

Supplementary Information

Mechanistic Insights into Ring Cleavage of Hydroquinone by PnpCD from Quantum Mechanical/Molecular Mechanical Calculations

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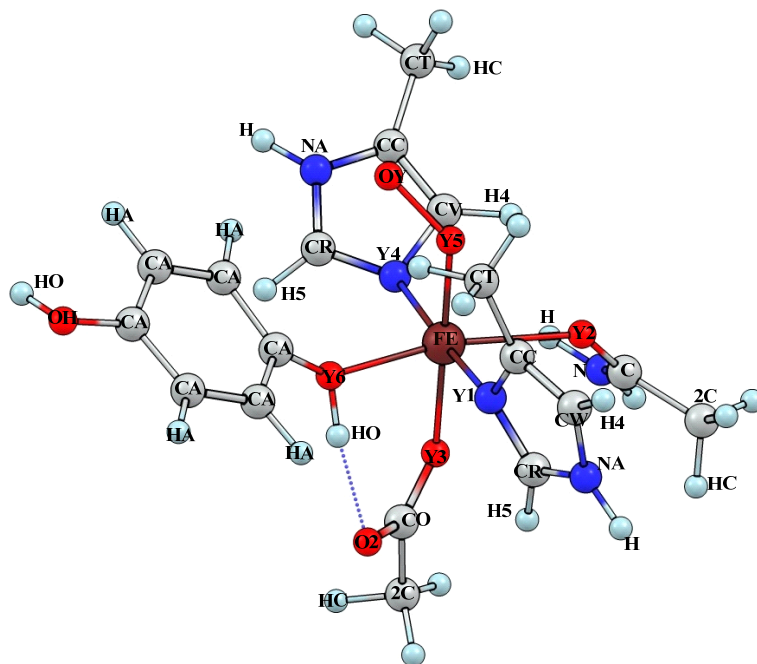
The Force Field for the Iron Center

BOND

FE-Y6	22.5	2.1007
Y1-FE	36.6	2.1751
Y2-FE	23.1	2.0671
Y3-FE	26.9	2.1110
Y4-FE	43.2	2.1564
Y5-FE	24.4	1.9100
C -Y2	570.0	1.229
CC-Y1	410.0	1.394
CO-Y3	656.0	1.2500
CR-Y4	488.0	1.335
Y1-CR	488.0	1.335
Y4-CV	410.0	1.394
Y5-OY	384.3	1.4300
Y6-CA	384.0	1.3637
Y6-HO	371.4	0.9730

ANGLES

C -Y2-FE	72.89	136.17
CC-Y1-FE	68.02	130.87
CO-Y3-FE	81.90	131.58
CR-Y4-FE	74.97	127.65
FE-Y1-CR	64.60	122.47
FE-Y4-CV	75.95	125.93
FE-Y4-Y5	28.40	41.56
FE-Y5-OY	11.98	130.67
FE-Y6-CA	92.38	135.86
FE-Y6-HO	65.59	104.48
Y1-FE-Y2	48.25	91.68
Y1-FE-Y3	59.36	91.31
Y1-FE-Y4	54.71	178.61
Y1-FE-Y5	46.05	91.38
Y1-FE-Y6	33.59	90.38
Y2-FE-Y3	64.31	91.90
Y2-FE-Y4	37.88	87.96
Y2-FE-Y5	54.74	88.10
Y2-FE-Y6	51.83	176.36
Y3-FE-Y4	61.66	87.35
Y3-FE-Y5	49.67	177.30
Y3-FE-Y6	55.11	85.06
Y4-FE-Y5	47.51	89.95
Y4-FE-Y6	28.17	89.90
Y4-Y5-FE	25.83	48.50
Y5-FE-Y6	48.71	94.852



