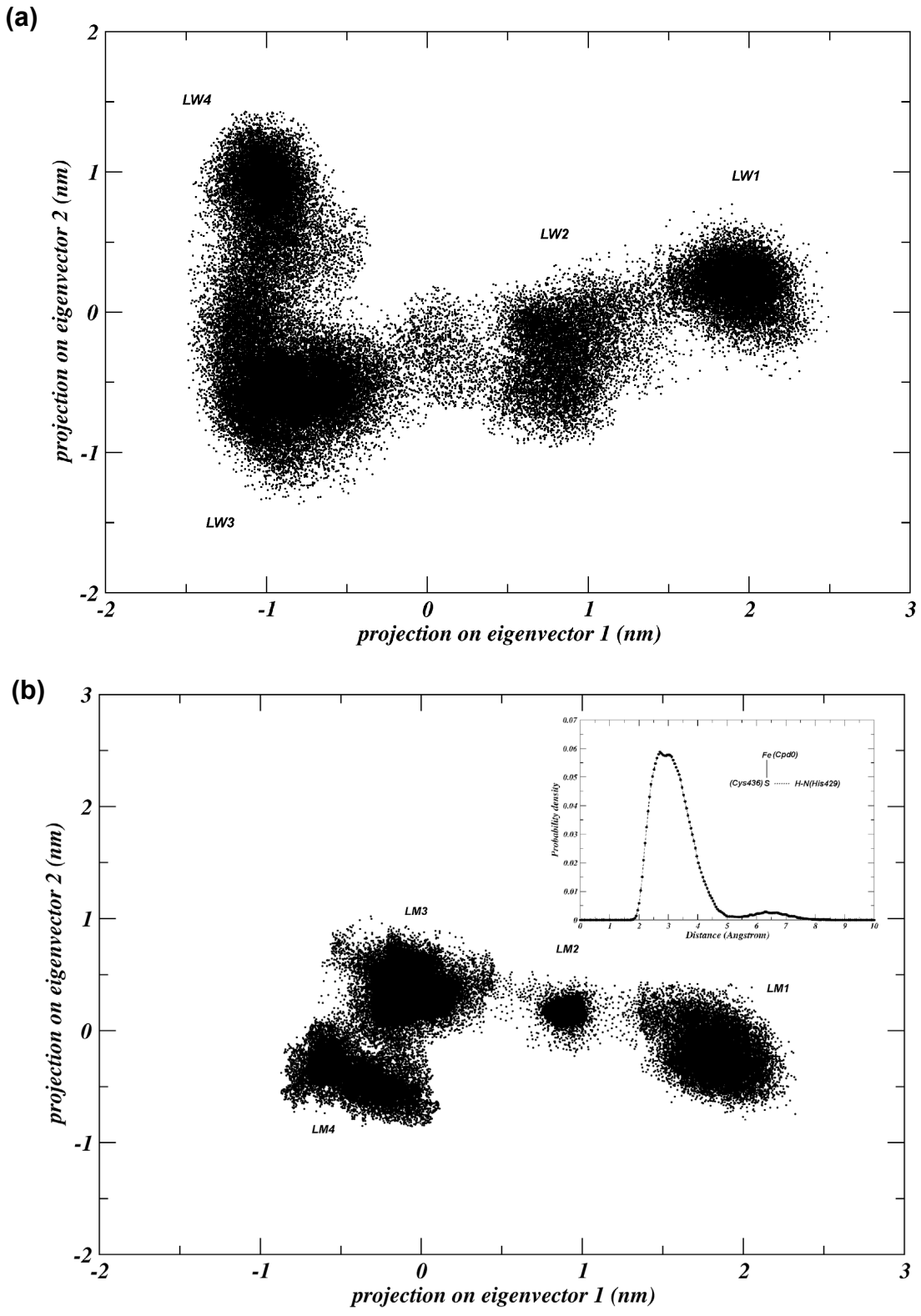

Figure S1. Projection of the trajectory of the active site residues and Cpd 0 species onto the essential plane as obtained from the diagonalization of the related covariance matrix extracted from the 60 ns MD sampling of (a) WT and (b) MT enzymes in physiological conditions (i.e. wet CYP 2B4 enzymes at 298 K) .

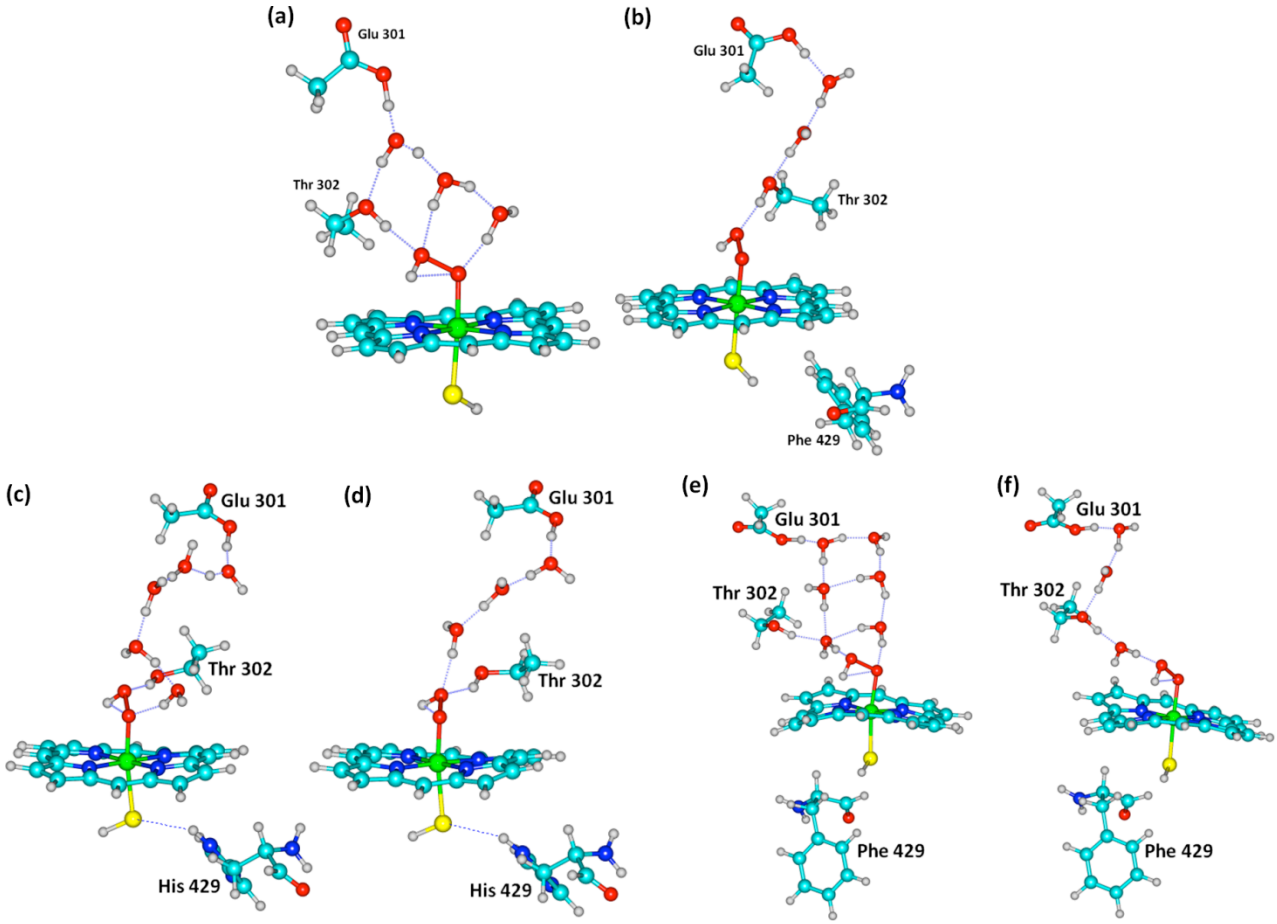

Figure S2. Water cluster arrangement of 2B4 **WT** and **MT** snapshots in Conf S (a), Conf S1 (b), Conf LM2 (c), Conf LM2 with substrate (d), Conf LW3 (e) and Conf LW3 with substrate (e). Only the QM region is shown. Note that water structure of the active site in the presence of substrate prefers the protonation of the distal OH group. On the other hand in the absence of the substrate, waters are close also to the proximal oxygen, thus prepared for uncoupling and H_2O_2 production.

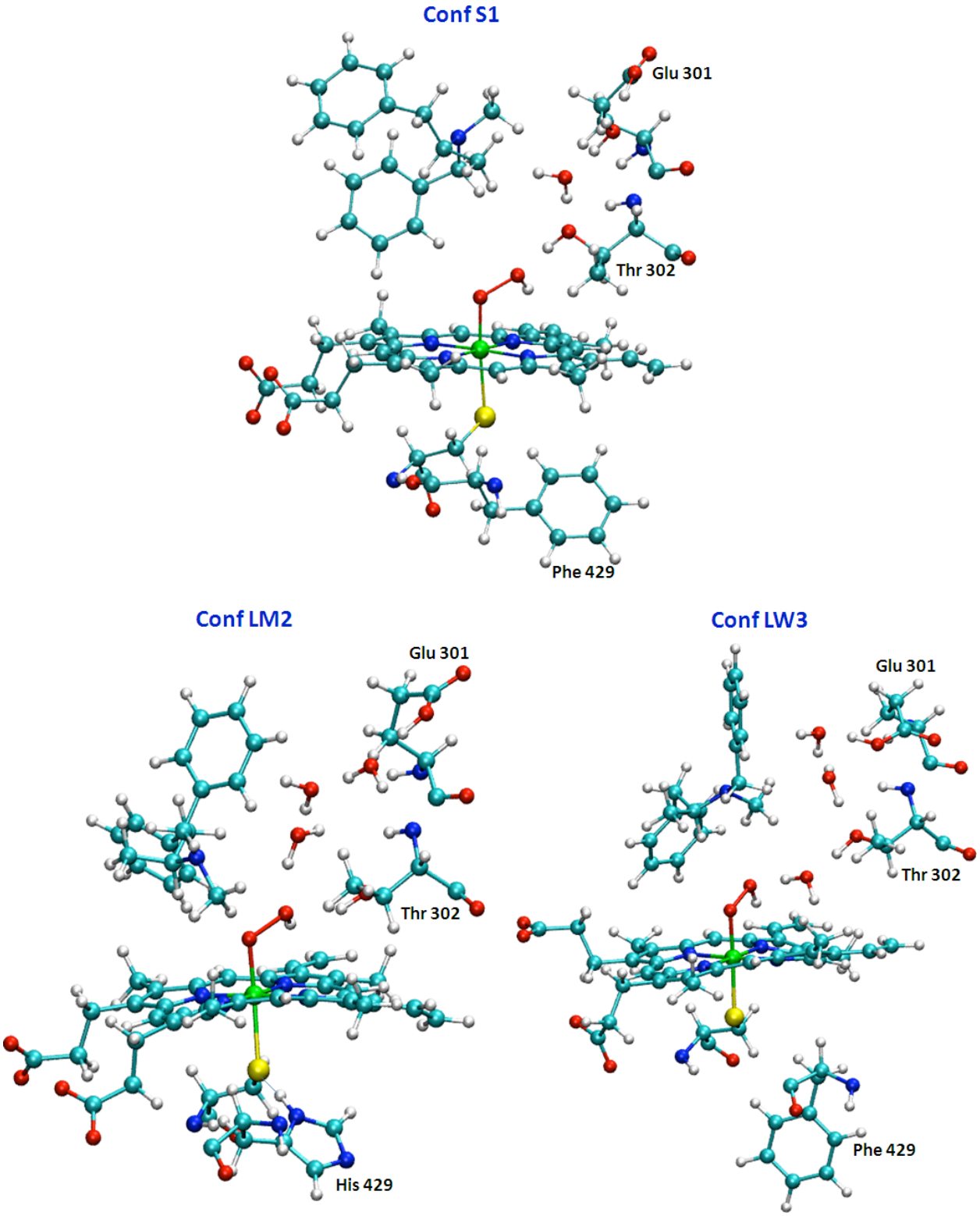

Figure S3. Benzphetamine in the active site region of **WT** and **MT** 2B4 enzymes

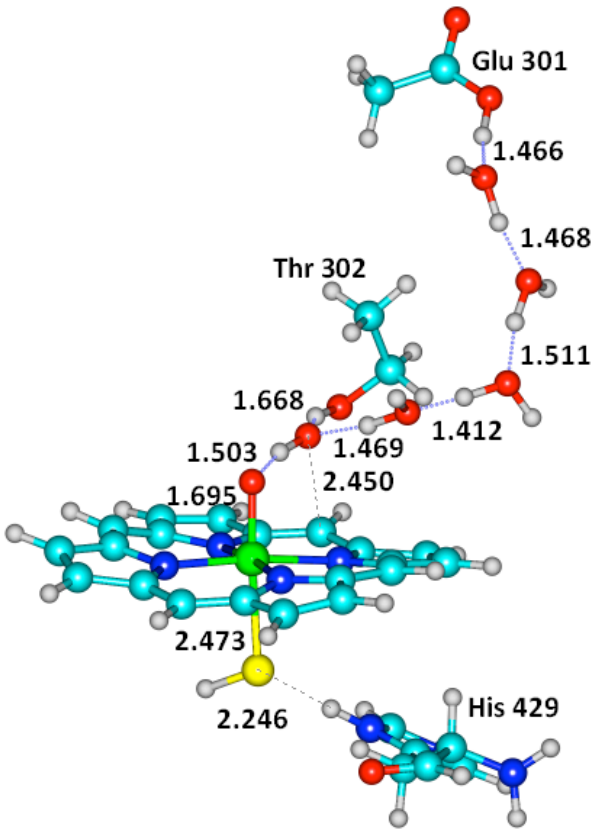

Figure S4. Key bond distances (in Å) in the $\mathbf{I_H}$ LM1 of 2B4 enzyme at (UB3LYP/B1/CHARMM) level. Only the QM region is shown. The spin density of the nascent OH is -0.52 (See Table S6).

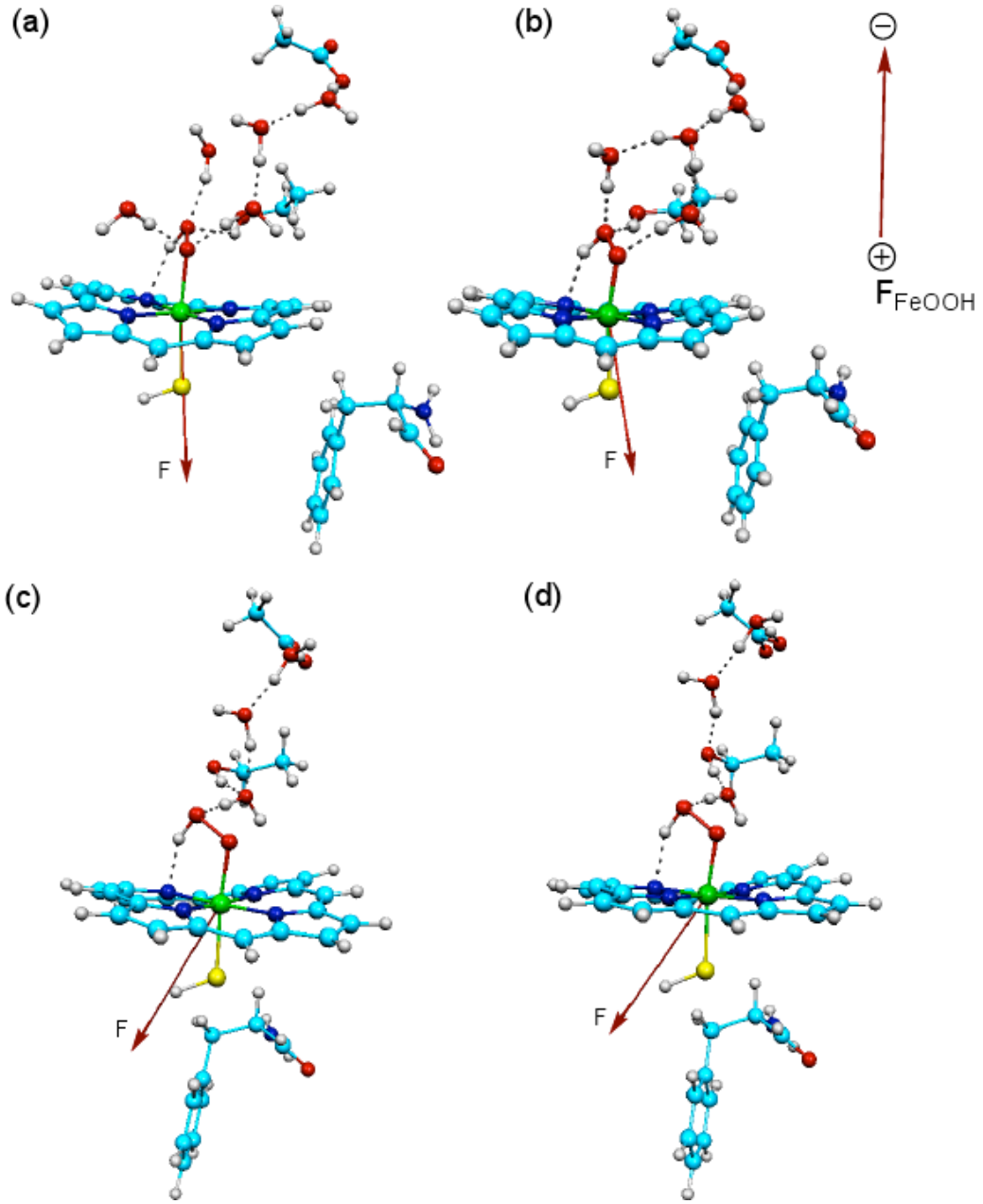

Figure S5: The protein electrical field closest to S-Fe-OOH axis, in various CYP 2B4 **WT** snapshots Conf LW1 (a), Conf LW1 with substrate (b) Conf LW3 (c), Conf LW3 with substrate (d). The conventional direction of electric field is also represented. In all WT cases the negative pole is away from the FeOOH moiety.

Figure S6 shows the intrinsic electric field vector for the mutant conformations LM1-LM3. It is apparent that in LM1 and LM3, in the presence of substrate the intrinsic field switches direction: Now, the negative pole is pointing towards OOH group. This will retard the electron flow from the heme to the nascent OH radical and will retard the PCET step thus preferring meso hydroxylation by the OH•. Note also, that in the unimportant LM2 conformation this change does not occur.

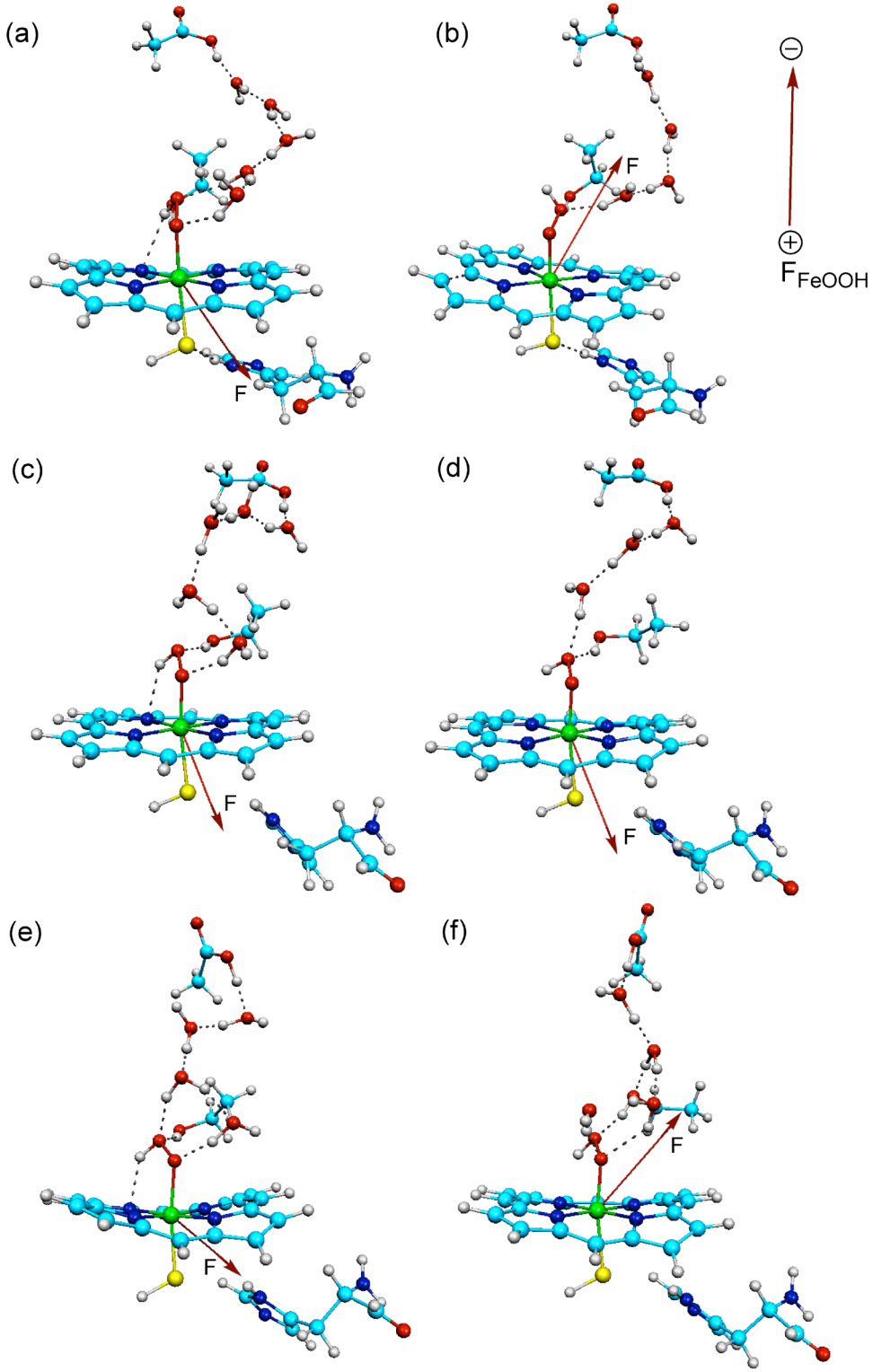

Figure S6: The protein electrical field or its component closest to S-Fe-OOH axis, various CYP 2B4 **MT** snapshots Conf LM1 (a), Conf LM1 with substrate (b) Conf LM2 (c), Conf LM2 with substrate (d) Conf LM3 (e), Conf LM3 with substrate (f) are shown. The conventional direction of electric field is also represented.

3. Cartesian coordinates of the QM region

Conf LW1-^{2}Cpd 0

N -2.444071 -8.312338 -0.168943
H -3.121662 -8.975618 0.163945
C -1.238758 -8.090481 0.605464
H -0.521548 -7.504482 0.005819
C -1.480462 -7.224346 1.914967
H -0.659771 -7.404929 2.623602
H -1.405090 -6.171583 1.628351
C -2.814726 -7.448584 2.581778
C -3.022739 -8.485235 3.506489
H -2.203992 -9.156853 3.749876
C -4.264134 -8.639510 4.134325
H -4.412883 -9.427158 4.865232
C -5.318223 -7.772339 3.828753
H -6.281687 -7.891958 4.310734
C -3.882637 -6.587131 2.279792
H -3.736242 -5.776979 1.572572
C -5.127081 -6.753946 2.890468
H -5.941401 -6.090057 2.628187
C -0.516815 -9.423802 0.895946
O -1.091453 -10.520290 0.742846
S -0.525713 -3.521057 5.371785
H 0.710267 0.540111 3.012833
O 1.900858 -0.978020 2.787590
O 1.184481 0.230626 2.204047
FE 0.814790 -1.972236 4.018546
N 1.697958 -3.655402 3.371063
N -0.642160 -2.118653 2.654233
N -0.037362 -0.256954 4.707838
N 2.259818 -1.832288 5.401821
C 2.639945 -4.436083 4.018741
C 2.975266 -5.604638 3.197365
C 2.254867 -5.472316 2.029243
C 1.408849 -4.286189 2.180585
C -0.652656 -2.999008 1.595355
C -1.888631 -2.845348 0.822192
C -2.625031 -1.839642 1.423876
C -1.818792 -1.395617 2.580302
C -1.318709 0.206212 4.428983
C -1.595748 1.414254 5.198796
C -0.451781 1.709933 5.925739
C 0.509232 0.637286 5.621462
C 2.553819 -0.700530 6.143820
C 3.687015 -0.961639 7.028296
C 3.999115 -2.298658 6.883334
C 3.136708 -2.823369 5.826782
C 3.251404 -4.071048 5.215910
H 3.935603 -4.787465 5.654796
C 0.355373 -3.931832 1.333892
H 0.256251 -4.518532 0.425612
C -2.133864 -0.349515 3.448067
H -3.083976 0.141473 3.283278
C 1.766707 0.449403 6.198477
H 2.139866 1.233747 6.849956
h -0.776239 -2.941534 6.598870
h 3.690351 -6.381588 3.467677
h 2.273034 -6.068681 1.117056
h -2.123636 -3.489959 -0.024753
h -3.561130 -1.352539 1.150898
h -2.531822 1.968760 5.132811
h -0.205400 2.523180 6.608375
h 4.167769 -0.192298 7.632495
h 4.705659 -2.874248 7.481296
h -2.609597 -7.898878 -1.064278
h 0.530028 -9.355143 1.191703

Conf LW1-^{4}Cpd 0

N -2.447651 -8.310790 -0.167305
H -3.126748 -8.973462 0.163892
C -1.244379 -8.091925 0.610768
H -0.526984 -7.501710 0.015628
C -1.490758 -7.231485 1.922356
H -0.663498 -7.401937 2.625791
H -1.430363 -6.177924 1.635065
C -2.817287 -7.469188 2.600109
C -3.001265 -8.488433 3.548903
H -2.170199 -9.141875 3.799875
C -4.232231 -8.643475 4.196731
H -4.359244 -9.413224 4.950545
C -5.301627 -7.797576 3.885038
H -6.256418 -7.918142 4.384028
C -3.900627 -6.629467 2.292418
H -3.773369 -5.832409 1.566952
C -5.135386 -6.798622 2.921388
H -5.959582 -6.148935 2.654357
C -0.520729 -9.425325 0.896860
O -1.093531 -10.521802 0.738037
S -0.656760 -3.602097 5.422810
H 0.815671 0.594816 2.924464
O 2.019534 -0.890658 2.559509
O 1.247967 0.330406 2.081087
FE 0.860315 -1.991161 3.993917
N 1.728568 -3.677663 3.332650
N -0.595127 -2.137120 2.617298
N 0.045174 -0.244037 4.658306
N 2.307147 -1.842932 5.365951
C 2.665721 -4.459024 3.987597
C 2.992326 -5.630929 3.172953
C 2.272459 -5.501798 2.002216
C 1.433972 -4.313303 2.143677
C -0.623901 -3.024821 1.565870
C -1.868728 -2.870279 0.810067
C -2.590015 -1.853328 1.412165
C -1.763965 -1.400260 2.550354
C -1.229187 0.229943 4.367491
C -1.490622 1.451281 5.118672
C -0.341599 1.743815 5.842385
C 0.602445 0.655072 5.559522
C 2.620032 -0.708602 6.100601
C 3.745183 -0.984590 6.985258
C 4.030155 -2.330020 6.854761
C 3.167091 -2.847332 5.797643
C 3.273040 -4.096477 5.188006
H 3.947742 -4.816824 5.633900
C 0.378418 -3.962556 1.299762
H 0.271096 -4.555064 0.396507
C -2.056295 -0.333933 3.400499
H -2.995962 0.173592 3.227459
C 1.856186 0.455089 6.141828
H 2.242671 1.240098 6.783857
h -0.871667 -3.017605 6.654285
h 3.702335 -6.410197 3.449892
h 2.285888 -6.104934 1.094410
h -2.121652 -3.521685 -0.026453
h -3.531518 -1.369966 1.151397
h -2.423750 2.010610 5.051665
h -0.081620 2.564562 6.510854
h 4.237935 -0.222164 7.588556
h 4.723122 -2.911805 7.462535
h -2.610525 -7.898537 -1.063681
h 0.525552 -9.356991 1.194673

Conf LM1-^{2}Cpd 0

N -3.781801 -5.025591 4.007525
H -4.564263 -5.044218 4.655731
C -2.503266 -4.470957 4.495931
H -1.864613 -4.214314 3.637387
C -2.759745 -3.167121 5.306089
H -3.221571 -3.463763 6.257325
H -1.777527 -2.774659 5.579575
N -3.116729 -0.743317 4.718386
H -2.128146 -0.498439 4.875186
C -3.582130 -2.055004 4.713979
C -4.136103 0.087993 4.341671
H -4.020776 1.155150 4.250949
N -5.253779 -0.606460 4.099266
C -4.903438 -1.941384 4.318568
H -5.594111 -2.719280 4.076547
C -1.687157 -5.441241 5.416828
O -1.103349 -4.973796 6.415871
S 0.093084 -0.637594 5.235126
H 2.080538 0.967852 0.963473
O 2.914017 -0.514137 1.948548
O 2.535804 0.158916 0.635166
FE 1.605812 -0.400823 3.323203
N 1.881895 -2.353109 3.645904

N -0.030236 -0.758376 2.142599
N 1.315527 1.606694 3.011894
N 3.164476 -0.006074 4.504160
C 2.677844 -2.954943 4.610853
C 2.499629 -4.409934 4.560427
C 1.634796 -4.667505 3.523595
C 1.219658 -3.370866 2.993855
C -0.461795 -2.010209 1.760858
C -1.742517 -1.918446 1.066155
C -2.097850 -0.581642 1.020476
C -1.011485 0.136561 1.715046
C 0.176768 2.194998 2.484153
C 0.304035 3.644772 2.492992
C 1.544413 3.947402 3.041792
C 2.163521 2.657695 3.383408
C 3.803304 1.220442 4.606800
C 4.929337 1.113745 5.530749
C 4.923565 -0.182030 6.008229
C 3.840607 -0.885401 5.335039
C 3.565620 -2.253604 5.418747
H 4.156334 -2.832816 6.121009
C 0.185154 -3.200230 2.079883
H -0.218221 -4.107168 1.645135
C -0.911446 1.502538 1.948570
H -1.752461 2.126193 1.696297
C 3.374114 2.420587 4.030479
H 4.059964 3.247270 4.151431
h 0.304418 0.432538 6.080407
h 2.927534 -5.125664 5.262349
h 1.275492 -5.612398 3.115987
h -2.281103 -2.791596 0.697914
h -3.008317 -0.238984 0.528846
h -0.488363 4.302724 2.136241
h 1.897977 4.971233 3.163567
h 5.599598 1.938537 5.772692
h 5.544974 -0.605775 6.797126
h -3.851284 -5.641168 3.222534
h -1.675361 -6.510855 5.207418

Conf LM1-^{4}Cpd 0

N -3.786072 -5.026299 4.007590
H -4.573725 -5.041903 4.649054
C -2.513950 -4.464528 4.504114
H -1.878294 -4.187198 3.649397
C -2.793132 -3.178353 5.333384
H -3.269222 -3.495994 6.270759
H -1.819466 -2.782569 5.631695
N -3.155956 -0.747469 4.803806
H -2.169965 -0.507789 5.002859
C -3.613091 -2.060192 4.747627
C -4.166086 0.089283 4.418918
H -4.055995 1.159563 4.364316
N -5.272144 -0.602567 4.120268
C -4.922389 -1.942650 4.312538
H -5.602427 -2.714653 4.026037
C -1.686486 -5.436237 5.414088
O -1.088369 -4.967750 6.403878
S 0.008345 -0.657297 5.327678
H 2.312476 0.893390 0.670895
O 3.164787 -0.490668 1.794663
O 2.762915 0.057265 0.426084
FE 1.603676 -0.380058 3.246597
N 1.880261 -2.343528 3.572584
N -0.012966 -0.757380 2.069629
N 1.323398 1.619681 2.954873
N 3.170367 0.023770 4.434330
C 2.673928 -2.931466 4.548974
C 2.496522 -4.387153 4.515201
C 1.637297 -4.658353 3.475963
C 1.224850 -3.370244 2.928620
C -0.452324 -2.013941 1.696450
C -1.740621 -1.919472 1.025971
C -2.097725 -0.580788 0.988441
C -1.005488 0.138701 1.664559
C 0.177622 2.199454 2.437330
C 0.295172 3.648938 2.452575
C 1.540725 3.958182 2.988597
C 2.172406 2.674016 3.317965
C 3.819787 1.244646 4.529415
C 4.937422 1.135140 5.458712
C 4.913999 -0.156479 5.952518
C 3.834232 -0.857687 5.274004
C 3.554268 -2.224802 5.359981
H 4.135290 -2.800995 6.072264
C 0.190533 -3.205509 2.014398
H -0.220431 -4.113464 1.590298
C -0.912414 1.502875 1.910086
H -1.764127 2.120375 1.680046
C 3.391096 2.442985 3.951231
H 4.076195 3.270606 4.066981
h 0.250113 0.431666 6.140116
h 2.925594 -5.096939 5.222425
h 1.271194 -5.608478 3.086993
h -2.285969 -2.792348 0.667154
h -3.015475 -0.238687 0.510142
h -0.506006 4.303560 2.109573
h 1.886958 4.984154 3.113377
h 5.613983 1.955791 5.697172
h 5.526937 -0.576994 6.749727
h -3.852470 -5.641662 3.222166
h -1.678674 -6.506440 5.207518

WT Conf S –RC

C 1.973546 3.027600 -5.884230
H 1.698849 3.683102 -6.714525
H 1.074564 2.480414 -5.574464
C 3.001385 2.031174 -6.403667
O 3.473827 2.178531 -7.564138
O 3.326104 1.003412 -5.634677
H 2.924488 0.928769 -4.572338
C -1.083558 1.434020 -2.057735
H -1.472737 1.832303 -1.112967
O 0.353193 1.189199 -1.873611
H 0.554963 0.822983 -0.969176
C -1.818964 0.146895 -2.437339
H -1.391497 -0.294791 -3.345054
H -2.887918 0.326535 -2.603836
H -1.739121 -0.574236 -1.621018
S -1.010929 -0.924642 5.076340
H 1.100222 1.166635 1.465517
O 1.543336 -0.744887 1.579056
O 1.379144 0.549121 0.746176
FE 0.434073 -0.873923 3.167615
N 0.428774 -2.863031 2.807438
N -1.224070 -0.598039 2.017011
N 0.496071 1.145204 3.527112
N 2.072571 -1.168398 4.373705
C 1.318705 -3.826920 3.262112
C 0.980145 -5.131899 2.703468
C -0.152557 -4.955620 1.943001
C -0.494547 -3.535859 2.024574
C -1.939510 -1.600794 1.390028
C -3.096937 -1.040898 0.685501
C -3.079244 0.327350 0.900444
C -1.896989 0.580569 1.754839
C -0.440351 2.092196 3.123733
C -0.137420 3.389073 3.718689
C 0.981350 3.222437 4.520953
C 1.359504 1.802722 4.399413
C 2.723003 -0.187284 5.097562
C 3.780741 -0.779616 5.923239
C 3.755077 -2.139421 5.694933
C 2.690953 -2.365423 4.714135
C 2.346635 -3.593077 4.168300
H 2.916815 -4.455801 4.490632
C -1.600926 -2.951816 1.417854
H -2.264796 -3.639352 0.905068
C -1.515436 1.815805 2.280538
H -2.162049 2.653732 2.047330
C 2.396800 1.165596 5.083316
H 3.020460 1.786601 5.720051
O 3.545721 0.299078 -1.092062
H 3.676130 -0.654287 -0.777308
H 2.927323 0.686031 -0.427929
O 3.405816 -1.938220 0.173106
H 3.206802 -2.859036 -0.061915
H 2.710699 -1.571485 0.811021
O 2.526355 0.802442 -3.349278
H 1.586822 0.872508 -3.032795
H 3.092052 0.581467 -2.507825
h -1.346052 -2.209098 5.453448
h 1.550477 -6.042290 2.887797
h -0.715302 -5.688827 1.365254
h -3.774105 -1.658707 0.095738
h -3.735454 1.130056 0.564115
h -0.735763 4.279662 3.526587
h 1.530759 3.914336 5.159305
h 4.460669 -0.206608 6.553657

h 4.393315 -2.908059 6.130724
h 2.308619 3.646370 -5.051814
h -1.168657 2.191685 -2.836688

