Supporting information

Mechanical insights into the oxidative cleavage of resveratrol catalyzed by dioxygenase NOV1 from *Novosphingobium aromaticivorans*: confirmation of dioxygenase mechanism by QM/MM calculations

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Table S1 Key coordinate distances of optimized reactant models at the triplet and quintet (showed in parentheses) spin states calculated at B3LYP/6-31G (d,p) basis set.

species	side-on	end-on I	end-on II	end-on III
r (Fe-H284)	2.00 (2.12)	2.05 (2.15)	2.07 (2.15)	2.06 (2.14)
r (Fe-H476)	1.98 (1.96)	1.98 (1.99)	1.99 (2.01)	1.99 (1.99)
r (Fe-H167)	1.99 (2.12)	2.00 (1.99)	2.01 (1.97)	2.01 (2.00)
r (Fe-H218)	2.02 (1.98)	2.01 (2.02)	2.02 (2.02)	2.02 (2.02)

Table S2 Spin densities of key atoms in involved species in path_a, path_b1 and path_b2 at the B3LYP/6-311++G (2d,2p) basis set.

	Fe	O1	O2	C1	C2
^3R_e	3.34	-0.65	-0.83	0	-0.02
^{3}IM1a	0.87	0.14	0.05	0.61	-0.01
^{3}IM2a	1.97	0	0.01	0	0
^{3}IM3a	0.93	0.75	0.08	0.01	0.02
^{3}Pa	1.96	0	0	0	0

	Fe	O1	O2	C1	C2
^5R_e	2.43	0.71	0.76	0	0
^{5}IM1a	3.57	-0.26	-0.17	0.45	-0.01
^{5}IM2a	3.73	0	0.03	0	0
^{5}IM3a	2.77	0.75	0.15	0.01	0.04

^{5}Pa	3.73	0	0.03	0	0

	Fe	O1	O2	C1	C2
^{3}Re	3.34	-0.65	-0.83	-0.02	0
^{3}IM1$_b$	2.69	0.10	0.01	0	-0.62
^{3}IM2$_{b1}$	2.82	0.06	-0.03	-0.01	-0.56
^{3}IM3$_{b1}$	1.98	0.01	0	0	0
^{3}IM4$_{b1}$	0.93	0.09	0.76	0	0.01
^{3}P$_{b1}$	1.96	0	0	0	0

	Fe	O1	O2	C1	C2
^{5}Re	2.43	0.71	0.76	0	0
^{5}IM1$_b$	3.71	0.28	0.19	0	-0.23
^{5}IM2$_{b1}$	3.87	0.54	0.23	0	-0.55
^{5}IM3$_{b1}$	3.73	0.03	0	0	0
^{5}IM4$_{b1}$	2.78	0.14	0.76	0.01	0.04
^{5}P$_{b1}$	3.73	0.03	0	0	0

	Fe	O1	O2	C1	C2
^{3}Re	3.34	-0.65	-0.83	0	-0.02
^{3}IM1$_b$	2.61	0.16	0.02	0	-0.65
^{3}IM2$_{b2}$	1.43	0.58	0	0	0
^{3}IM3$_{b2}$	0.97	0.04	0.78	0	0.07
^{3}P$_{b2}$	1.96	0	0	0	0

	Fe	O1	O2	C1	C2
^{5}Re	2.43	0.71	0.76	0	0
^{5}IM1$_b$	3.67	0.32	0.20	0.01	-0.27
^{5}IM2$_{b2}$	3.16	0.65	0	0	0
^{5}IM3$_{b2}$	2.77	0.14	0.78	-0.01	0.07
^{5}P$_{b2}$	3.73	0.03	0	0	0

Table S3 Natural population atomic charges of key atoms in involved species in path_a, path_b1 and path_b2 at the B3LYP/6-311++G (2d,2p) basis set.

	Fe	O1	O2	Sub
^{3}Re	1.45	-0.19	-0.04	0.17
^{3}TS1a	1.46	-0.31	-0.22	0.50
^{3}IM1a	1.21	-0.38	-0.34	0.48
^{3}TS2a	1.35	-0.41	-0.35	0.74
^{3}IM2a	1.20	-0.29	-0.36	0.85
^{3}TS3a	1.35	-0.39	-0.50	0.77
^{3}IM3a	1.28	-0.37	-0.68	0.77
^{3}TS4a	1.29	-0.51	-0.68	0.84

^{3}Pa	1.21	-0.62	-0.66	1.44

	Fe	O1	O2	Sub
^{5}Re	1.36	-0.17	-0.11	0.14
^{5}TS1a	1.48	-0.32	-0.16	0.58
^{5}IM1a	1.49	-0.41	-0.20	0.70
^{5}TS2a	1.51	-0.46	-0.33	0.82
^{5}IM2a	1.50	-0.31	-0.36	0.82
^{5}TS3a	1.77	-0.39	-0.62	0.73
^{5}IM3a	1.48	-0.36	-0.72	0.77
^{5}TS4a	1.49	-0.51	-0.71	0.84
^{5}Pa	1.51	-0.61	-0.68	1.41

	Fe	O1	O2	Sub
^{3}Re	1.45	-0.19	-0.04	0.17
^{3}TS1b	1.46	-0.32	-0.20	0.46
^{3}IM1b	1.42	-0.41	-0.35	0.49
^{3}TS2b1	1.47	-0.39	-0.34	0.48
^{3}IM2b1	1.48	-0.39	-0.34	0.48
^{3}TS3b1	1.44	-0.40	-0.33	0.52
^{3}IM3b1	1.20	-0.36	-0.29	0.85
^{3}TS4b1	1.36	-0.51	-0.39	0.77
^{3}IM4b1	1.38	-0.69	-0.36	0.77
^{3}TS5b1	1.37	-0.69	-0.48	0.83
^{3}Pb1	1.20	-0.65	-0.63	1.43

	Fe	O1	O2	Sub
^{5}Re	1.36	-0.17	-0.11	0.14
^{5}TS1b	1.48	-0.31	-0.16	0.62
^{5}IM1b	1.48	-0.47	-0.22	0.85
^{5}TS2b1	1.59	-0.35	-0.19	0.51
^{5}IM2b1	1.59	-0.33	-0.20	0.50
^{5}TS3b1	1.61	-0.49	-0.29	0.74
^{5}IM3b1	1.49	-0.35	-0.31	0.80
^{5}TS4b1	1.77	-0.62	-0.40	0.72
^{5}IM4b1	1.48	-0.72	-0.36	0.77
^{5}TS5b1	1.50	-0.72	-0.51	0.84
^{5}Pb1	1.51	-0.67	-0.61	1.38

	Fe	O1	O2	Sub
^{3}IM1b	1.42	-0.41	-0.35	0.49
^{3}TS2b2	1.21	-0.50	-0.28	0.97
^{3}IM2b2	1.17	-0.42	-0.55	0.69

$^{3}TS3_{b2}$	1.20	-0.54	-0.52	0.94
$^{3}IM3_{b2}$	1.29	-0.70	-0.35	0.76
$^{3}TS4_{b2}$	1.46	-0.71	-0.48	0.85
P_{b2}	1.20	-0.65	-0.63	1.43

	Fe	O1	O2	Sub
$^{5}IM1_{b}$	1.48	-0.47	-0.22	0.85
$^{5}TS2_{b2}$	1.58	-0.61	-0.32	0.91
$^{5}IM2_{b2}$	1.47	-0.47	-0.55	0.69
$^{5}TS3_{b2}$	1.66	-0.71	-0.47	0.95
$^{5}IM3_{b2}$	1.47	-0.72	-0.35	0.77
$^{5}TS4_{b2}$	1.49	-0.72	-0.44	0.83
P_{b2}	1.51	-0.66	-0.62	1.38

Table S4 Spin densities of key atoms in involved species in path_a at the B3LYP/6-311++G (2d,2p) basis set.

	Fe	O1	O2	C1	C2	Sub
$^{3}R_{P}$	3.18	-0.59	-0.76	-0.01	0	-0.01
$^{3}TS1_{P}$	2.92	-0.17	-0.36	-0.38	0.08	-0.54
$^{3}IM1_{P}$	0.89	0.13	0.06	0.61	-0.01	0.94
$^{5}R_{P}$	3.12	0.29	0.42	0	0	0
$^{5}TS1_{P}$	3.56	-0.28	-0.13	0.42	-0.04	0.65
$^{5}IM1_{P}$	2.91	-0.03	0.03	0.61	-0.01	0.93

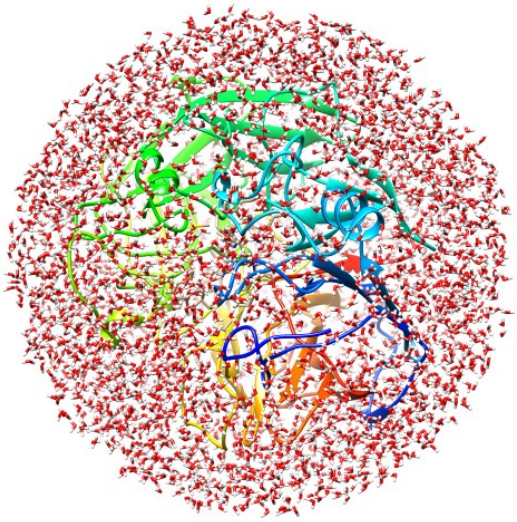

Figure S1 Constructed solvation model for the MD simulation.

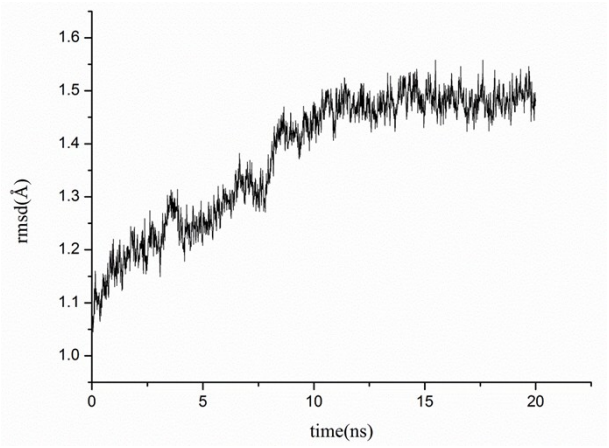

Figure S2 RMSD for the backbone atoms of the enzyme-substrate complex in 20 ns MD simulations.