2C-C -Y2	80.0	120.402
2C-CO-Y3	70.0	117.00
CC-CV-Y4	70.0	120.00
CC-Y1-CR	70.0	117.00
CR-Y4-CV	70.0	117.00
CT-CC-Y1	70.0	120.00
CW-CC-Y1	70.0	120.00
N -C -Y2	80.0	122.90
NA-CR-Y4	70.0	120.00
O2-CO-Y3	80.0	126.00
Y1-CR-H5	50.0	120.00
Y1-CR-NA	70.0	120.00
Y4-CR-H5	50.0	120.00
Y4-CV-H4	50.0	120.00
Y6-CA-CA	69.52	119.90
HO-Y6-CA	49.00	108.58

DIHE

X -CC-Y1-X	4.8	2	180.0
X -CR-Y4-X	10.0	2	180.0
X -CV-Y4-X	4.8	2	180.0
X -Y1-CR-X	10.0	2	180.0
X -Y6-CA-X	1.8	2	180.0
2C-2C-CO-Y3	0.39	1	180.0
2C-C -Y2-FE	0.00	3	0.00
2C-CO-Y3-FE	0.00	3	0.00
C -Y2-FE-Y3	0.00	3	0.00
C -Y2-FE-Y4	0.00	3	0.00
C -Y2-FE-Y5	0.00	3	0.00
C -Y2-FE-Y6	0.00	3	0.00
CC-CV-Y4-FE	0.00	3	0.00
CC-Y1-FE-Y2	0.00	3	0.00
CC-Y1-FE-Y3	0.00	3	0.00
CC-Y1-FE-Y4	0.00	3	0.00
CC-Y1-FE-Y5	0.00	3	0.00
CC-Y1-FE-Y6	0.00	3	0.00
CO-Y3-FE-Y4	0.00	3	0.00
CO-Y3-FE-Y5	0.00	3	0.00
CO-Y3-FE-Y6	0.00	3	0.00
CR-Y4-FE-Y5	0.00	3	0.00
CR-Y4-FE-Y6	0.00	3	0.00
CT-CC-Y1-FE	0.00	3	0.00
CW-CC-Y1-FE	0.00	3	0.00
H -N -C -Y2	2.0	1	0.00
FE-Y1-CR-H5	0.00	3	0.00
FE-Y1-CR-NA	0.00	3	0.00

FE-Y4-CR-H5	0.00	3	0.00
FE-Y4-CV-H4	0.00	3	0.00
FE-Y4-Y5-OY	0.00	3	0.00
FE-Y5-Y4-CV	0.00	3	0.00
FE-Y6-CA-CA	0.00	3	0.00
N -C -Y2-FE	0.00	3	0.00
NA-CR-Y4-FE	0.00	3	0.00
O2-CO-Y3-FE	0.00	3	0.00
Y1-FE-Y2-C	0.00	3	0.00
Y1-FE-Y3-CO	0.00	3	0.00
Y1-FE-Y4-CR	0.00	3	0.00
Y1-FE-Y4-CV	0.00	3	0.00
Y1-FE-Y4-Y5	0.00	3	0.00
Y1-FE-Y5-Y4	0.00	3	0.00
Y1-FE-Y5-OY	0.00	3	0.00
Y1-FE-Y6-CA	0.00	3	0.00
Y1-FE-Y6-HO	0.00	3	0.00
Y2-C -2C-HC	0.8	1	0.00
Y2-FE-Y1-CR	0.00	3	0.00
Y2-FE-Y3-CO	0.00	3	0.00
Y2-FE-Y4-CR	0.00	3	0.00
Y2-FE-Y4-CV	0.00	3	0.00
Y2-FE-Y4-Y5	0.00	3	0.00
Y2-FE-Y5-Y4	0.00	3	0.00
Y2-FE-Y5-OY	0.00	3	0.00
Y2-FE-Y6-CA	0.00	3	0.00
Y2-FE-Y6-HO	0.00	3	0.00
Y3-CO-2C-HC	0.00	1	0.00
Y3-FE-Y1-CR	0.00	3	0.00
Y3-FE-Y4-CR	0.00	3	0.00
Y3-FE-Y4-CV	0.00	3	0.00
Y3-FE-Y5-OY	0.00	3	0.00
Y3-FE-Y6-CA	0.00	3	0.00
Y3-FE-Y6-HO	0.00	3	0.00
Y4-FE-Y1-CR	0.00	3	0.00
Y4-FE-Y5-OY	0.00	3	0.00
Y4-FE-Y6-CA	0.00	3	0.00
Y4-FE-Y6-HO	0.00	3	0.00
Y5-FE-Y1-CR	0.00	3	0.00
Y5-FE-Y4-CV	0.00	3	0.00
Y5-FE-Y6-CA	0.00	3	0.00
Y5-FE-Y6-HO	0.00	3	0.00
Y6-FE-Y1-CR	0.00	3	0.00
Y6-FE-Y4-CV	0.00	3	0.00
Y6-FE-Y5-OY	0.00	3	0.00