Conf S -TSoo

C 1.988692 2.994370 -5.849001
H 1.714959 3.636292 -6.691113
H 1.088743 2.450913 -5.531644
C 3.032504 1.982182 -6.339711
O 3.491568 2.140855 -7.518943
O 3.354599 0.994748 -5.551241
H 2.888751 0.853419 -4.224157
C -1.076447 1.426380 -2.117755
H -1.467106 1.806776 -1.165457
O 0.354224 1.185673 -1.936929
H 0.586585 0.886611 -0.993755
C -1.810476 0.143876 -2.516895
H -1.400379 -0.270139 -3.445354
H -2.884420 0.317565 -2.656735
H -1.701935 -0.598589 -1.723262
S -0.977518 -0.934971 5.076098
H 1.135384 1.304565 1.189815
O 1.566263 -0.720789 1.776484
O 1.385371 0.702162 0.457493
FE 0.496026 -0.847281 3.123776
N 0.433293 -2.856150 2.823000
N -1.185143 -0.602907 2.013521
N 0.499172 1.128515 3.584294
N 2.087987 -1.156454 4.407122
C 1.331490 -3.814176 3.279901
C 0.998717 -5.118582 2.720698
C -0.132609 -4.948586 1.955610
C -0.480011 -3.533153 2.032221
C -1.902368 -1.602087 1.379043
C -3.050114 -1.035026 0.667987
C -3.031120 0.330726 0.890738
C -1.853187 0.578623 1.751657
C -0.411184 2.076995 3.140857
C -0.101437 3.380839 3.717680
C 1.001913 3.216326 4.539780
C 1.367408 1.791999 4.446524
C 2.739300 -0.182310 5.136494
C 3.798657 -0.780203 5.952728
C 3.770843 -2.137796 5.713978
C 2.704158 -2.356947 4.734891
C 2.358478 -3.581389 4.185118
H 2.929509 -4.444761 4.502810
C -1.576693 -2.952478 1.408647
H -2.235946 -3.637760 0.888072
C -1.474250 1.808778 2.282233
H -2.107976 2.650907 2.033458
C 2.406965 1.166593 5.132707
H 3.029851 1.790272 5.766342
O 3.495982 0.241800 -1.040355
H 3.650002 -0.703397 -0.713935
H 2.822520 0.614192 -0.388194
O 3.367435 -1.952817 0.280419
H 3.151251 -2.878818 0.083400
H 2.698829 -1.563847 0.924299
O 2.550612 0.722100 -3.213710
H 1.588033 0.851488 -2.963692
H 3.118571 0.470747 -2.281043
h -1.333907 -2.214070 5.451917
h 1.568909 -6.028665 2.906966
h -0.690989 -5.685347 1.378149
h -3.723589 -1.648937 0.069981
h -3.688505 1.133634 0.557198
h -0.681874 4.277188 3.499238
h 1.548322 3.913653 5.174790
h 4.480887 -0.210529 6.583680
h 4.406352 -2.910407 6.146723
h 2.316801 3.627327 -5.024516
h -1.171347 2.199376 -2.880341

Conf S -TShooh

C 1.970622 3.029501 -5.894627
H 1.696895 3.685232 -6.725237
H 1.070083 2.485188 -5.583394
C 2.997382 2.027199 -6.412915
O 3.472221 2.183928 -7.574538
O 3.310779 1.000254 -5.647536
H 2.900555 0.906369 -4.538460
C -1.062566 1.445544 -2.057808
H -1.446962 1.847899 -1.112647
O 0.378409 1.211002 -1.883842
H 0.587036 0.844035 -0.982280
C -1.791416 0.153186 -2.428564
H -1.375999 -0.280857 -3.345496
H -2.864657 0.321995 -2.576787
H -1.689994 -0.571245 -1.617722
S -1.019054 -0.929457 5.074894
H 1.065179 1.178219 1.497429
O 1.552792 -0.705831 1.569143
O 1.369059 0.590689 0.762321
FE 0.425739 -0.880670 3.180768
N 0.428366 -2.866260 2.807632
N -1.227553 -0.603446 2.021680
N 0.483682 1.139446 3.538957
N 2.064579 -1.173366 4.379999
C 1.318226 -3.830956 3.262873
C 0.980585 -5.135210 2.703554
C -0.151198 -4.959128 1.941783
C -0.493574 -3.539706 2.022729
C -1.938984 -1.605812 1.388489
C -3.094668 -1.046423 0.681613
C -3.082385 0.320814 0.902880
C -1.905027 0.574428 1.762981
C -0.456456 2.085952 3.139838
C -0.150732 3.382929 3.731816
C 0.973140 3.217735 4.527833
C 1.350842 1.798507 4.407115
C 2.716351 -0.191213 5.102232
C 3.777116 -0.782790 5.923865
C 3.752543 -2.142651 5.694898
C 2.686105 -2.369851 4.717850
C 2.345348 -3.597096 4.169241
H 2.918070 -4.458946 4.488941
C -1.597781 -2.956027 1.412421
H -2.257462 -3.643027 0.893897
C -1.530942 1.808548 2.296180
H -2.179278 2.645120 2.063272
C 2.390090 1.161581 5.088212
H 3.016546 1.783138 5.721503
O 3.594987 0.279090 -1.172576
H 3.572564 -0.672953 -0.734126
H 3.095320 0.827761 -0.532353
O 3.217229 -1.742241 0.226232
H 3.081189 -2.683743 0.036262
H 2.458478 -1.317680 0.904078
O 2.533369 0.768680 -3.371442
H 1.596896 0.860370 -3.053227
H 3.113703 0.525612 -2.522843
h -1.347645 -2.215631 5.451896
h 1.550058 -6.045930 2.888913
h -0.712545 -5.693010 1.363534
h -3.768625 -1.663956 0.087895
h -3.740265 1.122108 0.566447
h -0.747911 4.274448 3.540410
h 1.526569 3.911187 5.161006
h 4.459781 -0.209751 6.551290
h 4.391243 -2.911103 6.130341
h 2.307260 3.647974 -5.062622
h -1.157842 2.200245 -2.838458

Conf S -CpdI

C 1.836171 3.330454 -6.269875
H 1.771401 4.133967 -7.013112
H 0.824150 2.947987 -6.086300
C 2.649812 2.173315 -6.874803
O 3.326019 2.415337 -7.937398
O 2.539170 1.010954 -6.315734
H 2.649515 0.723759 -4.654854
C -1.046168 1.410556 -2.268807
H -1.320473 1.799143 -1.276304
O 0.354264 1.052172 -2.256387
H 0.777997 1.068580 -1.313602
C -1.898732 0.182861 -2.610095
H -1.590749 -0.236881 -3.573960
H -2.972046 0.407748 -2.651443
H -1.746613 -0.576696 -1.839321
S -1.108267 -0.898517 5.174251
H 1.568963 0.577592 0.676646
O 1.611565 -0.701585 1.983509
O 1.665462 1.151712 -0.114833
FE 0.552409 -0.893518 3.261427
N 0.424955 -2.888268 2.980115
N -1.115722 -0.632591 2.103336
N 0.545115 1.081527 3.741071

N 2.048375 -1.208138 4.615970
C 1.331564 -3.850413 3.406108
C 1.014254 -5.143814 2.822119
C -0.120419 -4.971123 2.063159
C -0.473655 -3.562831 2.165314
C -1.852599 -1.609702 1.464055
C -2.973439 -1.027664 0.726478
C -2.921247 0.338819 0.932755
C -1.748676 0.563026 1.803779
C -0.288278 2.041802 3.214073
C 0.031429 3.359087 3.754700
C 1.066601 3.187355 4.656258
C 1.387787 1.751776 4.618441
C 2.715963 -0.241784 5.347591
C 3.799824 -0.837444 6.120770
C 3.786897 -2.189082 5.844273
C 2.700169 -2.401884 4.895324
C 2.365977 -3.614923 4.305287
H 2.964258 -4.473539 4.584332
C -1.550488 -2.967464 1.519390
H -2.207630 -3.642916 0.982609
C -1.333768 1.783115 2.323587
H -1.919404 2.647505 2.034412
C 2.388986 1.110062 5.342378
H 3.008861 1.730282 5.981819
O 3.856476 0.592257 -1.391122
H 3.871098 -0.332089 -1.038122
H 2.599437 1.070601 -0.527732
O 3.106941 -1.764346 -0.134428
H 2.383716 -1.989948 -0.749478
H 2.702638 -1.454946 0.714385
O 2.604494 0.578551 -3.664277
H 1.673955 0.655230 -3.334323
H 3.519707 0.607946 -2.352067
h -1.447887 -2.183396 5.545856
h 1.589413 -6.053444 2.994842
h -0.664992 -5.701526 1.464813
h -3.643950 -1.630826 0.114370
h -3.553890 1.153288 0.579954
h -0.467873 4.264066 3.408609
h 1.585456 3.885148 5.313480
h 4.499616 -0.272658 6.736703
h 4.434365 -2.962201 6.257963
h 2.209136 3.763590 -5.341782
h -1.172308 2.212001 -2.996709

Conf S –Fe RS

C 1.798276 3.326209 -6.259630
H 1.735602 4.116771 -7.015953
H 0.783551 2.957987 -6.063478
C 2.592396 2.150417 -6.848331
O 3.274866 2.363141 -7.908676
O 2.458103 0.993998 -6.271792
H 2.403833 0.781680 -4.686612
C -1.025580 1.468472 -2.090462
H -1.395510 1.873741 -1.139859
O 0.420487 1.250546 -1.949766
H 0.653789 0.918337 -1.045300
C -1.749900 0.168311 -2.441929
H -1.343969 -0.265733 -3.362607
H -2.826714 0.327429 -2.575264
H -1.628422 -0.551911 -1.629866
S -1.052464 -0.920361 5.095979
H 0.887966 1.283312 1.482110
O 1.609863 -0.504705 1.544094
O 1.261531 0.742162 0.745632
FE 0.403365 -0.855873 3.237796
N 0.433342 -2.830740 2.824662
N -1.224670 -0.577807 2.047004
N 0.445144 1.157805 3.606581
N 2.050175 -1.145738 4.416301
C 1.320348 -3.799750 3.286253
C 0.986389 -5.102019 2.724460
C -0.141955 -4.926162 1.956822
C -0.485247 -3.508416 2.035298
C -1.926849 -1.577368 1.396023
C -3.073020 -1.016898 0.676556
C -3.068669 0.348194 0.907319
C -1.909211 0.599352 1.790213
C -0.505863 2.100669 3.222104
C -0.212761 3.392772 3.830085
C 0.936119 3.236852 4.591923
C 1.321441 1.820734 4.461880
C 2.703344 -0.162302 5.139217
C 3.769958 -0.752287 5.951927
C 3.745418 -2.113160 5.723955
C 2.677313 -2.341962 4.751903
C 2.340311 -3.568755 4.200123
H 2.909971 -4.431306 4.523172
C -1.585020 -2.926296 1.416947
H -2.238924 -3.611514 0.889404
C -1.559678 1.827487 2.351079
H -2.197562 2.664886 2.097907
C 2.372740 1.189124 5.128402
H 3.006328 1.813295 5.751550
O 4.067596 -0.134647 -2.035838
H 3.504170 -0.931760 -0.926874
H 4.577145 0.632785 -1.723546
O 3.106271 -1.484301 -0.134877
H 3.149141 -2.441836 -0.273039
H 2.278130 -0.993169 0.832621
O 2.420764 0.693533 -3.675299
H 1.561416 0.835787 -3.209297
H 3.393105 0.171271 -2.801459
h -1.363836 -2.213435 5.463882
h 1.556184 -6.012800 2.908516
h -0.698990 -5.661750 1.376573
h -3.732449 -1.631941 0.064231
h -3.722912 1.148963 0.562645
h -0.848297 4.270247 3.710920
h 1.507841 3.938446 5.199349
h 4.455738 -0.179570 6.576240
h 4.388549 -2.880960 6.153991
h 2.186747 3.771580 -5.343770
h -1.142435 2.218927 -2.872273

MT Conf S –RC

C 1.886526 3.000914 -5.764405
H 1.553152 3.616554 -6.604169
H 1.019902 2.436889 -5.396254
C 2.929174 2.020340 -6.282957
O 3.356844 2.168884 -7.471207
O 3.298439 1.038829 -5.492191
H 2.809984 0.890946 -4.160362
C -1.075800 1.515050 -1.930606
H -1.451864 1.902205 -0.978681
O 0.368979 1.279715 -1.759949
H 0.569115 0.922147 -0.854614
C -1.787348 0.222064 -2.332500
H -1.382992 -0.172760 -3.272360
H -2.865456 0.377625 -2.455493
H -1.660524 -0.529686 -1.550926
S -1.204592 -0.998757 5.011104
H 1.190649 1.189008 1.576046
O 1.553404 -0.736204 1.664733
O 1.451000 0.571655 0.848360
FE 0.385132 -0.872382 3.198684
N 0.397046 -2.852871 2.808813
N -1.231909 -0.572290 2.007241
N 0.463840 1.146470 3.564505
N 1.994897 -1.179596 4.447909
C 1.288061 -3.818407 3.258199
C 0.967533 -5.112260 2.665997
C -0.155337 -4.927131 1.890169
C -0.507815 -3.512656 1.993566
C -1.946780 -1.568143 1.365967
C -3.106707 -0.998303 0.673161
C -3.089612 0.367241 0.907643
C -1.902800 0.610916 1.756811
C -0.449156 2.109133 3.136439
C -0.126504 3.411207 3.711842
C 0.984163 3.233874 4.522673
C 1.333774 1.803358 4.431762
C 2.655468 -0.201244 5.167716
C 3.725216 -0.797089 5.973772
C 3.705681 -2.155176 5.729703
C 2.629228 -2.377267 4.762119
C 2.301845 -3.594763 4.184633
H 2.883494 -4.456174 4.489109
C -1.604717 -2.918786 1.375509
H -2.258615 -3.597489 0.838505
C -1.520077 1.842946 2.288665
H -2.143431 2.689625 2.034369
C 2.346785 1.156542 5.141156
H 2.974726 1.776012 5.775025
O 3.473338 0.128511 -1.015119
H 3.581659 -0.832407 -0.699792
H 2.923864 0.560840 -0.314755

O 3.321342 -2.063487 0.280107
H 3.084197 -2.984851 0.086544
H 2.653219 -1.646349 0.918783
O 2.476787 0.758045 -3.151951
H 1.540221 0.963277 -2.844514
H 3.051074 0.443543 -2.287069
h -1.460889 -2.293583 5.413700
h 1.544718 -6.020579 2.838858
h -0.708915 -5.648244 1.288825
h -3.787909 -1.605379 0.076932
h -3.746382 1.172726 0.579142
h -0.703899 4.310951 3.499375
h 1.543841 3.926628 5.151099
h 4.418283 -0.227995 6.593334
h 4.362859 -2.920256 6.143025
h 2.232280 3.662456 -4.970124
h -1.188006 2.283762 -2.695170

Conf S -TSoo

C 1.899198 3.013054 -5.796328
H 1.567198 3.636646 -6.631111
H 1.031741 2.445048 -5.435656
C 2.944130 2.036131 -6.322124
O 3.362615 2.191110 -7.515375
O 3.321429 1.057592 -5.536483
H 2.830400 0.889982 -4.147470
C -1.056463 1.518497 -1.970508
H -1.411738 1.906132 -1.009667
O 0.382092 1.275673 -1.833758
H 0.625408 0.973026 -0.899815
C -1.786782 0.230219 -2.357819
H -1.404206 -0.165553 -3.306424
H -2.866938 0.389496 -2.457732
H -1.640479 -0.522792 -1.580838
S -1.184796 -1.010144 5.007882
H 1.189526 1.317452 1.305615
O 1.513268 -0.751577 1.804896
O 1.436339 0.736605 0.553913
FE 0.414926 -0.861736 3.129448
N 0.365519 -2.870104 2.807475
N -1.237939 -0.598790 1.991012
N 0.431125 1.113225 3.585424
N 1.986128 -1.184197 4.440925
C 1.263905 -3.829400 3.259764
C 0.945619 -5.125762 2.674014
C -0.175099 -4.946689 1.893418
C -0.531597 -3.534788 1.989340
C -1.956053 -1.595010 1.349699
C -3.113202 -1.022255 0.657488
C -3.092402 0.342675 0.890167
C -1.906789 0.585038 1.739116
C -0.465326 2.073953 3.131578
C -0.136202 3.382293 3.690336
C 0.973122 3.210724 4.502664
C 1.314365 1.777325 4.432838
C 2.651625 -0.210181 5.157751
C 3.722693 -0.808722 5.956685
C 3.697230 -2.166520 5.712658
C 2.615785 -2.384980 4.749764
C 2.281200 -3.602553 4.179073
H 2.864731 -4.462993 4.480889
C -1.623191 -2.944832 1.361530
H -2.274342 -3.623358 0.822125
C -1.526932 1.813955 2.272568
H -2.141837 2.662113 2.006391
C 2.337689 1.144323 5.135172
H 2.971039 1.768968 5.757449
O 3.496662 0.210623 -1.016729
H 3.618431 -0.737790 -0.692551
H 2.869544 0.616961 -0.345036
O 3.316982 -1.995923 0.314464
H 3.020933 -2.889789 0.073871
H 2.663815 -1.585394 0.960549
O 2.500966 0.749103 -3.161067
H 1.554084 0.956814 -2.869139
H 3.085073 0.466209 -2.263414
h -1.465292 -2.297794 5.417304
h 1.524644 -6.033073 2.846012
h -0.723797 -5.671886 1.292514
h -3.793861 -1.625832 0.057100
h -3.747949 1.148241 0.559429
h -0.709781 4.283246 3.472716
h 1.538266 3.910285 5.118532
h 4.419890 -0.239202 6.571200
h 4.352306 -2.933772 6.125291
h 2.239580 3.667305 -4.993730
h -1.183379 2.292858 -2.727029

Conf S -CpdI

C 1.850863 3.226362 -6.106360
H 1.608990 3.980126 -6.863632
H 0.924022 2.699580 -5.844445
C 2.807613 2.213129 -6.737690
O 3.318216 2.491750 -7.878786
O 2.996913 1.089510 -6.111730
H 2.708806 0.787877 -4.451826
C -1.063543 1.463138 -2.138107
H -1.342246 1.823264 -1.139438
O 0.339425 1.110259 -2.126910
H 0.769549 1.172124 -1.194416
C -1.896611 0.237230 -2.534407
H -1.585885 -0.133434 -3.518105
H -2.973019 0.448692 -2.565524
H -1.734361 -0.557042 -1.801774
S -1.372000 -0.992170 5.102220
H 1.556509 0.655980 0.795507
O 1.555067 -0.695087 2.068142
O 1.673612 1.248428 0.021793
FE 0.453278 -0.900757 3.302556
N 0.331477 -2.893802 2.991238
N -1.173655 -0.609062 2.105537
N 0.446241 1.070024 3.800741
N 1.932387 -1.238391 4.681167
C 1.234995 -3.863770 3.415244
C 0.924320 -5.146632 2.804529
C -0.197166 -4.956143 2.027560
C -0.551481 -3.549648 2.150251
C -1.914191 -1.580040 1.449840
C -3.022118 -0.979006 0.707381
C -2.948973 0.387497 0.911647
C -1.777392 0.595438 1.787493
C -0.361007 2.047193 3.261092
C -0.037983 3.359606 3.815522
C 1.031204 3.179429 4.674787
C 1.314761 1.733966 4.660346
C 2.619379 -0.275476 5.396951
C 3.722095 -0.872281 6.138945
C 3.706303 -2.224194 5.854049
C 2.598310 -2.431921 4.930475
C 2.267800 -3.635817 4.317235
H 2.884318 -4.489320 4.568699
C -1.616893 -2.936606 1.492111
H -2.262343 -3.601984 0.929133
C -1.349637 1.816566 2.301869
H -1.836637 2.700876 1.912320
C 2.311890 1.083804 5.378641
H 2.959455 1.703877 5.990426
O 3.859449 0.635787 -1.243581
H 3.900019 -0.280355 -0.876562
H 2.605110 1.141255 -0.389204
O 3.127469 -1.750156 0.017524
H 2.424197 -1.904269 -0.642048
H 2.694822 -1.434622 0.850166
O 2.576701 0.576583 -3.485317
H 1.642710 0.719698 -3.180128
H 3.494796 0.628779 -2.197710
h -1.616795 -2.284856 5.518615
h 1.506049 -6.056557 2.951817
h -0.728506 -5.668528 1.396488
h -3.705874 -1.567657 0.095798
h -3.571428 1.210288 0.560036
h -0.622467 4.254505 3.601980
h 1.612987 3.884904 5.267999
h 4.441484 -0.308205 6.732548
h 4.372700 -2.993138 6.244828
h 2.201701 3.746316 -5.214942
h -1.202292 2.284538 -2.841041

WT-Conf S1 –RC

C 2.855527 3.380949 -5.250311
H 2.048109 2.661831 -5.100134
H 3.786079 2.794764 -5.256956
C 2.733215 4.034702 -6.611606
O 3.097912 5.184936 -6.921188
O 2.226623 3.225098 -7.574440
H 1.729053 2.380684 -7.241154
C -0.866901 1.609147 -2.031624
H -1.167262 1.981077 -1.047245

O 0.566237 1.257462 -1.962764
H 0.807049 0.892633 -1.053771
C -1.678155 0.375213 -2.435529
H -1.325869 -0.017861 -3.396330
H -2.748811 0.593959 -2.514542
H -1.563700 -0.397368 -1.671966
N -5.169558 -5.639488 2.547888
H -6.055130 -5.949745 2.924640
C -4.140273 -5.135485 3.476138
H -3.453340 -4.452454 2.956248
C -4.825685 -4.326759 4.625436
H -4.022907 -4.004579 5.296248
H -5.458002 -5.012756 5.203533
C -5.655825 -3.150547 4.152133
C -5.047084 -2.005586 3.606210
H -3.965142 -1.943699 3.530045
C -5.822831 -0.925292 3.169034
H -5.327639 -0.059334 2.742108
C -7.219996 -0.968617 3.276868
H -7.821307 -0.121927 2.954858
C -7.058568 -3.182252 4.255221
H -7.541732 -4.053963 4.690571
C -7.837490 -2.101025 3.822647
H -8.918254 -2.139982 3.917887
C -3.267785 -6.273356 4.105265
O -2.414973 -5.974938 4.964482
S -1.018476 -0.817408 5.021796
H 0.948151 1.279545 1.316281
O 1.468788 -0.629755 1.497984
O 1.220178 0.622935 0.635813
Fe 0.436805 -0.757047 3.073345
N 0.411377 -2.758266 2.720184
N -1.226202 -0.458790 1.958274
N 0.496272 1.244010 3.500275
N 2.096999 -1.083049 4.266933
C 1.287088 -3.735431 3.168538
C 0.924215 -5.038125 2.612227
C -0.192573 -4.834439 1.834209
C -0.515553 -3.408359 1.928707
C -1.938270 -1.445810 1.309056
C -3.063600 -0.859496 0.572511
C -3.011369 0.510161 0.772034
C -1.854669 0.735682 1.668479
C -0.428722 2.205074 3.111316
C -0.132947 3.486867 3.748202
C 1.001187 3.301856 4.523828
C 1.373325 1.881127 4.369264
C 2.778747 -0.111839 4.972364
C 3.873854 -0.711777 5.742427
C 3.829179 -2.070200 5.509660
C 2.720409 -2.284705 4.575083
C 2.341612 -3.510272 4.046028
H 2.917019 -4.376911 4.349564
C -1.612472 -2.801797 1.322312
H -2.277571 -3.475051 0.793602
C -1.469034 1.961795 2.215636
H -2.060636 2.821584 1.928242
C 2.437552 1.237072 5.004325
H 3.085259 1.851029 5.624658
O 0.833346 1.190596 -6.765519
H 0.956664 0.850653 -5.808638
H 0.854299 0.488403 -7.441632
O 1.257796 0.419121 -4.333307
H 1.008331 0.774044 -3.405334
H 1.886991 -0.316579 -4.221688
h -1.349919 -2.104838 5.391952
h 1.466974 -5.963859 2.803262
h -0.748333 -5.546359 1.223991
h -3.743811 -1.460368 -0.031088
h -3.623165 1.328461 0.392351
h -0.771416 4.364185 3.644580
h 1.571135 3.979424 5.159539
h 4.593176 -0.142580 6.331203
h 4.467496 -2.846372 5.931768
h -5.087079 -5.625941 1.551402
h -3.480988 -7.287028 3.766030
h 2.900602 4.030986 -4.376533
h -0.941965 2.419769 -2.756416

Conf S1 –TSoo

C 2.866219 3.377042 -5.250016
H 2.074263 2.640790 -5.098096
H 3.809046 2.810203 -5.261401
C 2.733387 4.028570 -6.610949
O 3.098764 5.179098 -6.921660
O 2.227291 3.218760 -7.571768
H 1.725331 2.370507 -7.243136
C -0.860960 1.600583 -2.086036
H -1.130815 1.963653 -1.088659
O 0.559650 1.224422 -2.063102
H 0.849452 0.915373 -1.125651
C -1.705203 0.384837 -2.478543
H -1.389405 -0.002700 -3.453992
H -2.774908 0.618394 -2.519775
H -1.573056 -0.398669 -1.728970
N -5.170206 -5.639279 2.547931
H -6.055650 -5.950702 2.924073
C -4.141743 -5.136254 3.477110
H -3.455230 -4.451815 2.958646
C -4.827820 -4.329416 4.627487
H -4.025244 -4.008210 5.299067
H -5.460087 -5.016474 5.204289
C -5.657902 -3.152510 4.155857
C -5.049001 -2.005264 3.614866
H -3.966879 -1.942120 3.541915
C -5.824660 -0.924459 3.178810
H -5.329482 -0.056354 2.756133
C -7.222071 -0.969527 3.282774
H -7.823476 -0.122787 2.961260
C -7.060885 -3.185697 4.255569
H -7.544337 -4.059011 4.687289
C -7.839713 -2.104008 3.824026
H -8.920658 -2.144240 3.916259
C -3.268423 -6.274156 4.105193
O -2.414894 -5.975328 4.963613
S -1.020476 -0.820760 5.028323
H 0.785594 1.333159 1.065253
O 1.472456 -0.661358 1.675309
O 1.308200 0.809814 0.417308
Fe 0.463573 -0.739886 3.066089
N 0.397617 -2.760810 2.748693
N -1.205667 -0.459469 1.963923
N 0.492431 1.229748 3.548760
N 2.090996 -1.081726 4.308125
C 1.276250 -3.735467 3.198532
C 0.920300 -5.036160 2.634541
C -0.193617 -4.833708 1.852091
C -0.520702 -3.410352 1.948479
C -1.925243 -1.445398 1.317642
C -3.049577 -0.854511 0.585516
C -2.989552 0.514925 0.781468
C -1.830723 0.737157 1.674831
C -0.416103 2.192267 3.138152
C -0.116474 3.478870 3.765847
C 1.015319 3.295477 4.542931
C 1.379079 1.871002 4.403296
C 2.784212 -0.114879 5.005369
C 3.883872 -0.719363 5.762986
C 3.829236 -2.077343 5.530749
C 2.710812 -2.287018 4.607102
C 2.328438 -3.510776 4.077136
H 2.904351 -4.377820 4.377594
C -1.611627 -2.802241 1.334998
H -2.276954 -3.472863 0.803766
C -1.444156 1.958622 2.226909
H -2.025776 2.821867 1.931105
C 2.446578 1.233657 5.035466
H 3.102633 1.850979 5.642832
O 0.837745 1.185870 -6.801350
H 0.953496 0.825685 -5.845905
H 0.855389 0.499480 -7.493709
O 1.220516 0.374471 -4.398415
H 0.974899 0.743897 -3.465776
H 1.829485 -0.376799 -4.279885
h -1.362581 -2.104377 5.402004
h 1.466069 -5.960843 2.822060
h -0.744699 -5.544113 1.235894
h -3.736228 -1.452741 -0.013398
h -3.598073 1.335355 0.401121
h -0.752444 4.357706 3.659759
h 1.587777 3.976679 5.172473
h 4.611572 -0.152851 6.344004
h 4.466842 -2.856751 5.947941
h -5.087258 -5.625886 1.551481
h -3.481655 -7.287771 3.765806
h 2.905937 4.027333 -4.376168
h -0.944502 2.424947 -2.794210

Conf S1 –IC1

C 2.741751 3.375854 -5.345399
H 1.852481 2.745935 -5.243428
H 3.597020 2.685116 -5.345075
C 2.726751 4.062542 -6.699713
O 3.053800 5.243665 -6.935490
O 2.358469 3.263507 -7.723940
H 1.931471 2.329675 -7.481613
C -0.802202 1.563341 -2.312244
H -0.903967 1.853136 -1.260567
O 0.584141 1.130560 -2.543928
H 1.043113 0.937172 -1.655363
C -1.743671 0.408889 -2.657654
H -1.581005 0.080428 -3.689746
H -2.798247 0.676531 -2.533795
H -1.540871 -0.426879 -1.983304
N -5.169423 -5.637878 2.547852
H -6.053331 -5.951397 2.925971
C -4.139817 -5.133707 3.474771
H -3.451978 -4.451811 2.954018
C -4.822830 -4.316660 4.618791
H -4.021283 -4.006685 5.296889
H -5.470718 -4.993418 5.190394
C -5.629236 -3.127014 4.137284
C -4.995864 -1.995361 3.591302
H -3.912436 -1.953291 3.521795
C -5.747877 -0.901194 3.147917
H -5.233404 -0.045215 2.723093
C -7.146168 -0.916305 3.250835
H -7.728676 -0.057729 2.925838
C -7.032678 -3.131384 4.233093
H -7.534934 -3.992807 4.667324
C -7.788253 -2.035322 3.795986
H -8.869950 -2.052402 3.887845
C -3.266975 -6.270933 4.105694
O -2.414565 -5.969854 4.964345
S -1.045191 -0.791359 5.078904
H 1.561132 0.324720 0.730841
O 1.585266 -0.401928 1.892553
O 1.691459 0.853340 -0.200385
Fe 0.595748 -0.714626 3.219939
N 0.512204 -2.716183 2.876303
N -1.044290 -0.426010 2.040282
N 0.584792 1.250495 3.749398
N 2.158507 -1.052545 4.509696
C 1.391295 -3.691343 3.325978
C 1.042298 -4.987942 2.753448
C -0.074895 -4.789153 1.974974
C -0.400718 -3.367088 2.064726
C -1.762072 -1.399643 1.377574
C -2.853858 -0.793891 0.610132
C -2.778932 0.574406 0.808514
C -1.639434 0.781973 1.732706
C -0.287863 2.212715 3.278468
C -0.000817 3.506163 3.902679
C 1.111433 3.327642 4.707702
C 1.462046 1.897572 4.602054
C 2.856190 -0.085897 5.209240
C 3.969922 -0.692077 5.939239
C 3.925354 -2.045425 5.680840
C 2.797775 -2.254941 4.773378
C 2.432505 -3.473381 4.218503
H 3.009024 -4.342116 4.513895
C -1.472524 -2.760792 1.418934
H -2.128333 -3.430365 0.872737
C -1.265581 1.993701 2.311866
H -1.809973 2.871317 1.985207
C 2.521988 1.261805 5.247563
H 3.181344 1.880441 5.849800
O 1.159874 1.120137 -7.229987
H 1.096073 0.663889 -6.318147
H 1.044352 0.555230 -8.020222
O 0.992485 0.104583 -4.877951
H 0.843032 0.566906 -3.971104
H 1.443578 -0.742190 -4.713936
h -1.376469 -2.083829 5.431212
h 1.592255 -5.911359 2.934875
h -0.639183 -5.502795 1.374674
h -3.535370 -1.388845 0.002154
h -3.378999 1.400253 0.426462
h -0.648508 4.376720 3.799268
h 1.680380 4.016310 5.332283
h 4.701070 -0.131376 6.521565
h 4.564858 -2.829818 6.085597
h -5.087039 -5.625510 1.551342
h -3.478369 -7.284887 3.766168
h 2.832623 4.001008 -4.457148
h -0.933972 2.452857 -2.928251

Conf S1 -CpdI

C 2.693520 3.404852 -5.422171
H 1.786968 2.796028 -5.324994
H 3.527014 2.687102 -5.419014
C 2.696174 4.067841 -6.808812
O 2.955449 5.299445 -6.990560
O 2.438014 3.240972 -7.794577
H 1.702097 1.908838 -7.481331
C -0.794766 1.553644 -2.342612
H -0.869471 1.839491 -1.291159
O 0.587959 1.112791 -2.515488
H 1.253430 1.238128 -0.890735
C -1.749488 0.406306 -2.687091
H -1.608296 0.090314 -3.725437
H -2.802991 0.669962 -2.538481
H -1.523057 -0.439873 -2.032404
N -5.170961 -5.638543 2.548316
H -6.054461 -5.955923 2.924648
C -4.145547 -5.135915 3.477121
H -3.463422 -4.445062 2.961177
C -4.833514 -4.329199 4.626298
H -4.034921 -4.019198 5.308210
H -5.478132 -5.012563 5.192849
C -5.645955 -3.141744 4.149044
C -5.019277 -2.007752 3.600855
H -3.936104 -1.963660 3.528381
C -5.775164 -0.915410 3.160269
H -5.267180 -0.055888 2.734255
C -7.172876 -0.935221 3.268318
H -7.759657 -0.079567 2.944364
C -7.048777 -3.150586 4.249812
H -7.547159 -4.013803 4.684493
C -7.808823 -2.056635 3.815202
H -8.889980 -2.077748 3.908842
C -3.261220 -6.268571 4.101226
O -2.399430 -5.957963 4.948093
S -1.087414 -0.782877 5.114286
H 1.473750 0.685088 0.623704
O 1.711928 -0.556231 2.015783
O 1.333584 1.478720 0.064730
Fe 0.653203 -0.760172 3.272151
N 0.522698 -2.762236 2.957194
N -0.967532 -0.457340 2.081296
N 0.652613 1.197358 3.795870
N 2.170559 -1.109958 4.606586
C 1.400429 -3.746724 3.399738
C 1.055075 -5.035264 2.818046
C -0.058968 -4.829480 2.035553
C -0.375497 -3.409856 2.131718
C -1.705111 -1.421282 1.415472
C -2.783277 -0.805787 0.639327
C -2.682049 0.560662 0.823941
C -1.542075 0.751918 1.746787
C -0.199275 2.167708 3.321313
C 0.067424 3.454135 3.961823
C 1.167829 3.274297 4.780005
C 1.515585 1.847754 4.669840
C 2.888070 -0.151160 5.295483
C 4.005563 -0.754240 6.009330
C 3.956750 -2.107471 5.743363
C 2.819126 -2.310899 4.856978
C 2.444632 -3.523837 4.287720
H 3.031397 -4.391501 4.566286
C -1.429961 -2.782148 1.466277
H -2.085583 -3.443001 0.908576
C -1.151672 1.959760 2.321443
H -1.648292 2.851171 1.958810
C 2.562829 1.203164 5.317425
H 3.227832 1.820565 5.913984
O 1.143005 1.053900 -7.331484
H 0.925493 0.495555 -5.922717
H 0.983117 0.601926 -8.188960
O 0.811799 0.114901 -4.977510
H 0.728545 0.806896 -3.464311
H 1.410022 -0.643439 -4.851664
h -1.415038 -2.076106 5.467228
h 1.600318 -5.961314 3.000276
h -0.617924 -5.540788 1.427542
h -3.461077 -1.392408 0.019223

h -3.261826 1.394441 0.428040
h -0.585035 4.320242 3.851266
h 1.734170 3.966276 5.403295
h 4.741716 -0.194787 6.586528
h 4.596155 -2.893502 6.145087
h -5.087486 -5.625693 1.551903
h -3.473898 -7.283919 3.766707
h 2.800866 4.017118 -4.526809
h -0.934516 2.449354 -2.947790