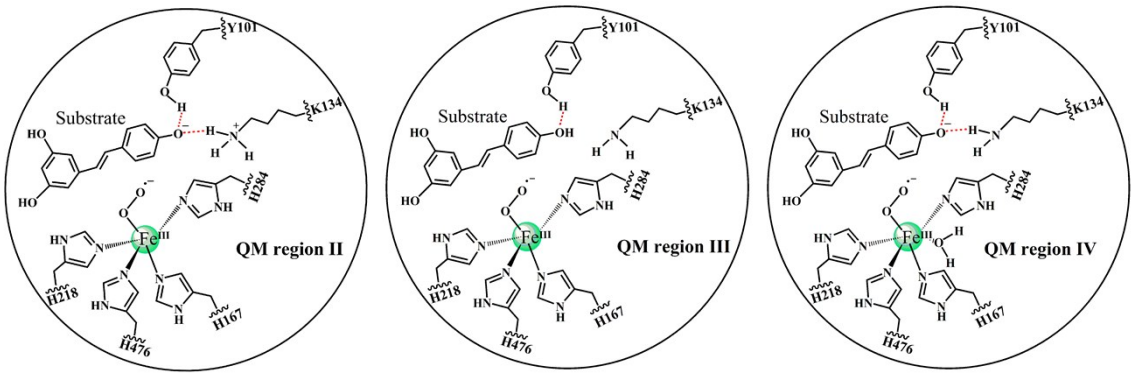

Figure S3 QM-region II (contains a protonated K134), QM-region III (4′-OH of substrate in neutral form) and QM-region IV (contains a coordinate water molecule) created in the QM/MM calculation. Possible hydrogen bonds are shown by red dashed lines.

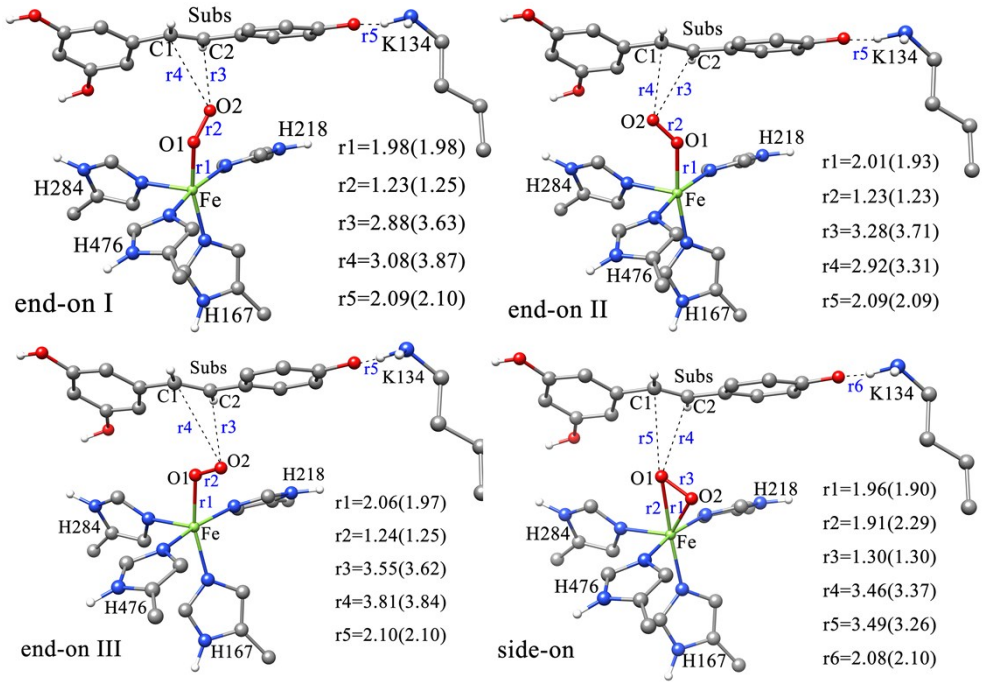

Figure S4 Optimized geometries for different binding modes (one side on mode and three side on

modes) at triplet state and quintet state (in brackets). All distances are shown in angstrom.

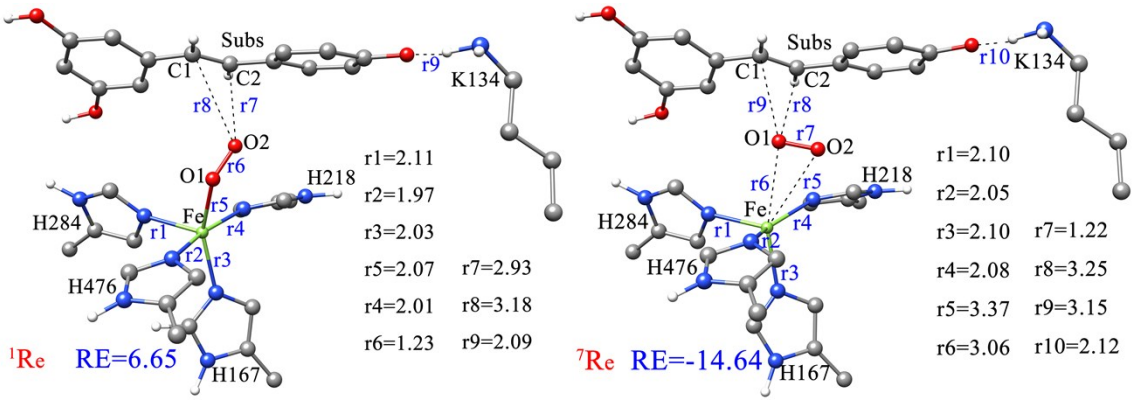

Figure S5 Optimized geometries of the end-on I mode at the open-shell singlet and septet spin states. The relative energies (RE) are given in kcal/mol, and distances are shown in angstrom.

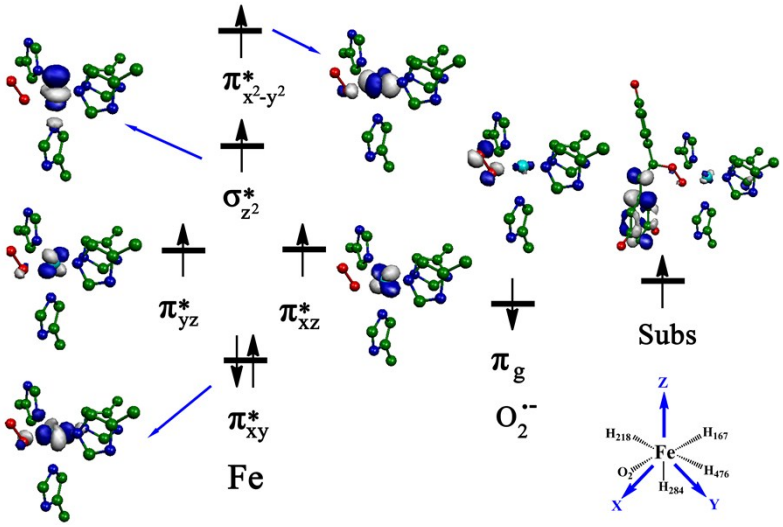

Figure S6 Valence electron orbital diagrams of ^{5}IM1$_{a}$.

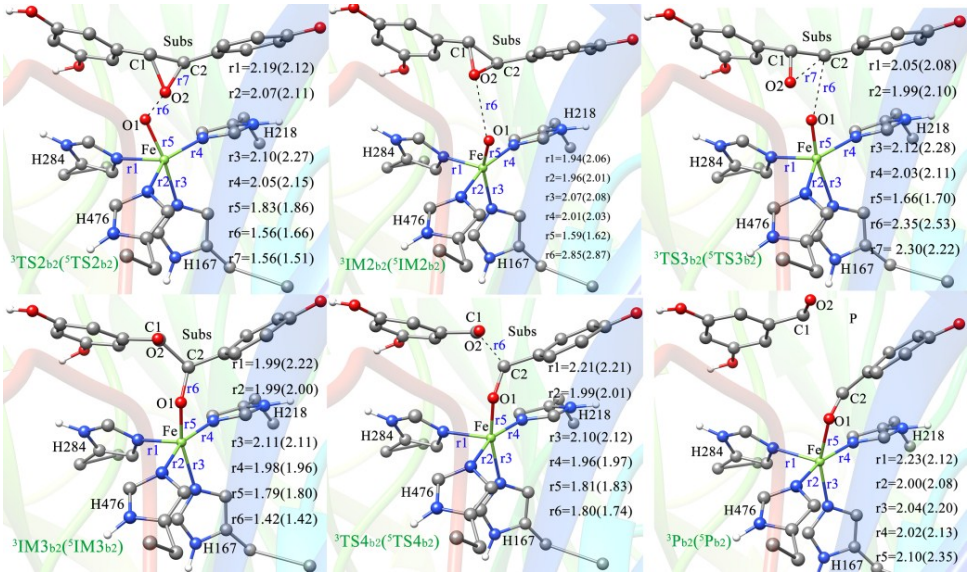

Figure S7 Optimized structures of transition states and intermediates at triplet and quintet (showed in parentheses) spin states in path_b2. All distances are shown in angstrom.

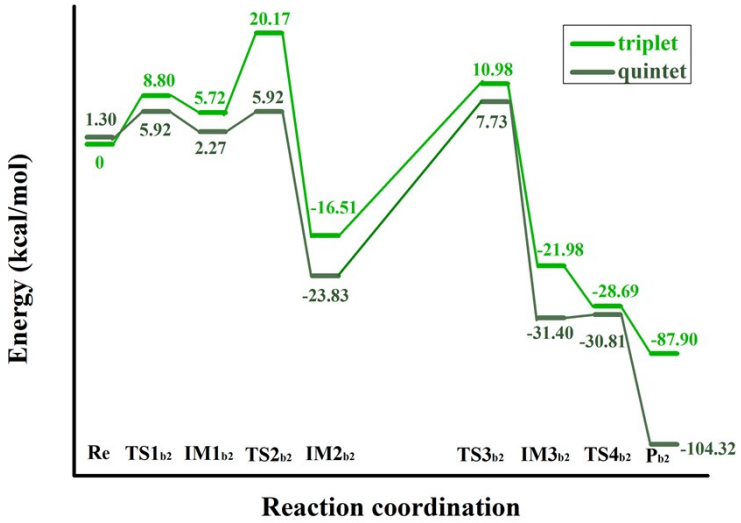

Figure S8 Energy profiles of path-b2 at the triplet and quintet spin states. All energies are given in kcal/mol relative to ^{3}Re. Note that the optimized transition state ^{3}TS4$_{b2}$ is higher than ^{3}IM3$_{b2}$ at the UB3LYP/6-31G (d,p) level, after single point calculation and DFT-D3 correction, ^{3}TS4$_{b2}$ is slightly lower than ^{3}IM3$_{b2}$.