Solvation Procedure

To attain equilibrium of the inner solvent layer, the following four steps were carried out: (1) optimization of the inner 8 Å solvent layer for 1000 steps of steepest descent and 1000 steps of adapted basis Newton-Raphson minimization; (2) heating gently the system from 0 to 300 K for 15 ps with a time step of 1 fs; (3) equilibrating the solvent layer for 15 ps at 300 K; and (4) resolution of the protein to fill up the interspace of solvent layer. These four steps were repeated three times until no more than 100 additional water molecules were incorporated into the system.

MD Simulation Results

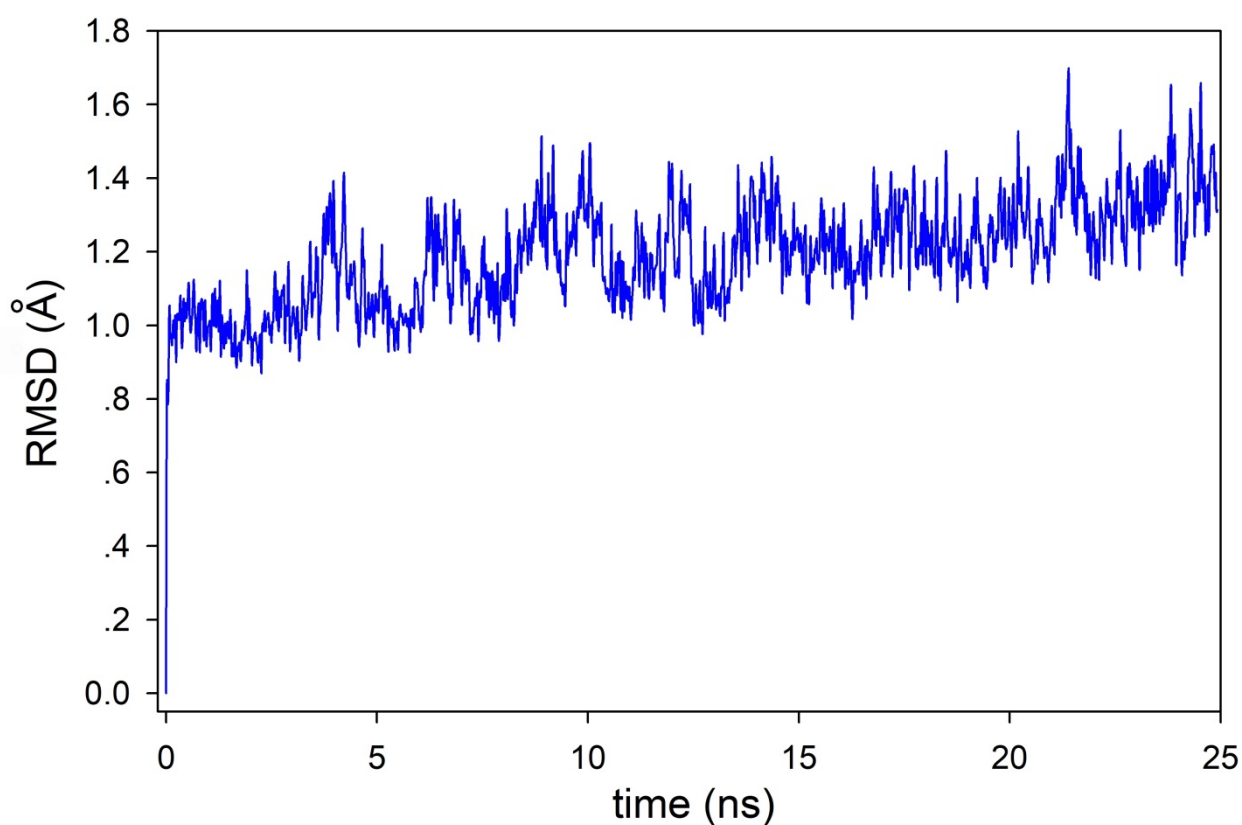


Figure S1. The RMSD plot of backbone during MD simulations.

Energies and Spin Density of the Involved Species

(1) Model A Using Neutral Substrate.

Table S1. Absolute energies (in a.u.) for the key species.

Species	B3LYP/Def2-SVP		B3LYP/Def2-TZVP		dispersion	ZPE
	QM	QM/MM	QM	QM/MM		
³ N-1	-2992.902805	-3155.469978	-2995.039665	-3157.606838	-0.071560	0.458210
⁵ N-1	-2992.898248	-3155.466250	-2995.036051	-3157.604053	-0.071521	0.458182
⁷ N-1	-2992.896481	-3155.464171	-2995.033669	-3157.601358	-0.071195	0.458079
⁵ N-TS1	-2992.885490	-3155.454949	-2995.023695	-3157.593154	-0.070694	0.458139
⁵ N-2	-2992.899109	-3155.469159	-2995.038415	-3157.608465	-0.069500	0.460757