MT-Conf S1 –RC

C 2.867322 3.397346 -5.232230
H 2.060937 2.676182 -5.086219
H 3.801700 2.817354 -5.260448
C 2.732715 4.094821 -6.572801
O 3.246448 5.189512 -6.873102
O 2.042844 3.413692 -7.520151
H 1.528177 2.561837 -7.232354
C -0.854994 1.661381 -2.074813
H -1.110563 2.021119 -1.073466
O 0.569683 1.260109 -2.063152
H 0.825572 0.886182 -1.168631
C -1.718439 0.465164 -2.481979
H -1.418575 0.091098 -3.467276
H -2.783701 0.718346 -2.511633
H -1.602756 -0.332348 -1.745062
N -5.163106 -5.584652 2.434035
H -6.038500 -5.920908 2.813230
C -4.142728 -5.071288 3.365298
H -3.404657 -4.460154 2.825505
C -4.817542 -4.146474 4.436787
H -5.623582 -4.716187 4.915387
H -4.067748 -3.960474 5.211514
N -4.646753 -1.730105 3.611182
H -3.659241 -1.568730 3.807096
C -5.388948 -2.880317 3.886954
C -5.495463 -0.809816 3.041423
H -5.160210 0.154680 2.702695
N -6.735135 -1.295119 2.932756
C -6.672855 -2.581997 3.469238
H -7.551547 -3.202724 3.541859
C -3.333575 -6.208619 4.074955
O -2.540953 -5.905923 4.989015
S -1.167697 -0.865796 4.953061
H 0.960614 1.283219 1.280060
O 1.493970 -0.615261 1.510323
O 1.230067 0.608976 0.615291
FE 0.407317 -0.759919 3.043981
N 0.373928 -2.761798 2.704584
N -1.232382 -0.453012 1.906066
N 0.470953 1.241732 3.472799
N 2.043308 -1.089180 4.270085
C 1.236202 -3.742726 3.171900
C 0.872611 -5.046080 2.617927
C -0.232038 -4.838763 1.822270
C -0.547277 -3.409787 1.904586
C -1.944002 -1.438327 1.251733
C -3.067301 -0.849370 0.515667
C -3.019987 0.518628 0.726173
C -1.863320 0.742603 1.621483
C -0.448693 2.206204 3.078276
C -0.144055 3.491078 3.703971
C 0.995249 3.307783 4.472065
C 1.356373 1.883004 4.330242
C 2.736312 -0.116358 4.963462
C 3.834973 -0.715722 5.727574
C 3.788189 -2.074264 5.497177
C 2.668798 -2.290311 4.576875
C 2.282713 -3.517150 4.058520
H 2.854665 -4.382169 4.372350
C -1.631213 -2.797081 1.279911
H -2.292703 -3.465407 0.741020
C -1.488549 1.964763 2.182863
H -2.084555 2.823253 1.902463
C 2.410982 1.236310 4.977667
H 3.064401 1.850930 5.591025
O 0.671721 1.340310 -6.913890
H 0.765546 0.943446 -5.978481
H 0.633133 0.675948 -7.627402
O 1.072233 0.405967 -4.506184
H 0.920522 0.776635 -3.567908
H 1.480590 -0.473171 -4.417995
h -1.431885 -2.156273 5.364427
h 1.413109 -5.972833 2.810429
h -0.779565 -5.548217 1.201822
h -3.752623 -1.448213 -0.084156
h -3.642329 1.336482 0.363032
h -0.783857 4.367028 3.597060
h 1.575555 3.988135 5.095308
h 4.556294 -0.146063 6.313452
h 4.443571 -2.846958 5.899029
h -5.074477 -5.588566 1.437993
h -3.516223 -7.226142 3.729481
h 2.931348 4.035542 -4.350940
h -0.922505 2.494167 -2.774796

Conf S1 –TSoo

C 2.859350 3.390983 -5.240046
H 2.048550 2.674643 -5.091994
H 3.788861 2.802885 -5.268514
C 2.730571 4.088049 -6.582009
O 3.249284 5.182068 -6.879046
O 2.043205 3.411119 -7.532861
H 1.522463 2.555771 -7.255312
C -0.843742 1.650146 -2.159717
H -1.068919 1.987216 -1.142515
O 0.567845 1.232305 -2.196717
H 0.882471 0.941295 -1.267260
C -1.733818 0.473044 -2.568412
H -1.464829 0.119505 -3.569947
H -2.797872 0.733860 -2.562268
H -1.598590 -0.342973 -1.855150
N -5.164485 -5.584629 2.434061
H -6.040652 -5.919714 2.812498
C -4.146004 -5.071868 3.366762
H -3.408023 -4.459164 2.828834
C -4.821930 -4.148508 4.438335
H -5.627233 -4.718060 4.918359
H -4.072419 -3.960714 5.212918
N -4.646917 -1.733587 3.611197
H -3.661093 -1.571106 3.815347
C -5.391819 -2.882451 3.886656
C -5.491654 -0.815071 3.032495
H -5.155292 0.149690 2.695164
N -6.730889 -1.300049 2.918377
C -6.672753 -2.585111 3.459564
H -7.552374 -3.204890 3.528767
C -3.335136 -6.208771 4.075190
O -2.539878 -5.905084 4.986672
S -1.179045 -0.869272 4.962215
H 0.797673 1.353224 0.958403
O 1.504063 -0.607759 1.693050
O 1.367823 0.884773 0.308068
FE 0.478230 -0.752050 3.018539
N 0.378827 -2.770343 2.729278
N -1.177002 -0.467603 1.897759
N 0.489546 1.213337 3.532157
N 2.053121 -1.094902 4.318126
C 1.244786 -3.747955 3.198722
C 0.885573 -5.050741 2.643263
C -0.215390 -4.846186 1.841608
C -0.533522 -3.420337 1.921410
C -1.900627 -1.448664 1.246438
C -3.015937 -0.850845 0.508807
C -2.957380 0.516478 0.717421
C -1.799305 0.732567 1.612587
C -0.408200 2.178154 3.104400
C -0.109868 3.467122 3.727742
C 1.020141 3.287594 4.507624
C 1.376114 1.859720 4.382508
C 2.754141 -0.129306 5.011481
C 3.855026 -0.735185 5.761272
C 3.801548 -2.091795 5.522920
C 2.676171 -2.300377 4.609839
C 2.287885 -3.523946 4.087447
H 2.858167 -4.390199 4.399493
C -1.608251 -2.808475 1.284013
H -2.272798 -3.474819 0.747095
C -1.424686 1.949799 2.180595
H -2.002646 2.813531 1.882139
C 2.430787 1.221536 5.032167
H 3.086452 1.837201 5.640979
O 0.664171 1.342705 -6.965134
H 0.765776 0.924700 -6.034352
H 0.615845 0.695429 -7.694176
O 1.064999 0.377337 -4.593705
H 0.904440 0.748607 -3.646830
H 1.502293 -0.487687 -4.509360

h -1.451876 -2.157123 5.376159
h 1.425899 -5.977435 2.836533
h -0.760149 -5.557112 1.220410
h -3.704689 -1.443564 -0.093165
h -3.576891 1.336991 0.355438
h -0.750770 4.342299 3.621078
h 1.598513 3.972284 5.127909
h 4.581623 -0.169705 6.344672
h 4.453213 -2.869219 5.921683
h -5.074857 -5.588559 1.438107
h -3.518632 -7.226413 3.730515
h 2.929261 4.030221 -4.359958
h -0.922764 2.505068 -2.831230

Conf S1 –IC1

C 2.774437 3.368212 -5.266182
H 1.909018 2.715708 -5.123477
H 3.655011 2.709317 -5.285655
C 2.700876 4.062246 -6.615067
O 3.221183 5.162037 -6.890772
O 2.062799 3.378682 -7.592622
H 1.525371 2.513867 -7.354512
C -0.802688 1.626322 -2.341262
H -0.895184 1.907159 -1.286045
O 0.572568 1.164419 -2.576572
H 1.053428 1.023279 -1.688448
C -1.769683 0.496899 -2.699901
H -1.624361 0.189111 -3.740615
H -2.818158 0.781590 -2.562530
H -1.579177 -0.355578 -2.043525
N -5.164488 -5.583306 2.434081
H -6.039830 -5.919404 2.813668
C -4.146512 -5.067810 3.365503
H -3.406299 -4.459468 2.825464
C -4.819661 -4.133923 4.429514
H -5.633419 -4.693588 4.906793
H -4.072769 -3.949955 5.207472
N -4.613673 -1.725884 3.589036
H -3.630198 -1.567827 3.807510
C -5.373194 -2.864491 3.868190
C -5.444467 -0.801766 2.999109
H -5.094795 0.157622 2.659381
N -6.688600 -1.273438 2.881665
C -6.648126 -2.555399 3.431491
H -7.535032 -3.164806 3.498572
C -3.336733 -6.203232 4.078785
O -2.543371 -5.896904 4.990930
S -1.216823 -0.845232 5.021067
H 1.554813 0.506728 0.594319
O 1.595138 -0.462460 1.896801
O 1.698850 1.087916 -0.237239
FE 0.566294 -0.750176 3.185345
N 0.449492 -2.751242 2.854244
N -1.052442 -0.435766 1.992781
N 0.572023 1.209184 3.727496
N 2.095608 -1.107040 4.508431
C 1.310187 -3.739636 3.314378
C 0.951204 -5.031527 2.736785
C -0.150435 -4.814931 1.939247
C -0.460849 -3.389392 2.032418
C -1.783980 -1.400364 1.327133
C -2.864156 -0.779813 0.556432
C -2.775597 0.586346 0.761214
C -1.632995 0.778251 1.683212
C -0.286167 2.182339 3.254768
C 0.006737 3.469979 3.884783
C 1.122737 3.285125 4.680824
C 1.453332 1.851664 4.580920
C 2.810822 -0.148128 5.203528
C 3.928116 -0.762207 5.916438
C 3.875580 -2.113187 5.648084
C 2.734305 -2.312822 4.758249
C 2.350998 -3.528222 4.208242
H 2.926440 -4.398364 4.500720
C -1.521211 -2.765234 1.381039
H -2.186848 -3.423684 0.833455
C -1.251849 1.983956 2.272413
H -1.777607 2.874133 1.947733
C 2.498708 1.204579 5.234774
H 3.167156 1.818799 5.831267
O 0.634221 1.327512 -7.171827
H 0.726170 0.813691 -6.282532
H 0.551267 0.756761 -7.963032
O 0.911124 0.171762 -4.912963
H 0.816964 0.598156 -3.977649
H 1.056101 -0.784041 -4.824949
h -1.478374 -2.140334 5.419374
h 1.489434 -5.961484 2.919963
h -0.700357 -5.513886 1.309077
h -3.554660 -1.362997 -0.052803
h -3.376062 1.419272 0.395508
h -0.654858 4.331895 3.798411
h 1.709271 3.977616 5.284563
h 4.664219 -0.206726 6.497523
h 4.529087 -2.896718 6.031586
h -5.074859 -5.588204 1.438132
h -3.517707 -7.221262 3.733922
h 2.880766 4.006046 -4.388726
h -0.920621 2.527799 -2.942508

Conf S1 –CpdI

C 2.759185 3.416110 -5.342270
H 1.902011 2.748060 -5.213110
H 3.647187 2.765147 -5.375149
C 2.670099 4.112569 -6.709959
O 3.178982 5.261363 -6.913805
O 2.091759 3.416148 -7.656440
H 1.251095 2.185130 -7.439031
C -0.814618 1.589194 -2.367637
H -0.887011 1.863425 -1.311896
O 0.547843 1.101530 -2.541571
H 1.390995 1.211446 -1.018880
C -1.809075 0.482178 -2.735785
H -1.691705 0.197525 -3.785894
H -2.852619 0.770559 -2.564914
H -1.599827 -0.392930 -2.114769
N -5.168239 -5.583041 2.434184
H -6.043176 -5.924090 2.810828
C -4.157007 -5.067997 3.369066
H -3.421805 -4.449722 2.833979
C -4.839921 -4.144186 4.437049
H -5.648827 -4.712841 4.910906
H -4.096854 -3.955954 5.218143
N -4.648107 -1.739889 3.586088
H -3.668409 -1.578014 3.806783
C -5.403846 -2.879228 3.876134
C -5.485228 -0.819309 2.995934
H -5.143181 0.141876 2.652667
N -6.726418 -1.295830 2.888072
C -6.681020 -2.574934 3.444021
H -7.566470 -3.185362 3.516893
C -3.335052 -6.199180 4.076703
O -2.530607 -5.882920 4.976385
S -1.240179 -0.847077 5.022629
H 1.641813 0.645945 0.484850
O 1.676229 -0.582106 1.974289
O 1.700580 1.425924 -0.103400
FE 0.601067 -0.779926 3.215923
N 0.452458 -2.780662 2.901832
N -1.008119 -0.456795 2.017401
N 0.609033 1.175952 3.750025
N 2.099991 -1.143003 4.565551
C 1.315272 -3.774877 3.350949
C 0.961094 -5.060374 2.765113
C -0.138223 -4.838687 1.964266
C -0.445474 -3.416854 2.066857
C -1.753932 -1.412870 1.349114
C -2.828750 -0.787781 0.577295
C -2.723013 0.577079 0.771519
C -1.580071 0.759502 1.690559
C -0.233917 2.153833 3.278101
C 0.044784 3.438664 3.915753
C 1.150947 3.253191 4.723858
C 1.480910 1.822222 4.620283
C 2.826066 -0.190657 5.253902
C 3.945376 -0.799764 5.957316
C 3.894903 -2.150996 5.680069
C 2.748805 -2.346936 4.803754
C 2.363142 -3.556757 4.236766
H 2.951678 -4.424493 4.510185
C -1.493910 -2.777440 1.402842
H -2.158575 -3.429894 0.845933
C -1.189818 1.960137 2.277527
H -1.683078 2.858122 1.926538
C 2.516134 1.168150 5.274126
H 3.186654 1.779990 5.869911
O 0.598725 1.376657 -7.326166
H 0.674341 0.684848 -5.937326

H 0.519243 0.853533 -8.151697
O 0.816133 0.225118 -5.032793
H 0.686490 0.795892 -3.492646
H 1.572736 -0.383147 -5.086502
h -1.497771 -2.141177 5.426728
h 1.497020 -5.991419 2.949520
h -0.687969 -5.531662 1.327374
h -3.515067 -1.366055 -0.041278
h -3.308353 1.414771 0.392422
h -0.614337 4.300447 3.811081
h 1.732951 3.946706 5.330796
h 4.683956 -0.244595 6.535548
h 4.547733 -2.935068 6.063618
h -5.075896 -5.588131 1.438484
h -3.517279 -7.218553 3.736500
h 2.866610 4.032965 -4.450072
h -0.928500 2.500141 -2.955237

WT-Conf S2 –RC-

C 2.429143 3.138050 -5.295100
H 1.476517 2.607727 -5.189917
H 3.204823 2.359749 -5.270858
C 2.474727 3.801321 -6.660033
O 2.762394 4.985152 -6.898398
O 2.171278 2.975810 -7.702699
H 1.892492 2.026715 -7.447358
C -0.990974 1.535119 -1.976119
H -1.201936 1.884910 -0.960815
O 0.441857 1.149671 -2.037048
H 0.741859 0.812346 -1.144058
C -1.857004 0.328179 -2.336596
H -1.587431 -0.049900 -3.329771
H -2.924842 0.571212 -2.330702
H -1.704875 -0.461605 -1.597608
N -5.215937 -5.820105 2.647495
H -6.136168 -6.016233 3.008922
C -4.185527 -5.302711 3.568038
H -3.467603 -4.673475 3.023102
C -4.870992 -4.414779 4.653165
H -4.083650 -4.121549 5.353524
H -5.572050 -5.043082 5.219253
C -5.596942 -3.197783 4.116509
C -4.903072 -2.015861 3.795554
H -3.823277 -1.964694 3.900768
C -5.593558 -0.877587 3.361907
H -5.033696 0.017417 3.115638
C -6.988612 -0.901420 3.234131
H -7.521250 -0.009154 2.912905
C -6.996239 -3.210662 3.973138
H -7.548882 -4.110124 4.234295
C -7.691473 -2.076503 3.532549
H -8.772599 -2.108470 3.429545
C -3.360396 -6.430308 4.283655
O -2.517473 -6.093228 5.137772
S -1.084065 -0.863640 5.187463
H 0.968568 1.272853 1.393252
O 1.486638 -0.623886 1.680371
O 1.199547 0.568976 0.745159
Fe 0.407912 -0.755952 3.231334
N 0.377671 -2.751423 2.885571
N -1.248315 -0.457508 2.102639
N 0.470426 1.245193 3.652860
N 2.031621 -1.084127 4.474830
C 1.259026 -3.725295 3.331543
C 0.915848 -5.023969 2.756589
C -0.208971 -4.827884 1.989387
C -0.546586 -3.405989 2.094085
C -1.973536 -1.447946 1.472699
C -3.114733 -0.867047 0.757610
C -3.062625 0.503766 0.953332
C -1.882258 0.735856 1.817043
C -0.422109 2.214632 3.215499
C -0.109301 3.508303 3.819920
C 0.980650 3.314333 4.653332
C 1.331195 1.883441 4.537400
C 2.698689 -0.116436 5.199447
C 3.770853 -0.722314 5.997105
C 3.728134 -2.080291 5.759014
C 2.641149 -2.289600 4.799999
C 2.285363 -3.509502 4.243042
H 2.854881 -4.378366 4.549253
C -1.650967 -2.804730 1.495596
H -2.322548 -3.481446 0.977764
C -1.477961 1.966343 2.338870
H -2.079203 2.825597 2.066882
C 2.367454 1.235306 5.213685
H 2.998524 1.848556 5.851634
O 1.369502 0.570752 -7.063353
H 1.207599 0.395444 -6.074097
H 0.657688 0.223183 -7.635630
O 0.914210 0.082613 -4.488150
H 0.824396 0.565780 -3.601887
H 0.918812 -0.872386 -4.298167
h -1.386029 -2.158981 5.555233
h 1.483377 -5.939617 2.922623
h -0.760000 -5.548410 1.385005
h -3.811508 -1.473944 0.179469
h -3.695177 1.318046 0.599929
h -0.685813 4.409365 3.610667
h 1.526667 3.989440 5.312242
h 4.477789 -0.161956 6.608911
h 4.361656 -2.858754 6.184117
h -5.130978 -5.888179 1.653453
h -3.583634 -7.457319 3.994726
h 2.576699 3.774152 -4.422364
h -1.111467 2.367835 -2.669033

Conf S2 –TSoo

C 2.434154 3.140480 -5.297993
H 1.484492 2.606211 -5.187983
H 3.212368 2.364750 -5.273291
C 2.473908 3.800546 -6.664440
O 2.759927 4.984614 -6.906094
O 2.168394 2.973093 -7.704370
H 1.888296 2.023339 -7.445167
C -0.988304 1.528172 -2.023929
H -1.183850 1.868427 -1.001751
O 0.432877 1.131712 -2.107619
H 0.764154 0.839609 -1.186389
C -1.870586 0.331016 -2.380653
H -1.616166 -0.041775 -3.379562
H -2.937410 0.578370 -2.357644
H -1.706946 -0.465328 -1.651069
N -5.215529 -5.820446 2.647649
H -6.135227 -6.018065 3.009609
C -4.184974 -5.303250 3.567687
H -3.467025 -4.674401 3.022418
C -4.869047 -4.414444 4.653017
H -4.080528 -4.120392 5.351722
H -5.568735 -5.042440 5.221059
C -5.596800 -3.198634 4.116061
C -4.904630 -2.016039 3.794089
H -3.824899 -1.963810 3.899516
C -5.596480 -0.879005 3.359404
H -5.038171 0.017019 3.112863
C -6.991595 -0.904546 3.232243
H -7.525661 -0.013332 2.910540
C -6.996083 -3.213257 3.973126
H -7.547763 -4.113115 4.234868
C -7.692765 -2.080294 3.531703
H -8.773779 -2.113791 3.428492
C -3.359040 -6.430569 4.282971
O -2.515105 -6.092725 5.135917
S -1.074709 -0.866224 5.193736
H 0.783900 1.312074 1.079518
O 1.481747 -0.618567 1.847937
O 1.264821 0.744486 0.435734
Fe 0.452895 -0.738012 3.197352
N 0.369437 -2.751462 2.898797
N -1.222324 -0.462253 2.100143
N 0.469957 1.231321 3.694959
N 2.035743 -1.078730 4.497885
C 1.255674 -3.721711 3.346259
C 0.916189 -5.020104 2.770213
C -0.206694 -4.826875 1.999124
C -0.548136 -3.408017 2.102714
C -1.956319 -1.450193 1.471659
C -3.093449 -0.862761 0.758839
C -3.035821 0.506752 0.956808
C -1.854608 0.733811 1.818894
C -0.406247 2.200346 3.236414
C -0.091060 3.498457 3.832096
C 0.993794 3.307294 4.670588
C 1.338262 1.874036 4.567795
C 2.709736 -0.116551 5.220524
C 3.783371 -0.727321 6.008813
C 3.734417 -2.084171 5.766785
C 2.642397 -2.287755 4.812748

C 2.282641 -3.505674 4.255141
H 2.852715 -4.374586 4.559328
C -1.647151 -2.807116 1.497002
H -2.320084 -3.481047 0.978077
C -1.450685 1.960059 2.345681
H -2.045641 2.821325 2.068462
C 2.378050 1.233380 5.240726
H 3.013656 1.848312 5.871586
O 1.371549 0.575697 -7.059540
H 1.208736 0.400713 -6.065389
H 0.659673 0.227737 -7.631210
O 0.923477 0.086400 -4.506162
H 0.809597 0.569504 -3.612417
H 0.966132 -0.867113 -4.314384
h -1.391715 -2.157697 5.562450
h 1.484988 -5.935115 2.935409
h -0.754499 -5.548734 1.393404
h -3.792430 -1.464897 0.178387
h -3.666096 1.323184 0.604303
h -0.662898 4.400095 3.612740
h 1.540367 3.985772 5.325564
h 4.493618 -0.168951 6.618597
h 4.366698 -2.864895 6.189582
h -5.130875 -5.888265 1.653564
h -3.582317 -7.457718 3.994563
h 2.581755 3.778659 -4.426782
h -1.114550 2.372173 -2.702008

Conf S2 -CpdI

C 2.367424 3.189251 -5.437137
H 1.403773 2.674582 -5.339279
H 3.122630 2.389782 -5.436635
C 2.420799 3.865360 -6.817894
O 2.713157 5.091097 -6.964110
O 2.149251 3.076422 -7.833961
H 1.671345 1.707686 -7.636602
C -0.939190 1.491483 -2.281688
H -0.926804 1.769031 -1.223955
O 0.409396 1.007504 -2.573493
H 1.697399 0.878360 -1.237325
C -1.957859 0.382045 -2.548099
H -1.942121 0.110419 -3.607085
H -2.980311 0.667892 -2.277760
H -1.684008 -0.492485 -1.952293
N -5.218015 -5.817252 2.647891
H -6.135879 -6.024081 3.009546
C -4.192269 -5.298468 3.567761
H -3.479489 -4.662251 3.023819
C -4.878242 -4.409975 4.652548
H -4.092571 -4.118246 5.356008
H -5.582210 -5.036282 5.216296
C -5.597953 -3.191974 4.109056
C -4.896018 -2.018345 3.775475
H -3.816168 -1.977313 3.883641
C -5.575652 -0.878094 3.331122
H -5.011208 0.013023 3.078947
C -6.971309 -0.891389 3.207491
H -7.497824 0.001699 2.879826
C -6.996914 -3.194421 3.967773
H -7.557128 -4.086880 4.235291
C -7.682551 -2.057824 3.518195
H -8.763529 -2.081885 3.415041
C -3.353696 -6.419376 4.281112
O -2.500629 -6.067147 5.119964
S -1.090557 -0.816672 5.284132
H 2.106293 0.439492 0.264190
O 1.650692 -0.433610 2.125852
O 2.414989 0.867001 -0.560175
Fe 0.614634 -0.699741 3.392349
N 0.511478 -2.698624 3.063186
N -1.030306 -0.414801 2.224833
N 0.589249 1.262148 3.928613
N 2.109147 -1.049756 4.748323
C 1.393738 -3.678378 3.500772
C 1.066741 -4.968187 2.907461
C -0.055235 -4.772214 2.135622
C -0.390968 -3.356452 2.243715
C -1.761764 -1.381803 1.568011
C -2.868641 -0.784153 0.819910
C -2.801378 0.581677 1.024556
C -1.643301 0.789777 1.920859
C -0.241415 2.234904 3.422217
C 0.054215 3.538170 4.016923
C 1.095169 3.345051 4.907933
C 1.429100 1.911062 4.824545
C 2.783701 -0.095010 5.486246
C 3.870450 -0.703162 6.246483
C 3.841367 -2.053962 5.965504
C 2.747875 -2.252595 5.023251
C 2.408788 -3.461568 4.424821
H 2.989519 -4.330017 4.712086
C -1.465420 -2.742828 1.607519
H -2.124951 -3.409651 1.061074
C -1.249914 1.999647 2.482516
H -1.823751 2.869220 2.186453
C 2.446200 1.256344 5.514327
H 3.073621 1.864992 6.158443
O 1.349600 0.701112 -7.543214
H 0.802591 0.364285 -6.066030
H 0.725558 0.449396 -8.260595
O 0.383722 0.096529 -5.173677
H 0.484681 0.739460 -3.537780
H 0.415466 -0.873059 -5.083761
h -1.403717 -2.118187 5.619299
h 1.633643 -5.884368 3.072686
h -0.613222 -5.485035 1.528496
h -3.540184 -1.383747 0.205432
h -3.415274 1.404084 0.657343
h -0.478167 4.444525 3.728554
h 1.617366 4.022620 5.583416
h 4.583832 -0.151772 6.858955
h 4.476780 -2.839723 6.374034
h -5.131582 -5.887377 1.654119
h -3.576736 -7.448601 4.000018
h 2.539747 3.796287 -4.548386
h -1.110094 2.398808 -2.861016

MT-Conf S2 –RC

C 2.363827 3.104497 -5.339711
H 1.404082 2.586531 -5.233088
H 3.128305 2.314987 -5.320188
C 2.414320 3.773642 -6.701945
O 2.712097 4.956858 -6.930683
O 2.104015 2.959921 -7.750994
H 1.805736 2.011775 -7.510665
C -1.055241 1.515571 -2.040038
H -1.243920 1.858851 -1.018140
O 0.369822 1.103185 -2.129927
H 0.678048 0.760109 -1.246744
C -1.946497 0.327429 -2.400915
H -1.712950 -0.031925 -3.409669
H -3.010396 0.583513 -2.358931
H -1.785784 -0.478706 -1.681627
N -5.170690 -5.791013 2.665451
H -6.090198 -5.978093 3.034661
C -4.128404 -5.297227 3.580182
H -3.382649 -4.708410 3.027041
C -4.787446 -4.356353 4.642454
H -5.578853 -4.920358 5.153774
H -4.027020 -4.152161 5.400913
N -4.657676 -1.936047 3.808051
H -3.669091 -1.757593 3.992815
C -5.376437 -3.101356 4.081436
C -5.529723 -1.018582 3.272386
H -5.214858 -0.042996 2.945115
N -6.766981 -1.518538 3.181627
C -6.672865 -2.815962 3.691312
H -7.538830 -3.454626 3.757622
C -3.337664 -6.442074 4.307037
O -2.491326 -6.119756 5.163551
S -1.264925 -0.945216 5.104388
H 0.920882 1.226769 1.381045
O 1.460608 -0.656750 1.703317
O 1.171223 0.515408 0.747825
Fe 0.353729 -0.795207 3.222592
N 0.335558 -2.788352 2.880154
N -1.277365 -0.493779 2.065647
N 0.412086 1.206567 3.649605
N 1.958669 -1.119812 4.497742
C 1.215880 -3.758885 3.334457
C 0.884331 -5.057961 2.754079
C -0.234568 -4.865445 1.977102
C -0.578217 -3.444607 2.077951
C -2.001052 -1.487476 1.437621
C -3.142181 -0.907754 0.721668
C -3.090018 0.463923 0.914880
C -1.910404 0.698791 1.777927
C -0.468966 2.178818 3.194548

C -0.150119 3.476685 3.787119
C 0.939725 3.285873 4.620840
C 1.277900 1.851044 4.524641
C 2.631847 -0.147894 5.211819
C 3.709425 -0.747632 6.005249
C 3.667537 -2.106804 5.774228
C 2.576541 -2.322597 4.821796
C 2.231302 -3.541966 4.258297
H 2.802616 -4.408631 4.566868
C -1.679416 -2.844733 1.470373
H -2.343667 -3.523232 0.946229
C -1.512183 1.930062 2.304064
H -2.109420 2.788855 2.023405
C 2.307077 1.205136 5.212444
H 2.946372 1.822256 5.837718
O 1.253076 0.561377 -7.176254
H 1.068015 0.367537 -6.196133
H 0.560339 0.220535 -7.777366
O 0.754163 0.036871 -4.615903
H 0.709505 0.510912 -3.724518
H 0.701350 -0.920074 -4.444441
h -1.483910 -2.243171 5.518762
h 1.456466 -5.969451 2.927037
h -0.775136 -5.589456 1.367462
h -3.848308 -1.512369 0.152553
h -3.724189 1.277826 0.563518
h -0.724122 4.378910 3.575985
h 1.492838 3.965913 5.268665
h 4.425520 -0.185684 6.604823
h 4.306449 -2.879681 6.201451
h -5.096191 -5.854008 1.670235
h -3.573890 -7.464991 4.013945
h 2.523234 3.736571 -4.466132
h -1.169108 2.359021 -2.720987

Conf S2–TSoo

C 2.381565 3.105866 -5.331505
H 1.429735 2.576235 -5.216498
H 3.156523 2.326674 -5.311793
C 2.416099 3.767824 -6.697374
O 2.704978 4.951341 -6.936919
O 2.102370 2.944578 -7.738111
H 1.816825 1.996270 -7.482117
C -1.050275 1.520807 -2.047939
H -1.245569 1.865182 -1.027359
O 0.371474 1.115286 -2.128025
H 0.691681 0.812446 -1.215215
C -1.938297 0.328001 -2.405226
H -1.685727 -0.046551 -3.403909
H -3.003584 0.581550 -2.383675
H -1.781366 -0.469016 -1.674858
N -5.170851 -5.791635 2.665439
H -6.089403 -5.982922 3.034937
C -4.130515 -5.295503 3.580810
H -3.386431 -4.703525 3.029025
C -4.794679 -4.356944 4.642966
H -5.586593 -4.923127 5.150784
H -4.037716 -4.150276 5.404345
N -4.666079 -1.936101 3.809638
H -3.677520 -1.758688 3.992456
C -5.384338 -3.102182 4.082302
C -5.539221 -1.017638 3.276851
H -5.225808 -0.040647 2.952600
N -6.776141 -1.517746 3.186823
C -6.681168 -2.816418 3.694294
H -7.546645 -3.455544 3.760501
C -3.336469 -6.437170 4.306661
O -2.489858 -6.110996 5.161769
S -1.260589 -0.938423 5.121062
H 0.774442 1.296912 1.116589
O 1.425741 -0.668997 1.832550
O 1.178823 0.684534 0.461098
Fe 0.364721 -0.780635 3.178724
N 0.303264 -2.792038 2.878534
N -1.292471 -0.505095 2.063287
N 0.385518 1.192923 3.662794
N 1.939810 -1.115903 4.496477
C 1.189640 -3.759118 3.333231
C 0.865886 -5.057070 2.747550
C -0.247820 -4.866598 1.962248
C -0.600527 -3.450042 2.068066
C -2.021292 -1.498209 1.434801
C -3.164286 -0.915869 0.726323
C -3.108144 0.455180 0.918639
C -1.927494 0.688132 1.778773
C -0.484874 2.163308 3.193627
C -0.161146 3.466019 3.773847
C 0.927281 3.279678 4.608622
C 1.259721 1.842158 4.525605
C 2.618114 -0.147683 5.207836
C 3.697385 -0.750026 5.994892
C 3.649460 -2.109097 5.764616
C 2.554550 -2.321080 4.815246
C 2.205854 -3.539981 4.253737
H 2.782624 -4.404491 4.556707
C -1.700087 -2.853085 1.457399
H -2.362046 -3.530692 0.930515
C -1.526565 1.917674 2.301727
H -2.119060 2.777487 2.016156
C 2.293045 1.203991 5.210473
H 2.931516 1.823160 5.833954
O 1.288314 0.547258 -7.102033
H 1.121652 0.372743 -6.110748
H 0.579619 0.200740 -7.679023
O 0.830460 0.059874 -4.542299
H 0.738878 0.542460 -3.649429
H 0.838468 -0.895402 -4.354686
h -1.496036 -2.234177 5.533290
h 1.439058 -5.968594 2.916857
h -0.780383 -5.590410 1.345370
h -3.877537 -1.515562 0.160897
h -3.738264 1.269811 0.561719
h -0.730111 4.368779 3.551657
h 1.483482 3.964551 5.248665
h 4.416913 -0.184907 6.587333
h 4.288046 -2.883685 6.189219
h -5.096232 -5.854176 1.670205
h -3.569510 -7.461282 4.015197
h 2.537308 3.743953 -4.461646
h -1.167866 2.363389 -2.729330

Conf S2 –IC1

C 2.343862 3.103734 -5.378079
H 1.377213 2.597052 -5.276133
H 3.098834 2.304750 -5.362930
C 2.410936 3.783167 -6.735292
O 2.724171 4.967385 -6.945383
O 2.104085 2.990092 -7.797923
H 1.776046 2.034025 -7.600387
C -1.007360 1.492855 -2.248073
H -1.022065 1.779895 -1.190960
O 0.353536 1.026134 -2.591735
H 0.841944 0.721455 -1.762410
C -2.003013 0.367476 -2.524323
H -1.930517 0.051242 -3.569683
H -3.036774 0.663481 -2.320215
H -1.777468 -0.481111 -1.874026
N -5.171745 -5.789870 2.665462
H -6.090290 -5.981982 3.034937
C -4.132870 -5.291152 3.580717
H -3.388005 -4.700865 3.028011
C -4.795106 -4.346269 4.638655
H -5.592386 -4.906188 5.144884
H -4.038626 -4.142137 5.401391
N -4.643686 -1.931900 3.791201
H -3.656937 -1.757751 3.985160
C -5.373403 -3.089199 4.070934
C -5.506633 -1.010111 3.247164
H -5.182754 -0.037506 2.918966
N -6.747295 -1.500968 3.156502
C -6.666133 -2.795247 3.675220
H -7.537645 -3.425943 3.743161
C -3.338708 -6.431239 4.309843
O -2.492289 -6.102130 5.163803
S -1.271390 -0.912742 5.169426
H 1.537878 0.055686 0.643351
O 1.499649 -0.457143 2.029144
O 1.680544 0.389340 -0.354897
Fe 0.483684 -0.748543 3.333456
N 0.404016 -2.744525 2.992447
N -1.147785 -0.457584 2.146127
N 0.474980 1.221923 3.857881
N 1.997717 -1.090438 4.680582
C 1.291870 -3.715250 3.435211
C 0.966855 -5.006938 2.839070
C -0.155995 -4.814358 2.066950
C -0.505179 -3.398772 2.179382
C -1.886080 -1.437190 1.511923