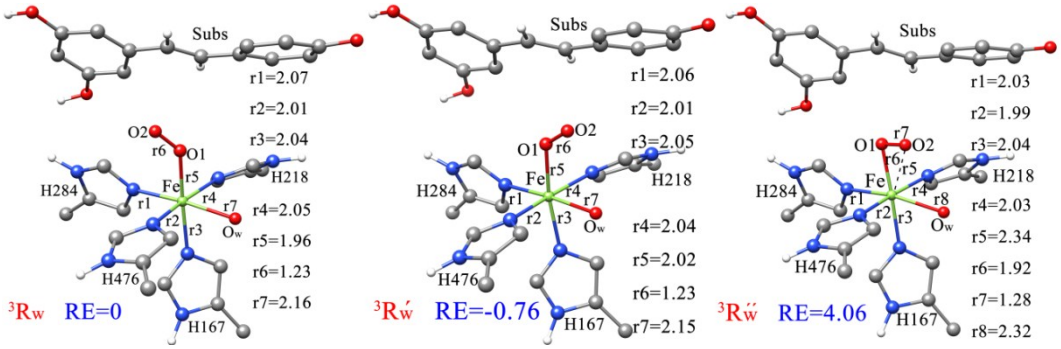

Figure S9 Optimized geometries of Fe-O2 complex at triplet state with a water molecule coordinated with the iron center. ^{3}Rw and $^3R_w^{'}$ represent the two end-on modes, and $^3R_w^{''}$ represents the side-on mode. All distances are shown in angstroms, and relative energies are given in kcal/mol.

Absolute QM/MM single-point energies (E, a.u.) at the B3LYP/6-311++G(2d,2p) level, as well as Cartesian coordinates of QM regions:

^{5}Re

E=-2747.071758 (a.u.)

C	2.61300000	14.16700000	-6.18100000
H	1.57300000	14.17400000	-6.52700000

H	3.25300000	14.27400000	-7.06100000
C	2.91500000	12.90300000	-5.39700000
C	1.98000000	12.40300000	-4.48100000
H	1.01200000	12.89200000	-4.37900000
C	2.27500000	11.32300000	-3.66200000
H	1.54800000	10.98500000	-2.93100000
C	3.52300000	10.68200000	-3.75100000
O	3.82200000	9.62600000	-2.96900000
H	2.92500000	9.08700000	-2.72300000
C	4.16000000	12.26300000	-5.48000000
H	4.90900000	12.65000000	-6.16900000
C	4.46400000	11.16000000	-4.67900000
H	5.43100000	10.66600000	-4.74000000
C	1.22200000	9.59700000	3.80700000
H	0.17100000	9.29400000	3.84900000
H	1.41600000	10.24800000	4.66000000
C	1.49300000	10.32000000	2.48100000
H	1.18500000	11.36600000	2.61300000
H	2.56600000	10.37600000	2.25200000
C	0.73700000	9.75000000	1.27800000
H	1.01800000	8.70500000	1.09700000
H	-0.34000000	9.74900000	1.50700000
C	0.96200000	10.59700000	0.02300000
H	0.88300000	11.65300000	0.31700000
H	1.98400000	10.46900000	-0.35100000
N	0.03700000	10.34700000	-1.09900000
H	-0.91400000	10.24500000	-0.72500000
H	0.30300000	9.46200000	-1.53500000
C	5.13600000	-0.93400000	3.05800000
H	5.96000000	-0.23900000	2.88900000
H	5.55500000	-1.93600000	3.15000000
N	3.39300000	-2.05600000	1.65500000
H	3.35300000	-2.88000000	2.26100000
C	4.20000000	-0.95800000	1.89500000
C	2.67400000	-1.84300000	0.54400000
H	1.99900000	-2.57100000	0.12100000
N	2.97600000	-0.64300000	0.03800000
C	3.93100000	-0.08500000	0.87700000
H	4.35600000	0.88800000	0.70200000
C	7.29000000	2.11200000	-2.09500000
H	7.57400000	3.01500000	-2.64600000
H	7.61600000	1.26200000	-2.70000000
N	5.04400000	3.08100000	-1.39400000
H	5.40100000	3.96000000	-0.96200000

C	5.81100000	2.04600000	-1.90100000
C	3.76200000	2.67300000	-1.33600000
H	2.95100000	3.27200000	-0.94900000
N	3.65700000	1.42800000	-1.79100000
C	4.92800000	1.02800000	-2.15300000
H	5.12000000	0.04900000	-2.56400000
C	3.87900000	-4.52400000	-3.97300000
H	3.69300000	-4.94600000	-4.96500000
H	3.50500000	-5.22400000	-3.21600000
N	2.15000000	-2.78700000	-4.60500000
H	1.84800000	-3.28700000	-5.47000000
C	3.17500000	-3.21600000	-3.78700000
C	1.65500000	-1.63800000	-4.09900000
H	0.85500000	-1.07900000	-4.55900000
N	2.30800000	-1.29900000	-2.98500000
C	3.26000000	-2.28500000	-2.78600000
H	3.90400000	-2.29500000	-1.91900000
C	-2.33200000	-0.60600000	1.85200000
H	-2.16000000	0.31400000	2.41200000
H	-2.22300000	-1.44600000	2.54200000
N	-1.23500000	-1.76700000	-0.13100000
H	-1.79000000	-2.65500000	-0.10700000
C	-1.33800000	-0.69200000	0.73300000
C	-0.25200000	-1.53500000	-1.01300000
H	0.04300000	-2.23900000	-1.77700000
N	0.30600000	-0.35300000	-0.76000000
C	-0.36300000	0.18700000	0.32600000
H	-0.10800000	1.15300000	0.73300000
Fe	2.05900000	0.23100000	-1.50200000
O	1.02600000	1.58900000	-2.50300000
O	0.65800000	2.70800000	-2.09500000
C	0.07100000	0.02100000	-8.25000000
O	-1.00600000	-0.20200000	-9.04500000
H	-0.91000000	-1.03000000	-9.56800000
C	2.25000000	-0.50900000	-7.35700000
O	3.35900000	-1.29700000	-7.24900000
H	3.18600000	-2.22600000	-7.53800000
C	1.85800000	7.16900000	-3.17000000
O	1.76600000	8.34800000	-2.54900000
C	1.14400000	1.53800000	-6.68100000
C	1.07800000	2.79800000	-5.94200000
H	0.08800000	3.25200000	-5.91800000
C	2.10200000	3.43900000	-5.34100000
H	3.10600000	3.02200000	-5.41900000

C	2.00000000	4.68700000	-4.59200000
C	1.16900000	-0.84300000	-8.18400000
H	1.18200000	-1.74700000	-8.78200000
C	2.25100000	0.67400000	-6.61800000
H	3.10900000	0.89400000	-5.99400000
C	0.04700000	1.18600000	-7.48000000
H	-0.83100000	1.82200000	-7.53300000
C	3.16200000	5.36900000	-4.19000000
H	4.13400000	4.94300000	-4.43300000
C	3.10400000	6.58000000	-3.50000000
H	4.02100000	7.07800000	-3.20000000
C	0.69000000	6.46700000	-3.55300000
H	-0.27500000	6.89600000	-3.29500000
C	0.76400000	5.26700000	-4.23500000
H	-0.15800000	4.76000000	-4.49500000

^{5}TS1$_{b}$

E=-2747.064871 (a.u.)

C	2.60400000	14.17100000	-6.18400000
H	1.56200000	14.17900000	-6.52400000
H	3.23800000	14.28000000	-7.06800000
C	2.91100000	12.90800000	-5.40500000
C	1.98100000	12.40300000	-4.48600000
H	1.01100000	12.88500000	-4.38100000
C	2.28700000	11.32700000	-3.66500000
H	1.56600000	10.98500000	-2.93000000
C	3.54000000	10.70200000	-3.76000000
O	3.85900000	9.64900000	-2.97200000
H	2.99200000	9.13700000	-2.70900000
C	4.16000000	12.27600000	-5.49300000
H	4.90400000	12.66800000	-6.18500000
C	4.47600000	11.17800000	-4.69100000
H	5.44600000	10.69100000	-4.75100000
C	1.21900000	9.60100000	3.82200000
H	0.17000000	9.29500000	3.86800000
H	1.41500000	10.25000000	4.67600000
C	1.48200000	10.33000000	2.49800000
H	1.17000000	11.37400000	2.63500000
H	2.55400000	10.39100000	2.26600000
C	0.72400000	9.76200000	1.29500000
H	1.00900000	8.71900000	1.11000000
H	-0.35300000	9.75600000	1.52400000
C	0.94500000	10.61600000	0.04400000

H	0.85300000	11.67000000	0.33900000
H	1.97100000	10.50300000	-0.32500000
N	0.02900000	10.36200000	-1.08400000
H	-0.92600000	10.27300000	-0.71700000
H	0.28700000	9.46800000	-1.50500000
C	5.11800000	-0.94300000	3.06800000
H	5.93000000	-0.23500000	2.88900000
H	5.55800000	-1.93500000	3.16600000
N	3.37500000	-2.09500000	1.68700000
H	3.32700000	-2.90100000	2.31500000
C	4.18000000	-0.99100000	1.90400000
C	2.68400000	-1.91000000	0.54700000
H	2.01200000	-2.64900000	0.13700000
N	2.98900000	-0.73300000	0.00600000
C	3.92300000	-0.15400000	0.85100000
H	4.36000000	0.81000000	0.64400000
C	7.22200000	2.15900000	-2.10100000
H	7.52800000	3.06600000	-2.63600000
H	7.53800000	1.31300000	-2.71800000
N	4.97400000	3.12300000	-1.36800000
H	5.33500000	3.97800000	-0.89200000
C	5.73800000	2.11300000	-1.93100000
C	3.68100000	2.73600000	-1.38700000
H	2.87300000	3.31400000	-0.96400000
N	3.55900000	1.53800000	-1.94800000
C	4.83900000	1.14500000	-2.29400000
H	5.02800000	0.19300000	-2.76700000
C	3.96600000	-4.67100000	-3.99100000
H	3.80500000	-5.10600000	-4.98200000
H	3.60700000	-5.37700000	-3.23300000
N	2.19800000	-2.99100000	-4.64800000
H	1.91100000	-3.49500000	-5.51500000
C	3.22700000	-3.38500000	-3.81900000
C	1.67700000	-1.84700000	-4.16400000
H	0.87100000	-1.30300000	-4.62800000
N	2.31900000	-1.48000000	-3.05400000
C	3.28600000	-2.44000000	-2.82800000
H	3.91800000	-2.41600000	-1.95400000
C	-2.40200000	-0.54500000	1.83700000
H	-2.24400000	0.38000000	2.39400000
H	-2.27700000	-1.38300000	2.52700000
N	-1.29800000	-1.71000000	-0.13200000
H	-1.81800000	-2.61600000	-0.07700000
C	-1.42300000	-0.61400000	0.70400000