⁵ N-TS2	-2992.899255	-3155.468891	-2995.038150	-3157.607786	-0.069188	0.457972
⁵ N-3	-2992.902848	-3155.471951	-2995.041007	-3157.610111	-0.069381	0.462079
⁵ N-TS3	-2992.865921	-3155.433999	-2995.010496	-3157.578573	-0.071179	0.457440
⁵ N-4	-2992.879986	-3155.446625	-2995.022958	-3157.589597	-0.070886	0.457770
⁵ N-5	-2992.929211	-3155.500336	-2995.071156	-3157.642281	-0.069887	0.460671
⁵ N-TS4	-2992.908729	-3155.478815	-2995.049862	-3157.619948	-0.072244	0.458760
⁵ N-6	-2993.006766	-3155.578649	-2995.143827	-3157.715710	-0.070840	0.464018
⁵ N-TS5	-2993.007477	-3155.577262	-2995.144714	-3157.714498	-0.071195	0.462900
⁵ N-7	-2993.007917	-3155.577273	-2995.145326	-3157.714682	-0.071293	0.462910

Table S2. Relative energies (in kcal/mol) for the key species.

Species	B3LYP/Def2-SVP		B3LYP/Def2-TZVP		$\Delta E(\text{B3LYP-D3})$	$\Delta E(\text{B3LYP-D3})+\text{ZPE}$
	QM	QM/MM	QM	QM/MM		
³ N-1	0.0	0.0	0.0	0.0	0.0	0.0
⁵ N-1	2.9	2.3	2.3	1.7	1.8	1.8
⁷ N-1	4.0	3.6	3.8	3.4	3.7	3.6
⁵ N-TS1	10.9	9.4	10.0	8.6	9.1	9.1
⁵ N-2	2.3	0.5	0.8	-1.0	0.3	1.9
⁵ N-TS2	2.2	0.7	1.0	-0.6	0.9	0.7
⁵ N-3	0.0	-1.2	-0.8	-2.1	-0.7	1.7
⁵ N-TS3	23.1	22.6	18.3	17.7	18.0	17.5
⁵ N-4	14.3	14.7	10.5	10.8	11.2	11.0
⁵ N-5	-16.6	-19.0	-19.8	-22.2	-21.2	-19.6
⁵ N-TS4	-3.7	-5.5	-6.4	-8.2	-8.7	-8.3
⁵ N-6	-65.2	-68.2	-65.4	-68.3	-67.9	-64.2
⁵ N-TS5	-65.7	-67.3	-65.9	-67.6	-67.3	-64.4
⁵ N-7	-66.0	-67.3	-66.3	-67.7	-67.5	-64.6