C -3.000707 -0.837125 0.775212
C -2.923215 0.533146 0.965932
C -1.753560 0.747919 1.848007
C -0.351636 2.196226 3.331252
C -0.028569 3.504242 3.906312
C 1.022915 3.313045 4.784880
C 1.335385 1.869048 4.729447
C 2.673738 -0.128504 5.408554
C 3.766335 -0.738418 6.166618
C 3.733819 -2.090184 5.895118
C 2.635064 -2.294732 4.953665
C 2.303614 -3.505073 4.362117
H 2.883955 -4.371958 4.652173
C -1.595158 -2.798009 1.558116
H -2.263321 -3.470484 1.030892
C -1.357363 1.966071 2.397271
H -1.929495 2.834901 2.096071
C 2.348791 1.222123 5.433867
H 2.982858 1.833675 6.069094
O 1.201127 0.604601 -7.413365
H 0.944810 0.350119 -6.454759
H 0.558883 0.292359 -8.087675
O 0.509054 -0.031866 -4.993199
H 0.515583 0.434669 -4.081523
H 0.389121 -0.987209 -4.854188
h -1.504227 -2.214847 5.562688
h 1.539760 -5.920071 3.000422
h -0.701252 -5.534084 1.456412
h -3.705141 -1.433055 0.194947
h -3.541514 1.355354 0.605729
h -0.570249 4.411352 3.638354
h 1.564341 3.993298 5.442283
h 4.486187 -0.184110 6.768799
h 4.374599 -2.870904 6.304925
h -5.096482 -5.853695 1.670357
h -3.569691 -7.456039 4.019160
h 2.510596 3.727723 -4.500068
h -1.163468 2.388298 -2.849637

Conf S2 -CpdI

C 2.332677 3.182685 -5.505535
H 1.378158 2.656542 -5.381408
H 3.099228 2.393625 -5.511048
C 2.359379 3.849425 -6.888146
O 2.642202 5.075855 -7.041147
O 2.084842 3.057556 -7.902795
H 1.607117 1.710401 -7.718541
C -1.089323 1.376459 -2.433026
H -0.947345 1.602462 -1.372802
O 0.148499 0.733565 -2.873540
H 1.376806 1.467812 -2.009242
C -2.243999 0.392124 -2.632451
H -2.406064 0.210823 -3.698387
H -3.186713 0.743128 -2.199942
H -1.976607 -0.549989 -2.146150
N -5.177029 -5.787746 2.665367
H -6.094378 -5.991918 3.031324
C -4.146822 -5.289614 3.585442
H -3.407078 -4.686823 3.039321
C -4.821673 -4.356812 4.647367
H -5.615528 -4.926462 5.147241
H -4.071750 -4.149162 5.415995
N -4.683114 -1.941696 3.802053
H -3.703611 -1.761142 4.011636
C -5.408870 -3.103392 4.080870
C -5.550187 -1.022352 3.255973
H -5.234929 -0.044627 2.934428
N -6.785441 -1.520379 3.161898
C -6.700533 -2.815013 3.679924
H -7.569635 -3.448915 3.742881
C -3.338752 -6.424696 4.309169
O -2.483428 -6.083365 5.150352
S -1.325469 -0.901112 5.212757
H 1.705932 2.258036 -0.620567
O 1.616172 -0.496842 2.209959
O 1.869368 2.220517 -1.577669
Fe 0.533956 -0.751040 3.432612
N 0.435800 -2.747364 3.097232
N -1.085953 -0.460887 2.229268
N 0.514119 1.217783 3.952935
N 2.005991 -1.098344 4.813200
C 1.319493 -3.725647 3.540011
C 1.011488 -5.011393 2.927476
C -0.098797 -4.814465 2.138424
C -0.448223 -3.402445 2.258356
C -1.824238 -1.431048 1.578965
C -2.936891 -0.832940 0.838686
C -2.861487 0.533986 1.033100
C -1.695683 0.744396 1.919097
C -0.294864 2.194340 3.418986
C 0.019498 3.505066 3.987685
C 1.054024 3.314171 4.887110
C 1.360948 1.872671 4.838263
C 2.693075 -0.137542 5.533237
C 3.795124 -0.738003 6.275420
C 3.765299 -2.090244 5.999044
C 2.655957 -2.295980 5.077803
C 2.323718 -3.506648 4.473835
H 2.912074 -4.370429 4.758719
C -1.523773 -2.790062 1.617841
H -2.178168 -3.458320 1.067105
C -1.296317 1.956903 2.471349
H -1.856707 2.828759 2.157361
C 2.365316 1.216618 5.545329
H 2.999746 1.828639 6.179177
O 1.276230 0.698424 -7.640802
H 0.623029 0.329567 -6.266600
H 0.668313 0.448174 -8.373785
O 0.090607 0.022393 -5.442263
H 0.151816 0.543252 -3.866696
H 0.062418 -0.951453 -5.421001
h -1.549044 -2.206349 5.600979
h 1.584866 -5.923777 3.091369
h -0.637742 -5.524222 1.510850
h -3.624588 -1.429708 0.239514
h -3.477850 1.356111 0.669405
h -0.501070 4.413424 3.684433
h 1.586494 3.997376 5.548753
h 4.522651 -0.182894 6.867557
h 4.410522 -2.870516 6.402688
h -5.097921 -5.853105 1.670660
h -3.569336 -7.450977 4.023435
h 2.517477 3.804266 -4.629434
h -1.205564 2.329109 -2.949759

Conf LW1 –RC-

C 2.622693 3.071102 -4.372729
H 2.906651 4.006200 -4.860517
H 3.508734 2.430267 -4.308468
C 1.551957 2.424246 -5.221736
O 0.829256 3.080911 -5.993657
O 1.388022 1.079683 -5.112476
H 2.046581 0.561199 -4.477240
C -1.097757 0.098802 -1.104347
H -1.937696 -0.605169 -1.076352
O -0.936637 0.739034 0.198438
H -0.539682 0.113243 0.841748
C 0.151160 -0.669015 -1.547563
H 0.358068 -1.466792 -0.827463
H -0.006696 -1.137880 -2.528599
H 1.031123 -0.024434 -1.586401
N -2.605429 -8.397374 -0.253460
H -3.069859 -9.247637 0.017473
C -1.371759 -8.064269 0.415410
H -0.675593 -7.562264 -0.282137
C -1.538123 -7.065331 1.634878
H -0.610302 -7.061487 2.227149
H -1.629770 -6.060961 1.214494
C -2.726768 -7.320128 2.528119
C -2.730372 -8.339233 3.495606
H -1.867050 -8.991883 3.595370
C -3.821890 -8.496197 4.356787
H -3.806747 -9.264653 5.121906
C -4.934630 -7.655945 4.244933
H -5.781675 -7.791329 4.907785
C -3.851034 -6.485049 2.423516
H -3.861206 -5.690895 1.682451
C -4.950706 -6.656453 3.267602
H -5.812616 -6.010587 3.155593
C -0.662070 -9.370584 0.817583
O -1.262657 -10.463230 0.767074
S -0.551188 -3.398524 5.424427
H 0.677432 0.441906 2.956757
O 1.960199 -0.992776 2.676505
O 1.211546 0.233399 2.145269
Fe 0.806222 -1.985641 4.024591
N 1.673961 -3.674775 3.396904
N -0.641706 -2.126485 2.617500

N -0.024609 -0.230407 4.638250
N 2.237189 -1.839381 5.418408
C 2.624753 -4.445811 4.049673
C 2.964249 -5.613988 3.234154
C 2.230911 -5.503840 2.073444
C 1.384649 -4.319566 2.214307
C -0.653963 -3.023919 1.568693
C -1.870312 -2.854880 0.765935
C -2.601395 -1.832430 1.348927
C -1.807479 -1.384730 2.510863
C -1.296888 0.247922 4.326918
C -1.573829 1.468880 5.072544
C -0.443661 1.759053 5.822770
C 0.496567 0.653450 5.581803
C 2.501013 -0.717147 6.185065
C 3.615732 -0.980759 7.092849
C 3.945704 -2.314491 6.942128
C 3.109374 -2.831652 5.859411
C 3.232743 -4.077378 5.247236
H 3.912088 -4.794547 5.694478
C 0.345885 -3.972884 1.346391
H 0.248659 -4.593445 0.461855
C -2.105739 -0.303458 3.339548
H -3.034298 0.217946 3.147234
C 1.716917 0.435816 6.222237
H 2.065994 1.207327 6.900949
O 2.762748 -1.867535 0.353463
H 2.237059 -2.670183 0.193460
H 2.510051 -1.526303 1.281275
O 2.958513 -0.374135 -3.799179
H 3.299916 -0.298969 -2.806140
H 2.669328 -1.290172 -3.965882
O 4.466041 -0.300740 3.492219
H 4.510767 -0.366762 4.460637
H 3.538165 -0.515044 3.206315
O 3.697207 -0.251231 -1.382945
H 3.576692 0.658787 -1.027465
H 3.313672 -0.942273 -0.713205
O 1.716058 1.875198 -0.026140
H 2.665076 2.143966 -0.024763
H 1.561210 1.160867 0.639215
h -0.722389 -2.789597 6.650903
h 3.697514 -6.376821 3.495833
h 2.254480 -6.103247 1.163378
h -2.110509 -3.470897 -0.100607
h -3.539421 -1.352374 1.070142
h -2.527701 1.992344 5.007888
h -0.185609 2.603493 6.461830
h 4.075447 -0.215892 7.718714
h 4.664916 -2.887671 7.527162
h -2.977319 -7.895210 -1.034166
h 0.382944 -9.306365 1.120716
h 2.323563 3.318372 -3.354179
h -1.308476 0.902574 -1.809765

Conf LW1 –TSoo

C 2.619223 3.080870 -4.403897
H 2.903870 4.012900 -4.897083
H 3.503627 2.438429 -4.334522
C 1.544346 2.432096 -5.245151
O 0.821237 3.094654 -6.014411
O 1.375306 1.091929 -5.133281
H 2.034944 0.552162 -4.495433
C -1.097481 0.158459 -1.022941
H -1.961008 -0.507144 -0.912533
O -0.857509 0.873429 0.221973
H -0.224620 0.395171 0.824492
C 0.083787 -0.705215 -1.478207
H 0.344328 -1.413029 -0.686185
H -0.186767 -1.285934 -2.371237
H 0.974248 -0.115534 -1.695275
N -2.608459 -8.396220 -0.251697
H -3.078203 -9.241735 0.024662
C -1.376207 -8.063371 0.419267
H -0.681405 -7.556777 -0.276125
C -1.548743 -7.066370 1.638652
H -0.614536 -7.044813 2.220353
H -1.664705 -6.066291 1.214016
C -2.722782 -7.337629 2.547354
C -2.695123 -8.348447 3.523061
H -1.817712 -8.982718 3.618135
C -3.771250 -8.517059 4.401336
H -3.728751 -9.274875 5.175935
C -4.902516 -7.701134 4.296150
H -5.738616 -7.849421 4.970327
C -3.864681 -6.525208 2.450950
H -3.900533 -5.737783 1.703390
C -4.950419 -6.710806 3.310341
H -5.826111 -6.082719 3.203738
C -0.664987 -9.369992 0.818835
O -1.265882 -10.462408 0.768163
S -0.518784 -3.357621 5.415286
H 0.841083 0.646359 2.810771
O 1.921365 -1.161261 2.811023
O 1.174545 0.382781 1.924688
Fe 0.850549 -1.950736 3.978632
N 1.643097 -3.710356 3.413810
N -0.632322 -2.145226 2.625903
N 0.004727 -0.252441 4.656896
N 2.246379 -1.844986 5.431124
C 2.601139 -4.469930 4.070380
C 2.947685 -5.634130 3.254393
C 2.214737 -5.530441 2.092436
C 1.360738 -4.354586 2.230598
C -0.657758 -3.046252 1.580451
C -1.876219 -2.866350 0.784716
C -2.592938 -1.835646 1.367928
C -1.785606 -1.388154 2.519943
C -1.250756 0.240021 4.324187
C -1.517255 1.474880 5.051881
C -0.385183 1.766332 5.796784
C 0.541916 0.645532 5.577040
C 2.532954 -0.722852 6.186606
C 3.645536 -0.997204 7.090151
C 3.953979 -2.336805 6.945906
C 3.105413 -2.849250 5.869817
C 3.214473 -4.098338 5.263151
H 3.891676 -4.817057 5.710535
C 0.326858 -4.007361 1.359097
H 0.226155 -4.628733 0.476321
C -2.069876 -0.304688 3.343988
H -2.988957 0.231424 3.148888
C 1.762473 0.436575 6.215768
H 2.121702 1.216273 6.878775
O 2.765334 -2.047084 0.404289
H 2.193132 -2.828976 0.306326
H 2.522547 -1.636611 1.290721
O 2.894099 -0.394091 -3.832679
H 3.190545 -0.346787 -2.799105
H 2.584376 -1.298366 -4.026911
O 4.438022 -0.293750 3.460654
H 4.507619 -0.358002 4.427776
H 3.519361 -0.562103 3.197706
O 3.448472 -0.309635 -1.402479
H 2.944331 0.464854 -0.997510
H 3.254069 -1.101001 -0.793602
O 2.134888 1.638821 -0.151271
H 2.987428 2.144725 -0.131367
H 1.908621 1.193048 0.724838
h -0.695030 -2.765091 6.649058
h 3.687376 -6.390897 3.515594
h 2.256111 -6.117400 1.174922
h -2.122401 -3.475022 -0.085329
h -3.530413 -1.350362 1.096440
h -2.471488 1.997795 4.988109
h -0.118990 2.619233 6.421098
h 4.116453 -0.234489 7.710288
h 4.668447 -2.914263 7.532544
h -2.978217 -7.894783 -1.033880
h 0.379942 -9.305363 1.122173
h 2.324390 3.332238 -3.385097
h -1.302759 0.919168 -1.776100

Conf LW1 -CpdI

C 2.549046 3.054987 -4.435643
H 2.871760 3.979219 -4.923981
H 3.406158 2.374452 -4.378354
C 1.437792 2.445426 -5.286929
O 0.772406 3.219476 -6.041359
O 1.218534 1.154351 -5.196116
H 2.120559 0.161417 -4.495743
C -1.089533 0.137376 -1.079407
H -1.892173 -0.607967 -1.099520
O -1.058814 0.714464 0.243934
H -0.116205 0.846803 0.600358
C 0.214425 -0.579940 -1.469794
H 0.396188 -1.395788 -0.761760
H 0.145912 -1.015386 -2.474667
H 1.088579 0.077115 -1.448810

N -2.599786 -8.397314 -0.255755
H -3.065064 -9.243906 0.025288
C -1.356425 -8.067315 0.394719
H -0.663555 -7.574906 -0.312255
C -1.508783 -7.053825 1.605541
H -0.572752 -7.043628 2.186028
H -1.614194 -6.056828 1.168848
C -2.686805 -7.304735 2.515060
C -2.677469 -8.322683 3.483875
H -1.809137 -8.969111 3.580151
C -3.764439 -8.488625 4.349143
H -3.738170 -9.255825 5.115052
C -4.887121 -7.661297 4.238896
H -5.732596 -7.808391 4.901296
C -3.820000 -6.480929 2.413244
H -3.845597 -5.692657 1.666181
C -4.915778 -6.662348 3.261051
H -5.786465 -6.028111 3.148502
C -0.653794 -9.375056 0.809074
O -1.270168 -10.459255 0.794773
S -0.584428 -3.318242 5.468494
H 1.474549 0.454964 1.939821
O 1.857850 -0.919802 3.037099
O 1.275560 1.102061 1.221351
Fe 0.894664 -1.856756 4.055724
N 1.689280 -3.613272 3.488673
N -0.585501 -2.069334 2.691540
N -0.025535 -0.232919 4.804864
N 2.227110 -1.799771 5.561942
C 2.630693 -4.396710 4.156383
C 2.981745 -5.555936 3.340852
C 2.275632 -5.430319 2.163383
C 1.437159 -4.248832 2.298847
C -0.597106 -2.964752 1.630597
C -1.813281 -2.801852 0.830938
C -2.537800 -1.777528 1.408943
C -1.735696 -1.322483 2.562487
C -1.242994 0.290148 4.409927
C -1.516900 1.537865 5.117352
C -0.401799 1.821972 5.885993
C 0.511109 0.683261 5.696874
C 2.508426 -0.682447 6.329316
C 3.608545 -0.955288 7.240775
C 3.934061 -2.288847 7.077989
C 3.097087 -2.792089 5.993545
C 3.218676 -4.035056 5.363020
H 3.883797 -4.762008 5.816692
C 0.405713 -3.897882 1.415841
H 0.346248 -4.489768 0.510325
C -2.026559 -0.235430 3.388415
H -2.926370 0.320045 3.158447
C 1.733018 0.474854 6.338646
H 2.097644 1.265900 6.985238
O 3.263813 -2.275708 0.192852
H 3.829426 -1.874568 0.916761
H 2.335017 -2.211356 0.483380
O 2.702871 -0.646554 -4.201191
H 3.428018 -0.704454 -2.744499
H 2.223067 -1.472741 -4.391662
O 4.371617 -1.063892 2.344150
H 4.801636 -1.689767 2.955085
H 3.446366 -0.864208 2.696964
O 3.823193 -0.669773 -1.820020
H 3.371272 0.565865 -1.037875
H 3.595818 -1.428968 -1.210284
O 3.087170 1.396419 -0.513552
H 3.772641 2.093711 -0.608492
H 2.061119 1.232259 0.582744
h -0.762123 -2.769337 6.722078
h 3.708579 -6.324688 3.603148
h 2.322256 -6.015079 1.244717
h -2.046411 -3.415791 -0.039003
h -3.478548 -1.301594 1.132273
h -2.465771 2.065468 5.020681
h -0.139216 2.675289 6.511266
h 4.068987 -0.195362 7.872101
h 4.662638 -2.865534 7.647790
h -2.975730 -7.895301 -1.034613
h 0.398045 -9.315866 1.088713
h 2.272764 3.314597 -3.413715
h -1.310657 0.907205 -1.818687

Conf LW2 –RC

C -0.565605 4.256094 -4.224035
H -1.274943 4.944052 -4.689026
H 0.448685 4.645569 -4.375459
C -0.686079 2.924682 -4.934893
O -1.674302 2.621850 -5.625434
O 0.358728 2.059790 -4.847478
H 1.194222 2.355230 -4.288371
C -0.673071 -0.341232 -1.088855
H -0.821948 -1.419040 -0.927543
O -0.488265 0.350687 0.176612
H 0.480298 0.373655 0.440351
C 0.540774 -0.165894 -2.018084
H 1.414844 -0.640654 -1.562261
H 0.381640 -0.628387 -2.999908
H 0.768040 0.892590 -2.185696
N 2.685307 -8.499796 -0.834679
H 2.789950 -9.405528 -0.389420
C 3.714110 -7.504059 -0.607896
H 3.658432 -6.708295 -1.365469
C 3.569320 -6.762719 0.790860
H 4.410328 -6.070092 0.927266
H 2.667558 -6.147826 0.717610
C 3.472675 -7.705286 1.964940
C 4.620329 -8.118393 2.666148
H 5.594001 -7.718320 2.397578
C 4.516773 -9.038130 3.719285
H 5.407951 -9.341261 4.259254
C 3.268132 -9.564636 4.079329
H 3.191273 -10.296649 4.875820
C 2.221598 -8.213840 2.361647
H 1.329516 -7.879510 1.843491
C 2.116340 -9.139869 3.403852
H 1.146425 -9.531114 3.692476
C 5.108454 -8.139155 -0.764846
O 5.252366 -9.380259 -0.749330
S 5.076078 -3.438612 3.508767
H 3.856080 -0.776787 -0.337143
O 4.539620 0.245075 1.202619
O 4.458613 0.005008 -0.319763
Fe 4.824242 -1.457398 2.253388
N 6.263805 -2.174659 1.051974
N 3.443389 -2.345151 1.075460
N 3.378736 -0.703863 3.425114
N 6.185497 -0.485711 3.319985
C 7.611819 -2.264509 1.368710
C 8.337947 -2.924322 0.278921
C 7.420803 -3.138262 -0.729862
C 6.115691 -2.739348 -0.202032
C 3.635846 -2.920611 -0.174051
C 2.387294 -3.502893 -0.654209
C 1.461790 -3.389445 0.373665
C 2.126974 -2.606217 1.430442
C 2.071690 -1.149445 3.463572
C 1.313017 -0.401992 4.468249
C 2.162121 0.564160 4.983223
C 3.475785 0.321017 4.354423
C 5.954242 0.546577 4.215114
C 7.223590 1.052140 4.723358
C 8.213643 0.248104 4.193441
C 7.554963 -0.706028 3.302213
C 8.191183 -1.624785 2.462020
H 9.251592 -1.790349 2.615239
C 4.885453 -3.020294 -0.799057
H 4.910251 -3.457112 -1.792557
C 1.527909 -2.079336 2.575291
H 0.487013 -2.332304 2.742373
C 4.690538 0.941827 4.656333
H 4.675706 1.766443 5.363614
O 4.040138 2.161701 -1.735790
H 4.920794 2.568563 -1.863334
H 4.147092 1.294992 -1.224693
O 2.457747 2.787389 -3.740892
H 3.000382 2.520206 -2.937324
H 2.988255 3.246482 -4.438801
O 1.998145 0.991315 0.714341
H 2.293937 1.623691 0.033710
H 2.817517 0.647846 1.178127
h 4.682255 -3.268760 4.820407
h 9.370664 -3.270979 0.316225
h 7.587009 -3.447756 -1.761683
h 2.280225 -3.883826 -1.669834
h 0.460018 -3.801376 0.495456
h 0.286377 -0.664486 4.723538
h 1.989852 1.406957 5.652614
h 7.303959 1.927453 5.367899

h 9.284106 0.315834 4.387314
h 1.870434 -8.370242 -1.399630
h 5.990207 -7.511647 -0.894509
h -0.731063 4.288180 -3.147159
h -1.555340 0.098108 -1.554310

Conf LW2 -TSoo

C -0.606782 4.269861 -4.249956
H -1.329634 4.954171 -4.699056
H 0.402240 4.666606 -4.416807
C -0.727716 2.940330 -4.966101
O -1.718237 2.644139 -5.658761
O 0.314649 2.076681 -4.881329
H 1.167043 2.382112 -4.334017
C -0.662961 -0.334211 -1.100200
H -0.813018 -1.409414 -0.922141
O -0.452282 0.372593 0.153707
H 0.524416 0.411395 0.389114
C 0.534616 -0.174363 -2.053134
H 1.418627 -0.639100 -1.606536
H 0.357339 -0.654106 -3.023688
H 0.759582 0.880420 -2.243541
N 2.684084 -8.499842 -0.833297
H 2.788440 -9.405656 -0.388091
C 3.713503 -7.505155 -0.607861
H 3.656990 -6.708608 -1.364630
C 3.571833 -6.764786 0.791964
H 4.415744 -6.075353 0.927383
H 2.671792 -6.147210 0.719852
C 3.473399 -7.707426 1.966011
C 4.619914 -8.121834 2.668256
H 5.594456 -7.723760 2.399778
C 4.514382 -9.041247 3.721515
H 5.404760 -9.345722 4.262113
C 3.264794 -9.566246 4.080461
H 3.186315 -10.298587 4.876509
C 2.221343 -8.214476 2.361598
H 1.330116 -7.879694 1.842291
C 2.114116 -9.140322 3.403736
H 1.143554 -9.530845 3.691148
C 5.106835 -8.141805 -0.765315
O 5.249895 -9.382816 -0.743687
S 5.068360 -3.403762 3.526544
H 3.790666 -0.606484 -0.538988
O 4.569913 0.124123 1.328584
O 4.457912 0.105273 -0.612748
FE 4.810748 -1.398101 2.190109
N 6.246800 -2.184517 1.069920
N 3.440607 -2.359439 1.095899
N 3.370620 -0.723046 3.432041
N 6.189649 -0.494955 3.320434
C 7.598062 -2.284379 1.393727
C 8.316280 -2.951520 0.307739
C 7.400205 -3.156886 -0.704413
C 6.098818 -2.743065 -0.187336
C 3.628277 -2.907268 -0.160995
C 2.380515 -3.492866 -0.641285
C 1.460630 -3.401259 0.392530
C 2.126270 -2.627972 1.456369
C 2.068711 -1.173172 3.480681
C 1.314632 -0.418651 4.480664
C 2.163647 0.556464 4.980512
C 3.474378 0.313811 4.348089
C 5.951586 0.544530 4.204066
C 7.219873 1.052025 4.712956
C 8.211324 0.242410 4.194119
C 7.554892 -0.717146 3.309270
C 8.185961 -1.648001 2.480382
H 9.243996 -1.823042 2.635576
C 4.871509 -3.006656 -0.790551
H 4.894725 -3.428435 -1.789987
C 1.526831 -2.113662 2.602946
H 0.489940 -2.376419 2.776478
C 4.687660 0.938942 4.642663
H 4.671765 1.767635 5.344533
O 3.903210 2.269036 -1.767795
H 4.753695 2.744021 -1.874996
H 4.087066 1.348863 -1.299352
O 2.405858 2.815205 -3.806895
H 2.932113 2.572995 -2.972644
H 2.949111 3.273786 -4.494368
O 2.059322 0.999782 0.658339
H 2.390511 1.613024 -0.025414
H 2.861037 0.603649 1.103729
h 4.674979 -3.254299 4.840796
h 9.350336 -3.294481 0.341973
h 7.569805 -3.473075 -1.733649
h 2.272256 -3.864355 -1.660275
h 0.460852 -3.818374 0.513053
h 0.288142 -0.678626 4.739116
h 1.991214 1.404953 5.642630
h 7.299562 1.932112 5.351048
h 9.281928 0.310241 4.387176
h 1.869978 -8.370235 -1.399341
h 5.988800 -7.515657 -0.900007
h -0.753926 4.295202 -3.170246
h -1.550826 0.100944 -1.558896

Conf LW2 -CpdI

C -0.644921 4.215281 -4.272372
H -1.389105 4.874178 -4.726985
H 0.351437 4.639187 -4.456549
C -0.712496 2.857112 -4.974958
O -1.733585 2.566805 -5.662430
O 0.336017 2.062182 -4.875818
H 1.504642 2.468437 -4.171213
C -0.673149 -0.364752 -1.147060
H -0.830062 -1.442813 -0.983801
O -0.437027 0.309115 0.121523
H 0.552935 0.410303 0.297044
C 0.505964 -0.199023 -2.121981
H 1.403997 -0.648142 -1.686780
H 0.310853 -0.684728 -3.086091
H 0.720040 0.852288 -2.333529
N 2.685396 -8.498888 -0.835000
H 2.791165 -9.402687 -0.385202
C 3.717931 -7.506050 -0.627879
H 3.661366 -6.720262 -1.396577
C 3.583141 -6.745802 0.763019
H 4.432799 -6.060127 0.886897
H 2.684762 -6.125756 0.686358
C 3.484811 -7.674854 1.948102
C 4.632849 -8.093085 2.644959
H 5.608903 -7.705003 2.367471
C 4.528018 -9.007304 3.702487
H 5.419848 -9.316555 4.237936
C 3.277030 -9.522046 4.071667
H 3.198740 -10.252382 4.869595
C 2.231397 -8.171394 2.353071
H 1.339239 -7.836149 1.835573
C 2.124686 -9.091404 3.400269
H 1.153721 -9.476064 3.693984
C 5.110314 -8.148940 -0.777625
O 5.252900 -9.388547 -0.734171
S 4.985653 -3.478635 3.615562
H 4.955882 0.901357 -0.027574
O 4.717195 0.168309 1.481381
O 5.099134 1.343513 -0.902761
FE 4.806873 -1.277942 2.334552
N 6.273633 -2.099904 1.249949
N 3.458468 -2.224508 1.210238
N 3.367093 -0.695436 3.585734
N 6.175874 -0.548221 3.581500
C 7.616500 -2.252130 1.596798
C 8.340504 -2.903788 0.508458
C 7.442166 -3.046417 -0.529450
C 6.147983 -2.594493 -0.028514
C 3.665191 -2.708565 -0.066885
C 2.442776 -3.322167 -0.579194
C 1.514545 -3.292998 0.450287
C 2.155142 -2.534507 1.538927
C 2.055453 -1.132917 3.602784
C 1.282790 -0.372724 4.578494
C 2.126617 0.603420 5.090568
C 3.447913 0.339373 4.498449
C 5.940656 0.508515 4.459535
C 7.205557 1.018311 4.964785
C 8.197993 0.220000 4.433206
C 7.543253 -0.744928 3.561386
C 8.184554 -1.657095 2.712676
H 9.237812 -1.842201 2.883175
C 4.919406 -2.783629 -0.670337
H 4.960579 -3.142618 -1.693726
C 1.535373 -2.059985 2.700301
H 0.498389 -2.336136 2.851754
C 4.671583 0.937573 4.833743
H 4.646037 1.782602 5.515439
O 2.846883 2.827561 -1.318516

H 2.589938 3.703145 -0.973117
H 4.291547 1.857822 -1.159657
O 2.416209 2.780338 -3.724784
H 2.653525 2.794655 -2.396708
H 2.973644 3.257712 -4.383254
O 2.051652 0.995538 0.496459
H 2.312418 1.640114 -0.224508
H 2.845048 0.609887 0.928984
h 4.624013 -3.325553 4.938486
h 9.367105 -3.267836 0.548779
h 7.618794 -3.364010 -1.557071
h 2.355191 -3.682555 -1.604141
h 0.527712 -3.744126 0.553772
h 0.247807 -0.624452 4.809817
h 1.943372 1.462819 5.735488
h 7.286363 1.908974 5.587887
h 9.274705 0.323196 4.567773
h 1.870324 -8.369974 -1.399810
h 5.991470 -7.524873 -0.926525
h -0.781872 4.256027 -3.191794
h -1.565340 0.078746 -1.589068

Conf LW3 –RC-

C 4.613350 4.525950 -0.900430
H 4.640099 5.566538 -1.225963
H 5.557086 4.291817 -0.395653
C 4.466424 3.644927 -2.120621
O 4.009255 4.077808 -3.201790
O 4.863570 2.372882 -2.026093
H 5.267865 2.007276 -1.099550
C 0.972724 0.304157 -1.268932
H 0.203325 -0.383647 -1.649920
O 0.957527 0.331714 0.184726
H 1.239279 -0.555085 0.531228
C 2.316897 -0.151192 -1.848913
H 2.524701 -1.183608 -1.549301
H 2.306047 -0.132527 -2.945126
H 3.146679 0.475213 -1.512486
N -3.347020 -7.969678 -2.174464
H -3.330484 -8.870158 -2.629847
C -2.705851 -7.861794 -0.876488
H -2.019811 -6.998552 -0.822492
C -3.726905 -7.673870 0.318640
H -3.137593 -7.396063 1.195730
H -4.340568 -6.801419 0.062693
C -4.610435 -8.863121 0.629197
C -4.325176 -9.709419 1.715359
H -3.450012 -9.524551 2.330024
C -5.148459 -10.798281 2.017324
H -4.914325 -11.425934 2.870579
C -6.272847 -11.068615 1.230578
H -6.916333 -11.908174 1.473606
C -5.746805 -9.145196 -0.148008
H -5.980497 -8.499130 -0.984809
C -6.566182 -10.241409 0.139886
H -7.435228 -10.440143 -0.481333
C -1.843061 -9.121915 -0.697948
O -1.936523 -10.038579 -1.542267
S -0.522311 -7.242306 2.663101
H 0.914809 -3.004956 3.464763
O 2.466440 -4.169308 3.143061
O 1.880887 -2.747567 3.345026
Fe 0.987943 -5.472226 2.903345
N 2.450115 -6.774210 2.445487
N 0.870701 -4.936421 0.950926
N -0.478552 -4.103190 3.341463
N 1.144747 -5.887643 4.837960
C 2.978417 -7.729247 3.294560
C 3.974483 -8.539785 2.592597
C 4.020891 -8.065032 1.299139
C 3.066036 -6.961961 1.220223
C 1.798489 -5.239732 -0.035338
C 1.438271 -4.567424 -1.274406
C 0.212343 -3.940474 -1.065444
C -0.127532 -4.182748 0.344634
C -1.422172 -3.663463 2.411034
C -2.525610 -2.994929 3.088644
C -2.222209 -2.966969 4.441434
C -0.993845 -3.754051 4.595267
C 0.489146 -5.276042 5.892232
C 0.827638 -5.944767 7.143650
C 1.692132 -6.968298 6.819660
C 1.873107 -6.939753 5.375106
C 2.666476 -7.820663 4.644749
H 3.107222 -8.661971 5.163830
C 2.811952 -6.185689 0.096407
H 3.411488 -6.394244 -0.782894
C -1.256456 -3.734061 1.034791
H -2.085711 -3.372510 0.447815
C -0.451339 -4.249561 5.777051
H -0.881117 -3.897067 6.710120
O 2.205684 -1.947258 0.947825
H 2.011122 -2.259695 1.916376
H 1.878419 -2.595841 0.289944
O 3.826104 0.127619 1.353266
H 3.312949 -0.667484 1.034765
H 3.178484 0.817237 1.628875
O 5.663155 1.443246 0.086479
H 4.966290 0.876272 0.550581
H 6.574025 1.077778 0.227689
h -1.628147 -7.117653 3.479149
h 4.655501 -9.251105 3.059828
h 4.628129 -8.412746 0.463422
h 2.069921 -4.552081 -2.162578
h -0.325417 -3.420928 -1.858510
h -3.424039 -2.673170 2.561992
h -2.699116 -2.468583 5.285375
h 0.398236 -5.652452 8.101894
h 2.293500 -7.591384 7.481616
h -3.676460 -7.171593 -2.678945
h -1.151766 -9.247195 0.135407
h 3.837234 4.432887 -0.140791
h 0.751204 1.324951 -1.580343

Conf LW3 -TSoo

C 4.609949 4.522038 -0.906289
H 4.638528 5.561236 -1.236223
H 5.554631 4.287963 -0.402953
C 4.459110 3.635682 -2.122405
O 4.014254 4.069886 -3.208371
O 4.838210 2.359219 -2.019060
H 5.233625 1.989475 -1.089963
C 0.959369 0.279742 -1.203008
H 0.184215 -0.407488 -1.574362
O 0.930706 0.344394 0.247822
H 1.196307 -0.530039 0.641237
C 2.303850 -0.211105 -1.754901
H 2.489083 -1.236490 -1.416174
H 2.306945 -0.227415 -2.851302
H 3.137882 0.414923 -1.428519
N -3.347265 -7.970788 -2.176623
H -3.331728 -8.870368 -2.633888
C -2.704154 -7.866079 -0.879888
H -2.016884 -7.003907 -0.825246
C -3.723789 -7.679102 0.316559
H -3.133106 -7.402240 1.192820
H -4.337499 -6.806245 0.061911
C -4.607749 -8.867817 0.627964
C -4.324373 -9.711890 1.716340
H -3.448941 -9.527258 2.330673
C -5.149624 -10.798510 2.020895
H -4.917369 -11.423908 2.876329
C -6.273881 -11.069238 1.234128
H -6.918896 -11.907044 1.479147
C -5.743609 -9.150692 -0.149726
H -5.975353 -8.506915 -0.988829
C -6.564752 -10.244940 0.140564
H -7.433216 -10.444517 -0.481160
C -1.842458 -9.127540 -0.705841
O -1.939183 -10.043383 -1.550201
S -0.517471 -7.269617 2.645225
H 1.112785 -2.876504 3.806809
O 2.426665 -4.420506 2.988867
O 2.053445 -2.628380 3.633162
Fe 1.038300 -5.468794 2.857807
N 2.422658 -6.870702 2.373378
N 0.865662 -4.998099 0.883910
N -0.448243 -4.176294 3.278669
N 1.170791 -5.940594 4.783315
C 2.969552 -7.806329 3.232030
C 3.976988 -8.602416 2.531606
C 4.017409 -8.130521 1.236690
C 3.044386 -7.044197 1.149810
C 1.789460 -5.310420 -0.103738
C 1.430645 -4.632936 -1.340987
C 0.211871 -3.998882 -1.130949
C -0.126673 -4.238219 0.279332
C -1.387087 -3.718184 2.357637