C	-0.36600000	-1.44900000	-1.05900000
H	-0.06600000	-2.16300000	-1.81200000
N	0.14000000	-0.22900000	-0.87300000
C	-0.51300000	0.29900000	0.22900000
H	-0.28200000	1.28300000	0.60900000
Fe	1.97900000	0.14800000	-1.75300000
O	0.89600000	0.90400000	-3.66600000
O	0.79600000	2.17200000	-3.89900000
C	0.06800000	0.07900000	-8.15300000
O	-0.99500000	-0.10400000	-8.97300000
H	-0.90000000	-0.91700000	-9.52200000
C	2.25100000	-0.49200000	-7.27600000
O	3.35600000	-1.28100000	-7.20900000
H	3.18300000	-2.19700000	-7.54000000
C	1.87200000	7.20000000	-3.17400000
O	1.76800000	8.35000000	-2.53900000
C	1.12400000	1.49800000	-6.49200000
C	1.03500000	2.69600000	-5.64900000
H	0.07100000	3.19200000	-5.71800000
C	2.15500000	3.51000000	-5.33500000
H	3.15300000	3.12500000	-5.53200000
C	2.04300000	4.74800000	-4.65000000
C	1.17200000	-0.78100000	-8.12000000
H	1.19400000	-1.65800000	-8.76000000
C	2.24500000	0.65700000	-6.47800000
H	3.09800000	0.85500000	-5.84000000
C	0.03000000	1.19600000	-7.31500000
H	-0.85400000	1.82400000	-7.32800000
C	3.20900000	5.45300000	-4.24600000
H	4.18200000	5.03600000	-4.49400000
C	3.13400000	6.63500000	-3.53100000
H	4.04300000	7.14000000	-3.21800000
C	0.70600000	6.48800000	-3.57000000
H	-0.26100000	6.90200000	-3.29700000
C	0.78900000	5.31300000	-4.27800000
H	-0.12900000	4.80500000	-4.54400000

^{5}IM1$_{b}$

E=-2747.06964 (a.u.)

C	2.61000000	14.18500000	-6.22100000
H	1.56300000	14.18700000	-6.54500000
H	3.22900000	14.31700000	-7.11200000
C	2.94700000	12.91200000	-5.47100000

C	2.06600000	12.41100000	-4.50300000
H	1.10900000	12.90300000	-4.33600000
C	2.40500000	11.32200000	-3.71500000
H	1.72000000	10.97500000	-2.94900000
C	3.64100000	10.68300000	-3.89800000
O	3.99200000	9.60600000	-3.15100000
H	3.14500000	9.15600000	-2.80200000
C	4.17800000	12.26600000	-5.64500000
H	4.87800000	12.63900000	-6.38900000
C	4.52600000	11.15400000	-4.87700000
H	5.47700000	10.64800000	-5.01400000
C	1.27300000	9.59800000	3.84100000
H	0.22100000	9.30500000	3.90000000
H	1.48100000	10.25400000	4.68700000
C	1.52800000	10.31600000	2.51000000
H	1.23300000	11.36500000	2.65000000
H	2.59800000	10.36000000	2.26200000
C	0.74800000	9.76100000	1.31400000
H	1.05500000	8.73200000	1.08800000
H	-0.32200000	9.71900000	1.57000000
C	0.91300000	10.66200000	0.08800000
H	0.73900000	11.69700000	0.40900000
H	1.94900000	10.63900000	-0.26900000
N	0.03500000	10.37800000	-1.06200000
H	-0.92600000	10.26900000	-0.71800000
H	0.32300000	9.49000000	-1.47500000
C	5.10400000	-0.92000000	3.04300000
H	5.90900000	-0.20600000	2.85900000
H	5.55700000	-1.90700000	3.14900000
N	3.34900000	-2.08700000	1.68600000
H	3.27900000	-2.87200000	2.34000000
C	4.17400000	-0.99200000	1.87500000
C	2.68100000	-1.93000000	0.52700000
H	1.99700000	-2.66800000	0.13500000
N	3.01900000	-0.78200000	-0.05300000
C	3.95200000	-0.19400000	0.78300000
H	4.41900000	0.74500000	0.53700000
C	7.22600000	2.22100000	-2.11800000
H	7.53300000	3.13700000	-2.63600000
H	7.55400000	1.38500000	-2.74300000
N	4.94600000	3.15000000	-1.42100000
H	5.26400000	4.02100000	-0.94600000
C	5.74100000	2.15500000	-1.96700000
C	3.66400000	2.71900000	-1.44100000

H	2.84400000	3.26700000	-1.00200000
N	3.58000000	1.51300000	-1.98900000
C	4.87100000	1.15700000	-2.32500000
H	5.09200000	0.20600000	-2.78700000
C	4.03600000	-4.75400000	-4.00600000
H	3.89300000	-5.18500000	-5.00200000
H	3.69100000	-5.47700000	-3.25600000
N	2.21800000	-3.11700000	-4.64300000
H	1.94800000	-3.60500000	-5.52500000
C	3.26400000	-3.48900000	-3.82400000
C	1.67500000	-1.98800000	-4.14800000
H	0.85600000	-1.45500000	-4.60400000
N	2.31400000	-1.61400000	-3.04000000
C	3.30400000	-2.54900000	-2.82700000
H	3.94300000	-2.51300000	-1.95800000
C	-2.38700000	-0.55200000	1.86400000
H	-2.22900000	0.37600000	2.41500000
H	-2.26900000	-1.38500000	2.56300000
N	-1.28800000	-1.73500000	-0.09500000
H	-1.81700000	-2.63500000	-0.04200000
C	-1.40200000	-0.63600000	0.73700000
C	-0.35400000	-1.48300000	-1.02400000
H	-0.05900000	-2.20200000	-1.77500000
N	0.16500000	-0.27000000	-0.84100000
C	-0.48200000	0.26600000	0.25800000
H	-0.24400000	1.25000000	0.63500000
Fe	1.97800000	0.09300000	-1.82600000
O	1.03200000	0.76100000	-3.62100000
O	0.83600000	2.09700000	-3.81000000
C	0.09800000	0.18700000	-8.06300000
O	-0.95200000	0.08000000	-8.91500000
H	-0.86600000	-0.71400000	-9.49400000
C	2.25200000	-0.47500000	-7.18600000
O	3.34800000	-1.27900000	-7.15600000
H	3.16800000	-2.17200000	-7.54000000
C	1.92300000	7.22000000	-3.10900000
O	1.84200000	8.39300000	-2.54000000
C	1.11600000	1.44200000	-6.25900000
C	0.98900000	2.54900000	-5.26100000
H	0.07800000	3.11400000	-5.46100000
C	2.15600000	3.39900000	-4.99000000
H	3.14000000	2.94800000	-5.09200000
C	2.06100000	4.68000000	-4.42700000
C	1.19100000	-0.68500000	-8.07500000

H	1.22600000	-1.50800000	-8.78300000
C	2.23400000	0.60400000	-6.29500000
H	3.06300000	0.72300000	-5.60700000
C	0.05100000	1.23600000	-7.13900000
H	-0.83500000	1.86100000	-7.10900000
C	3.24100000	5.37100000	-4.01900000
H	4.20600000	4.90300000	-4.19900000
C	3.18300000	6.59400000	-3.38900000
H	4.09600000	7.08300000	-3.06500000
C	0.74300000	6.52600000	-3.51400000
H	-0.21600000	6.98800000	-3.29700000
C	0.80800000	5.31300000	-4.15000000
H	-0.11600000	4.81800000	-4.42000000

$^{5}TS2_{b1}$

E=-2747.068358 (a.u.)

C	2.61700000	14.18100000	-6.21600000
H	1.57100000	14.18100000	-6.54200000
H	3.23800000	14.31000000	-7.10700000
C	2.95300000	12.90900000	-5.46300000
C	2.06700000	12.41000000	-4.49800000
H	1.11200000	12.90600000	-4.33300000
C	2.39800000	11.31800000	-3.71100000
H	1.70900000	10.97000000	-2.94900000
C	3.63000000	10.66700000	-3.89200000
O	3.96400000	9.58400000	-3.15100000
H	3.09600000	9.12000000	-2.81900000
C	4.18200000	12.25700000	-5.63200000
H	4.88600000	12.62800000	-6.37400000
C	4.52000000	11.14100000	-4.86600000
H	5.46800000	10.62800000	-5.00500000
C	1.26800000	9.59800000	3.83700000
H	0.21600000	9.30200000	3.89200000
H	1.47200000	10.25500000	4.68300000
C	1.52600000	10.31500000	2.50500000
H	1.22700000	11.36400000	2.64300000
H	2.59600000	10.36200000	2.26200000
C	0.75200000	9.75800000	1.30500000
H	1.06600000	8.73200000	1.07800000
H	-0.31800000	9.71100000	1.55700000
C	0.92000000	10.66200000	0.08100000
H	0.73800000	11.69600000	0.40500000
H	1.95800000	10.64300000	-0.26800000