Table S3. Spin density distribution and the spin expectation value $\langle S^2 \rangle$ for the key species.

Species ^a	Spin density						$\langle S^2 \rangle$
	Fe	O1	O2	Sub	L ^b	other	
³ N-1	3.75	-0.48	-0.78	-0.56	0.05	0.03	3.84
⁵ N-1	3.78	0.36	0.39	-0.62	0.05	0.04	6.87
⁷ N-1	3.82	0.58	0.79	0.71	0.05	0.03	12.02
⁵ N-TS1	3.76	0.17	0.12	-0.13	0.05	0.03	6.23
⁵ N-2	3.78	0.11	0.01	0.04	0.04	0.01	6.01
⁵ N-TS2	3.78	0.10	0.01	0.02	0.05	0.04	6.01
⁵ N-3	3.79	0.09	0.02	0.01	0.07	0.05	6.01
⁵ N-TS3	4.01	0.63	-0.39	-0.42	0.13	0.03	6.90
⁵ N-4	3.92	0.78	-0.07	-0.79	0.11	0.03	6.90
⁵ N-5	3.92	0.89	-0.06	-0.85	0.07	0.05	6.97
⁵ N-TS4	3.87	0.65	-0.04	-0.56	0.06	0.06	6.59
⁵ N-6	3.81	0.06	0.00	0.01	0.07	0.06	6.01
⁵ N-TS5	3.82	0.03	0.01	0.01	0.07	0.04	6.01
⁵ N-7	3.82	0.03	0.01	0.01	0.07	0.04	6.01

^a The QM/MM-optimized geometries can be found in Fig 3 for N-1, Fig 6 for ⁵N-TS1 and ⁵N-2, Fig. 7 for the others.

^b The ligated N atoms of His256, His303, and O atom of Glu262.

(2) Model B Using Monoanionized Substrate.

Table S4. Absolute energies (in a.u.) for the key species.

Species	B3LYP/Def2-SVP		B3LYP/Def2-TZVP		dispersion	ZPE
	QM	QM/MM	QM	QM/MM		
³ M-1	-2992.356486	-3158.855596	-2994.503879	-3161.002988	-0.068167	0.445357
⁵ M-1	-2992.348332	-3158.847675	-2994.496514	-3160.995857	-0.068031	0.444613
⁷ M-1	-2992.353595	-3158.853318	-2994.501592	-3161.001315	-0.067943	0.445549
⁵ M-TS1	-2992.317302	-3158.817436	-2994.466464	-3160.966598	-0.066175	0.443543
⁵ M-2	-2992.320098	-3158.819377	-2994.469911	-3160.969190	-0.066777	0.444351
⁵ M-TS2	-2992.299841	-3158.797823	-2994.453429	-3160.951411	-0.069148	0.442823
⁵ M-3	-2992.301994	-3158.810468	-2994.457203	-3160.965677	-0.069165	0.443622
⁵ M-4	-2992.351461	-3158.843340	-2994.505027	-3160.996906	-0.070011	0.446104
⁵ M-TS3	-2992.293888	-3158.801439	-2994.448387	-3160.955938	-0.068604	0.441433
⁵ M-4'	-2992.310988	-3158.810418	-2994.463966	-3160.963396	-0.067652	0.444604
⁵ M-TS4	-2992.345061	-3158.838712	-2994.498257	-3160.991907	-0.069062	0.444340
⁵ M-5	-2992.373598	-3158.872969	-2994.526491	-3161.025861	-0.066742	0.444180
⁵ M-TS5	-2992.373120	-3158.862274	-2994.524426	-3161.013580	-0.068765	0.444968
⁵ M-6	-2992.460526	-3158.952716	-2994.609298	-3161.101488	-0.065553	0.447589