C -2.470031 -3.021861 3.043456
C -2.147450 -2.984118 4.389300
C -0.926801 -3.789532 4.532211
C 0.542052 -5.308626 5.838015
C 0.887850 -5.967329 7.090991
C 1.738360 -7.002904 6.767047
C 1.898818 -6.992776 5.318878
C 2.675465 -7.884985 4.586481
H 3.126636 -8.716913 5.110947
C 2.791949 -6.266500 0.025993
H 3.391518 -6.475176 -0.853056
C -1.245562 -3.787723 0.979112
H -2.077708 -3.414491 0.404318
C -0.379994 -4.269579 5.718284
H -0.788705 -3.889861 6.649424
O 2.117149 -1.895754 1.219375
H 2.047716 -2.169457 2.242167
H 1.755258 -2.608366 0.656227
O 3.800385 0.134253 1.401482
H 3.259827 -0.668213 1.147925
H 3.169462 0.845233 1.662566
O 5.624859 1.418470 0.093525
H 4.929909 0.852981 0.563753
H 6.536829 1.055136 0.233084
h -1.620156 -7.134343 3.463841
h 4.665395 -9.304232 3.002368
h 4.636419 -8.466281 0.404729
h 2.072929 -4.597401 -2.220915
h -0.324822 -3.470654 -1.918985
h -3.369797 -2.690643 2.525012
h -2.610672 -2.478737 5.236697
h 0.464558 -5.659845 8.047204
h 2.344978 -7.619916 7.429902
h -3.676593 -7.171723 -2.679623
h -1.148520 -9.254181 0.125109
h 3.835779 4.433274 -0.144155
h 0.751646 1.294823 -1.541428

Conf LW3 –IC1

C 4.605536 4.532659 -0.917689
H 4.622322 5.575268 -1.238599
H 5.550565 4.304378 -0.412693
C 4.472271 3.654050 -2.144377
O 3.999658 4.095588 -3.219678
O 4.900178 2.398430 -2.062139
H 5.338464 2.019303 -1.115979
C 0.970162 0.291664 -1.218242
H 0.218294 -0.405257 -1.627107
O 0.916024 0.328933 0.222680
H 1.399212 -0.471714 0.630500
C 2.330985 -0.153148 -1.777469
H 2.552418 -1.170871 -1.442592
H 2.332790 -0.159599 -2.874216
H 3.146393 0.491975 -1.440192
N -3.348431 -7.974076 -2.182627
H -3.330087 -8.868852 -2.649413
C -2.702919 -7.879975 -0.888468
H -2.013336 -7.019280 -0.830050
C -3.719346 -7.697984 0.310743
H -3.127048 -7.427344 1.187962
H -4.332306 -6.822996 0.060838
C -4.605216 -8.885491 0.620654
C -4.320177 -9.732149 1.706603
H -3.440316 -9.552019 2.316193
C -5.149477 -10.814812 2.013954
H -4.916773 -11.442080 2.867899
C -6.278624 -11.079087 1.231989
H -6.926733 -11.913723 1.479324
C -5.745622 -9.161795 -0.152542
H -5.978689 -8.515457 -0.989326
C -6.570337 -10.252649 0.140238
H -7.442425 -10.447491 -0.477760
C -1.836920 -9.141117 -0.730244
O -1.922494 -10.044383 -1.587403
S -0.565345 -7.356965 2.642700
H 1.234096 -2.633490 3.692181
O 2.513419 -4.612155 2.800556
O 2.117796 -2.224010 3.690964
Fe 1.166119 -5.595036 2.687349
N 2.450298 -7.076291 2.234583
N 0.956735 -5.195452 0.715399
N -0.339607 -4.292073 3.082705
N 1.251414 -6.058400 4.626539
C 3.015518 -7.979577 3.119794
C 4.059699 -8.753575 2.453141
C 4.126025 -8.282572 1.158605
C 3.121373 -7.232565 1.042074
C 1.893728 -5.497593 -0.260624
C 1.557308 -4.816006 -1.503505
C 0.345581 -4.172010 -1.301288
C -0.007444 -4.423610 0.100882
C -1.283739 -3.857166 2.164345
C -2.363773 -3.139434 2.832617
C -2.028849 -3.063865 4.173560
C -0.796475 -3.855037 4.315960
C 0.644888 -5.375724 5.667908
C 0.965359 -6.008120 6.939051
C 1.789179 -7.073806 6.645407
C 1.952577 -7.100741 5.197595
C 2.722881 -8.017182 4.476867
H 3.184475 -8.824845 5.028618
C 2.895349 -6.445922 -0.091277
H 3.551956 -6.628041 -0.934313
C -1.140993 -3.976451 0.788473
H -1.980934 -3.646683 0.195789
C -0.238228 -4.312463 5.511388
H -0.615549 -3.878085 6.431814
O 2.419627 -1.599976 1.133039
H 2.290521 -1.972722 2.724781
H 2.223351 -2.323751 0.508511
O 3.986650 0.279063 1.327133
H 3.410366 -0.584445 1.091000
H 3.346466 0.953126 1.650694
O 5.737422 1.502979 0.015067
H 5.018535 0.955227 0.528412
H 6.645735 1.134982 0.150425
h -1.655848 -7.171256 3.467723
h 4.740605 -9.451046 2.940961
h 4.784008 -8.586273 0.344423
h 2.220207 -4.768526 -2.367437
h -0.179239 -3.603064 -2.068707
h -3.257860 -2.809477 2.303653
h -2.494155 -2.549769 5.014548
h 0.535950 -5.668862 7.881695
h 2.362612 -7.696724 7.331857
h -3.677087 -7.172150 -2.681499
h -1.146519 -9.275330 0.102462
h 3.830785 4.429699 -0.157934
h 0.749792 1.304173 -1.556370

Conf LW3 -CpdI

C 4.558884 4.634359 -1.014705
H 4.454202 5.655388 -1.390416
H 5.536239 4.537332 -0.530095
C 4.500312 3.657732 -2.184999
O 3.941123 4.016842 -3.274315
O 5.067751 2.495685 -2.022722
H 6.011240 2.324927 -0.853324
C 0.792179 0.206840 -0.953286
H -0.077476 -0.018523 -0.322553
O 1.918196 0.118215 -0.051252
H 2.757094 -0.207507 -0.531265
C 0.898730 -0.827740 -2.080677
H 1.040582 -1.818207 -1.643193
H -0.007274 -0.852682 -2.698115
H 1.754987 -0.625243 -2.735222
N -3.348469 -7.971912 -2.178235
H -3.334826 -8.870225 -2.637953
C -2.712432 -7.870531 -0.879260
H -2.026498 -7.007027 -0.820763
C -3.738093 -7.688361 0.312764
H -3.154055 -7.410826 1.193641
H -4.353639 -6.817475 0.055362
C -4.620211 -8.879878 0.618783
C -4.331561 -9.732267 1.699555
H -3.452254 -9.554281 2.310181
C -5.156632 -10.819462 2.001462
H -4.920656 -11.450521 2.851635
C -6.285264 -11.083367 1.218774
H -6.929943 -11.921705 1.462044
C -5.760004 -9.156297 -0.155040
H -5.996712 -8.506014 -0.987636
C -6.580568 -10.251868 0.131886
H -7.452267 -10.446163 -0.486738
C -1.846075 -9.128731 -0.705715
O -1.932185 -10.041732 -1.553191
S -0.553754 -7.286193 2.678506
H 1.916456 -2.309401 2.412375
O 2.106521 -4.116327 3.118150

O 2.392189 -1.497143 2.143212
Fe 1.020751 -5.356194 2.854255
N 2.432396 -6.728096 2.422350
N 0.792992 -5.005081 0.882310
N -0.577365 -4.205564 3.223951
N 1.101826 -5.868648 4.775606
C 2.964412 -7.683541 3.273747
C 4.014738 -8.441378 2.600208
C 4.122105 -7.908700 1.331344
C 3.122636 -6.851186 1.236518
C 1.743511 -5.259765 -0.084153
C 1.301955 -4.750258 -1.373579
C 0.006980 -4.279639 -1.208410
C -0.280867 -4.414618 0.228599
C -1.520149 -3.793713 2.306279
C -2.576435 -3.032114 2.966845
C -2.214815 -2.911646 4.298789
C -0.996083 -3.721352 4.452854
C 0.467413 -5.216205 5.816944
C 0.789661 -5.860902 7.081263
C 1.633141 -6.910740 6.778193
C 1.815612 -6.908392 5.336820
C 2.617877 -7.793833 4.611866
H 3.054726 -8.632741 5.137567
C 2.852505 -6.081908 0.105626
H 3.521126 -6.213090 -0.737909
C -1.406906 -3.980616 0.926656
H -2.276173 -3.704240 0.354416
C -0.434963 -4.164521 5.651152
H -0.824975 -3.737977 6.570435
O 4.202659 -0.646705 -0.974601
H 1.971763 -0.991235 1.406562
H 4.416119 -0.305786 -1.872447
O 4.702442 0.745062 1.095903
H 4.574345 -0.062554 -0.218290
H 3.816454 1.028183 1.397855
O 6.423964 2.197683 0.081599
H 5.356517 1.500608 0.792227
H 7.235675 1.635598 0.118206
h -1.668940 -7.163340 3.482005
h 4.676893 -9.165682 3.074550
h 4.795467 -8.184267 0.519733
h 1.980011 -4.697892 -2.225380
h -0.598824 -3.907068 -2.034399
h -3.478122 -2.707927 2.447298
h -2.649739 -2.351165 5.126296
h 0.360933 -5.544902 8.032264
h 2.208772 -7.546711 7.450693
h -3.676988 -7.171841 -2.680165
h -1.156427 -9.253552 0.129073
h 3.824014 4.493693 -0.222086
h 0.703213 1.209323 -1.371831

Conf LW3 –RC1-
C 4.629092 4.503001 -0.876787
H 4.666867 5.540726 -1.210294
H 5.566695 4.265090 -0.361935
C 4.484182 3.613699 -2.090762
O 4.036127 4.043206 -3.177270
O 4.868099 2.337136 -1.986305
H 5.269984 1.961422 -1.065206
C 0.956472 0.258753 -1.200548
H 0.212639 -0.429098 -1.627484
O 0.841934 0.306371 0.250006
H 1.023615 -0.589962 0.632691
C 2.336049 -0.226376 -1.652981
H 2.491140 -1.248375 -1.284116
H 2.415656 -0.262764 -2.745395
H 3.145470 0.407938 -1.281365
N -3.345317 -7.969243 -2.174759
H -3.329789 -8.870128 -2.629410
C -2.697374 -7.859206 -0.880088
H -2.007627 -6.998432 -0.832416
C -3.712564 -7.664851 0.319083
H -3.117980 -7.389966 1.193455
H -4.323295 -6.789675 0.065700
C -4.598960 -8.850995 0.633018
C -4.316327 -9.694253 1.722292
H -3.442695 -9.507041 2.338529
C -5.139989 -10.782747 2.024823
H -4.907699 -11.408619 2.879870
C -6.262593 -11.054979 1.236149
H -6.906311 -11.894374 1.479181
C -5.733731 -9.134805 -0.145900
H -5.964471 -8.491583 -0.985636
C -6.553885 -10.230078 0.143173
H -7.421649 -10.430411 -0.479335
C -1.839267 -9.122435 -0.700736
O -1.939267 -10.041494 -1.541565
S -0.500241 -7.234018 2.644496
H 1.190051 -3.150516 3.933972
O 2.595609 -4.258275 3.108802
O 2.157616 -2.955565 3.821309
Fe 1.043142 -5.493355 2.870026
N 2.473184 -6.818033 2.395402
N 0.941202 -4.929982 0.919225
N -0.401743 -4.117601 3.326428
N 1.198653 -5.911408 4.814547
C 3.006669 -7.765330 3.251452
C 4.010810 -8.568986 2.553796
C 4.064669 -8.090375 1.261790
C 3.099179 -6.996882 1.174964
C 1.845569 -5.261328 -0.082179
C 1.464295 -4.611031 -1.326228
C 0.248176 -3.974826 -1.110156
C -0.064203 -4.178086 0.311518
C -1.324655 -3.641246 2.400301
C -2.420620 -2.958886 3.080051
C -2.124269 -2.951052 4.433305
C -0.909530 -3.760615 4.580705
C 0.548607 -5.305182 5.874529
C 0.886301 -5.980297 7.122562
C 1.747563 -7.004355 6.790654
C 1.922056 -6.968835 5.343722
C 2.703595 -7.852927 4.603886
H 3.146123 -8.693834 5.121770
C 2.848099 -6.219098 0.049591
H 3.443117 -6.436464 -0.830384
C -1.170073 -3.705969 1.020054
H -1.997756 -3.319337 0.448602
C -0.379896 -4.269151 5.764012
H -0.808428 -3.916819 6.697441
O 7.613523 -0.089249 0.896973
H 7.137771 -0.599924 1.618886
H 8.299943 -0.613300 0.436099
O 5.906939 -1.130664 2.640264
H 5.511187 -2.028853 2.402989
H 5.163605 -0.501790 2.483802
O 4.452638 -3.153185 1.659781
H 3.970643 -2.742281 0.917073
H 3.748650 -3.612101 2.252899
O 5.665178 1.350624 0.115837
H 4.933673 0.880109 0.583696
H 6.550094 0.866907 0.300007
h -1.598279 -7.103877 3.470161
h 4.688083 -9.281043 3.025329
h 4.688065 -8.425195 0.432731
h 2.090472 -4.597842 -2.218301
h -0.305092 -3.478220 -1.907240
h -3.318205 -2.627901 2.557694
h -2.599951 -2.460272 5.282379
h 0.453606 -5.690086 8.079964
h 2.360241 -7.620429 7.448791
h -3.675990 -7.171515 -2.678999
h -1.145600 -9.247754 0.130641
h 3.845078 4.422790 -0.123823
h 0.755926 1.277120 -1.533377

Conf LW3 -TShooh
C 4.605491 4.511392 -0.926058
H 4.622719 5.542103 -1.286451
H 5.554629 4.304337 -0.416524
C 4.473167 3.560370 -2.112809
O 4.036505 4.013553 -3.220575
O 4.831059 2.319929 -1.936095
H 5.512149 1.760040 -0.699416
C 0.989470 0.310695 -1.367003
H 0.262259 -0.374704 -1.826431
O 0.881525 0.254815 0.090488
H 1.133165 -0.660281 0.372918
C 2.377799 -0.080214 -1.869583
H 2.606497 -1.105366 -1.552185
H 2.412734 -0.073299 -2.964819
H 3.167725 0.589972 -1.518266
N -3.346299 -7.970825 -2.176035
H -3.333779 -8.870645 -2.632866
C -2.699839 -7.865436 -0.881596
H -2.012062 -7.003083 -0.830327
C -3.716868 -7.678238 0.317674

H -3.125606 -7.404093 1.194998
H -4.328359 -6.803140 0.065971
C -4.602687 -8.865468 0.630268
C -4.323885 -9.706158 1.722376
H -3.451859 -9.518930 2.341006
C -5.150275 -10.791948 2.026964
H -4.922110 -11.415309 2.884898
C -6.271934 -11.064027 1.237090
H -6.917973 -11.900773 1.482515
C -5.736392 -9.149344 -0.150195
H -5.965518 -8.508212 -0.991979
C -6.559213 -10.242059 0.140768
H -7.426411 -10.442584 -0.482155
C -1.838827 -9.127354 -0.706483
O -1.940448 -10.047375 -1.544700
S -0.484655 -7.258708 2.655855
H 0.937435 -2.987769 3.426175
O 2.575244 -4.005387 3.225188
O 1.874936 -2.641721 3.301138
Fe 1.007977 -5.510114 2.868913
N 2.499503 -6.781144 2.432289
N 0.938006 -4.964377 0.918772
N -0.427276 -4.126385 3.293918
N 1.188187 -5.880391 4.809276
C 3.025223 -7.733249 3.291153
C 4.026819 -8.543997 2.602226
C 4.084881 -8.075722 1.306658
C 3.125413 -6.981542 1.210753
C 1.854622 -5.290097 -0.078280
C 1.479761 -4.650201 -1.328883
C 0.263062 -4.009494 -1.117611
C -0.068800 -4.225674 0.297307
C -1.372120 -3.696585 2.355447
C -2.476793 -3.024506 3.022174
C -2.176759 -2.978842 4.376331
C -0.949821 -3.760288 4.544481
C 0.527113 -5.264179 5.860810
C 0.856092 -5.927395 7.115910
C 1.717615 -6.956169 6.801373
C 1.907235 -6.935114 5.358653
C 2.703958 -7.820038 4.638515
H 3.140968 -8.658566 5.164065
C 2.871279 -6.227551 0.073056
H 3.478740 -6.450852 -0.795526
C -1.202460 -3.780196 0.981034
H -2.035806 -3.439523 0.386825
C -0.411806 -4.240077 5.733840
H -0.845995 -3.879326 6.661123
O 7.513731 -0.268744 1.098214
H 6.587272 -0.927053 1.974440
H 8.229144 -0.689183 0.583424
O 5.768024 -1.226369 2.584004
H 5.052664 -2.366962 2.195515
H 5.056000 -0.548308 2.489906
O 4.366302 -3.110509 1.777661
H 3.828854 -2.709840 1.057456
H 3.509967 -3.641653 2.529927
O 5.790860 1.291468 0.177768
H 4.987015 0.898260 0.589470
H 6.969136 0.458212 0.596149
h -1.587789 -7.117763 3.472907
h 4.696878 -9.262122 3.074860
h 4.708536 -8.416923 0.480399
h 2.107847 -4.635717 -2.219593
h -0.274980 -3.477335 -1.902076
h -3.372839 -2.706577 2.489174
h -2.658086 -2.471215 5.212217
h 0.425192 -5.628149 8.071338
h 2.308003 -7.581905 7.470673
h -3.676180 -7.172110 -2.679229
h -1.140595 -9.251028 0.121312
h 3.834546 4.434724 -0.159356
h 0.752913 1.340480 -1.634680

Conf LW3 –FeRS

C 4.605453 4.509045 -0.926026
H 4.627371 5.543863 -1.274479
H 5.553013 4.290845 -0.418542
C 4.469770 3.571545 -2.123906
O 4.016021 4.034141 -3.221821
O 4.843485 2.334450 -1.965411
H 5.600652 1.783985 -0.740962
C 1.003975 0.318582 -1.413581
H 0.258862 -0.364592 -1.846475
O 0.967022 0.236430 0.046520
H 1.272978 -0.671102 0.295389
C 2.367960 -0.052349 -1.990341
H 2.621583 -1.083039 -1.713802
H 2.349792 -0.015682 -3.085999
H 3.170133 0.614051 -1.659192
N -3.347515 -7.970821 -2.175660
H -3.338060 -8.871363 -2.631144
C -2.701599 -7.865415 -0.881487
H -2.013222 -7.003368 -0.830480
C -3.718038 -7.676526 0.318589
H -3.126511 -7.401911 1.195838
H -4.329219 -6.801310 0.066432
C -4.603749 -8.863427 0.632393
C -4.325634 -9.701772 1.726415
H -3.454781 -9.512164 2.346195
C -5.150813 -10.788364 2.031504
H -4.922940 -11.409904 2.890864
C -6.270664 -11.063404 1.239999
H -6.915984 -11.900854 1.485001
C -5.735850 -9.149962 -0.149377
H -5.964294 -8.510242 -0.992356
C -6.557404 -10.243532 0.142030
H -7.423089 -10.446135 -0.482347
C -1.842146 -9.128173 -0.706527
O -1.947474 -10.049793 -1.542158
S -0.493068 -7.262125 2.657334
H 0.850492 -2.956257 3.224298
O 2.550524 -3.861851 3.230369
O 1.775245 -2.553742 3.110152
Fe 0.976124 -5.506419 2.855066
N 2.484683 -6.753689 2.419840
N 0.913208 -4.939631 0.916027
N -0.442199 -4.106961 3.279818
N 1.188599 -5.853045 4.792753
C 3.015861 -7.707117 3.274975
C 4.014275 -8.517005 2.581519
C 4.069002 -8.044996 1.286899
C 3.108756 -6.951659 1.195612
C 1.838345 -5.250307 -0.078548
C 1.472570 -4.590357 -1.321187
C 0.249953 -3.959937 -1.111411
C -0.091512 -4.197235 0.295961
C -1.403767 -3.689350 2.347839
C -2.504436 -3.023196 3.022057
C -2.190508 -2.967648 4.373566
C -0.956289 -3.736621 4.534708
C 0.530802 -5.233889 5.846621
C 0.857635 -5.898554 7.100616
C 1.714219 -6.931607 6.785583
C 1.904831 -6.910715 5.343967
C 2.700052 -7.795519 4.623217
H 3.139990 -8.633093 5.147869
C 2.853823 -6.190527 0.063155
H 3.459100 -6.405359 -0.809596
C -1.233528 -3.766176 0.974130
H -2.066557 -3.426010 0.379389
C -0.406909 -4.208924 5.720995
H -0.834919 -3.844779 6.649737
O 7.694460 -0.190767 1.052993
H 6.748234 -0.803838 2.013606
H 8.347095 -0.675114 0.508997
O 5.952599 -1.062081 2.645088
H 5.159042 -2.338000 2.222960
H 5.213667 -0.432860 2.467042
O 4.509590 -3.032294 1.806795
H 3.977186 -2.603320 1.099850
H 3.390397 -3.609728 2.653191
O 5.911761 1.330018 0.125925
H 5.123917 0.923576 0.555567
H 7.140952 0.510962 0.543805
h -1.592051 -7.114256 3.478746
h 4.685688 -9.234635 3.052984
h 4.694024 -8.379980 0.459131
h 2.100892 -4.569637 -2.211607
h -0.285704 -3.425152 -1.895721
h -3.405994 -2.712944 2.493850
h -2.669432 -2.460597 5.211180
h 0.422906 -5.603834 8.055716
h 2.291376 -7.568100 7.456278
h -3.676556 -7.171983 -2.679209
h -1.141719 -9.251258 0.119499
h 3.833378 4.427742 -0.160940
h 0.753641 1.350765 -1.658522

Conf LM1–RC-

C 2.367306 4.354233 -7.347954
H 2.290212 5.439831 -7.460219
H 3.436957 4.126644 -7.419326
C 1.715677 3.721246 -8.562044
O 1.847520 4.251947 -9.687868
O 1.039538 2.554762 -8.491683
H 0.903898 2.025253 -7.612888
C -0.507047 1.573202 -1.947125
H -1.164735 0.757962 -1.613303
O -0.415894 2.610710 -0.928292
H -0.340647 2.202478 -0.039803
C 0.876785 1.007330 -2.287602
H 1.281355 0.477002 -1.420380
H 0.828309 0.302163 -3.125511
H 1.577966 1.809375 -2.542031
N -3.972986 -5.119365 4.199493
H -4.706179 -5.196096 4.895862
C -2.678487 -4.522005 4.593758
H -2.079009 -4.299149 3.697357
C -2.869695 -3.184760 5.356353
H -3.359811 -3.418999 6.312346
H -1.869066 -2.835231 5.624085
N -3.113885 -0.774147 4.654575
H -2.132281 -0.541288 4.855512
C -3.618334 -2.072934 4.678226
C -4.077549 0.058508 4.152118
H -3.929633 1.116252 4.014340
N -5.191188 -0.620276 3.855185
C -4.898099 -1.951658 4.166173
H -5.600515 -2.726028 3.944400
C -1.823251 -5.481199 5.487343
O -1.094253 -5.006179 6.380058
S 0.103354 -0.659304 5.204287
H 1.982593 0.838568 0.878266
O 2.904722 -0.598067 1.860940
O 2.525054 0.089945 0.535859
Fe 1.592474 -0.469126 3.276188
N 1.904733 -2.416855 3.605125
N -0.039986 -0.859789 2.092189
N 1.274636 1.525296 2.949957
N 3.156206 -0.049128 4.443421
C 2.711270 -2.992796 4.580650
C 2.546631 -4.445836 4.564417
C 1.663281 -4.733929 3.550270
C 1.224211 -3.455343 2.995879
C -0.469529 -2.123076 1.732357
C -1.752922 -2.038060 1.036186
C -2.118877 -0.701536 0.992559
C -1.031970 0.024481 1.673328
C 0.107600 2.099380 2.468308
C 0.202190 3.550185 2.506448
C 1.448452 3.868921 3.033771
C 2.106987 2.587042 3.323995
C 3.791135 1.180962 4.516135
C 4.928948 1.096842 5.430431
C 4.926857 -0.184140 5.948887
C 3.842737 -0.905415 5.292104
C 3.586815 -2.273557 5.386923
H 4.172649 -2.836890 6.105377
C 0.170995 -3.307244 2.095776
H -0.267595 -4.229973 1.732847
C -0.971723 1.389840 1.937277
H -1.853138 1.981157 1.741854
C 3.341106 2.367646 3.932234
H 4.025645 3.199302 4.012795
O 0.480025 -1.123402 -5.193564
H 0.831071 -1.597443 -4.386772
H -0.464289 -1.390634 -5.319166
O 0.297860 1.021514 -6.614526
H -0.638803 1.264688 -6.435902
H 0.593006 0.290749 -5.977392
O 3.679835 -3.191080 1.030318
H 4.618707 -2.926353 0.856222
H 3.300803 -2.506997 1.641071
O 2.159819 -2.227934 -0.853136
H 2.664223 -2.815118 -0.203579
H 2.014975 -1.360410 -0.398290
O 0.974912 -2.674040 -3.057734
H 1.410946 -2.517909 -2.137561
H 1.015374 -3.615868 -3.299020
h 0.334793 0.417371 6.035884
h 2.989623 -5.129489 5.288601
h 1.310501 -5.698927 3.186413
h -2.326366 -2.902260 0.700947
h -3.050759 -0.349893 0.549829
h -0.602077 4.206726 2.174520
h 1.773621 4.898472 3.183292
h 5.608514 1.924227 5.634613
h 5.547644 -0.584085 6.750594
h -4.096408 -5.585726 3.323567
h -1.922924 -6.555216 5.330434
h 2.050448 4.079457 -6.341890
h -0.941508 2.031768 -2.835397

Conf LM1 -TSoo

C 2.369784 4.354307 -7.352235
H 2.297346 5.440159 -7.465366
H 3.438457 4.122301 -7.422284
C 1.716857 3.721803 -8.566172
O 1.850130 4.253502 -9.692074
O 1.041929 2.555861 -8.496238
H 0.904621 2.020696 -7.617113
C -0.504867 1.559529 -2.009013
H -1.157546 0.744410 -1.665298
O -0.393381 2.591033 -0.982778
H -0.046312 2.196761 -0.157315
C 0.863908 0.994905 -2.397426
H 1.313473 0.476298 -1.545321
H 0.779726 0.279713 -3.223729
H 1.556398 1.792328 -2.689609
N -3.970066 -5.119239 4.199186
H -4.700387 -5.195511 4.898831
C -2.673888 -4.522457 4.587579
H -2.076262 -4.303349 3.688983
C -2.862133 -3.181950 5.346101
H -3.354253 -3.412129 6.301841
H -1.860857 -2.834530 5.614538
N -3.096061 -0.776511 4.614279
H -2.117181 -0.542507 4.809620
C -3.607824 -2.072282 4.661998
C -4.060561 0.055650 4.109914
H -3.907543 1.109946 3.952876
N -5.180068 -0.621210 3.834931
C -4.891969 -1.949649 4.162391
H -5.601115 -2.722757 3.958239
C -1.815708 -5.478724 5.481715
O -1.080945 -4.999165 6.367373
S 0.147146 -0.657625 5.187374
H 2.406013 0.723971 0.501928
O 2.822904 -0.687114 1.983607
O 2.971324 0.245812 -0.140591
Fe 1.657100 -0.493669 3.209548
N 1.866345 -2.444473 3.627367
N -0.009587 -0.886875 2.088476
N 1.314576 1.501118 2.977616
N 3.156389 -0.057297 4.469548
C 2.685218 -3.012296 4.594105
C 2.535745 -4.468293 4.565974
C 1.664322 -4.760009 3.544040
C 1.216293 -3.484265 2.993752
C -0.448465 -2.145323 1.722584
C -1.722310 -2.045263 1.016632
C -2.074200 -0.705055 0.969356
C -0.983211 0.011414 1.651153
C 0.175838 2.073360 2.438696
C 0.280901 3.525100 2.454795
C 1.508111 3.841865 3.021240
C 2.148225 2.561595 3.345555
C 3.815986 1.160558 4.539326
C 4.950865 1.054884 5.448954
C 4.930312 -0.227641 5.960779
C 3.833018 -0.931188 5.306500
C 3.565937 -2.296694 5.395762
H 4.157428 -2.865651 6.104396
C 0.178155 -3.336389 2.081094
H -0.253966 -4.255152 1.701955
C -0.898500 1.375492 1.889097
H -1.742731 1.989008 1.624523
C 3.381160 2.348270 3.954293
H 4.070806 3.177706 4.022658
O 0.522443 -1.137121 -5.259064
H 0.924507 -1.605489 -4.466694
H -0.422796 -1.416609 -5.339393
O 0.308036 1.024444 -6.625867
H -0.626547 1.267854 -6.439975
H 0.603997 0.273296 -6.006343
O 3.751561 -3.106082 1.008611

H 4.705471 -2.867373 0.891578
H 3.336358 -2.378560 1.550500
O 2.614397 -2.135899 -1.154369
H 2.939625 -2.728184 -0.409836
H 2.586998 -1.198798 -0.777928
O 1.188927 -2.643858 -3.167139
H 1.742407 -2.441324 -2.307867
H 1.310610 -3.572683 -3.431528
h 0.356335 0.416327 6.028334
h 2.979183 -5.151766 5.290055
h 1.318946 -5.725185 3.173612
h -2.298364 -2.905087 0.674681
h -3.004619 -0.351793 0.524843
h -0.513938 4.177894 2.094020
h 1.839365 4.867677 3.182628
h 5.638088 1.875057 5.656573
h 5.546548 -0.633841 6.762852
h -4.095606 -5.585640 3.323582
h -1.918642 -6.553126 5.329625
h 2.051214 4.081369 -6.346211
h -0.954281 2.034470 -2.881094

Conf LM1 -CpdI
C 2.361248 4.424903 -7.467343
H 2.263144 5.511650 -7.570160
H 3.434873 4.219586 -7.560802
C 1.689043 3.766370 -8.682049
O 1.920594 4.310562 -9.817660
O 0.970713 2.686509 -8.559156
H 0.685713 1.768557 -7.343390
C -0.436506 1.727091 -1.921996
H -1.116324 1.019846 -1.440744
O -0.268090 2.812782 -0.950574
H 0.489354 3.381121 -1.220852
C 0.894084 1.033068 -2.230641
H 1.321690 0.615600 -1.314260
H 0.763007 0.222130 -2.957189
H 1.633785 1.727338 -2.651241
N -3.974773 -5.117216 4.198663
H -4.707294 -5.193054 4.896463
C -2.684410 -4.515088 4.589069
H -2.093019 -4.281092 3.689645
C -2.882375 -3.184184 5.361727
H -3.375596 -3.427295 6.313547
H -1.883714 -2.834586 5.637420
N -3.143628 -0.764472 4.699456
H -2.176371 -0.520531 4.930488
C -3.631407 -2.071144 4.686621
C -4.105176 0.065603 4.185895
H -3.970846 1.128251 4.074400
N -5.198875 -0.623094 3.847522
C -4.898237 -1.956445 4.142696
H -5.588886 -2.733758 3.895797
C -1.807886 -5.469379 5.469528
O -1.043718 -4.980153 6.324321
S 0.098702 -0.610797 5.221651
H 3.357231 0.058024 0.179023
O 2.616900 -0.415403 1.869240
O 3.913072 -0.168357 -0.592616
Fe 1.588486 -0.383197 3.189633
N 1.829541 -2.345376 3.580306
N -0.107007 -0.783545 2.119840
N 1.197307 1.609975 3.046329
N 3.102796 0.034595 4.440044
C 2.654412 -2.928177 4.531519
C 2.504364 -4.382770 4.505714
C 1.621747 -4.668334 3.489392
C 1.172954 -3.387503 2.955009
C -0.538770 -2.031409 1.735833
C -1.810943 -1.938963 1.026581
C -2.166265 -0.599962 0.982157
C -1.077855 0.116870 1.668866
C 0.091932 2.180925 2.472341
C 0.204803 3.633759 2.455552
C 1.431011 3.953492 3.017016
C 2.053232 2.672783 3.375686
C 3.750252 1.251674 4.528978
C 4.889528 1.153868 5.428537
C 4.885255 -0.137637 5.929022
C 3.797742 -0.839930 5.266883
C 3.539519 -2.210365 5.332765
H 4.134336 -2.783722 6.035702
C 0.112024 -3.225190 2.068586
H -0.318063 -4.138981 1.673821
C -0.980502 1.476495 1.905759
H -1.803283 2.099785 1.604738
C 3.293717 2.445682 3.950419
H 3.993039 3.268923 3.998282
O 0.457451 -1.062085 -5.295443
H 0.974223 -1.943256 -4.216392
H -0.494633 -1.296025 -5.408476
O 0.284012 1.063751 -6.701642
H -0.652432 1.305786 -6.526376
H 0.634754 -0.192314 -5.795194
O 3.541284 -3.018742 0.790371
H 4.477366 -2.706979 0.673553
H 3.066786 -2.284310 1.247834
O 3.010356 -2.306658 -1.761566
H 3.029878 -2.810512 -0.908395
H 3.462860 -0.868487 -1.155653
O 1.066940 -2.654996 -3.463419
H 2.200102 -2.429209 -2.339874
H 1.251925 -3.533728 -3.839105
h 0.313022 0.453447 6.073589
h 2.951875 -5.069913 5.223791
h 1.271731 -5.630726 3.116087
h -2.367168 -2.805737 0.669673
h -3.094234 -0.249330 0.530497
h -0.583686 4.281791 2.072923
h 1.778464 4.977731 3.152216
h 5.580424 1.972476 5.630057
h 5.510301 -0.548734 6.721728
h -4.096885 -5.585127 3.323380
h -1.922994 -6.544442 5.331478
h 2.065783 4.134485 -6.459164
h -0.885142 2.105097 -2.840639

Conf LM2–RC-
C 0.133878 -2.917021 -6.268890
H -0.188966 -2.544498 -7.242304
H 1.221791 -3.065621 -6.301571
C -0.524497 -4.259214 -6.057962
O -1.259116 -4.772152 -6.944599
O -0.252321 -4.980303 -4.975734
H 0.271260 -4.570236 -4.129082
C -0.951236 -1.335713 -0.195317
H -1.295240 -1.575486 0.818322
O -0.973041 0.101492 -0.415120
H -0.149923 0.497630 -0.040675
C 0.469524 -1.892296 -0.381330
H 1.143170 -1.439228 0.354917
H 0.512819 -2.978644 -0.228717
H 0.865879 -1.663240 -1.376493
N 1.039653 -2.475795 8.887533
H 0.781545 -2.747104 9.823654
C 2.048832 -1.452507 8.783291
H 2.620595 -1.538821 7.854275
C 1.477828 0.048533 8.843578
H 1.560681 0.398857 9.877199
H 2.134596 0.686477 8.238956
N -0.349973 0.656417 7.171698
H 0.234281 1.059470 6.446646
C 0.055742 0.220836 8.430774
C -1.717606 0.672100 7.143229
H -2.274522 0.981753 6.277025
N -2.218530 0.265024 8.313477
C -1.117157 -0.007463 9.125229
H -1.241167 -0.338718 10.142997
C 2.994142 -1.661886 9.996075
O 2.538515 -2.282550 10.979791
S 0.734353 3.182597 5.152178
H 0.970211 2.384158 0.261609
O 2.415153 1.742838 1.418359
O 1.500617 1.550763 0.191362
FE 1.576202 2.518219 2.984286
N 2.904681 1.414480 4.026766
N 0.204236 1.020810 3.067210
N 0.260475 3.628803 1.881120
N 2.904644 4.037874 2.936539
C 4.069970 1.856367 4.621478
C 4.689764 0.763995 5.368591
C 3.909966 -0.360016 5.165524
C 2.767122 0.076952 4.365745
C 0.437871 -0.251945 3.555093
C -0.791616 -1.037289 3.513149
C -1.795246 -0.206778 3.039564
C -1.136420 1.069010 2.713415
C -1.075320 3.323357 1.639445