N	0.05100000	10.37600000	-1.07500000
H	-0.90900000	10.24600000	-0.73700000
H	0.36200000	9.49900000	-1.49900000
C	5.10600000	-0.93500000	3.05800000
H	5.90500000	-0.21700000	2.86100000
H	5.56500000	-1.91700000	3.16900000
N	3.34200000	-2.12000000	1.72300000
H	3.27600000	-2.90000000	2.38400000
C	4.16900000	-1.02300000	1.89700000
C	2.66200000	-1.97300000	0.57100000
H	1.97500000	-2.71300000	0.18900000
N	2.99800000	-0.82700000	-0.01900000
C	3.94000000	-0.23200000	0.80500000
H	4.40400000	0.70500000	0.55200000
C	7.25500000	2.22600000	-2.10100000
H	7.55000000	3.14800000	-2.61400000
H	7.58700000	1.39600000	-2.73100000
N	4.97100000	3.13800000	-1.40400000
H	5.28200000	4.02400000	-0.95000000
C	5.77400000	2.14300000	-1.93500000
C	3.70000000	2.68400000	-1.38100000
H	2.87400000	3.23200000	-0.95100000
N	3.63300000	1.45800000	-1.88400000
C	4.92100000	1.11500000	-2.23900000
H	5.15300000	0.15600000	-2.68000000
C	4.03100000	-4.73800000	-3.99900000
H	3.87900000	-5.16500000	-4.99500000
H	3.68200000	-5.45700000	-3.24900000
N	2.25200000	-3.05900000	-4.64400000
H	1.97100000	-3.54500000	-5.52600000
C	3.27600000	-3.46300000	-3.81300000
C	1.72800000	-1.92300000	-4.14800000
H	0.92100000	-1.37900000	-4.61200000
N	2.36100000	-1.57100000	-3.02800000
C	3.32800000	-2.53300000	-2.80900000
H	3.95600000	-2.52000000	-1.93100000
C	-2.36100000	-0.53600000	1.84800000
H	-2.20400000	0.39000000	2.40200000
H	-2.23100000	-1.37300000	2.54000000
N	-1.27500000	-1.70300000	-0.12800000
H	-1.80700000	-2.60200000	-0.07600000
C	-1.38600000	-0.60800000	0.71200000
C	-0.34400000	-1.44900000	-1.05700000
H	-0.05100000	-2.16800000	-1.81000000

N	0.17800000	-0.23600000	-0.86900000
C	-0.46400000	0.29500000	0.23800000
H	-0.22000000	1.27500000	0.62100000
Fe	2.03000000	0.06900000	-1.76000000
O	1.38600000	1.00600000	-3.50600000
O	0.46600000	1.84900000	-3.95700000
C	0.06700000	0.14800000	-8.13700000
O	-0.97900000	0.02500000	-8.99000000
H	-0.88800000	-0.77000000	-9.56500000
C	2.23200000	-0.48000000	-7.26500000
O	3.34400000	-1.26500000	-7.23900000
H	3.17000000	-2.17100000	-7.59500000
C	1.89100000	7.19900000	-3.10400000
O	1.83300000	8.39800000	-2.55100000
C	1.06800000	1.42300000	-6.33500000
C	0.91900000	2.50900000	-5.31200000
H	0.00800000	3.08000000	-5.50200000
C	2.07500000	3.37400000	-5.04100000
H	3.06900000	2.96200000	-5.19000000
C	1.97900000	4.63200000	-4.40400000
C	1.17100000	-0.71000000	-8.14900000
H	1.21700000	-1.53000000	-8.86000000
C	2.20000000	0.60000000	-6.37600000
H	3.03900000	0.74500000	-5.70800000
C	0.00200000	1.19500000	-7.21100000
H	-0.89100000	1.81000000	-7.18500000
C	3.16800000	5.32600000	-4.02700000
H	4.12700000	4.85600000	-4.23000000
C	3.13100000	6.55600000	-3.39600000
H	4.05700000	7.04000000	-3.10100000
C	0.70400000	6.50500000	-3.47100000
H	-0.24900000	6.97900000	-3.24700000
C	0.74400000	5.27600000	-4.09000000
H	-0.19400000	4.79100000	-4.33400000

$^{5}IM2_{b1}$

E=-2747.070621 (a.u.)

C	2.60200000	14.17500000	-6.20100000
H	1.55600000	14.18300000	-6.53100000
H	3.22700000	14.29500000	-7.09000000
C	2.92200000	12.90300000	-5.44000000
C	2.01800000	12.40000000	-4.49400000
H	1.06100000	12.89600000	-4.34600000

C	2.33400000	11.30400000	-3.70600000
H	1.63100000	10.95600000	-2.95600000
C	3.57000000	10.65500000	-3.86200000
O	3.89600000	9.57500000	-3.11400000
H	3.02400000	9.07400000	-2.83300000
C	4.15400000	12.25100000	-5.58800000
H	4.87200000	12.62500000	-6.31500000
C	4.47800000	11.13400000	-4.81800000
H	5.43000000	10.62400000	-4.93800000
C	1.27500000	9.60200000	3.83800000
H	0.22200000	9.31100000	3.89200000
H	1.48000000	10.26000000	4.68500000
C	1.53800000	10.31700000	2.50600000
H	1.23600000	11.36600000	2.63900000
H	2.60900000	10.36500000	2.26700000
C	0.77000000	9.75100000	1.30700000
H	1.08100000	8.72100000	1.09500000
H	-0.30200000	9.71100000	1.55500000
C	0.94500000	10.63800000	0.07200000
H	0.78600000	11.67900000	0.38400000
H	1.97900000	10.59600000	-0.28800000
N	0.05900000	10.35200000	-1.07200000
H	-0.89800000	10.23200000	-0.72000000
H	0.35300000	9.47000000	-1.49600000
C	5.10100000	-0.96400000	3.06900000
H	5.91000000	-0.25600000	2.87500000
H	5.54700000	-1.95200000	3.18000000
N	3.32600000	-2.11800000	1.71700000
H	3.25200000	-2.90500000	2.36900000
C	4.16700000	-1.03500000	1.90500000
C	2.65700000	-1.95300000	0.56100000
H	1.96100000	-2.68000000	0.16900000
N	3.01200000	-0.80800000	-0.01900000
C	3.95800000	-0.23300000	0.81600000
H	4.43800000	0.69900000	0.57400000
C	7.32000000	2.23100000	-2.06300000
H	7.61800000	3.15800000	-2.56600000
H	7.65600000	1.40700000	-2.69700000
N	5.03400000	3.15900000	-1.40300000
H	5.34400000	4.04800000	-0.95300000
C	5.83900000	2.15000000	-1.90500000
C	3.76400000	2.70800000	-1.37000000
H	2.93700000	3.26900000	-0.96100000
N	3.69800000	1.46800000	-1.83900000

C	4.98700000	1.11400000	-2.18500000
H	5.21800000	0.14500000	-2.59900000
C	3.97500000	-4.67700000	-4.00100000
H	3.81700000	-5.10900000	-4.99400000
H	3.61700000	-5.38600000	-3.24600000
N	2.19800000	-2.99600000	-4.64900000
H	1.91500000	-3.49100000	-5.52400000
C	3.23200000	-3.39300000	-3.82500000
C	1.67900000	-1.85400000	-4.15800000
H	0.86400000	-1.31900000	-4.61900000
N	2.32400000	-1.49200000	-3.04800000
C	3.29200000	-2.45300000	-2.83000000
H	3.92700000	-2.43300000	-1.95700000
C	-2.32000000	-0.52000000	1.84200000
H	-2.16200000	0.40500000	2.39800000
H	-2.17600000	-1.36000000	2.52700000
N	-1.25600000	-1.66300000	-0.16100000
H	-1.79000000	-2.56200000	-0.11200000
C	-1.36000000	-0.57700000	0.69200000
C	-0.33200000	-1.40100000	-1.09400000
H	-0.04400000	-2.11300000	-1.85400000
N	0.19100000	-0.18900000	-0.90000000
C	-0.44500000	0.33200000	0.21800000
H	-0.19800000	1.30900000	0.60800000
Fe	2.05800000	0.15000000	-1.74600000
O	1.51700000	1.28500000	-3.42700000
O	0.42100000	1.72500000	-4.03200000
C	0.04500000	0.07700000	-8.22200000
O	-0.98500000	-0.06100000	-9.09100000
H	-0.88500000	-0.86400000	-9.65400000
C	2.19700000	-0.52300000	-7.29800000
O	3.31700000	-1.29400000	-7.23900000
H	3.16200000	-2.20500000	-7.59300000
C	1.83300000	7.14300000	-3.18700000
O	1.78200000	8.33200000	-2.61000000
C	0.98900000	1.36700000	-6.40300000
C	0.82200000	2.44600000	-5.37300000
H	-0.11300000	2.98700000	-5.54000000
C	1.97500000	3.33400000	-5.15800000
H	2.95500000	2.96400000	-5.44300000
C	1.89800000	4.59000000	-4.51800000
C	1.16100000	-0.76700000	-8.20800000
H	1.23300000	-1.58600000	-8.91600000
C	2.13000000	0.55600000	-6.41200000

H	2.94300000	0.71000000	-5.71400000
C	-0.05100000	1.12800000	-7.30200000
H	-0.95400000	1.73100000	-7.29600000
C	3.08900000	5.32400000	-4.24100000
H	4.04300000	4.89200000	-4.53400000
C	3.06500000	6.54500000	-3.59100000
H	3.99400000	7.06100000	-3.36900000
C	0.64300000	6.41600000	-3.46700000
H	-0.30300000	6.86000000	-3.17000000
C	0.67300000	5.19000000	-4.09500000
H	-0.26400000	4.67500000	-4.27200000

$^{5}TS3_{b1}$

E=-2747.068633 (a.u.)

C	2.59600000	14.17500000	-6.19600000
H	1.55000000	14.18100000	-6.52100000
H	3.21800000	14.29500000	-7.08800000
C	2.92300000	12.90100000	-5.44000000
C	2.02700000	12.39100000	-4.49200000
H	1.07000000	12.88500000	-4.33300000
C	2.34800000	11.28600000	-3.71600000
H	1.65000000	10.93300000	-2.96400000
C	3.58200000	10.64200000	-3.89100000
O	3.91700000	9.54600000	-3.15900000
H	3.06400000	9.06500000	-2.86900000
C	4.15600000	12.25300000	-5.60100000
H	4.86900000	12.63400000	-6.32800000
C	4.48600000	11.12900000	-4.84400000
H	5.43800000	10.62100000	-4.97300000
C	1.27500000	9.60000000	3.83900000
H	0.22200000	9.30700000	3.89200000
H	1.47900000	10.26000000	4.68300000
C	1.53900000	10.31200000	2.50500000
H	1.23800000	11.36000000	2.63500000
H	2.61000000	10.35800000	2.26600000
C	0.77000000	9.74400000	1.30800000
H	1.07900000	8.71200000	1.09800000
H	-0.30200000	9.70500000	1.55600000
C	0.94400000	10.62900000	0.07100000
H	0.78400000	11.66900000	0.38200000
H	1.97700000	10.58800000	-0.29100000
N	0.05400000	10.34500000	-1.07100000
H	-0.90400000	10.24100000	-0.71800000