C -1.723926 4.411693 0.913441
C -0.769834 5.394994 0.708299
C 0.461250 4.900370 1.351131
C 2.782166 5.216566 2.219524
C 3.965538 6.050809 2.409165
C 4.783481 5.385390 3.294556
C 4.116519 4.124384 3.615726
C 4.623799 3.124821 4.434598
H 5.559993 3.335487 4.942207
C 1.643035 -0.696342 4.097065
H 1.677376 -1.728059 4.428383
C -1.694505 2.136929 2.013805
H -2.692841 1.997203 1.627651
C 1.666571 5.592842 1.479188
H 1.740046 6.556638 0.986582
O 4.305048 0.373695 -0.759857
H 3.461775 0.869518 -0.849707
H 4.225310 -0.125251 0.141340
O 2.812718 -2.701108 -3.456639
H 3.533704 -2.072695 -3.102843
H 3.202224 -3.338596 -4.099478
O 4.747856 -1.239528 -2.672146
H 5.625658 -1.647180 -2.601794
H 4.589136 -0.548510 -1.930096
O 0.951252 -4.254475 -2.980918
H 0.529083 -4.515178 -2.133100
H 1.665220 -3.499173 -2.958786
O 3.820745 -0.554328 1.507600
H 3.185248 0.199603 1.695586
H 4.557922 -0.562682 2.164385
h 0.446669 4.532115 5.132517
h 5.500118 0.925089 6.079535
h 4.091751 -1.389756 5.473184
h -0.833315 -2.065944 3.871196
h -2.842989 -0.497201 2.962393
h -2.793198 4.415215 0.701987
h -0.815943 6.363859 0.211065
h 4.146861 6.991305 1.888918
h 5.740790 5.724871 3.690005
h 0.748041 -3.091211 8.155277
h 4.022583 -1.302295 10.028765
h -0.029238 -2.122514 -5.540730
h -1.635241 -1.772064 -0.923191

Conf LM2 –TSoo

C 0.134493 -2.929987 -6.269464
H -0.185026 -2.565605 -7.247124
H 1.223287 -3.072890 -6.294415
C -0.519773 -4.273564 -6.051809
O -1.254862 -4.791553 -6.936666
O -0.245879 -4.988901 -4.967653
H 0.296477 -4.582230 -4.124950
C -0.984367 -1.291875 -0.219678
H -1.346777 -1.495639 0.795388
O -1.005690 0.134808 -0.471930
H -0.081639 0.512587 -0.452642
C 0.431612 -1.879899 -0.347717
H 1.095638 -1.410411 0.385188
H 0.444098 -2.961511 -0.155521
H 0.862400 -1.695947 -1.338039
N 1.043317 -2.480096 8.888240
H 0.780899 -2.747501 9.824247
C 2.055951 -1.460695 8.782956
H 2.633100 -1.552975 7.857436
C 1.477254 0.036167 8.830091
H 1.534879 0.392761 9.863097
H 2.137801 0.678558 8.233661
N -0.339363 0.438071 7.086930
H 0.262022 0.691196 6.314635
C 0.059496 0.183066 8.396191
C -1.707892 0.470991 7.052183
H -2.261906 0.663949 6.150352
N -2.213548 0.240274 8.267016
C -1.116492 0.067338 9.112057
H -1.245771 -0.127852 10.164115
C 2.994967 -1.664377 10.000700
O 2.532680 -2.275737 10.986929
S 0.671009 3.202841 5.151868
H 1.753824 1.850627 0.247551
O 2.344601 1.907265 1.533906
O 1.570444 1.123435 -0.463136
FE 1.611329 2.516804 2.982650
N 2.887898 1.430404 4.110842
N 0.240220 1.016889 3.114843
N 0.272631 3.661551 1.978220
N 2.893693 4.079546 3.020219
C 4.059081 1.880039 4.693276
C 4.697844 0.781439 5.411816
C 3.932728 -0.350096 5.194626
C 2.779200 0.081426 4.414897
C 0.473931 -0.263487 3.584419
C -0.753743 -1.047671 3.526448
C -1.754915 -0.212317 3.058493
C -1.096855 1.065866 2.745675
C -1.033967 3.316289 1.679252
C -1.669938 4.372121 0.895319
C -0.720315 5.357664 0.687500
C 0.489197 4.903620 1.397069
C 2.785441 5.248880 2.286375
C 3.976429 6.068280 2.468875
C 4.786536 5.399768 3.359863
C 4.106711 4.150357 3.694894
C 4.610234 3.147987 4.511565
H 5.554212 3.351095 5.005740
C 1.673927 -0.708572 4.128923
H 1.721805 -1.745837 4.438902
C -1.650944 2.126085 2.039233
H -2.632533 1.968125 1.619435
C 1.683204 5.610123 1.525127
H 1.766843 6.552330 0.996423
O 4.098453 0.117408 -0.885712
H 3.176004 0.497490 -0.957716
H 4.145444 -0.238232 0.069644
O 2.834463 -2.736377 -3.624187
H 3.564280 -2.089838 -3.308108
H 3.222556 -3.415977 -4.224943
O 4.749487 -1.255612 -2.873548
H 5.636813 -1.644376 -2.816416
H 4.519413 -0.671643 -2.044438
O 0.994371 -4.252353 -3.004918
H 0.578962 -4.464558 -2.142434
H 1.715537 -3.498665 -3.045122
O 3.874007 -0.356781 1.571179
H 3.277666 0.433288 1.728180
H 4.637866 -0.360630 2.193500
h 0.410386 4.557983 5.148364
h 5.514028 0.937811 6.117122
h 4.131525 -1.383198 5.479664
h -0.797083 -2.081294 3.869686
h -2.803426 -0.499080 2.978140
h -2.731889 4.357583 0.650135
h -0.758437 6.303750 0.147561
h 4.168737 6.999336 1.935753
h 5.750052 5.729713 3.748241
h 0.748792 -3.092829 8.154902
h 4.025204 -1.309917 10.032896
h -0.032187 -2.130322 -5.547786
h -1.652458 -1.762829 -0.940736

Conf LM2 –IC1

C 0.136000 -2.934000 -6.275000
H -0.184000 -2.573000 -7.254000
H 1.225000 -3.078000 -6.301000
C -0.519000 -4.276000 -6.052000
O -1.256000 -4.796000 -6.932000
O -0.243000 -4.987000 -4.965000
H 0.298000 -4.577000 -4.127000
C -0.999000 -1.253000 -0.242000
H -1.357000 -1.440000 0.776000
O -1.050000 0.172000 -0.512000
H -0.136000 0.551000 -0.611000
C 0.426000 -1.819000 -0.359000
H 1.077000 -1.342000 0.383000
H 0.455000 -2.900000 -0.162000
H 0.861000 -1.635000 -1.348000
N 1.043000 -2.479000 8.888000
H 0.780000 -2.747000 9.824000
C 2.054000 -1.459000 8.782000
H 2.630000 -1.549000 7.855000
C 1.476000 0.039000 8.833000
H 1.537000 0.392000 9.867000
H 2.137000 0.682000 8.238000
N -0.340000 0.481000 7.100000
H 0.258000 0.770000 6.337000
C 0.058000 0.191000 8.402000
C -1.709000 0.509000 7.065000
H -2.263000 0.725000 6.168000
N -2.215000 0.243000 8.272000

C -1.118000 0.052000 9.113000
H -1.247000 -0.170000 10.160000
C 2.995000 -1.664000 9.999000
O 2.533000 -2.275000 10.985000
S 0.693000 3.203000 5.153000
H 1.834000 1.471000 0.400000
O 2.395000 1.911000 1.566000
O 1.585000 1.019000 -0.568000
Fe 1.627000 2.518000 2.997000
N 2.897000 1.427000 4.132000
N 0.261000 1.006000 3.109000
N 0.292000 3.654000 1.980000
N 2.903000 4.082000 3.042000
C 4.067000 1.877000 4.713000
C 4.710000 0.775000 5.426000
C 3.948000 -0.357000 5.202000
C 2.794000 0.075000 4.423000
C 0.495000 -0.276000 3.577000
C -0.732000 -1.060000 3.517000
C -1.734000 -0.223000 3.051000
C -1.076000 1.055000 2.740000
C -1.013000 3.307000 1.677000
C -1.649000 4.364000 0.894000
C -0.701000 5.352000 0.693000
C 0.508000 4.898000 1.403000
C 2.799000 5.246000 2.302000
C 3.991000 6.065000 2.484000
C 4.799000 5.397000 3.378000
C 4.115000 4.150000 3.716000
C 4.617000 3.146000 4.533000
H 5.561000 3.349000 5.027000
C 1.694000 -0.719000 4.126000
H 1.742000 -1.756000 4.435000
C -1.630000 2.116000 2.034000
H -2.611000 1.959000 1.614000
C 1.700000 5.606000 1.536000
H 1.786000 6.547000 1.005000
O 4.233000 0.135000 -0.905000
H 3.314000 0.479000 -1.054000
H 4.241000 -0.170000 0.076000
O 2.855000 -2.734000 -3.589000
H 3.616000 -2.141000 -3.247000
H 3.221000 -3.407000 -4.211000
O 4.858000 -1.383000 -2.801000
H 5.723000 -1.814000 -2.730000
H 4.665000 -0.743000 -2.010000
O 0.995000 -4.245000 -2.998000
H 0.578000 -4.469000 -2.139000
H 1.722000 -3.498000 -3.023000
O 3.948000 -0.276000 1.553000
H 3.365000 0.521000 1.746000
H 4.700000 -0.335000 2.188000
h 0.421334 4.555958 5.146093
h 5.525358 0.932311 6.132053
h 4.146843 -1.390537 5.485425
h -0.777838 -2.094312 3.857828
h -2.783142 -0.508417 2.974157
h -2.710452 4.347716 0.646772
h -0.740959 6.301616 0.159428
h 4.184611 6.995225 1.949900
h 5.762945 5.725884 3.766215
h 0.748795 -3.092356 8.155054
h 4.025162 -1.309382 10.031851
h -0.030790 -2.132123 -5.555805
h -1.657661 -1.747712 -0.955788

Conf LM2 -CpdI

C -0.028000 -2.983000 -6.388000
H -0.455000 -2.622000 -7.327000
H 1.054000 -3.108000 -6.538000
C -0.610000 -4.361000 -6.088000
O -1.367000 -4.909000 -6.972000
O -0.256000 -4.992000 -5.016000
H 0.482000 -4.459000 -3.823000
C -0.962000 -1.274000 -0.214000
H -1.353000 -1.450000 0.796000
O -0.917000 0.155000 -0.448000
H 0.024000 0.462000 -0.669000
C 0.427000 -1.930000 -0.299000
H 1.113000 -1.445000 0.402000
H 0.384000 -2.996000 -0.040000
H 0.864000 -1.848000 -1.299000
N 1.042000 -2.480000 8.889000
H 0.780000 -2.750000 9.824000
C 2.057000 -1.463000 8.788000
H 2.634000 -1.552000 7.863000
C 1.482000 0.036000 8.846000
H 1.551000 0.388000 9.879000
H 2.139000 0.680000 8.247000
N -0.342000 0.486000 7.125000
H 0.256000 0.778000 6.366000
C 0.061000 0.191000 8.425000
C -1.711000 0.518000 7.095000
H -2.270000 0.739000 6.203000
N -2.212000 0.249000 8.302000
C -1.113000 0.052000 9.140000
H -1.241000 -0.174000 10.186000
C 2.995000 -1.671000 10.007000
O 2.526000 -2.276000 10.993000
S 0.601000 3.220000 5.220000
H 1.737000 1.437000 0.227000
O 2.401000 1.932000 1.679000
O 1.567000 1.047000 -0.664000
Fe 1.610000 2.506000 3.045000
N 2.859000 1.439000 4.215000
N 0.249000 0.997000 3.156000
N 0.270000 3.637000 2.030000
N 2.862000 4.087000 3.122000
C 4.037000 1.883000 4.789000
C 4.699000 0.779000 5.473000
C 3.945000 -0.355000 5.239000
C 2.783000 0.084000 4.481000
C 0.483000 -0.289000 3.619000
C -0.731000 -1.087000 3.539000
C -1.731000 -0.260000 3.056000
C -1.076000 1.019000 2.759000
C -1.023000 3.283000 1.697000
C -1.662000 4.334000 0.911000
C -0.715000 5.320000 0.706000
C 0.485000 4.871000 1.429000
C 2.777000 5.233000 2.353000
C 3.970000 6.048000 2.515000
C 4.775000 5.392000 3.423000
C 4.081000 4.163000 3.785000
C 4.580000 3.154000 4.601000
H 5.533000 3.354000 5.080000
C 1.686000 -0.718000 4.168000
H 1.752000 -1.761000 4.453000
C -1.618000 2.068000 2.019000
H -2.580000 1.889000 1.562000
C 1.684000 5.566000 1.556000
H 1.790000 6.479000 0.984000
O 4.200000 0.152000 -0.917000
H 2.432000 0.674000 -0.993000
H 4.078000 -0.339000 -0.065000
O 2.922000 -2.588000 -3.814000
H 4.082000 -1.804000 -3.273000
H 3.227000 -3.298000 -4.428000
O 4.923000 -1.354000 -2.882000
H 5.629000 -2.009000 -2.753000
H 4.494000 -0.436000 -1.684000
O 1.073000 -4.219000 -3.008000
H 0.634000 -4.492000 -2.174000
H 2.165000 -3.019000 -3.303000
O 3.730000 -0.568000 1.595000
H 3.206000 0.268000 1.695000
H 4.575000 -0.481000 2.101000
h 0.356731 4.578075 5.202333
h 5.525822 0.931348 6.166702
h 4.156697 -1.393431 5.493779
h -0.768025 -2.127412 3.861861
h -2.776869 -0.549517 2.954002
h -2.719929 4.306569 0.650039
h -0.743245 6.255998 0.148167
h 4.168987 6.964976 1.960360
h 5.742927 5.720993 3.801085
h 0.748491 -3.092700 8.155227
h 4.027163 -1.322171 10.039018
h -0.124679 -2.193927 -5.642290
h -1.632683 -1.741835 -0.934681

Conf LM3 –RC

C -1.232754 -5.382907 -4.487271
H -1.627576 -5.305471 -3.468836
H -2.048831 -5.682204 -5.151892
C -0.180683 -6.475240 -4.562278
O -0.051184 -7.202780 -5.571374
O 0.610094 -6.663493 -3.488259

H 0.419558 -6.090520 -2.632950
C -1.871312 -1.238696 -0.586499
H -2.423015 -0.964248 0.321816
O -1.332514 -0.045093 -1.222000
H -0.396663 0.083864 -0.933783
C -0.751242 -2.211927 -0.204565
H -0.124846 -1.756010 0.568655
H -1.136670 -3.163254 0.182449
H -0.110714 -2.417247 -1.066035
N -0.094767 -0.051106 8.431627
H -0.501063 0.111204 9.338584
C 1.213048 0.516642 8.198987
H 1.634878 0.168277 7.253489
C 1.166937 2.100839 8.150356
H 0.884857 2.442352 9.153050
H 2.186611 2.470163 7.966958
N 0.412368 2.778066 5.801798
H 1.269793 2.612611 5.291583
C 0.196724 2.666841 7.175102
C -0.710068 3.307144 5.228182
H -0.777891 3.517344 4.175926
N -1.641803 3.535620 6.157237
C -1.079274 3.147907 7.374813
H -1.608578 3.256668 8.306046
C 2.123843 0.154366 9.387433
O 1.615496 0.150822 10.530219
S 2.000860 3.909915 3.127562
H 1.463563 1.412011 -0.973672
O 2.472583 0.530035 0.432984
O 1.525197 0.446030 -0.763056
Fe 2.283691 2.143498 1.501878
N 3.046140 1.103880 3.024604
N 0.431858 1.521982 1.976031
N 1.535064 3.204873 -0.056699
N 4.130716 2.711468 1.005783
C 4.255480 1.353072 3.649315
C 4.349985 0.568502 4.876772
C 3.261099 -0.277229 4.891513
C 2.406960 0.136058 3.771858
C 0.147744 0.439348 2.785334
C -1.291443 0.189751 2.783396
C -1.886323 1.188760 2.031119
C -0.777463 1.984708 1.475022
C 0.195295 3.496560 -0.266795
C 0.042901 4.347937 -1.444414
C 1.315327 4.539498 -1.977817
C 2.244252 3.836564 -1.074177
C 4.521660 3.259955 -0.209400
C 5.980988 3.353984 -0.260629
C 6.452304 2.949962 0.975605
C 5.287254 2.554406 1.758831
C 5.303176 2.047989 3.057256
H 6.239119 2.106779 3.602023
C 1.076227 -0.236881 3.586302
H 0.690740 -1.017385 4.235937
C -0.856712 2.929740 0.455265
H -1.839158 3.143598 0.064524
C 3.641550 3.770298 -1.164223
H 4.109159 4.199711 -2.044910
O 0.237675 -5.206910 -1.432503
H 0.713320 -4.351580 -1.780808
H 0.755009 -5.457865 -0.618031
O 3.654835 -2.461043 -0.938671
H 3.225963 -2.507175 -0.030926
H 4.155158 -1.609586 -0.948978
O 2.513686 -1.904390 1.310191
H 2.404075 -0.926935 1.017754
H 1.828437 -2.125686 1.961296
O 1.682541 -3.380188 -2.366907
H 2.091035 -3.689194 -3.211104
H 2.355206 -2.843815 -1.842013
h 2.533933 5.102386 2.682373
h 5.098221 0.756794 5.646679
h 3.097706 -1.170160 5.494874
h -1.727802 -0.641706 3.336872
h -2.963770 1.307139 1.916404
h -0.936503 4.682299 -1.786520
h 1.666652 5.038713 -2.880824
h 6.547836 3.652160 -1.142582
h 7.481220 2.850023 1.321165
h -0.595656 -0.683323 7.840540
h 3.186467 -0.046432 9.251139
h -0.901930 -4.393071 -4.801669
h -2.551079 -1.713908 -1.293716

Conf LM3 –TShooh

C -1.321470 -5.454907 -4.667819
H -1.800455 -5.395438 -3.684183
H -2.076105 -5.755972 -5.402830
C -0.227486 -6.534011 -4.637772
O -0.062441 -7.270590 -5.662495
O 0.478529 -6.640305 -3.538752
H 0.073976 -6.006779 -2.287604
C -1.885568 -1.283070 -0.592638
H -2.440692 -1.033787 0.320788
O -1.363007 -0.063482 -1.204681
H -0.464612 0.111017 -0.850900
C -0.757861 -2.251917 -0.233270
H -0.138724 -1.809150 0.556025
H -1.133893 -3.217011 0.123802
H -0.120991 -2.436560 -1.100013
N -0.094888 -0.054816 8.434766
H -0.502466 0.104475 9.341810
C 1.214248 0.510028 8.207996
H 1.639167 0.162743 7.263356
C 1.164596 2.092875 8.162912
H 0.878930 2.433451 9.164654
H 2.182667 2.467929 7.982210
N 0.399638 2.724384 5.808632
H 1.247448 2.508807 5.304902
C 0.192881 2.653027 7.186164
C -0.718912 3.257820 5.229264
H -0.797414 3.443583 4.173376
N -1.638012 3.527183 6.158670
C -1.072998 3.160592 7.382290
H -1.595950 3.297301 8.313189
C 2.122800 0.146161 9.398694
O 1.611654 0.150387 10.539617
S 1.969899 3.994282 3.126660
H 1.580636 1.435933 -0.836630
O 2.683042 0.564270 0.480628
O 1.722143 0.458669 -0.702808
FE 2.319152 2.263281 1.633096
N 3.060529 1.184323 3.123743
N 0.494155 1.514521 2.033873
N 1.587143 3.201515 -0.007880
N 4.154569 2.810884 1.101640
C 4.271677 1.438071 3.749768
C 4.380438 0.625256 4.956371
C 3.309815 -0.244031 4.952080
C 2.448587 0.172992 3.845381
C 0.209844 0.412565 2.822142
C -1.222578 0.137249 2.793417
C -1.823100 1.143075 2.055451
C -0.719860 1.964579 1.522746
C 0.241674 3.478336 -0.225448
C 0.086313 4.314493 -1.409370
C 1.359335 4.517471 -1.941635
C 2.292133 3.841053 -1.030954
C 4.559377 3.305038 -0.133995
C 6.018951 3.355843 -0.191183
C 6.480122 2.977451 1.057028
C 5.305501 2.640397 1.855968
C 5.315840 2.138960 3.158712
H 6.254628 2.186802 3.699122
C 1.138800 -0.249066 3.630605
H 0.769880 -1.055886 4.256211
C -0.806233 2.903652 0.498319
H -1.789738 3.103873 0.102412
C 3.689122 3.786847 -1.109899
H 4.161342 4.191720 -1.999038
O -0.103942 -5.383448 -1.441463
H 0.689646 -4.288061 -2.076974
H 0.537083 -5.560109 -0.703396
O 2.674281 -2.096825 -1.178377
H 2.650937 -2.102498 0.108570
H 2.438133 -1.172215 -1.413614
O 2.624110 -1.744815 1.188484
H 2.582046 -0.487405 0.960505
H 1.936034 -2.088350 1.779375
O 1.416443 -3.677781 -2.468752
H 1.862053 -4.044632 -3.267605
H 2.075896 -2.812734 -1.739429
h 2.527981 5.173695 2.677355
h 5.138322 0.793721 5.721419
h 3.159807 -1.153220 5.534266
h -1.656971 -0.711707 3.321283
h -2.901013 1.256861 1.940457

h -0.896074 4.637057 -1.754239
h 1.707395 5.011502 -2.848748
h 6.590107 3.609769 -1.084138
h 7.507241 2.864683 1.403980
h -0.595887 -0.684570 7.841149
h 3.184527 -0.060668 9.264448
h -0.976909 -4.456789 -4.938199
h -2.560922 -1.745808 -1.312246

Conf LM3 –Fe RS

C -1.322928 -5.455331 -4.668120
H -1.799778 -5.395357 -3.683331
H -2.079686 -5.755720 -5.401299
C -0.229069 -6.535128 -4.640871
O -0.066458 -7.271281 -5.666738
O 0.477436 -6.643320 -3.542822
H 0.068038 -6.010519 -2.285400
C -1.885770 -1.286399 -0.592369
H -2.440621 -1.039784 0.322118
O -1.367092 -0.063051 -1.201778
H -0.467253 0.108765 -0.851248
C -0.754795 -2.253318 -0.238118
H -0.135192 -1.810599 0.551166
H -1.128493 -3.219655 0.118189
H -0.118770 -2.435829 -1.106049
N -0.094754 -0.054786 8.434993
H -0.502187 0.104062 9.342232
C 1.214479 0.510460 8.208848
H 1.638947 0.162659 7.264334
C 1.164861 2.093394 8.164269
H 0.879361 2.433029 9.166395
H 2.183256 2.467817 7.983365
N 0.399529 2.723525 5.810156
H 1.247111 2.506180 5.307030
C 0.193057 2.653499 7.187708
C -0.718986 3.257384 5.230549
H -0.797646 3.442174 4.174512
N -1.637721 3.527072 6.160036
C -1.072847 3.160925 7.383684
H -1.595662 3.298467 8.314450
C 2.122772 0.145887 9.399381
O 1.611749 0.150391 10.540311
S 1.966060 4.000372 3.130034
H 1.577713 1.448264 -0.827417
O 2.682061 0.564091 0.470987
O 1.713577 0.467086 -0.704689
Fe 2.318056 2.272619 1.639568
N 3.059650 1.189122 3.125140
N 0.494065 1.518754 2.035362
N 1.586576 3.203696 -0.006007
N 4.153694 2.814164 1.104409
C 4.271251 1.441896 3.751659
C 4.379595 0.628209 4.957434
C 3.308938 -0.240987 4.952186
C 2.447845 0.176600 3.846059
C 0.209467 0.416458 2.823734
C -1.222366 0.140265 2.793949
C -1.823082 1.145927 2.056146
C -0.720579 1.968251 1.524162
C 0.240470 3.480874 -0.224676
C 0.086041 4.316251 -1.408698
C 1.359421 4.518722 -1.940808
C 2.292071 3.843778 -1.029426
C 4.558589 3.307614 -0.131848
C 6.018105 3.356924 -0.189783
C 6.479692 2.978960 1.058432
C 5.305475 2.643097 1.858022
C 5.315780 2.142036 3.160734
H 6.255236 2.188247 3.700316
C 1.138247 -0.244907 3.631799
H 0.770329 -1.054007 4.254949
C -0.807434 2.906336 0.498907
H -1.791105 3.105731 0.103112
C 3.688646 3.789380 -1.107958
H 4.161238 4.193080 -1.997647
O -0.115222 -5.391909 -1.440521
H 0.680945 -4.291211 -2.087359
H 0.529384 -5.562133 -0.704208
O 2.690910 -2.104413 -1.197611
H 2.660268 -2.114453 0.165628
H 2.449861 -1.182171 -1.428604
O 2.625523 -1.770285 1.198915
H 2.575089 -0.422917 0.935369
H 1.923287 -2.132622 1.760990
O 1.404393 -3.684509 -2.480723
H 1.853538 -4.059992 -3.273123
H 2.088180 -2.803878 -1.744508
h 2.526734 5.177668 2.678410
h 5.138047 0.795799 5.722110
h 3.159339 -1.151345 5.532646
h -1.656418 -0.709331 3.321065
h -2.901022 1.258393 1.940109
h -0.896215 4.638422 -1.754307
h 1.707666 5.012134 -2.848187
h 6.589146 3.610213 -1.082993
h 7.506799 2.865340 1.405143
h -0.595770 -0.684461 7.841306
h 3.184422 -0.061309 9.265089
h -0.978480 -4.457424 -4.939421
h -2.561555 -1.747811 -1.312425

Conf LM4 –RC

C -0.931816 -4.469177 -2.917540
H -1.610892 -5.147840 -3.438592
H -0.092145 -4.265446 -3.599679
C -0.366784 -5.209967 -1.726092
O -0.498305 -6.448945 -1.625039
O 0.343079 -4.525722 -0.814275
H 0.671491 -3.526122 -1.051237
C -0.733980 -1.698234 2.321815
H -0.851885 -1.579376 3.408808
O -0.824793 -0.377250 1.689220
H -0.315501 0.283349 2.223718
C 0.625393 -2.346752 2.046933
H 1.420076 -1.712122 2.451215
H 0.705000 -3.327596 2.531407
H 0.811454 -2.468951 0.978220
N 6.440598 2.253696 6.771388
H 6.873394 2.525531 7.641895
C 7.081987 2.691216 5.560775
H 7.114801 1.902975 4.793723
C 6.379587 3.973147 4.894607
H 6.955537 4.859862 5.183177
H 6.469889 3.894716 3.804117
N 3.910148 4.133689 4.338099
H 4.003820 3.957608 3.349283
C 4.948040 4.198966 5.266167
C 2.741408 4.474020 4.965850
H 1.798458 4.527873 4.453532
N 2.963465 4.753341 6.251156
C 4.334416 4.577394 6.446906
H 4.790617 4.729857 7.409840
C 8.541608 3.039164 5.927953
O 8.848895 3.143411 7.132919
S 2.363438 5.823272 1.754513
H 1.665649 1.012480 -0.835672
O 2.252161 2.816529 -1.458785
O 2.555530 1.367923 -1.096210
FE 2.266464 4.157489 0.023746
N 4.221066 3.807848 0.360265
N 1.809990 2.787353 1.445744
N 0.306207 4.553078 -0.276110
N 2.741173 5.488562 -1.370595
C 5.267574 4.665687 0.041549
C 6.527057 4.129282 0.563372
C 6.232299 2.898676 1.116977
C 4.779436 2.740496 1.044585
C 2.674136 1.884872 2.037151
C 2.000662 1.192716 3.128614
C 0.725695 1.743797 3.241528
C 0.597248 2.683307 2.111169
C -0.720086 4.100644 0.527133
C -1.995845 4.646758 0.067812
C -1.730764 5.453625 -1.026911
C -0.275072 5.363609 -1.243997
C 1.875799 6.078177 -2.274534
C 2.605149 7.024019 -3.115061
C 3.899300 7.056405 -2.634543
C 3.983874 6.083306 -1.549300
C 5.128989 5.755467 -0.816859
H 6.026535 6.335353 -1.000509
C 4.040345 1.795374 1.753546
H 4.601561 1.019860 2.262673
C -0.576391 3.260639 1.628924
H -1.499806 2.987417 2.122069
C 0.485299 5.965466 -2.245521
H -0.034567 6.424628 -3.075035
O 4.859421 0.593183 -3.791852

H 4.150690 1.317697 -3.854042
H 4.816594 -0.011409 -4.549916
O 2.947458 2.414510 -3.863758
H 2.230870 2.032491 -4.403706
H 2.603115 2.627124 -2.887886
O 1.311536 -2.326848 -1.333203
H 2.357993 -2.374122 -1.248743
H 0.947687 -1.427117 -1.173898
O 4.801685 -0.086339 -1.233106
H 4.119849 0.530209 -0.859790
H 4.795675 0.058148 -2.226852
O 3.777112 -2.428956 -1.096573
H 4.295453 -1.554867 -1.050335
H 4.299551 -3.243368 -0.942645
h 1.792049 7.012525 1.350115
h 7.478571 4.660843 0.574816
h 6.895593 2.133272 1.519797
h 2.510290 0.481319 3.778430
h 0.061635 1.578067 4.089834
h -2.928476 4.435617 0.590962
h -2.487411 6.036616 -1.551956
h 2.150109 7.624144 -3.903004
h 4.719615 7.684614 -2.981681
h 5.838553 1.455708 6.798347
h 9.290393 3.215743 5.155808
h -1.433477 -3.512816 -2.769971
h -1.549668 -2.310522 1.937338

Conf LM4 –TSoo

C -0.923992 -4.459490 -2.915187
H -1.597217 -5.134644 -3.447978
H -0.078648 -4.245381 -3.587097
C -0.367153 -5.209199 -1.725079
O -0.507346 -6.448666 -1.631339
O 0.343042 -4.533403 -0.809820
H 0.680366 -3.526168 -1.041252
C -0.733369 -1.711106 2.334330
H -0.853232 -1.596022 3.421620
O -0.822317 -0.388110 1.706548
H -0.284186 0.263394 2.221691
C 0.622481 -2.366862 2.058234
H 1.422430 -1.746365 2.473421
H 0.690756 -3.354074 2.531517
H 0.813176 -2.478372 0.989176
N 6.440999 2.253737 6.769058
H 6.876816 2.524582 7.638537
C 7.084494 2.685287 5.556873
H 7.118440 1.894119 4.792510
C 6.383875 3.964671 4.883694
H 6.956080 4.853135 5.175022
H 6.481816 3.884592 3.793770
N 3.916386 4.123666 4.312476
H 4.015142 3.951423 3.323443
C 4.949811 4.188898 5.245917
C 2.744407 4.463581 4.935500
H 1.803837 4.517865 4.418821
N 2.960544 4.741840 6.221982
C 4.330462 4.566387 6.423844
H 4.782463 4.718407 7.388823
C 8.543553 3.035903 5.925152
O 8.849202 3.141885 7.130327
S 2.354489 5.828303 1.733995
H 1.664564 0.923404 -0.976034
O 2.291362 3.060968 -1.427028
O 2.531841 1.111106 -1.417642
FE 2.284126 4.126716 -0.050715
N 4.236589 3.847371 0.333238
N 1.836634 2.790538 1.385329
N 0.317583 4.565442 -0.285087
N 2.752931 5.553057 -1.361004
C 5.279196 4.716227 0.026328
C 6.539541 4.170147 0.533715
C 6.250002 2.926510 1.060068
C 4.799659 2.762427 0.982639
C 2.704429 1.876312 1.953619
C 2.044923 1.183203 3.052349
C 0.778257 1.745326 3.193523
C 0.631763 2.687276 2.070455
C -0.704464 4.103081 0.513542
C -1.981772 4.645936 0.059154
C -1.720228 5.461255 -1.030049
C -0.263884 5.379785 -1.248900
C 1.881910 6.124332 -2.268815
C 2.606617 7.068957 -3.114585
C 3.899890 7.111868 -2.634789
C 3.991610 6.145342 -1.543874
C 5.138880 5.816548 -0.815483
H 6.034639 6.399888 -0.996143
C 4.067032 1.791393 1.660131
H 4.630342 1.000333 2.140990
C -0.549604 3.261648 1.611221
H -1.465295 2.985574 2.116725
C 0.493474 5.995986 -2.243352
H -0.029509 6.454625 -3.071107
O 5.011489 0.645579 -3.902269
H 4.272014 1.330372 -3.928696
H 5.060052 0.144650 -4.731923
O 2.946113 2.358569 -3.913665
H 2.263602 1.840247 -4.379338
H 2.645948 2.501296 -2.949777
O 1.313546 -2.344693 -1.312935
H 2.362413 -2.383489 -1.238653
H 0.940854 -1.443721 -1.174268
O 4.814106 -0.123964 -1.341456
H 4.029714 0.443237 -1.066866
H 4.887211 -0.006620 -2.330486
O 3.775552 -2.447662 -1.105429
H 4.309743 -1.580099 -1.115301
H 4.293724 -3.264367 -0.949226
h 1.785867 7.026223 1.351890
h 7.491306 4.701046 0.552600
h 6.913705 2.157296 1.454877
h 2.560934 0.468161 3.693062
h 0.129580 1.584126 4.054510
h -2.911862 4.423927 0.582327
h -2.480268 6.046088 -1.548100
h 2.148053 7.649848 -3.914805
h 4.719138 7.737011 -2.989888
h 5.838809 1.455917 6.797726
h 9.293043 3.213020 5.153815
h -1.427192 -3.504809 -2.762090
h -1.550122 -2.318738 1.944759

Conf LM4 –Cpd I

C -1.018969 -4.587892 -2.879965
H -1.745369 -5.246977 -3.364743
H -0.201158 -4.439335 -3.603780
C -0.410654 -5.334303 -1.690557
O -0.500778 -6.605760 -1.696566
O 0.242255 -4.658162 -0.785629
H 0.950141 -3.344721 -1.152951
C -0.704042 -1.752180 2.320726
H -0.804341 -1.645798 3.411222
O -0.788144 -0.417839 1.707025
H -0.260010 0.220810 2.234700
C 0.634877 -2.422394 2.005672
H 1.453464 -1.822554 2.418038
H 0.695422 -3.417652 2.461559
H 0.805143 -2.529136 0.932300
N 6.443889 2.252715 6.771595
H 6.885203 2.512815 7.642209
C 7.092586 2.686335 5.563480
H 7.125765 1.899292 4.794995
C 6.401620 3.974823 4.895095
H 6.997368 4.855014 5.163535
H 6.474836 3.884007 3.804358
N 3.936755 4.222297 4.358079
H 4.027181 4.089247 3.363418
C 4.979379 4.226208 5.284253
C 2.775427 4.559383 5.007345
H 1.828659 4.649786 4.507867
N 3.010175 4.782431 6.299319
C 4.377904 4.570243 6.481669
H 4.841037 4.674252 7.447202
C 8.553036 3.032739 5.935198
O 8.854925 3.140014 7.140484
S 2.172339 6.038601 1.996025
H 2.747936 2.143906 -1.766579
O 1.708860 2.958223 -0.873654
O 3.411978 1.796384 -2.422613
FE 1.962664 4.178700 0.218815
N 3.924356 3.833578 0.514535
N 1.548021 2.958852 1.771202
N 0.036126 4.733085 0.094626
N 2.456485 5.531014 -1.153724
C 4.994945 4.617472 0.120424
C 6.251186 4.040576 0.592014
C 5.929647 2.826288 1.167456

C 4.473197 2.735096 1.157833
C 2.384070 1.980245 2.266617
C 1.723986 1.247993 3.337628
C 0.469221 1.822308 3.512672
C 0.342982 2.833746 2.450411
C -0.991594 4.246823 0.870969
C -2.276685 4.719130 0.365159
C -2.016824 5.528622 -0.726828
C -0.559091 5.480665 -0.922548
C 1.583124 6.096979 -2.055609
C 2.300807 6.991301 -2.958970
C 3.614044 7.017801 -2.531141
C 3.711819 6.068977 -1.426592
C 4.872713 5.693752 -0.758952
H 5.790620 6.210006 -1.016020
C 3.721686 1.820427 1.889398
H 4.257853 0.983692 2.322801
C -0.833281 3.412677 1.978295
H -1.754146 3.118471 2.462414
C 0.187349 6.001656 -1.974172
H -0.351527 6.413116 -2.817564
O 5.287607 0.387215 -4.702601
H 4.156620 1.374546 -5.041779
H 5.602747 -0.237437 -5.376211
O 3.338752 2.004928 -5.072466
H 2.649037 1.621306 -5.646447
H 3.083864 1.843154 -3.360356
O 1.478780 -2.487182 -1.356141
H 2.972105 -2.411549 -1.277363
H 0.934472 -1.668936 -1.264434
O 4.882086 -0.294466 -2.384405
H 4.243991 0.468199 -2.191881
H 5.108810 -0.072717 -3.727204
O 3.997803 -2.332784 -1.262901
H 4.581723 -1.184489 -1.934509
H 4.438099 -3.185596 -1.063014
h 1.674832 7.242862 1.541506
h 7.217313 4.545005 0.577282
h 6.579391 2.044392 1.560569
h 2.234356 0.477169 3.915054
h -0.208071 1.586556 4.333503
h -3.218182 4.427975 0.830859
h -2.775708 6.100387 -1.260913
h 1.833235 7.523186 -3.787547
h 4.422399 7.669049 -2.863564
h 5.839953 1.456150 6.798378
h 9.301961 3.207110 5.162688
h -1.469055 -3.605954 -2.734073
h -1.537193 -2.342915 1.939993

With substrate

Conf LW1 –RC

C 1.899198 3.013054 -5.796328
H 1.567198 3.636646 -6.631111
H 1.031741 2.445048 -5.435656
C 2.944130 2.036131 -6.322124
O 3.362615 2.191110 -7.515375
O 3.321429 1.057592 -5.536483
H 2.830400 0.889982 -4.147470
C -1.056463 1.518497 -1.970508
H -1.411738 1.906132 -1.009667
O 0.382092 1.275673 -1.833758
H 0.625408 0.973026 -0.899815
C -1.786782 0.230219 -2.357819
H -1.404206 -0.165553 -3.306424
H -2.866938 0.389496 -2.457732
H -1.640479 -0.522792 -1.580838
S -1.184796 -1.010144 5.007882
H 1.189526 1.317452 1.305615
O 1.513268 -0.751577 1.804896
O 1.436339 0.736605 0.553913
FE 0.414926 -0.861736 3.129448
N 0.365519 -2.870104 2.807475
N -1.237939 -0.598790 1.991012
N 0.431125 1.113225 3.585424
N 1.986128 -1.184197 4.440925
C 1.263905 -3.829400 3.259764
C 0.945619 -5.125762 2.674014
C -0.175099 -4.946689 1.893418
C -0.531597 -3.534788 1.989340
C -1.956053 -1.595010 1.349699
C -3.113202 -1.022255 0.657488
C -3.092402 0.342675 0.890167
C -1.906789 0.585038 1.739116
C -0.465326 2.073953 3.131578
C -0.136202 3.382293 3.690336
C 0.973122 3.210724 4.502664
C 1.314365 1.777325 4.432838
C 2.651625 -0.210181 5.157751
C 3.722693 -0.808722 5.956685
C 3.697230 -2.166520 5.712658
C 2.615785 -2.384980 4.749764
C 2.281200 -3.602553 4.179073
H 2.864731 -4.462993 4.480889
C -1.623191 -2.944832 1.361530
H -2.274342 -3.623358 0.822125
C -1.526932 1.813955 2.272568
H -2.141837 2.662113 2.006391
C 2.337689 1.144323 5.135172
H 2.971039 1.768968 5.757449
O 3.496662 0.210623 -1.016729
H 3.618431 -0.737790 -0.692551
H 2.869544 0.616961 -0.345036
O 3.316982 -1.995923 0.314464
H 3.020933 -2.889789 0.073871
H 2.663815 -1.585394 0.960549
O 2.500966 0.749103 -3.161067
H 1.554084 0.956814 -2.869139
H 3.085073 0.466209 -2.263414
h -1.465292 -2.297794 5.417304
h 1.524644 -6.033073 2.846012
h -0.723797 -5.671886 1.292514
h -3.793861 -1.625832 0.057100
h -3.747949 1.148241 0.559429
h -0.709781 4.283246 3.472716
h 1.538266 3.910285 5.118532
h 4.419890 -0.239202 6.571200
h 4.352306 -2.933772 6.125291
h 2.239580 3.667305 -4.993730
h -1.183379 2.292858 -2.727029

Conf LW1 –TSoo

C 2.460586 3.305703 -4.736601
H 2.689035 4.255472 -5.222633
H 3.375170 2.702423 -4.702798
C 1.386579 2.616283 -5.537236
O 0.694593 3.234753 -6.374786
O 1.188545 1.301233 -5.324512
H 1.808318 0.786451 -4.645142
C -1.049591 0.350537 -0.904183
H -1.886614 -0.341439 -0.753866
O -0.797843 1.110523 0.309429
H -0.187053 0.608970 0.922086
C 0.159831 -0.478455 -1.329144
H 0.425764 -1.180020 -0.534696
H -0.058280 -1.068442 -2.231592
H 1.038629 0.139078 -1.517080
N -2.778673 -8.183543 -0.176223
H -3.283833 -9.001992 0.120337
C -1.540276 -7.893518 0.499151
H -0.828498 -7.395931 -0.183876
C -1.698400 -6.920411 1.736737
H -0.771525 -6.937428 2.327822
H -1.782584 -5.909933 1.332654
C -2.894441 -7.182513 2.617292
C -2.877696 -8.137050 3.647810
H -1.987589 -8.739345 3.810870
C -3.984935 -8.295199 4.489049
H -3.951589 -9.007405 5.306429
C -5.138803 -7.531900 4.285268
H -6.002312 -7.676541 4.924594
C -4.057079 -6.418086 2.427102
H -4.085026 -5.673752 1.636798
C -5.175174 -6.601161 3.242602
H -6.066891 -6.017822 3.053584
C -0.883178 -9.227654 0.883336
O -1.524345 -10.296333 0.797614
S -0.621628 -3.404654 5.459821
H 0.976631 0.565619 2.892081
O 1.823892 -1.337235 2.785806
O 1.176373 0.288900 1.971065
Fe 0.777350 -2.050936 3.977175
N 1.561559 -3.834371 3.453874
N -0.689269 -2.261179 2.615096
N -0.054095 -0.333303 4.621265
N 2.178465 -1.913013 5.426055
C 2.516014 -4.578819 4.129027
C 2.878391 -5.754354 3.332880

C 2.163317 -5.663742 2.156036
C 1.298787 -4.490295 2.272448
C -0.685707 -3.151048 1.560850
C -1.865591 -2.935258 0.715289
C -2.596940 -1.909648 1.291271
C -1.822449 -1.483141 2.473713
C -1.305543 0.155699 4.274383
C -1.578009 1.398875 4.986589
C -0.452067 1.697026 5.737582
C 0.479378 0.577323 5.529382
C 2.474048 -0.776121 6.152255
C 3.588457 -1.030640 7.058568
C 3.893068 -2.370496 6.942777
C 3.036267 -2.907565 5.882410
C 3.133035 -4.174374 5.310404
H 3.811361 -4.883032 5.771925
C 0.287942 -4.134740 1.375950
H 0.197793 -4.763819 0.497089
C -2.114106 -0.394890 3.289330
H -3.028279 0.144312 3.079265
C 1.704645 0.382587 6.164526
H 2.064595 1.174004 6.813544
O 2.580598 -2.292193 0.289747
H 1.939178 -3.026818 0.264165
H 2.422951 -1.831321 1.163731
O 2.500485 -0.297718 -3.909078
H 1.883501 -1.048894 -4.009346
H 2.880444 -0.327129 -2.900198
O 3.248891 0.914063 0.613730
H 4.096626 0.860293 1.090307
H 2.470713 0.624753 1.219272
O 3.287181 -0.530415 -1.559477
H 3.338849 0.187590 -0.852397
H 3.028182 -1.344908 -1.032579
h -0.775691 -2.796076 6.688741
h 3.623794 -6.498704 3.612851
h 2.267579 -6.230026 1.230553
h -2.068973 -3.502718 -0.192836
h -3.527419 -1.419162 1.005438
h -2.528838 1.925585 4.905553
h -0.194243 2.550302 6.364889
h 4.064178 -0.255510 7.659341
h 4.622642 -2.932870 7.525464
h -3.108218 -7.730350 -1.004466
h 0.156203 -9.223590 1.211569
h 2.194760 3.522559 -3.702011
h -1.291879 1.063305 -1.692425

Conf LW1 –Cpd I

C 2.380876 3.257894 -4.800515
H 2.631245 4.202697 -5.290591
H 3.282040 2.633027 -4.776519
C 1.292160 2.576946 -5.616002
O 0.639421 3.288075 -6.444220
O 1.089778 1.291208 -5.448908
H 1.929358 0.332487 -4.591110
C -1.026510 0.344591 -0.950088
H -1.777002 -0.455176 -0.958001
O -1.036055 0.960602 0.359726
H -0.118111 0.967202 0.788451
C 0.321733 -0.283055 -1.309012
H 0.591105 -1.035518 -0.563970
H 0.291324 -0.768681 -2.292210
H 1.136981 0.444530 -1.328142
N -2.776512 -8.186727 -0.178844
H -3.280039 -9.007014 0.115965
C -1.533832 -7.902668 0.487215
H -0.821272 -7.412325 -0.200785
C -1.683863 -6.923823 1.721766
H -0.755040 -6.943423 2.310908
H -1.770311 -5.916409 1.309679
C -2.879349 -7.176824 2.605864
C -2.866517 -8.132018 3.635567
H -1.979530 -8.739116 3.798150
C -3.976540 -8.288542 4.473479
H -3.947977 -9.003539 5.288460
C -5.128173 -7.522351 4.267373
H -5.994342 -7.667166 4.902761
C -4.039455 -6.409020 2.413236
H -4.066948 -5.667920 1.619727
C -5.159983 -6.590069 3.225933
H -6.051129 -6.006941 3.033836
C -0.882491 -9.238510 0.877352
O -1.532095 -10.302156 0.808085
S -0.720205 -3.399482 5.519135
H 1.355137 0.255813 2.204883
O 1.812438 -1.297054 2.883238
O 1.265686 0.988745 1.550627
FE 0.807529 -2.057057 3.986434
N 1.546186 -3.860361 3.511266
N -0.664420 -2.272601 2.616564
N -0.078474 -0.373251 4.657083
N 2.138420 -1.943562 5.490985
C 2.511721 -4.600225 4.185619
C 2.894353 -5.763123 3.388510
C 2.184663 -5.675362 2.207269
C 1.310679 -4.516365 2.328356
C -0.661554 -3.177621 1.563395
C -1.819057 -2.955733 0.692917
C -2.541626 -1.912469 1.241707
C -1.779516 -1.487352 2.431866
C -1.300172 0.145025 4.257840
C -1.580185 1.398874 4.950243
C -0.468881 1.693035 5.718620
C 0.448082 0.555296 5.541473
C 2.438412 -0.797137 6.205932
C 3.551753 -1.035898 7.111755
C 3.868400 -2.374253 6.999288
C 3.011489 -2.920603 5.948692
C 3.119017 -4.186361 5.367676
H 3.804678 -4.888161 5.829223
C 0.302776 -4.165388 1.416880
H 0.234458 -4.794369 0.536609
C -2.075354 -0.386407 3.238463
H -2.965638 0.175105 2.989540
C 1.669576 0.361896 6.186149
H 2.035963 1.170442 6.809501
O 2.600178 -2.315557 0.289797
H 1.825547 -2.905968 0.314353
H 2.549735 -1.764812 1.110127
O 2.403455 -0.505013 -4.205673
H 1.809912 -1.266298 -4.345875
H 3.047336 -0.631869 -2.662748
O 3.438422 0.994092 0.081202
H 4.290376 1.075998 0.541050
H 2.101852 1.016333 0.988645
O 3.421700 -0.732580 -1.738744
H 3.494146 0.349088 -0.727694
H 3.059168 -1.472786 -1.191797
h -0.850477 -2.806798 6.758531
h 3.642025 -6.505042 3.668884
h 2.302982 -6.233235 1.278374
h -2.006394 -3.522971 -0.218792
h -3.458027 -1.410587 0.931240
h -2.527257 1.927360 4.841504
h -0.212228 2.554239 6.335485
h 4.020731 -0.253623 7.708556
h 4.609033 -2.926213 7.577967
h -3.107648 -7.731191 -1.005166
h 0.160365 -9.237011 1.194391
h 2.137479 3.488654 -3.763417
h -1.288700 1.070636 -1.719620

Conf LW3 –RC

C 4.061287 5.052025 -1.300355
H 3.931697 6.040854 -1.745266
H 5.067310 5.002938 -0.873492
C 3.929624 4.014139 -2.397355
O 3.233120 4.188314 -3.412811
O 4.607606 2.859421 -2.234778
H 5.093739 2.708263 -1.293874
C 0.842482 0.412494 -1.467609
H 0.019023 -0.290914 -1.655684
O 1.159360 0.380574 -0.046391
H 1.280137 -0.594264 0.284659
C 2.055434 -0.032265 -2.293871
H 2.338735 -1.049842 -2.004446
H 1.847243 -0.032451 -3.370649
H 2.916579 0.620354 -2.121916
N -3.388949 -7.962215 -2.121861
H -3.381337 -8.855524 -2.591162
C -2.790808 -7.906788 -0.799433
H -2.093442 -7.058718 -0.697757
C -3.849293 -7.741297 0.368412
H -3.294611 -7.442405 1.262277
H -4.485261 -6.892748 0.089361
C -4.692797 -8.964028 0.661876
C -4.392993 -9.793197 1.757727

H -3.534700 -9.571026 2.382470
C -5.169670 -10.917581 2.049295
H -4.922070 -11.532083 2.908867
C -6.261930 -11.242727 1.239329
H -6.871236 -12.107726 1.478291
C -5.791534 -9.306994 -0.144555
H -6.035026 -8.681393 -0.994362
C -6.564640 -10.439435 0.132874
H -7.408412 -10.680491 -0.507628
C -1.966881 -9.197454 -0.623579
O -2.087760 -10.110727 -1.468874
S -0.692085 -7.457576 2.796632
H 0.803309 -3.171027 3.411594
O 2.246005 -4.373856 2.877937
O 1.746497 -2.949809 3.163559
FE 0.840926 -5.691694 2.915425
N 2.311423 -6.998881 2.416005
N 0.588604 -5.229262 0.954828
N -0.605316 -4.330387 3.414598
N 1.124933 -6.090412 4.863686
C 2.944874 -7.899372 3.254928
C 3.909005 -8.707203 2.501741
C 3.844195 -8.270648 1.196830
C 2.852955 -7.200235 1.158607
C 1.498713 -5.510152 -0.047569
C 1.143602 -4.788215 -1.256911
C -0.064420 -4.140783 -1.014426
C -0.392230 -4.425155 0.397357
C -1.563597 -3.842646 2.524121
C -2.607703 -3.128087 3.252152
C -2.262116 -3.149128 4.594950
C -1.057056 -3.986031 4.691082
C 0.480269 -5.508735 5.943532
C 0.884582 -6.171913 7.182081
C 1.784419 -7.154340 6.823458
C 1.918149 -7.112420 5.375353
C 2.731141 -7.958666 4.626940
H 3.259482 -8.743901 5.154359
C 2.525354 -6.444647 0.041899
H 3.105589 -6.621080 -0.858211
C -1.466940 -3.924282 1.139709
H -2.299896 -3.517925 0.586813
C -0.487536 -4.506590 5.851899
H -0.913302 -4.176525 6.794648
O 1.653100 -2.009226 0.690561
H 1.674531 -2.315172 1.658971
H 1.219698 -2.686332 0.129393
O 3.277217 1.604939 0.697816
H 2.557247 1.010114 0.301494
H 2.847167 2.125075 1.409567
O 5.558366 2.351504 -0.029581
H 4.733300 1.906234 0.376314
H 6.348415 1.779506 -0.049997
h -1.798473 -7.294335 3.605090
h 4.638486 -9.399427 2.922158
h 4.384195 -8.630156 0.320919
h 1.832267 -4.725856 -2.099478
h -0.590476 -3.568651 -1.778623
h -3.495157 -2.733604 2.757303
h -2.696060 -2.661340 5.467774
h 0.493502 -5.956739 8.176477
h 2.388091 -7.778708 7.482102
h -3.677849 -7.151831 -2.631553
h -1.288144 -9.334140 0.218264
h 3.366424 4.954077 -0.466306
h 0.540530 1.425682 -1.732828

Conf LW3 –TSoo

C 4.070923 5.046096 -1.284713
H 3.949304 6.034821 -1.732271
H 5.073654 4.995053 -0.849980
C 3.946185 4.007442 -2.380937
O 3.271293 4.188897 -3.409612
O 4.606349 2.843443 -2.202646
H 5.013189 2.655185 -1.230542
C 0.829891 0.423144 -1.574455
H 0.045601 -0.277568 -1.897996
O 0.982393 0.317798 -0.131479
H 1.168975 -0.673899 0.160645
C 2.129349 0.035442 -2.291143
H 2.413428 -0.981000 -1.999472
H 2.016361 0.054826 -3.381921
H 2.953890 0.705271 -2.029978
N -3.385421 -7.967203 -2.118689
H -3.384710 -8.861232 -2.586591
C -2.781878 -7.912705 -0.798718
H -2.080152 -7.067699 -0.700932
C -3.835407 -7.742963 0.373004
H -3.275381 -7.450044 1.265627
H -4.467562 -6.890322 0.097873
C -4.685588 -8.961424 0.665428
C -4.384088 -9.801002 1.752767
H -3.520364 -9.589742 2.373811
C -5.166051 -10.922828 2.040385
H -4.916708 -11.545389 2.893664
C -6.265470 -11.234797 1.234917
H -6.878696 -12.097825 1.470810
C -5.792066 -9.290729 -0.136045
H -6.037660 -8.656487 -0.978757
C -6.570293 -10.420728 0.136947
H -7.419445 -10.651330 -0.500257
C -1.962188 -9.206032 -0.623662
O -2.090829 -10.120807 -1.466020
S -0.662621 -7.478125 2.796796
H 0.807363 -2.941493 3.345450
O 2.191681 -4.520995 2.973294
O 1.670262 -2.550128 3.063820
FE 0.915343 -5.653687 2.937855
N 2.315469 -7.049783 2.423739
N 0.620675 -5.243160 0.970816
N -0.574306 -4.390972 3.417640
N 1.142004 -6.146058 4.873554
C 2.943005 -7.957250 3.259664
C 3.927231 -8.738310 2.507998
C 3.885238 -8.273288 1.211785
C 2.883730 -7.213485 1.173908
C 1.522261 -5.535253 -0.036198
C 1.135392 -4.850709 -1.258965
C -0.074269 -4.210944 -1.011945
C -0.379728 -4.469492 0.407797
C -1.535228 -3.901474 2.534562
C -2.553697 -3.157852 3.268253
C -2.180064 -3.154831 4.603151
C -0.987447 -4.010366 4.694292
C 0.520463 -5.546166 5.953291
C 0.915538 -6.217527 7.189814
C 1.792395 -7.217890 6.826783
C 1.919564 -7.181245 5.379038
C 2.722239 -8.032255 4.628493
H 3.244379 -8.824551 5.150296
C 2.560769 -6.453300 0.059689
H 3.151861 -6.620947 -0.834235
C -1.457445 -3.985317 1.150159
H -2.298935 -3.588960 0.603154
C -0.421083 -4.523175 5.858512
H -0.829479 -4.169065 6.799432
O 1.647405 -2.005781 0.564064
H 1.629636 -2.243087 1.578544
H 1.254225 -2.724060 0.027661
O 3.009461 1.603608 0.681923
H 2.287614 0.976406 0.318116
H 2.611966 2.116485 1.419147
O 5.352632 2.248945 0.058547
H 4.487891 1.829092 0.408345
H 6.135633 1.670856 0.107574
h -1.770452 -7.323097 3.604894
h 4.652811 -9.434495 2.928626
h 4.458452 -8.599476 0.343975
h 1.804268 -4.811225 -2.118681
h -0.615564 -3.643304 -1.768814
h -3.445263 -2.761474 2.782391
h -2.587985 -2.639891 5.472923
h 0.528504 -5.999064 8.185075
h 2.392832 -7.847182 7.483695
h -3.673022 -7.156062 -2.627912
h -1.280193 -9.344070 0.215322
h 3.368758 4.951525 -0.456409
h 0.539020 1.444347 -1.820635

Conf LW3 –IC1

C 4.103177 5.032877 -1.239711
H 4.004821 6.029083 -1.676200
H 5.095769 4.961517 -0.784501
C 3.989855 4.007909 -2.350740
O 3.347652 4.217680 -3.396569
O 4.621813 2.831386 -2.172520
H 5.032023 2.636784 -1.194434
C 0.820435 0.462890 -1.559195

H 0.024809 -0.240044 -1.851173
O 0.995674 0.397546 -0.118855
H 1.100914 -0.601864 0.195977
C 2.105030 0.043395 -2.284052
H 2.376985 -0.971475 -1.974573
H 1.981405 0.044022 -3.373987
H 2.941689 0.705612 -2.042886
N -3.380971 -7.984761 -2.111593
H -3.382162 -8.878123 -2.580484
C -2.783366 -7.932623 -0.788291
H -2.084027 -7.086318 -0.686237
C -3.844007 -7.765170 0.377685
H -3.289063 -7.471920 1.272918
H -4.474600 -6.912122 0.099489
C -4.698166 -8.982003 0.666376
C -4.405882 -9.819591 1.757950
H -3.546521 -9.608099 2.385044
C -5.194433 -10.937458 2.044380
H -4.950609 -11.559259 2.899906
C -6.291984 -11.246752 1.234819
H -6.910056 -12.107485 1.467966
C -5.803540 -9.307598 -0.138289
H -6.043146 -8.674116 -0.983297
C -6.588984 -10.432715 0.134585
H -7.438001 -10.659456 -0.504191
C -1.960554 -9.224554 -0.609034
O -2.087758 -10.142732 -1.447981
S -0.637181 -7.458004 2.760537
H 1.523134 -3.090767 3.288315
O 2.265483 -4.522482 3.080527
O 0.912738 -2.303510 3.095584
FE 1.046059 -5.683505 2.925628
N 2.414213 -7.087876 2.431510
N 0.764515 -5.280710 0.951406
N -0.449308 -4.387070 3.351626
N 1.198366 -6.190171 4.851913
C 3.019370 -8.005064 3.275979
C 4.040305 -8.755362 2.546353
C 4.045249 -8.261169 1.258186
C 3.033081 -7.217433 1.201859
C 1.692462 -5.545672 -0.041813
C 1.300502 -4.885382 -1.273496
C 0.051479 -4.312286 -1.056737
C -0.262862 -4.568713 0.361894
C -1.435950 -3.954784 2.458338
C -2.475309 -3.231126 3.180203
C -2.096027 -3.179154 4.511262
C -0.876933 -3.993759 4.620240
C 0.582443 -5.558848 5.911415
C 0.921307 -6.241580 7.158356
C 1.760278 -7.280837 6.817844
C 1.929795 -7.250337 5.373994
C 2.744194 -8.103723 4.638068
H 3.246341 -8.900694 5.174050
C 2.740633 -6.445814 0.082434
H 3.351868 -6.612300 -0.798670
C -1.368391 -4.108056 1.084942
H -2.228635 -3.780088 0.522234
C -0.325780 -4.503062 5.789365
H -0.732888 -4.127668 6.722399
O 1.408962 -1.951840 0.623313
H 1.133245 -2.112910 1.621133
H 1.043949 -2.651740 0.044022
O 3.065984 1.581473 0.753024
H 2.336001 0.995888 0.342411
H 2.648980 2.094387 1.478689
O 5.371714 2.263654 0.081193
H 4.514385 1.841108 0.457162
H 6.175164 1.721105 0.170651
h -1.740862 -7.312965 3.576134
h 4.755662 -9.460709 2.969221
h 4.657508 -8.557078 0.406340
h 1.975079 -4.793327 -2.124693
h -0.505453 -3.793760 -1.837137
h -3.375050 -2.866588 2.684578
h -2.519701 -2.660471 5.371224
h 0.527786 -6.019476 8.150262
h 2.296763 -7.943120 7.497279
h -3.669160 -7.171490 -2.617072
h -1.278168 -9.355447 0.230778
h 3.385969 4.938228 -0.424407
h 0.535559 1.482623 -1.818148

Conf LW3 –Cpd I

C 4.132828 4.945289 -1.142055
H 4.083093 5.954735 -1.557727
H 5.104786 4.827522 -0.651028
C 4.034908 3.933358 -2.277069
O 3.403770 4.258365 -3.331640
O 4.593796 2.763073 -2.103913
H 4.847069 2.299090 -0.666641
C 0.753498 0.494582 -1.835144
H 0.052045 -0.173780 -2.350992
O 0.610593 0.195456 -0.417145
H 1.343039 -1.212543 -0.040060
C 2.159261 0.181041 -2.350145
H 2.430915 -0.837880 -2.056866
H 2.197889 0.242913 -3.444310
H 2.919828 0.859863 -1.954234
N -3.382608 -7.995078 -2.119993
H -3.391213 -8.885396 -2.594197
C -2.786029 -7.950552 -0.798165
H -2.086331 -7.104309 -0.692739
C -3.846362 -7.788184 0.369906
H -3.293942 -7.495179 1.267396
H -4.478034 -6.935655 0.093314
C -4.697320 -9.007563 0.656796
C -4.401785 -9.848654 1.744449
H -3.539395 -9.642015 2.368994
C -5.188973 -10.967145 2.030836
H -4.944040 -11.589980 2.885228
C -6.287969 -11.274630 1.223003
H -6.904985 -12.135842 1.455979
C -5.803545 -9.332010 -0.146974
H -6.045970 -8.696522 -0.989663
C -6.587229 -10.458508 0.124934
H -7.436185 -10.685117 -0.513557
C -1.963769 -9.242458 -0.624321
O -2.098978 -10.163310 -1.456807
S -0.638660 -7.524418 2.785556
H 1.576356 -2.816070 3.287875
O 2.220473 -4.553312 3.134377
O 1.216008 -1.977410 2.929780
FE 1.029808 -5.713214 2.953043
N 2.407031 -7.123564 2.449954
N 0.750506 -5.311041 0.984143
N -0.503800 -4.503877 3.400841
N 1.172772 -6.263720 4.869459
C 3.017653 -8.050668 3.286223
C 4.041713 -8.792168 2.555810
C 4.045660 -8.289006 1.271034
C 3.029197 -7.251915 1.226269
C 1.651793 -5.605005 -0.025057
C 1.238334 -4.981119 -1.269855
C 0.018498 -4.360501 -1.030337
C -0.261747 -4.575588 0.398453
C -1.434765 -3.986576 2.516859
C -2.443634 -3.210112 3.233822
C -2.063146 -3.185858 4.562917
C -0.879175 -4.057311 4.653711
C 0.577913 -5.626745 5.946571
C 0.922196 -6.311025 7.184761
C 1.744749 -7.359383 6.830323
C 1.901183 -7.320212 5.388607
C 2.727179 -8.163620 4.641341
H 3.229912 -8.961704 5.174271
C 2.717538 -6.483166 0.106016
H 3.345881 -6.623257 -0.767098
C -1.349884 -4.096874 1.134802
H -2.191469 -3.718044 0.575518
C -0.304309 -4.555389 5.824437
H -0.659672 -4.136362 6.759493
O 1.815776 -2.069779 0.197944
H 1.410030 -1.983386 1.960239
H 1.391818 -2.800603 -0.290166
O 2.408965 1.529731 0.727387
H 1.312754 0.733685 0.104628
H 2.124238 2.071772 1.493475
O 4.844240 1.929029 0.292089
H 3.435174 1.547638 0.595030
H 5.628780 1.379498 0.462808
h -1.754144 -7.378190 3.584718
h 4.758090 -9.500551 2.971820
h 4.658528 -8.578599 0.417456
h 1.899851 -4.944780 -2.135385
h -0.539744 -3.816986 -1.792587
h -3.317905 -2.792359 2.734623
h -2.465582 -2.662356 5.430129

h 0.544001 -6.083722 8.181439
h 2.284816 -8.024911 7.503722
h -3.667606 -7.177972 -2.621079
h -1.273052 -9.372578 0.208773
h 3.379252 4.856976 -0.359501
h 0.490977 1.532629 -2.039125

Conf LM1 –RC

C 2.404854 4.622947 -7.409706
H 2.346995 5.704138 -7.561528
H 3.471597 4.370786 -7.484854
C 1.740915 3.959821 -8.604425
O 1.848886 4.486294 -9.734837
O 1.122180 2.769272 -8.515300
H 1.114577 2.178908 -7.652638
C -0.120319 1.898156 -2.068388
H -0.613051 0.940897 -1.864587
O -0.151304 2.745443 -0.894958
H 0.242548 2.278203 -0.129096
C 1.315999 1.649308 -2.563946
H 1.859009 1.018924 -1.857186
H 1.322409 1.123965 -3.527246
H 1.865867 2.589460 -2.671271
N -3.955367 -5.194950 4.270939
H -4.652964 -5.300602 5.000253
C -2.660996 -4.567977 4.611686
H -2.100951 -4.331283 3.693704
C -2.848181 -3.235958 5.385092
H -3.310653 -3.481333 6.352248
H -1.845148 -2.874097 5.626181
N -3.147442 -0.828651 4.686068
H -2.162546 -0.577781 4.866435
C -3.631766 -2.133529 4.734343
C -4.142132 -0.012125 4.224412
H -4.014272 1.047255 4.079440
N -5.258681 -0.708440 3.976150
C -4.931838 -2.035257 4.275398
H -5.626133 -2.827157 4.090307
C -1.756434 -5.509960 5.477002
O -0.976714 -5.010203 6.311745
S 0.027585 -0.628208 5.279934
H 2.995210 0.956514 0.342705
O 2.737881 -0.123682 1.963026
O 2.181435 0.533016 0.692622
FE 1.517663 -0.240629 3.380543
N 1.985081 -2.203314 3.652399
N -0.051150 -0.735195 2.202670
N 1.068539 1.725811 3.176566
N 3.069423 0.222395 4.583698
C 2.800748 -2.754035 4.634589
C 2.731393 -4.213905 4.582988
C 1.893380 -4.535310 3.539502
C 1.402129 -3.270009 2.995299
C -0.347017 -2.004251 1.753412
C -1.578114 -1.985284 0.967200
C -2.048460 -0.684213 0.962370
C -1.049189 0.100866 1.712949
C 0.001062 2.240941 2.470536
C 0.087791 3.698839 2.414830
C 1.242849 4.066399 3.087160
C 1.865538 2.810541 3.538161
C 3.628401 1.482471 4.711808
C 4.777460 1.431560 5.609866
C 4.852833 0.138071 6.084746
C 3.804778 -0.619716 5.408752
C 3.627721 -2.003704 5.468107
H 4.231100 -2.548385 6.186769
C 0.375870 -3.155533 2.063183
H 0.030137 -4.081820 1.614634
C -0.981834 1.486073 1.827205
H -1.691664 2.064390 1.256136
C 3.096442 2.654639 4.174736
H 3.729649 3.525921 4.272315
O -0.377540 -0.248772 -5.240963
H -0.414754 -0.589430 -4.274724
H -1.220859 0.210287 -5.482613
O 1.220493 1.030594 -6.718455
H 0.597890 0.558583 -6.038295
H 2.154569 0.826756 -6.508805
O 1.075495 -1.128937 -1.064938
H 1.286454 -0.509755 -0.310541
H 1.811021 -1.768157 -1.133151
O -0.626764 -1.315468 -2.913065
H -0.017632 -1.164598 -2.105425
H -1.553259 -1.537098 -2.660247
h 0.208064 0.439294 6.135629
h 3.184896 -4.879866 5.317084
h 1.568190 -5.514614 3.188387
h -2.009988 -2.898229 0.557221
h -2.990583 -0.383110 0.504322
h -0.661666 4.325602 1.931561
h 1.550984 5.103495 3.219645
h 5.444136 2.275131 5.788742
h 5.515434 -0.270333 6.847788
h -4.102628 -5.663137 3.399684
h -1.877056 -6.587068 5.361430
h 2.084326 4.394993 -6.393161
h -0.674911 2.402015 -2.859981

Conf LM1 –TSoo

C 2.411013 4.609788 -7.414798
H 2.364948 5.691021 -7.570146
H 3.475127 4.346751 -7.485854
C 1.742946 3.949019 -8.608175
O 1.847815 4.478059 -9.738279
O 1.125754 2.758437 -8.518694
H 1.117072 2.165848 -7.654811
C -0.106039 1.880174 -2.194923
H -0.580270 0.907240 -2.024202
O -0.084341 2.654577 -0.976607
H 0.589993 2.260748 -0.366201
C 1.305355 1.670810 -2.782756
H 1.882759 0.997620 -2.146718
H 1.268502 1.228727 -3.786233
H 1.852435 2.618684 -2.835608
N -3.953090 -5.196141 4.271416
H -4.648511 -5.302030 5.002791
C -2.656067 -4.573212 4.608935
H -2.099026 -4.336853 3.689021
C -2.838224 -3.241870 5.384834
H -3.295307 -3.487911 6.354314
H -1.833690 -2.880616 5.620848
N -3.149615 -0.831183 4.700247
H -2.168394 -0.576157 4.879102
C -3.626240 -2.139693 4.738958
C -4.147973 -0.016937 4.241181
H -4.026320 1.044275 4.104177
N -5.259020 -0.718488 3.986618
C -4.925530 -2.045261 4.278443
H -5.614954 -2.840015 4.089043
C -1.748900 -5.517825 5.469508
O -0.957975 -5.019317 6.294542
S 0.034531 -0.614193 5.272028
H 2.763629 0.996945 0.335683
O 2.661048 -0.229776 2.064569
O 1.797310 1.019476 0.161505
FE 1.571534 -0.277456 3.340310
N 1.959315 -2.241101 3.689815
N -0.033801 -0.787864 2.229804
N 1.096399 1.684907 3.167420
N 3.052251 0.211091 4.620436
C 2.782597 -2.777787 4.673367
C 2.736098 -4.238054 4.611521
C 1.913081 -4.568576 3.559062
C 1.407928 -3.311563 3.015664
C -0.324470 -2.053208 1.762856
C -1.555764 -2.030027 0.980823
C -2.032228 -0.732950 0.996513
C -1.032315 0.051046 1.742771
C 0.024331 2.189957 2.459130
C 0.109351 3.644278 2.387199
C 1.262045 4.024324 3.055876
C 1.889315 2.778663 3.519899
C 3.629266 1.464579 4.727861
C 4.779123 1.408087 5.618873
C 4.844157 0.116521 6.102231
C 3.784525 -0.637011 5.441796
C 3.602257 -2.020216 5.505760
H 4.208979 -2.561879 6.223744
C 0.397188 -3.203078 2.067828
H 0.067253 -4.126883 1.604027
C -0.964017 1.433601 1.835937
H -1.658278 2.001744 1.236795
C 3.112552 2.631510 4.167452
H 3.750893 3.500153 4.251557
O -0.382571 -0.277435 -5.282210
H -0.419566 -0.627036 -4.313077
H -1.223594 0.190354 -5.514616