H	0.32900000	9.45300000	-1.48500000
C	5.08300000	-0.96000000	3.04700000
H	5.90000000	-0.26100000	2.85800000
H	5.51800000	-1.95300000	3.15500000
N	3.30500000	-2.09900000	1.69000000
H	3.22900000	-2.88700000	2.33800000
C	4.15000000	-1.01900000	1.88200000
C	2.64000000	-1.92700000	0.53100000
H	1.94400000	-2.65100000	0.13400000
N	3.00000000	-0.78300000	-0.04700000
C	3.94500000	-0.21500000	0.79300000
H	4.43100000	0.71500000	0.55300000
C	7.35900000	2.24000000	-2.06100000
H	7.67100000	3.16500000	-2.56000000
H	7.69600000	1.41400000	-2.69200000
N	5.07500000	3.17500000	-1.41000000
H	5.38100000	4.06000000	-0.95100000
C	5.87800000	2.16700000	-1.91400000
C	3.80300000	2.72400000	-1.38500000
H	2.97600000	3.28200000	-0.97200000
N	3.73700000	1.48900000	-1.86100000
C	5.02300000	1.13500000	-2.20400000
H	5.25400000	0.16700000	-2.62100000
C	3.97000000	-4.67200000	-4.00000000
H	3.81200000	-5.10500000	-4.99200000
H	3.61300000	-5.38000000	-3.24400000
N	2.19600000	-2.98700000	-4.65000000
H	1.91100000	-3.48300000	-5.52300000
C	3.22800000	-3.38600000	-3.82600000
C	1.68000000	-1.84300000	-4.15800000
H	0.87000000	-1.29900000	-4.61700000
N	2.32400000	-1.48400000	-3.04900000
C	3.29000000	-2.44600000	-2.83100000
H	3.92500000	-2.42700000	-1.95800000
C	-2.30600000	-0.51900000	1.84300000
H	-2.14600000	0.40300000	2.40200000
H	-2.16000000	-1.36200000	2.52300000
N	-1.24800000	-1.64900000	-0.17200000
H	-1.77900000	-2.54900000	-0.12300000
C	-1.35200000	-0.56800000	0.68600000
C	-0.33500000	-1.37300000	-1.11400000
H	-0.04800000	-2.07900000	-1.88000000
N	0.18000000	-0.15900000	-0.91700000
C	-0.45000000	0.35100000	0.20700000

H	-0.21100000	1.32900000	0.59700000
Fe	2.04100000	0.20800000	-1.79900000
O	1.59300000	1.36100000	-3.43300000
O	0.35500000	1.65600000	-4.03400000
C	0.05300000	0.10900000	-8.23100000
O	-0.97500000	-0.01800000	-9.10600000
H	-0.88000000	-0.82200000	-9.66700000
C	2.19800000	-0.51100000	-7.30600000
O	3.32100000	-1.28000000	-7.26000000
H	3.16000000	-2.19300000	-7.60300000
C	1.80200000	7.10200000	-3.19600000
O	1.75600000	8.29100000	-2.65400000
C	0.97900000	1.35100000	-6.36900000
C	0.74800000	2.35000000	-5.25500000
H	-0.12900000	2.95700000	-5.50700000
C	1.94500000	3.20700000	-4.92600000
H	2.92400000	2.81700000	-5.18100000
C	1.86700000	4.50500000	-4.41800000
C	1.16800000	-0.73600000	-8.22800000
H	1.24500000	-1.54100000	-8.95200000
C	2.12000000	0.54300000	-6.39000000
H	2.91400000	0.66300000	-5.66400000
C	-0.04600000	1.14300000	-7.29400000
H	-0.95400000	1.73900000	-7.27400000
C	3.06900000	5.22700000	-4.12700000
H	4.02100000	4.75800000	-4.36200000
C	3.04500000	6.46900000	-3.53400000
H	3.97300000	6.97600000	-3.28700000
C	0.60100000	6.39500000	-3.51200000
H	-0.34300000	6.87600000	-3.27200000
C	0.63100000	5.15000000	-4.08800000
H	-0.30400000	4.64500000	-4.29800000

$^{5}IM3_{b1}$

E=-2747.109243 (a.u.)

C	2.61500000	14.17300000	-6.20500000
H	1.56500000	14.16700000	-6.52100000
H	3.22400000	14.31500000	-7.10300000
C	2.97000000	12.89000000	-5.47800000
C	2.09600000	12.34700000	-4.52600000
H	1.14400000	12.83600000	-4.32500000
C	2.42700000	11.20700000	-3.80600000
H	1.74300000	10.82500000	-3.05600000

C	3.64900000	10.55400000	-4.04000000
O	3.98300000	9.41700000	-3.38100000
H	3.11400000	8.92100000	-3.07300000
C	4.19600000	12.24400000	-5.68800000
H	4.89500000	12.64800000	-6.41800000
C	4.53600000	11.08700000	-4.98700000
H	5.48000000	10.57800000	-5.16400000
C	1.26400000	9.60400000	3.82000000
H	0.21200000	9.30600000	3.86400000
H	1.45700000	10.26900000	4.66300000
C	1.53600000	10.31100000	2.48500000
H	1.20100000	11.35100000	2.59900000
H	2.61100000	10.38700000	2.27200000
C	0.81300000	9.71000000	1.27500000
H	1.16700000	8.69100000	1.07500000
H	-0.26000000	9.62900000	1.50300000
C	0.97900000	10.59600000	0.03800000
H	0.77600000	11.63100000	0.34300000
H	2.02100000	10.58900000	-0.30200000
N	0.12300000	10.27600000	-1.12100000
H	-0.83500000	10.13200000	-0.78300000
H	0.44300000	9.39900000	-1.53700000
C	5.13600000	-0.93600000	3.08100000
H	5.94700000	-0.22800000	2.89900000
H	5.57900000	-1.92600000	3.18800000
N	3.36400000	-2.07700000	1.71800000
H	3.28300000	-2.86600000	2.36600000
C	4.20900000	-0.99800000	1.91100000
C	2.69900000	-1.90500000	0.56100000
H	2.00200000	-2.62800000	0.16300000
N	3.05900000	-0.75900000	-0.01300000
C	4.00500000	-0.19200000	0.82500000
H	4.49000000	0.74000000	0.58600000
C	7.32800000	2.23600000	-2.07900000
H	7.64100000	3.15400000	-2.59000000
H	7.65200000	1.40200000	-2.70600000
N	5.07100000	3.17600000	-1.35000000
H	5.40000000	4.04800000	-0.87800000
C	5.84600000	2.18100000	-1.92100000
C	3.79000000	2.76200000	-1.33700000
H	2.98300000	3.31600000	-0.88300000
N	3.68400000	1.55900000	-1.89400000
C	4.96300000	1.19100000	-2.26600000
H	5.16400000	0.24300000	-2.74100000

C	3.89800000	-4.55500000	-4.01000000
H	3.72900000	-4.99000000	-5.00000000
H	3.52100000	-5.24900000	-3.25000000
N	2.11500000	-2.87700000	-4.63800000
H	1.81700000	-3.38600000	-5.50000000
C	3.18200000	-3.25100000	-3.84700000
C	1.60700000	-1.72600000	-4.15100000
H	0.76700000	-1.20400000	-4.58000000
N	2.29500000	-1.33200000	-3.07900000
C	3.27800000	-2.28600000	-2.88000000
H	3.94100000	-2.24700000	-2.02800000
C	-2.28300000	-0.52000000	1.89700000
H	-2.12300000	0.39900000	2.46200000
H	-2.12900000	-1.36800000	2.57000000
N	-1.23700000	-1.62900000	-0.13700000
H	-1.77400000	-2.52700000	-0.09900000
C	-1.33600000	-0.55700000	0.73400000
C	-0.32500000	-1.34800000	-1.07600000
H	-0.04500000	-2.04500000	-1.85200000
N	0.19500000	-0.13600000	-0.86900000
C	-0.43300000	0.36500000	0.26300000
H	-0.19100000	1.33900000	0.66300000
Fe	2.06200000	0.24500000	-1.67700000
O	1.10000000	1.96400000	-3.14500000
O	0.10400000	1.36400000	-4.07000000
C	0.05400000	0.09500000	-8.27200000
O	-0.96600000	-0.02600000	-9.15600000
H	-0.85200000	-0.80700000	-9.74600000
C	2.20700000	-0.50300000	-7.34800000
O	3.34400000	-1.25100000	-7.31700000
H	3.18100000	-2.17500000	-7.63100000
C	1.84500000	6.95800000	-3.19700000
O	1.86300000	8.22200000	-2.79600000
C	0.93100000	1.28900000	-6.35600000
C	0.61500000	2.17500000	-5.18700000
H	-0.13700000	2.92000000	-5.46600000
C	1.71000000	2.74500000	-4.27100000
H	2.71000000	2.35400000	-4.46700000
C	1.75600000	4.21000000	-3.98800000
C	1.19000000	-0.72000000	-8.28600000
H	1.29600000	-1.49800000	-9.03500000
C	2.09400000	0.51500000	-6.39700000
H	2.88800000	0.62400000	-5.66900000
C	-0.07800000	1.09400000	-7.30000000

H	-1.00000000	1.66600000	-7.26600000
C	2.97900000	4.87900000	-3.83000000
H	3.90800000	4.33600000	-3.99000000
C	3.03300000	6.22200000	-3.45500000
H	3.99500000	6.70400000	-3.30600000
C	0.61400000	6.28600000	-3.41700000
H	-0.30700000	6.84000000	-3.25800000
C	0.57800000	4.95400000	-3.78900000
H	-0.38500000	4.47400000	-3.92100000

^{5}TS4$_{b1}$

E=-2747.094394 (a.u.)

C	2.60300000	14.16300000	-6.18200000
H	1.55200000	14.15600000	-6.49300000
H	3.20800000	14.29800000	-7.08300000
C	2.95700000	12.87700000	-5.45500000
C	2.07800000	12.32400000	-4.51300000
H	1.12800000	12.81400000	-4.30800000
C	2.40200000	11.17000000	-3.81100000
H	1.71200000	10.77900000	-3.07000000
C	3.62000000	10.51400000	-4.05200000
O	3.95200000	9.36400000	-3.41100000
H	3.09100000	8.85200000	-3.10800000
C	4.18200000	12.22900000	-5.66900000
H	4.88500000	12.64100000	-6.39100000
C	4.51300000	11.05900000	-4.98500000
H	5.45500000	10.54900000	-5.16800000
C	1.25800000	9.60900000	3.81900000
H	0.20800000	9.30700000	3.86100000
H	1.44700000	10.27600000	4.66100000
C	1.53200000	10.31400000	2.48300000
H	1.18300000	11.35000000	2.59000000
H	2.60700000	10.40200000	2.27600000
C	0.82300000	9.69700000	1.27300000
H	1.19100000	8.68100000	1.08100000
H	-0.25000000	9.60300000	1.49600000
C	0.98400000	10.57500000	0.02900000
H	0.76900000	11.61000000	0.32500000
H	2.02600000	10.57700000	-0.30900000
N	0.13200000	10.23700000	-1.12800000
H	-0.82600000	10.09800000	-0.79100000
H	0.45200000	9.35000000	-1.52600000

C	5.04900000	-0.91200000	2.97700000
H	5.89200000	-0.24000000	2.80500000
H	5.44300000	-1.92400000	3.06200000
N	3.22600000	-1.94700000	1.59500000
H	3.13300000	-2.75100000	2.22100000
C	4.11400000	-0.90500000	1.80800000
C	2.55600000	-1.72200000	0.45000000
H	1.82800000	-2.40900000	0.04700000
N	2.95700000	-0.57600000	-0.10500000
C	3.93600000	-0.06900000	0.73900000
H	4.45600000	0.84700000	0.52000000
C	7.40700000	2.24300000	-2.05700000
H	7.73800000	3.15300000	-2.57000000
H	7.72500000	1.40000000	-2.67700000
N	5.16100000	3.21100000	-1.34200000
H	5.49200000	4.08000000	-0.86500000
C	5.92400000	2.20700000	-1.91100000
C	3.87400000	2.81900000	-1.34200000
H	3.07100000	3.38900000	-0.90000000
N	3.75600000	1.62200000	-1.90400000
C	5.03000000	1.23100000	-2.26500000
H	5.22100000	0.28500000	-2.74800000
C	3.84900000	-4.46100000	-3.98000000
H	3.65800000	-4.91400000	-4.95800000
H	3.46000000	-5.12600000	-3.20100000
N	2.10800000	-2.75800000	-4.65700000
H	1.80100000	-3.29100000	-5.50200000
C	3.16300000	-3.13600000	-3.84800000
C	1.61600000	-1.59000000	-4.20500000
H	0.79100000	-1.05200000	-4.64800000
N	2.30700000	-1.18400000	-3.13500000
C	3.27200000	-2.15200000	-2.90200000
H	3.93000000	-2.10400000	-2.04800000
C	-2.23200000	-0.49600000	1.89100000
H	-2.07400000	0.41200000	2.47300000
H	-2.05800000	-1.35700000	2.54100000
N	-1.23400000	-1.53000000	-0.20600000
H	-1.77200000	-2.42800000	-0.18200000
C	-1.30600000	-0.49300000	0.70900000
C	-0.34200000	-1.21600000	-1.15600000
H	-0.08300000	-1.88600000	-1.96300000
N	0.19200000	-0.01800000	-0.90800000
C	-0.40600000	0.44100000	0.25500000
H	-0.15400000	1.40000000	0.68400000

Fe	2.00100000	0.44500000	-1.84800000
O	1.21500000	1.77900000	-3.05400000
O	-0.06400000	1.27200000	-4.27900000
C	0.07000000	0.10800000	-8.29200000
O	-0.97400000	-0.02600000	-9.14500000
H	-0.86500000	-0.80500000	-9.73900000
C	2.25600000	-0.46600000	-7.43600000
O	3.40300000	-1.20600000	-7.44500000
H	3.21900000	-2.15000000	-7.68100000
C	1.85000000	6.83600000	-3.16400000
O	1.86000000	8.11400000	-2.80800000
C	0.99100000	1.30900000	-6.39800000
C	0.64600000	2.13700000	-5.18400000
H	0.00300000	2.97500000	-5.48600000
C	1.73400000	2.58900000	-4.19200000
H	2.73600000	2.23500000	-4.44500000
C	1.78000000	4.05600000	-3.86600000
C	1.21200000	-0.69700000	-8.34000000
H	1.30200000	-1.47600000	-9.09000000
C	2.16300000	0.55100000	-6.48200000
H	2.98200000	0.67400000	-5.78500000
C	-0.04300000	1.10200000	-7.31300000
H	-0.97100000	1.66100000	-7.24500000
C	2.99700000	4.74600000	-3.74900000
H	3.93200000	4.21700000	-3.91700000
C	3.04100000	6.10000000	-3.41100000
H	4.00000000	6.59800000	-3.29300000
C	0.62400000	6.14300000	-3.34800000
H	-0.30200000	6.69500000	-3.20900000
C	0.59800000	4.79600000	-3.67100000
H	-0.36000000	4.30400000	-3.78700000

$^{5}IM4_{b1}$

E=-2747.114208 (a.u.)

C	2.67500000	14.17800000	-6.25500000
H	1.62700000	14.15600000	-6.57700000
H	3.28300000	14.35300000	-7.14700000
C	3.05100000	12.88200000	-5.55800000
C	2.18000000	12.29900000	-4.62900000
H	1.22300000	12.77400000	-4.42300000
C	2.51300000	11.13700000	-3.94700000
H	1.82700000	10.72600000	-3.21500000
C	3.73600000	10.49200000	-4.20000000

O	4.06800000	9.33000000	-3.59000000
H	3.19500000	8.81800000	-3.27700000
C	4.28400000	12.25200000	-5.78100000
H	4.98500000	12.68500000	-6.49200000
C	4.62500000	11.07200000	-5.12000000
H	5.57400000	10.57600000	-5.31100000
C	1.19300000	9.77000000	3.70800000
H	0.13400000	9.49300000	3.75400000
H	1.40100000	10.41800000	4.56000000
C	1.47600000	10.50400000	2.38600000
H	1.14000000	11.54100000	2.52300000
H	2.55300000	10.58200000	2.18700000
C	0.76200000	9.93700000	1.15400000
H	1.14800000	8.93900000	0.91400000
H	-0.30700000	9.81900000	1.38300000
C	0.89400000	10.86100000	-0.06300000
H	0.60500000	11.87600000	0.23700000
H	1.94100000	10.92100000	-0.38000000
N	0.08300000	10.49600000	-1.24600000
H	-0.88700000	10.36700000	-0.93500000
H	0.40900000	9.58900000	-1.58700000
C	5.10300000	-0.88900000	3.01000000
H	5.95000000	-0.22100000	2.84200000
H	5.48900000	-1.90500000	3.09500000
N	3.28600000	-1.91700000	1.61300000
H	3.20500000	-2.73900000	2.21900000
C	4.16700000	-0.87300000	1.84500000
C	2.58000000	-1.66000000	0.50200000
H	1.85400000	-2.34200000	0.08800000
N	2.95700000	-0.48600000	-0.01400000
C	3.95800000	0.00200000	0.81700000
H	4.46800000	0.92700000	0.62100000
C	7.44000000	2.15200000	-2.07800000
H	7.73400000	3.05600000	-2.62300000
H	7.77600000	1.30300000	-2.68000000
N	5.18900000	3.10500000	-1.37800000
H	5.50600000	4.00200000	-0.94700000
C	5.95900000	2.08300000	-1.91100000
C	3.91200000	2.69900000	-1.33300000
H	3.09600000	3.27700000	-0.92800000
N	3.80500000	1.46800000	-1.83000000
C	5.07600000	1.07200000	-2.19800000
H	5.26600000	0.10300000	-2.63200000
C	3.88700000	-4.44400000	-3.90200000

H	3.67600000	-4.88000000	-4.88400000
H	3.51300000	-5.12700000	-3.13000000
N	2.09100000	-2.77300000	-4.47000000
H	1.76900000	-3.28000000	-5.32200000
C	3.20200000	-3.12300000	-3.73200000
C	1.59700000	-1.62000000	-3.96800000
H	0.72500000	-1.11400000	-4.35200000
N	2.33800000	-1.19600000	-2.94500000
C	3.34200000	-2.13400000	-2.79000000
H	4.05300000	-2.08100000	-1.97900000
C	-2.16200000	-0.49600000	1.85800000
H	-1.97500000	0.41200000	2.43300000
H	-2.00200000	-1.35600000	2.51400000
N	-1.17600000	-1.58000000	-0.22500000
H	-1.74400000	-2.46000000	-0.19900000
C	-1.23700000	-0.52800000	0.67600000
C	-0.23400000	-1.32500000	-1.14400000
H	0.02900000	-2.01600000	-1.92900000
N	0.33500000	-0.14900000	-0.88600000
C	-0.28700000	0.36400000	0.24200000
H	-0.01100000	1.32100000	0.65900000
Fe	2.05000000	0.55300000	-1.57600000
O	1.29100000	1.96600000	-2.36100000
O	-0.29700000	0.98700000	-4.10500000
C	0.00200000	0.25100000	-7.95200000
O	-1.02000000	0.16000000	-8.83900000
H	-0.84200000	-0.53100000	-9.52000000
C	2.19200000	-0.33200000	-7.10400000
O	3.34500000	-1.05400000	-7.14800000
H	3.17800000	-1.96700000	-7.49100000
C	1.88900000	6.84500000	-3.19900000
O	1.95900000	8.15300000	-2.96400000
C	0.85400000	1.29900000	-5.93400000
C	0.44700000	2.02200000	-4.63900000
H	-0.18600000	2.88400000	-4.90100000
C	1.58600000	2.49200000	-3.66200000
H	2.55100000	2.10300000	-4.00000000
C	1.69000000	4.00600000	-3.58400000
C	1.17400000	-0.50200000	-8.05300000
H	1.31000000	-1.20400000	-8.87000000
C	2.05200000	0.58700000	-6.06300000
H	2.85200000	0.65700000	-5.33700000
C	-0.16900000	1.13100000	-6.87800000
H	-1.12400000	1.62900000	-6.75300000

C	2.91300000	4.67600000	-3.72500000
H	3.80900000	4.11000000	-3.97100000
C	3.02100000	6.05800000	-3.53500000
H	3.99600000	6.53800000	-3.60000000
C	0.64400000	6.17000000	-3.14700000
H	-0.24800000	6.75900000	-2.94800000
C	0.56100000	4.79400000	-3.29900000
H	-0.40100000	4.30900000	-3.18800000

^{5}TS5$_{b1}$

E=-2747.105636 (a.u.)