O 1.219797 1.021802 -6.723556
H 0.589711 0.532271 -6.056000
H 2.152461 0.830137 -6.496111
O 0.985568 -1.079357 -1.106100
H 1.227319 -0.271385 -0.534145
H 1.674818 -1.759309 -0.994263
O -0.633239 -1.358328 -2.978920
H -0.009890 -1.187089 -2.167444
H -1.564162 -1.538685 -2.713794
h 0.208679 0.448053 6.135539
h 3.194104 -4.901494 5.345103
h 1.603916 -5.550253 3.200182
h -1.981762 -2.935521 0.548767
h -2.979138 -0.426825 0.551862
h -0.639210 4.259072 1.887447
h 1.565358 5.063936 3.179469
h 5.452450 2.248119 5.789297
h 5.508680 -0.292098 6.863484
h -4.101993 -5.663391 3.399936
h -1.877197 -6.594467 5.357934
h 2.085030 4.388215 -6.398576
h -0.692892 2.411525 -2.944146

Conf LM1 –IH

C 2.427245 4.607945 -7.432888
H 2.390886 5.688976 -7.592211
H 3.488693 4.335255 -7.504540
C 1.750108 3.950636 -8.623113
O 1.851979 4.481444 -9.753295
O 1.129691 2.763450 -8.531144
H 1.126769 2.164991 -7.666544
C -0.122619 1.901912 -2.266597
H -0.597762 0.930050 -2.089711
O -0.092641 2.685998 -1.055319
H 0.587776 2.257642 -0.460957
C 1.291704 1.680890 -2.837635
H 1.864850 1.036226 -2.169962
H 1.261227 1.204425 -3.824990
H 1.835200 2.629106 -2.918842
N -3.946473 -5.203520 4.273991
H -4.641309 -5.305374 5.006882
C -2.641354 -4.596601 4.609979
H -2.087465 -4.357081 3.689089
C -2.808911 -3.267235 5.392786
H -3.261867 -3.512528 6.364314
H -1.800909 -2.911419 5.622161
N -3.121179 -0.854289 4.707354
H -2.140660 -0.598997 4.886333
C -3.597763 -2.162602 4.751744
C -4.122585 -0.040799 4.250939
H -4.004416 1.020864 4.113197
N -5.234292 -0.743424 4.002391
C -4.898891 -2.069291 4.295957
H -5.587198 -2.865723 4.110528
C -1.734711 -5.555373 5.456405
O -0.916012 -5.071677 6.263402
S 0.068573 -0.638963 5.290441
H 1.951584 0.634994 0.993717
O 2.655857 -0.153867 2.061303
O 1.352882 0.953807 0.244845
FE 1.644369 -0.330845 3.410044
N 2.033403 -2.299714 3.744729
N 0.046706 -0.875733 2.284878
N 1.163590 1.653260 3.258790
N 3.118839 0.173992 4.691068
C 2.873131 -2.828842 4.725394
C 2.820945 -4.286752 4.686989
C 1.972930 -4.629626 3.657325
C 1.460214 -3.381244 3.111674
C -0.287026 -2.152958 1.858576
C -1.482696 -2.103618 1.023049
C -1.860585 -0.778353 0.925515
C -0.840663 -0.025296 1.669830
C 0.194614 2.146766 2.430402
C 0.231102 3.603370 2.395203
C 1.291837 3.999127 3.192468
C 1.910405 2.760784 3.685744
C 3.672824 1.431353 4.836563
C 4.829789 1.374314 5.713481
C 4.918836 0.071387 6.161798
C 3.868251 -0.678642 5.491528
C 3.694965 -2.063238 5.545011
H 4.309719 -2.602988 6.257540
C 0.414192 -3.296209 2.190253
H 0.078018 -4.229527 1.751409
C -0.635909 1.361264 1.615856
H -1.177410 1.908431 0.856418
C 3.121916 2.616446 4.339453
H 3.739208 3.496497 4.461598
O -0.378311 -0.281649 -5.347192
H -0.439952 -0.639403 -4.375891
H -1.213660 0.194893 -5.584405
O 1.234664 1.032530 -6.742420
H 0.598356 0.530100 -6.083580
H 2.166233 0.850464 -6.503716
O 0.874842 -1.046994 -1.194739
H 0.985808 -0.216698 -0.563164
H 1.681311 -1.593820 -1.162743
O -0.686170 -1.361921 -3.072045
H -0.056821 -1.187331 -2.246601
H -1.618140 -1.532712 -2.808903
h 0.216236 0.431102 6.149221
h 3.280049 -4.945392 5.424202
h 1.661408 -5.615719 3.312884
h -1.947211 -2.996433 0.604511
h -2.760199 -0.426249 0.420754
h -0.501008 4.201566 1.852761
h 1.556315 5.040995 3.373104
h 5.500047 2.215071 5.892219
h 5.579215 -0.337080 6.926730
h -4.100228 -5.665443 3.400516
h -1.886965 -6.629263 5.348483
h 2.100743 4.392969 -6.415416
h -0.713713 2.433463 -3.012336

Conf LM1 –Heme-OH

C 2.442489 4.614491 -7.454146
H 2.411260 5.695336 -7.615560
H 3.502143 4.335805 -7.528182
C 1.757932 3.959976 -8.641190
O 1.857103 4.489521 -9.771521
O 1.132725 2.774944 -8.546494
H 1.132036 2.180802 -7.682803
C -0.122393 1.939620 -2.303522
H -0.601050 0.981740 -2.071189
O -0.081794 2.796558 -1.138062
H 0.649736 2.469313 -0.561818
C 1.285034 1.692245 -2.871369
H 1.858922 1.060180 -2.190941
H 1.245846 1.183445 -3.841067
H 1.832321 2.634182 -2.989675
N -3.944796 -5.206613 4.275535
H -4.639229 -5.309987 5.008627
C -2.637017 -4.605980 4.613915
H -2.082196 -4.366513 3.694169
C -2.797426 -3.275983 5.396369
H -3.248699 -3.517980 6.369511
H -1.787197 -2.923626 5.621362
N -3.101662 -0.864975 4.699067
H -2.116381 -0.616255 4.861349
C -3.584075 -2.170378 4.755119
C -4.102669 -0.050085 4.243941
H -3.980750 1.009942 4.097321
N -5.219857 -0.749139 4.008243
C -4.887935 -2.074449 4.308009
H -5.579469 -2.870357 4.131486
C -1.734901 -5.569490 5.458730
O -0.917358 -5.091701 6.270467
S 0.109293 -0.681146 5.265248
H 1.798302 0.651639 1.023966
O 2.746825 -0.192987 2.060659
O 1.049520 1.034079 0.440080
FE 1.736221 -0.384986 3.415935
N 2.100180 -2.349836 3.749767
N 0.141432 -0.938160 2.260118
N 1.237270 1.619110 3.269320
N 3.176366 0.139178 4.710247
C 2.955009 -2.874730 4.716448
C 2.884920 -4.329298 4.704966
C 2.001070 -4.680174 3.706157
C 1.486250 -3.441191 3.152504
C -0.300069 -2.227657 1.937254
C -1.507763 -2.138744 1.147841
C -1.795802 -0.781863 0.985181
C -0.705726 -0.086649 1.630038
C 0.297028 2.107654 2.430179
C 0.198795 3.534951 2.500352
C 1.196569 3.957967 3.387547

C 1.872875 2.749435 3.835247
C 3.692059 1.417034 4.901916
C 4.856636 1.356838 5.764818
C 4.983557 0.041647 6.168509
C 3.948659 -0.713319 5.483858
C 3.793089 -2.104646 5.522369
H 4.419241 -2.643499 6.225088
C 0.387881 -3.370488 2.294329
H 0.007925 -4.315101 1.917332
C -0.185891 1.261526 1.321069
H -0.830405 1.819991 0.653717
C 3.084796 2.606062 4.495298
H 3.659338 3.502239 4.692145
O -0.374876 -0.283939 -5.367337
H -0.438815 -0.639420 -4.401418
H -1.211666 0.188404 -5.609100
O 1.242341 1.043947 -6.754187
H 0.608492 0.537891 -6.101870
H 2.174580 0.851548 -6.526601
O 0.920602 -0.988009 -1.216949
H 0.886066 -0.214916 -0.571167
H 1.731269 -1.514776 -1.092842
O -0.682749 -1.356865 -3.078367
H -0.053395 -1.181195 -2.277601
H -1.610047 -1.539711 -2.801206
h 0.225025 0.391162 6.126124
h 3.336207 -4.982138 5.452098
h 1.677167 -5.669091 3.381819
h -2.035289 -3.009741 0.759065
h -2.678730 -0.380576 0.487715
h -0.547179 4.104402 1.945992
h 1.387890 5.007011 3.613310
h 5.514643 2.203113 5.962076
h 5.637749 -0.366303 6.939012
h -4.099755 -5.666215 3.401050
h -1.888453 -6.642751 5.346488
h 2.117877 4.403405 -6.435257
h -0.721130 2.455493 -3.054158

Conf LM2 –RC

C -0.278206 -2.768766 -6.528475
H -0.626557 -2.299272 -7.449568
H 0.800390 -2.943650 -6.628439
C -0.980975 -4.105065 -6.416920
O -1.822481 -4.474016 -7.265023
O -0.661879 -4.941556 -5.409152
H -0.072736 -4.589356 -4.634862
C -1.332177 -1.402969 -0.157038
H -1.863998 -1.408940 0.800702
O -1.089061 -0.029856 -0.582223
H -0.462375 0.419118 0.036338
C -0.035509 -2.199709 0.051490
H 0.575948 -1.698623 0.810409
H -0.268385 -3.201125 0.448276
H 0.564248 -2.298366 -0.854987
N 1.171903 -2.610789 8.886096
H 1.004225 -2.951537 9.820449
C 2.157178 -1.566084 8.773913
H 2.737874 -1.648605 7.848197
C 1.585378 -0.060570 8.835479
H 1.716990 0.306121 9.860579
H 2.218390 0.564253 8.193637
N -0.291779 0.697166 7.285757
H 0.266842 1.168058 6.579790
C 0.148974 0.121459 8.475776
C -1.658769 0.716224 7.299111
H -2.238859 1.120952 6.489107
N -2.127881 0.181934 8.431186
C -1.005139 -0.181815 9.174122
H -1.100945 -0.620058 10.153161
C 3.100695 -1.756798 9.992803
O 2.671291 -2.424120 10.958314
S 0.584058 3.265872 5.207355
H 0.623727 2.484867 0.290897
O 2.112800 1.853902 1.419831
O 1.083610 1.613072 0.303877
FE 1.386434 2.595191 2.985912
N 2.715752 1.458389 3.993364
N -0.008207 1.129162 3.069350
N 0.074023 3.764045 1.939521
N 2.749926 4.105081 2.982868
C 3.882465 1.865128 4.613450
C 4.507378 0.729356 5.304015
C 3.735719 -0.374847 5.026647
C 2.585397 0.108157 4.253576
C 0.221712 -0.153936 3.515660
C -1.020686 -0.925614 3.483025
C -2.019761 -0.080548 3.027004
C -1.348470 1.196969 2.713365
C -1.254025 3.468130 1.665365
C -1.885511 4.574679 0.951155
C -0.923467 5.564664 0.798518
C 0.299735 5.041120 1.436841
C 2.638223 5.304737 2.297880
C 3.821522 6.130372 2.537364
C 4.623527 5.433366 3.423057
C 3.939936 4.166498 3.690695
C 4.434061 3.138935 4.489926
H 5.355933 3.343525 5.027750
C 1.443694 -0.639417 3.987192
H 1.469129 -1.682184 4.285255
C -1.887115 2.275151 2.016068
H -2.886107 2.153539 1.623759
C 1.521433 5.706338 1.568742
H 1.601092 6.675576 1.087353
O 1.565475 0.124319 -1.897318
H 1.609043 0.580678 -1.015765
H 0.785061 0.476552 -2.381191
O 2.053023 -2.210633 -2.721303
H 1.856800 -1.268970 -2.351320
H 3.013804 -2.371891 -2.692234
O 0.721460 -4.277234 -3.354184
H 0.340853 -4.769550 -2.589075
H 1.171787 -3.398086 -3.063560
h 0.269674 4.609371 5.184544
h 5.348782 0.838919 5.988194
h 3.916656 -1.423076 5.264437
h -1.065316 -1.953812 3.842029
h -3.070663 -0.361795 2.959379
h -2.950894 4.579345 0.720926
h -0.970891 6.562545 0.362569
h 4.032854 7.100892 2.088482
h 5.597681 5.742520 3.801890
h 0.781763 -3.145355 8.136429
h 4.105981 -1.339787 10.052535
h -0.409677 -2.046896 -5.722444
h -1.947080 -1.850214 -0.938021

Conf LM2 –TSoo

C -0.281308 -2.791000 -6.533011
H -0.618227 -2.323562 -7.459513
H 0.798567 -2.966225 -6.615026
C -0.988890 -4.125561 -6.431153
O -1.831415 -4.480069 -7.286513
O -0.673363 -4.973482 -5.436279
H -0.089221 -4.638487 -4.638788
C -1.410581 -1.384763 -0.217420
H -1.912087 -1.439369 0.757557
O -1.306509 -0.005056 -0.655778
H -0.547017 0.476374 -0.199677
C -0.052308 -2.085721 -0.044218
H 0.551173 -1.523491 0.676104
H -0.195061 -3.095263 0.374946
H 0.517653 -2.159828 -0.971518
N 1.174352 -2.618563 8.888544
H 0.989522 -2.953784 9.821701
C 2.166060 -1.580243 8.786972
H 2.758022 -1.668971 7.869037
C 1.603075 -0.070320 8.835894
H 1.754717 0.314886 9.851684
H 2.226670 0.540075 8.171216
N -0.287269 0.672026 7.301829
H 0.273376 1.119791 6.585241
C 0.161686 0.110040 8.495171
C -1.654395 0.696241 7.324829
H -2.241070 1.092270 6.515115
N -2.115274 0.177635 8.466998
C -0.987983 -0.181265 9.206019
H -1.078828 -0.610449 10.189387
C 3.092741 -1.774809 10.017604
O 2.641005 -2.421875 10.986240
S 0.572949 3.283192 5.262742
H 1.004569 2.134168 0.113095
O 2.243915 2.114152 1.659724
O 0.905936 1.169616 -0.026652
Fe 1.480576 2.607048 3.065610
N 2.754537 1.477954 4.156526
N 0.114022 1.123344 3.139659

N 0.158577 3.795243 2.078582
N 2.792513 4.156030 3.149005
C 3.920572 1.895186 4.774983
C 4.568862 0.753039 5.429730
C 3.819201 -0.359888 5.127384
C 2.662163 0.115464 4.368203
C 0.342483 -0.171994 3.556537
C -0.893217 -0.947082 3.488686
C -1.892030 -0.092669 3.054809
C -1.224400 1.190469 2.768843
C -1.142391 3.467957 1.753524
C -1.775085 4.561118 1.018436
C -0.826872 5.565099 0.886305
C 0.386308 5.062708 1.559371
C 2.709948 5.336826 2.426797
C 3.913559 6.133216 2.641521
C 4.697208 5.435555 3.543160
C 3.985399 4.196505 3.848529
C 4.466961 3.170086 4.657220
H 5.392606 3.368987 5.189234
C 1.551432 -0.653784 4.051381
H 1.590766 -1.702238 4.323050
C -1.766037 2.265120 2.078423
H -2.749806 2.125247 1.655870
C 1.601285 5.735756 1.689738
H 1.687311 6.693204 1.187936
O 1.567303 -0.032260 -2.151432
H 1.528340 0.394416 -1.223396
H 0.835235 0.360702 -2.678693
O 2.068830 -2.353015 -2.849494
H 1.858414 -1.373976 -2.540164
H 3.022264 -2.525588 -2.746924
O 0.667398 -4.357513 -3.377972
H 0.279440 -4.829697 -2.604837
H 1.169462 -3.488492 -3.107059
h 0.253790 4.625716 5.252151
h 5.421339 0.859879 6.100502
h 4.019586 -1.410267 5.338613
h -0.942327 -1.988806 3.805651
h -2.944324 -0.369266 2.989721
h -2.833671 4.545734 0.759158
h -0.877652 6.560991 0.446209
h 4.151973 7.084704 2.166235
h 5.679816 5.725162 3.915552
h 0.786211 -3.149882 8.135538
h 4.106143 -1.378206 10.079162
h -0.422459 -2.066080 -5.731366
h -2.005987 -1.883442 -0.982192

Conf LM2 –Cpd I

C -0.341591 -2.837238 -6.573993
H -0.693953 -2.360026 -7.490875
H 0.737112 -3.014642 -6.675523
C -1.046510 -4.190572 -6.460340
O -1.906287 -4.489618 -7.352752
O -0.723779 -5.008482 -5.495179
H 0.005956 -4.691767 -4.327756
C -1.400160 -1.579188 -0.213528
H -1.857279 -1.788156 0.767082
O -1.335964 -0.157449 -0.449399
H -0.419651 0.223463 -0.190644
C -0.028889 -2.282127 -0.203855
H 0.614660 -1.802594 0.538778
H -0.146725 -3.339242 0.085181
H 0.491029 -2.231472 -1.162958
N 1.195097 -2.619916 8.909096
H 1.014332 -2.966585 9.838797
C 2.180082 -1.575824 8.813804
H 2.772538 -1.653962 7.894767
C 1.601167 -0.073064 8.875974
H 1.726517 0.298471 9.899498
H 2.230409 0.556730 8.234090
N -0.273471 0.565259 7.278353
H 0.302195 0.950080 6.542086
C 0.163989 0.091949 8.513946
C -1.642430 0.596121 7.287791
H -2.223941 0.935133 6.448773
N -2.112158 0.162215 8.459545
C -0.992241 -0.147359 9.232499
H -1.094528 -0.510494 10.241235
C 3.109883 -1.770711 10.041943
O 2.659292 -2.416216 11.011165
S 0.490966 3.308489 5.339103
H 1.519959 1.179416 0.569008
O 2.262240 2.179973 1.698115
O 1.018485 0.617628 -0.060755
FE 1.490231 2.626697 3.097843
N 2.760311 1.518709 4.211731
N 0.153968 1.100455 3.153263
N 0.130863 3.787108 2.152175
N 2.736358 4.209960 3.238832
C 3.926274 1.951641 4.834573
C 4.600078 0.819654 5.471991
C 3.869367 -0.305640 5.162753
C 2.709119 0.155661 4.407499
C 0.411212 -0.206188 3.536401
C -0.796625 -1.017198 3.431694
C -1.815443 -0.177412 3.021806
C -1.179539 1.127203 2.781762
C -1.162702 3.438755 1.824198
C -1.822651 4.517126 1.090100
C -0.887418 5.522180 0.922148
C 0.334642 5.044411 1.598238
C 2.654666 5.369742 2.483065
C 3.859148 6.168295 2.659912
C 4.655251 5.490400 3.568387
C 3.944804 4.265112 3.910985
C 4.444053 3.236673 4.711916
H 5.382488 3.439895 5.219404
C 1.623059 -0.646692 4.049563
H 1.697457 -1.699633 4.296757
C -1.746563 2.207757 2.111525
H -2.717663 2.040231 1.669340
C 1.543361 5.727659 1.720319
H 1.626847 6.665746 1.184239
O 1.749789 -0.124281 -2.362450
H 1.499993 0.318112 -0.900107
H 0.995733 0.274911 -2.850742
O 2.060834 -2.557702 -3.030618
H 1.882712 -1.085692 -2.657528
H 2.964263 -2.836487 -2.799658
O 0.576770 -4.546666 -3.432286
H 0.169297 -5.004891 -2.664534
H 1.405320 -3.350271 -3.155978
h 0.190896 4.655354 5.323076
h 5.456438 0.934805 6.136411
h 4.085681 -1.353690 5.369792
h -0.816756 -2.073951 3.698027
h -2.861296 -0.472383 2.936660
h -2.881384 4.478636 0.833838
h -0.937970 6.491449 0.426135
h 4.094533 7.105431 2.155496
h 5.646436 5.778775 3.918328
h 0.801440 -3.137793 8.149617
h 4.123713 -1.374391 10.098033
h -0.462543 -2.122047 -5.760397
h -2.024193 -2.000656 -1.001573

Conf LM3 –RC

C -1.286981 -5.092634 -4.924527
H -1.445888 -5.103032 -3.837145
H -2.234164 -5.370229 -5.395924
C -0.285209 -6.186081 -5.273660
O -0.659465 -7.198331 -5.919815
O 0.961959 -6.076518 -4.828120
H 1.332605 -5.165659 -4.222545
C -1.861644 -1.380664 -0.637540
H -2.127241 -0.365309 -0.315571
O -0.556148 -1.326004 -1.293072
H 0.057548 -0.609356 -0.963628
C -1.808823 -2.327938 0.565287
H -1.075862 -1.955085 1.284246
H -2.781716 -2.396467 1.066361
H -1.504738 -3.334455 0.258572
N -0.053737 -0.033009 8.533270
H -0.464255 0.125260 9.438903
C 1.247038 0.551930 8.301035
H 1.692296 0.171985 7.376605
C 1.177597 2.133944 8.194126
H 0.871296 2.503744 9.179590
H 2.195293 2.512840 8.018701
N 0.460713 2.746631 5.813268
H 1.328800 2.582405 5.320369
C 0.218968 2.657883 7.184547
C -0.656799 3.251085 5.208003
H -0.703135 3.443967 4.151300
N -1.609692 3.484801 6.114302
C -1.066428 3.127248 7.349797

H -1.614165 3.252421 8.268798
C 2.153986 0.251257 9.511404
O 1.635780 0.234321 10.649177
S 2.035131 3.874619 3.084943
H 1.141986 1.504081 -0.965882
O 2.440325 0.631434 0.219472
O 1.320952 0.544468 -0.822464
FE 2.303416 2.181190 1.354449
N 3.130071 1.099560 2.823529
N 0.451007 1.558793 1.868253
N 1.492158 3.304805 -0.140696
N 4.146583 2.805122 0.852253
C 4.354082 1.330740 3.423821
C 4.461020 0.552377 4.657140
C 3.355273 -0.269718 4.700592
C 2.494247 0.141154 3.584871
C 0.192179 0.500807 2.716133
C -1.249128 0.289366 2.814689
C -1.867026 1.257798 2.040067
C -0.774642 2.023590 1.411959
C 0.141454 3.566133 -0.334924
C -0.043411 4.438467 -1.492424
C 1.220089 4.683809 -2.024997
C 2.174653 3.988869 -1.140175
C 4.486526 3.485810 -0.304420
C 5.935319 3.690066 -0.353872
C 6.456038 3.186550 0.820434
C 5.326420 2.639758 1.570893
C 5.387589 2.046663 2.828266
H 6.336916 2.084879 3.352904
C 1.149895 -0.196629 3.458770
H 0.788407 -0.987928 4.107047
C -0.888395 2.967595 0.392202
H -1.882476 3.185832 0.031645
C 3.573343 4.007190 -1.221803
H 4.016665 4.521248 -2.069636
O 0.997187 -3.440382 -1.381148
H 1.623090 -3.104305 -0.648456
H 0.309642 -2.718535 -1.482439
O 4.472917 -0.870677 -0.674035
H 5.338057 -0.729615 -0.248740
H 3.852216 -0.113566 -0.470923
O 2.472742 -2.223407 0.372814
H 2.074398 -1.385355 0.687269
H 3.360783 -1.959098 -0.006638
O 1.859119 -4.246958 -3.557124
H 2.754059 -3.958178 -3.841760
H 1.548569 -3.901613 -2.606646
h 2.541590 5.093761 2.683026
h 5.192520 0.764323 5.436917
h 3.151491 -1.114570 5.358440
h -1.670134 -0.461481 3.483305
h -2.948384 1.372889 1.965998
h -1.035652 4.762309 -1.806512
h 1.553760 5.219525 -2.913670
h 6.458650 4.122188 -1.206786
h 7.498555 3.103268 1.127499
h -0.541747 -0.671255 7.937906
h 3.224835 0.099603 9.375941
h -1.035816 -4.071262 -5.210501
h -2.571520 -1.752021 -1.376619

Conf LM3–TSoo

C -1.323246 -5.117260 -4.975372
H -1.502205 -5.145840 -3.891253
H -2.266083 -5.375173 -5.467374
C -0.325729 -6.220239 -5.321950
O -0.723972 -7.225575 -5.973957
O 0.912437 -6.123516 -4.872948
H 1.352750 -5.162415 -4.227244
C -1.916034 -1.456056 -0.675365
H -2.084012 -0.392476 -0.455135
O -0.584942 -1.584562 -1.240943
H -0.033203 -0.738888 -1.188277
C -2.020607 -2.291854 0.601295
H -1.254504 -1.960475 1.304471
H -3.003520 -2.177255 1.073862
H -1.859211 -3.355489 0.394774
N -0.053518 -0.032079 8.532334
H -0.461581 0.124263 9.439451
C 1.247379 0.551906 8.298567
H 1.691512 0.170786 7.374240
C 1.178838 2.133989 8.190756
H 0.872421 2.504487 9.175898
H 2.196715 2.512538 8.015728
N 0.465434 2.752839 5.809849
H 1.333873 2.588193 5.318268
C 0.221016 2.658945 7.180677
C -0.651774 3.258039 5.204207
H -0.698566 3.453838 4.148120
N -1.606418 3.487730 6.109457
C -1.065108 3.126780 7.344721
H -1.614493 3.249096 8.263135
C 2.155575 0.251172 9.508801
O 1.637199 0.235057 10.646383
S 2.046979 3.916109 3.063041
H 0.868903 1.390467 -0.831430
O 2.681048 0.901610 0.278242
O 0.871786 0.537910 -1.319220
FE 2.412410 2.185859 1.337052
N 3.210427 1.181014 2.871975
N 0.569621 1.546511 1.871867
N 1.584992 3.370275 -0.093917
N 4.229145 2.916571 0.891220
C 4.437510 1.426464 3.461823
C 4.558872 0.635310 4.685890
C 3.467560 -0.205919 4.725752
C 2.601028 0.191926 3.613420
C 0.312611 0.484781 2.717322
C -1.127006 0.279812 2.829032
C -1.747585 1.259602 2.072356
C -0.661151 2.024833 1.435934
C 0.236127 3.597000 -0.292479
C 0.032780 4.448118 -1.465022
C 1.288679 4.696395 -2.008601
C 2.254504 4.027030 -1.114787
C 4.567393 3.545518 -0.292415
C 6.017678 3.713251 -0.363514
C 6.536857 3.245344 0.826052
C 5.405451 2.739692 1.603737
C 5.465219 2.147800 2.863517
H 6.417869 2.173050 3.381779
C 1.273301 -0.194672 3.465880
H 0.927745 -1.002252 4.101428
C -0.786814 2.979079 0.430221
H -1.783425 3.184722 0.070334
C 3.649525 4.045315 -1.213646
H 4.082089 4.535196 -2.079889
O 1.015322 -3.574155 -1.450896
H 1.657255 -3.165700 -0.767694
H 0.258359 -2.908812 -1.485108
O 4.527706 -0.811778 -0.577262
H 5.372193 -0.811261 -0.090247
H 3.997207 0.008164 -0.364779
O 2.394262 -2.124411 0.160226
H 1.875352 -1.323260 0.363820
H 3.308255 -1.812560 -0.115493
O 1.859725 -4.318641 -3.604668
H 2.744217 -4.014746 -3.906432
H 1.523325 -3.974342 -2.622015
h 2.543352 5.149272 2.692543
h 5.295889 0.840385 5.462303
h 3.269224 -1.051687 5.384087
h -1.549360 -0.467750 3.500474
h -2.828707 1.389220 2.022939
h -0.966542 4.748900 -1.779590
h 1.612082 5.215681 -2.910720
h 6.547421 4.080654 -1.242407
h 7.581507 3.168915 1.127598
h -0.541637 -0.670938 7.937716
h 3.226476 0.099325 9.373966
h -1.056921 -4.093696 -5.238913
h -2.625895 -1.813313 -1.421376

Conf LM3 –IH

C -1.295363 -5.109454 -4.962498
H -1.477352 -5.132784 -3.878805
H -2.233033 -5.380880 -5.456394
C -0.287160 -6.203428 -5.298423
O -0.662248 -7.216409 -5.946815
O 0.952213 -6.094021 -4.841771
H 1.346815 -5.163067 -4.219507
C -1.932033 -1.448989 -0.670435
H -2.116963 -0.389197 -0.446018
O -0.593070 -1.549733 -1.226762
H -0.130856 -0.651582 -1.268882
C -2.025075 -2.289797 0.602664
H -1.276526 -1.936676 1.314321

H -3.015489 -2.203625 1.065274
H -1.831536 -3.348115 0.397262
N -0.053958 -0.033242 8.533857
H -0.464131 0.122900 9.440062
C 1.246459 0.552668 8.302899
H 1.690929 0.175450 7.377022
C 1.174602 2.134901 8.201907
H 0.864447 2.500311 9.187772
H 2.191822 2.517308 8.031321
N 0.462330 2.749021 5.820612
H 1.330656 2.579884 5.330849
C 0.217694 2.660220 7.191588
C -0.653989 3.253667 5.212975
H -0.700814 3.446410 4.156428
N -1.608323 3.487507 6.117299
C -1.067818 3.129952 7.354073
H -1.617571 3.255040 8.271848
C 2.154988 0.249526 9.512068
O 1.637284 0.230376 10.649892
S 2.030755 3.945747 3.085428
H 1.362010 0.900684 -0.684465
O 2.551764 1.010944 0.186577
O 0.523397 0.813279 -1.314037
FE 2.404048 2.256013 1.345523
N 3.208219 1.201571 2.852990
N 0.562132 1.593962 1.889759
N 1.581669 3.477580 -0.051893
N 4.223608 2.969427 0.897795
C 4.437834 1.440935 3.445397
C 4.558281 0.647006 4.666569
C 3.464173 -0.191421 4.705601
C 2.597134 0.213311 3.598031
C 0.304401 0.524696 2.725591
C -1.135541 0.313277 2.827278
C -1.754106 1.285550 2.059056
C -0.664609 2.055040 1.432681
C 0.236239 3.645213 -0.281076
C 0.020937 4.486903 -1.460170
C 1.273921 4.767857 -1.988856
C 2.246458 4.129731 -1.075206
C 4.559450 3.627461 -0.271220
C 6.008790 3.789886 -0.345284
C 6.531706 3.292149 0.831132
C 5.403087 2.774397 1.601755
C 5.465855 2.165018 2.852920
H 6.419570 2.183683 3.369610
C 1.266153 -0.167360 3.460241
H 0.920457 -0.975547 4.095157
C -0.784559 3.000017 0.417814
H -1.777422 3.171736 0.030735
C 3.640291 4.153423 -1.176906
H 4.070760 4.650461 -2.039685
O 0.993774 -3.570285 -1.388906
H 1.606605 -3.215346 -0.657215
H 0.261132 -2.882402 -1.440750
O 4.343075 -0.807447 -0.343530
H 5.204758 -0.793729 0.110734
H 3.826743 0.042274 -0.183233
O 2.306019 -2.235508 0.385444
H 1.730602 -1.565590 0.792900
H 3.180727 -1.803464 0.120384
O 1.859801 -4.276677 -3.569189
H 2.750903 -3.977730 -3.853934
H 1.537500 -3.960319 -2.594515
h 2.527750 5.179664 2.718289
h 5.294027 0.850294 5.444656
h 3.263172 -1.035488 5.365310
h -1.559262 -0.429205 3.503479
h -2.835416 1.407552 1.996209
h -0.982286 4.761873 -1.785751
h 1.594402 5.289297 -2.890776
h 6.535907 4.173148 -1.218968
h 7.576864 3.205460 1.128110
h -0.541774 -0.671275 7.938104
h 3.225976 0.099649 9.375734
h -1.038061 -4.084923 -5.231196
h -2.635176 -1.812155 -1.419947

Conf LM3–Heme-OH

C -1.271286 -5.099673 -4.943232
H -1.452183 -5.116698 -3.859193
H -2.205499 -5.385796 -5.434916
C -0.249288 -6.180979 -5.273051
O -0.602884 -7.204025 -5.914132
O 0.990703 -6.050325 -4.814243
H 1.349283 -5.129842 -4.206659
C -1.945837 -1.478817 -0.645739
H -2.240931 -0.490031 -0.275391
O -0.635625 -1.342520 -1.263952
H -0.326019 -0.381341 -1.272824
C -1.864471 -2.459715 0.525366
H -1.231903 -2.033358 1.309318
H -2.854541 -2.662916 0.949061
H -1.426803 -3.410857 0.205469
N -0.056764 -0.029269 8.532819
H -0.467071 0.124335 9.439476
C 1.241807 0.560729 8.303167
H 1.687601 0.184492 7.378413
C 1.168406 2.142412 8.195755
H 0.852678 2.512599 9.177995
H 2.186081 2.524889 8.028432
N 0.461704 2.733150 5.804941
H 1.329370 2.558290 5.315213
C 0.215702 2.659708 7.176989
C -0.656530 3.225177 5.189681
H -0.703088 3.399883 4.129622
N -1.612760 3.466564 6.090773
C -1.071574 3.126725 7.332302
H -1.622901 3.260491 8.247945
C 2.152327 0.258404 9.511057
O 1.635739 0.233093 10.649090
S 2.062470 3.841649 3.018087
H 1.144586 1.038475 -0.821251
O 2.642267 0.992955 0.006053
O 0.184243 1.123811 -1.131890
FE 2.480901 2.173233 1.217227
N 3.262178 1.123329 2.755324
N 0.630038 1.440899 1.709626
N 1.647943 3.442001 -0.181668
N 4.275986 2.981745 0.826533
C 4.504535 1.353714 3.329708
C 4.621662 0.623557 4.583304
C 3.490099 -0.163007 4.690648
C 2.619141 0.216560 3.585695
C 0.308258 0.551953 2.745492
C -1.123881 0.386844 2.806649
C -1.672928 1.172713 1.784516
C -0.540858 1.738824 1.089307
C 0.353291 3.430245 -0.569158
C 0.068180 4.443190 -1.544885
C 1.303155 5.032497 -1.868863
C 2.285083 4.386975 -1.000961
C 4.601017 3.786941 -0.259582
C 6.046521 3.949116 -0.334652
C 6.582755 3.322221 0.772086
C 5.463392 2.730892 1.494493
C 5.536422 2.059132 2.716012
H 6.496110 2.059320 3.222374
C 1.253908 -0.071308 3.546244
H 0.885130 -0.790808 4.270803
C -0.462346 2.214195 -0.318683
H -1.443225 2.305382 -0.776128
C 3.678396 4.466843 -1.051961
H 4.104215 5.121210 -1.806473
O 0.947456 -3.402736 -1.398048
H 1.524630 -3.124852 -0.605951
H 0.279479 -2.656800 -1.488369
O 4.318032 -1.001026 -0.262283
H 5.176793 -0.973701 0.197021
H 3.852168 -0.111789 -0.236027
O 2.220844 -2.290128 0.559271
H 1.653977 -1.600735 0.946040
H 3.109570 -1.887889 0.291078
O 1.861416 -4.208321 -3.543188
H 2.761505 -3.925999 -3.815061
H 1.529216 -3.856223 -2.598083
h 2.537327 5.094680 2.688283
h 5.360398 0.850993 5.351816
h 3.289739 -0.979719 5.384119
h -1.608911 -0.216098 3.574291
h -2.739306 1.323404 1.616595
h -0.957488 4.663392 -1.840830
h 1.583175 5.749484 -2.640605
h 6.566850 4.388860 -1.185503
h 7.627973 3.224614 1.065441
h -0.542333 -0.669943 7.938066
h 3.223428 0.112052 9.371813
h -1.024369 -4.074637 -5.219637
h -2.645781 -1.831632 -1.403147