C	2.67700000	14.17900000	-6.25900000
H	1.63100000	14.15700000	-6.58400000
H	3.28800000	14.35500000	-7.14900000
C	3.05200000	12.88100000	-5.56400000
C	2.18100000	12.29700000	-4.63600000
H	1.22400000	12.77300000	-4.42800000
C	2.51300000	11.13400000	-3.95500000
H	1.82700000	10.72300000	-3.22400000
C	3.73600000	10.49100000	-4.21000000
O	4.07000000	9.32700000	-3.59900000
H	3.20300000	8.82400000	-3.29000000
C	4.28500000	12.25000000	-5.78800000
H	4.98600000	12.68300000	-6.49900000
C	4.62500000	11.06900000	-5.12900000
H	5.57300000	10.57200000	-5.32100000
C	1.19300000	9.77100000	3.70900000
H	0.13400000	9.49500000	3.75300000
H	1.40200000	10.41800000	4.56100000
C	1.47800000	10.50600000	2.38800000
H	1.14500000	11.54300000	2.52600000
H	2.55500000	10.58100000	2.18800000
C	0.76100000	9.94200000	1.15600000
H	1.14600000	8.94300000	0.91500000
H	-0.30800000	9.82500000	1.38700000
C	0.89100000	10.86600000	-0.06100000
H	0.60100000	11.88100000	0.23900000
H	1.93800000	10.92700000	-0.38100000
N	0.07800000	10.50000000	-1.24300000
H	-0.89200000	10.37200000	-0.93100000
H	0.40100000	9.59200000	-1.58400000
C	5.13100000	-0.90100000	3.04100000
H	5.97300000	-0.22700000	2.87100000

H	5.52600000	-1.91200000	3.13200000
N	3.31900000	-1.94200000	1.64600000
H	3.23600000	-2.76200000	2.25600000
C	4.19900000	-0.89700000	1.87400000
C	2.61300000	-1.69000000	0.53400000
H	1.88900000	-2.37400000	0.12000000
N	2.99100000	-0.51800000	0.01500000
C	3.99200000	-0.02600000	0.84400000
H	4.50300000	0.89800000	0.64400000
C	7.45900000	2.14900000	-2.07600000
H	7.74900000	3.05600000	-2.61900000
H	7.79800000	1.30200000	-2.67800000
N	5.20900000	3.09600000	-1.37100000
H	5.52300000	3.99800000	-0.94600000
C	5.97900000	2.07500000	-1.90300000
C	3.93500000	2.68300000	-1.30900000
H	3.12100000	3.26000000	-0.89800000
N	3.83100000	1.44600000	-1.79500000
C	5.10100000	1.05600000	-2.17400000
H	5.29300000	0.08500000	-2.60300000
C	3.86100000	-4.41700000	-3.92100000
H	3.64800000	-4.84200000	-4.90700000
H	3.48000000	-5.10500000	-3.15600000
N	2.07300000	-2.72300000	-4.47000000
H	1.74500000	-3.22600000	-5.32200000
C	3.18400000	-3.09300000	-3.73900000
C	1.59000000	-1.57000000	-3.95500000
H	0.72300000	-1.04500000	-4.32700000
N	2.34200000	-1.16700000	-2.92900000
C	3.33900000	-2.11600000	-2.78800000
H	4.05300000	-2.08000000	-1.97900000
C	-2.15700000	-0.49300000	1.85600000
H	-1.97000000	0.41300000	2.43200000
H	-2.00100000	-1.35500000	2.51200000
N	-1.16100000	-1.58000000	-0.22200000
H	-1.73600000	-2.45500000	-0.20300000
C	-1.22300000	-0.52900000	0.68100000
C	-0.20600000	-1.33400000	-1.12900000
H	0.06100000	-2.02400000	-1.91300000
N	0.37100000	-0.16300000	-0.86000000
C	-0.26100000	0.35500000	0.26100000
H	0.02000000	1.30900000	0.68200000
Fe	2.08600000	0.52400000	-1.53500000
O	1.31000000	1.97000000	-2.32000000

O	-0.43200000	1.15300000	-4.00800000
C	0.02400000	0.19900000	-8.07500000
O	-0.97800000	0.09200000	-8.98700000
H	-0.80200000	-0.62800000	-9.63500000
C	2.18200000	-0.35900000	-7.15600000
O	3.34600000	-1.07500000	-7.15200000
H	3.18800000	-1.99400000	-7.48100000
C	1.87500000	6.84200000	-3.19600000
O	1.94200000	8.14800000	-2.97700000
C	0.78500000	1.25200000	-6.02200000
C	0.25500000	1.94000000	-4.76600000
H	-0.18100000	2.93500000	-4.97700000
C	1.64100000	2.51400000	-3.53200000
H	2.51200000	2.05600000	-4.00400000
C	1.69800000	4.00300000	-3.52400000
C	1.20400000	-0.54700000	-8.13700000
H	1.37200000	-1.24800000	-8.94900000
C	1.99600000	0.56500000	-6.12100000
H	2.77000000	0.63100000	-5.36600000
C	-0.18400000	1.09000000	-7.01800000
H	-1.15100000	1.57500000	-6.93700000
C	2.90500000	4.68600000	-3.75600000
H	3.79200000	4.12500000	-4.04500000
C	3.00300000	6.06800000	-3.58200000
H	3.96500000	6.56200000	-3.69900000
C	0.64000000	6.15100000	-3.07400000
H	-0.24900000	6.73800000	-2.85400000
C	0.57100000	4.77300000	-3.18000000
H	-0.36900000	4.26000000	-3.01300000

$^{5}P_{b1}$

E=-2747.237887 (a.u.)

C	2.69000000	14.20200000	-6.31100000
H	1.65300000	14.20100000	-6.66700000
H	3.33300000	14.37200000	-7.17800000
C	3.01500000	12.90800000	-5.59100000
C	2.08100000	12.34400000	-4.71400000
H	1.10000000	12.80400000	-4.60800000
C	2.38600000	11.23000000	-3.94700000
H	1.65300000	10.83800000	-3.25300000
C	3.65100000	10.63100000	-4.05400000
O	3.97400000	9.54200000	-3.31400000
H	3.10500000	9.04200000	-3.08000000

C	4.27400000	12.30000000	-5.69300000
H	5.01900000	12.72100000	-6.36500000
C	4.59400000	11.17200000	-4.93800000
H	5.56700000	10.69500000	-5.02000000
C	1.19100000	9.80200000	3.78000000
H	0.13300000	9.52300000	3.80700000
H	1.39000000	10.42600000	4.65100000
C	1.48700000	10.57200000	2.48200000
H	1.16600000	11.60900000	2.64900000
H	2.56600000	10.64300000	2.28600000
C	0.77100000	10.05400000	1.23100000
H	1.14100000	9.05500000	0.96700000
H	-0.30100000	9.94900000	1.45000000
C	0.92800000	11.00700000	0.03900000
H	0.67500000	12.02200000	0.37000000
H	1.97600000	11.04000000	-0.28100000
N	0.10300000	10.70700000	-1.14700000
H	-0.86900000	10.57400000	-0.84600000
H	0.41200000	9.82400000	-1.55700000
C	5.17100000	-0.94600000	3.11200000
H	5.98600000	-0.24300000	2.92600000
H	5.61200000	-1.93600000	3.23200000
N	3.38500000	-2.07900000	1.75100000
H	3.29000000	-2.86200000	2.40300000
C	4.25100000	-1.01500000	1.93900000
C	2.72600000	-1.89800000	0.59000000
H	2.01400000	-2.60800000	0.19600000
N	3.11200000	-0.76500000	0.00900000
C	4.06800000	-0.21400000	0.84700000
H	4.57700000	0.70400000	0.61000000
C	7.54100000	2.22800000	-1.98100000
H	7.83500000	3.15600000	-2.48400000
H	7.87500000	1.40600000	-2.62000000
N	5.27400000	3.13300000	-1.25800000
H	5.57600000	4.02500000	-0.80200000
C	6.06100000	2.14400000	-1.81700000
C	4.00300000	2.69300000	-1.22100000
H	3.19000000	3.24400000	-0.77300000
N	3.91200000	1.48000000	-1.75500000
C	5.19300000	1.12900000	-2.13200000
H	5.40800000	0.17700000	-2.59300000
C	3.93100000	-4.57600000	-3.95300000
H	3.74300000	-5.03600000	-4.92800000
H	3.56000000	-5.24400000	-3.16800000

N	2.24400000	-2.82800000	-4.67200000
H	1.93000000	-3.35900000	-5.51300000
C	3.24200000	-3.25500000	-3.82000000
C	1.77900000	-1.64400000	-4.22000000
H	1.00000000	-1.07900000	-4.70600000
N	2.42500000	-1.28400000	-3.11100000
C	3.33900000	-2.28900000	-2.85300000
H	3.96200000	-2.27700000	-1.97200000
C	-2.25600000	-0.48100000	1.82400000
H	-2.08900000	0.42600000	2.40500000
H	-2.11100000	-1.34000000	2.48500000
N	-1.18700000	-1.58900000	-0.19500000
H	-1.73500000	-2.48000000	-0.15900000
C	-1.29800000	-0.51300000	0.66900000
C	-0.24700000	-1.31900000	-1.11300000
H	0.04700000	-2.02500000	-1.87700000
N	0.27700000	-0.11100000	-0.89800000
C	-0.37500000	0.40000000	0.21500000
H	-0.13200000	1.37100000	0.62100000
Fe	2.16700000	0.27700000	-1.69400000
O	1.37600000	1.95800000	-3.14500000
O	1.75300000	3.65900000	-6.48800000
C	-0.20700000	-0.22200000	-8.43600000
O	-1.28300000	-0.65300000	-9.12800000
H	-1.08800000	-1.45700000	-9.66500000
C	2.04100000	-0.47900000	-7.53400000
O	3.18100000	-1.18300000	-7.33000000
H	3.08500000	-2.13800000	-7.57100000
C	1.86700000	7.03800000	-3.12100000
O	1.79400000	8.31700000	-2.85100000
C	0.83900000	1.58700000	-7.23800000
C	0.79500000	3.00500000	-6.87400000
H	-0.19700000	3.48900000	-7.00800000
C	2.18100000	2.78600000	-3.60600000
H	3.11100000	2.43700000	-4.08600000
C	2.03800000	4.22300000	-3.51500000
C	0.94600000	-0.99100000	-8.24900000
H	0.98300000	-1.98500000	-8.67800000
C	1.99800000	0.82700000	-7.03800000
H	2.86400000	1.25300000	-6.54300000
C	-0.27800000	1.06200000	-7.89300000
H	-1.17800000	1.65100000	-8.03300000
C	3.14500000	5.05600000	-3.78400000
H	4.07400000	4.60800000	-4.13000000

C	3.07400000	6.42500000	-3.58300000
H	3.94500000	7.05400000	-3.74200000
C	0.72600000	6.19200000	-2.97300000
H	-0.21700000	6.66300000	-2.70900000
C	0.82900000	4.82400000	-3.10900000
H	-0.01600000	4.17300000	-2.92100000