Table S5. Relative energies (in kcal/mol) for the key species.

Species	B3LYP/Def2-SVP		B3LYP/Def2-TZVP		$\Delta E(\text{B3LYP-D3})$	$\Delta E(\text{B3LYP-D3})+\text{ZPE}$
	QM	QM/MM	QM	QM/MM		
³ M-1	0.0	0.0	0.0	0.0	0.0	0.0
⁵ M-1	5.1	5.0	4.6	4.5	4.6	4.1
⁷ M-1	1.8	1.4	1.4	1.0	1.2	1.3
⁵ M-TS1	24.6	23.9	23.5	22.8	24.1	22.9
⁵ M-2	22.8	22.7	21.3	21.2	22.1	21.5
⁵ M-TS2	35.5	36.3	31.7	32.4	31.7	30.2
⁵ M-3	34.2	28.3	29.3	23.4	22.8	21.7
⁵ M-4	3.2	7.7	-0.7	3.8	2.7	3.1
⁵ M-TS3	39.3	34.0	34.8	29.5	29.2	26.8
⁵ M-4'	28.6	28.3	25.0	24.8	25.2	24.7
⁵ M-TS4	7.2	10.6	3.5	7.0	6.4	5.8
⁵ M-5	-10.7	-10.9	-14.2	-14.4	-13.5	-14.2
⁵ M-TS5	-10.4	-4.2	-12.9	-6.6	-7.0	-7.3
⁵ M-6	-65.3	-60.9	-66.2	-61.8	-60.2	-58.8

Table S6. Spin density distribution and the spin expectation value $\langle S^2 \rangle$ for the key species.

Species ^a	Spin density						$\langle S^2 \rangle$
	Fe	O1	O2	Sub	L ^b	other	
³ M-1	3.72	-0.66	-0.83	-0.31	0.05	0.03	3.82
⁵ M-1	3.76	0.25	0.29	-0.40	0.06	0.03	6.80
⁷ M-1	3.81	0.84	0.88	0.37	0.06	0.04	12.02
⁵ M-TS1	3.79	0.11	0.07	-0.05	0.06	0.01	6.07
⁵ M-2	3.82	0.10	0.02	-0.01	0.05	0.02	6.06
⁵ M-TS2	4.03	0.13	-0.30	0.02	0.10	0.02	6.56
⁵ M-3	4.07	0.06	-0.40	0.14	0.11	0.02	6.74
⁵ M-4	3.15	0.63	0.00	0.12	0.07	0.03	6.06
⁵ M-TS3	4.10	-0.20	-0.30	0.24	0.13	0.03	6.76
⁵ M-4'	4.13	-0.51	-0.06	0.26	0.16	0.02	6.83
⁵ M-TS4	3.22	0.61	0.00	0.06	0.07	0.03	6.09
⁵ M-5	3.95	0.84	-0.07	-0.84	0.09	0.03	6.97
⁵ M-TS5	4.05	0.62	-0.05	-0.77	0.12	0.03	6.92
⁵ M-6	3.84	0.03	0.00	0.04	0.06	0.03	6.01

^a The QM/MM-optimized geometries can be found in Fig 4 for **M-1**, Fig 9 for the others.^b The ligated N atoms of His256, His303, and O atom of Glu262.

Spin Natural Orbital Analysis for the Fe-O₂ Species.

(1) Model A Using Neutral Substrate..

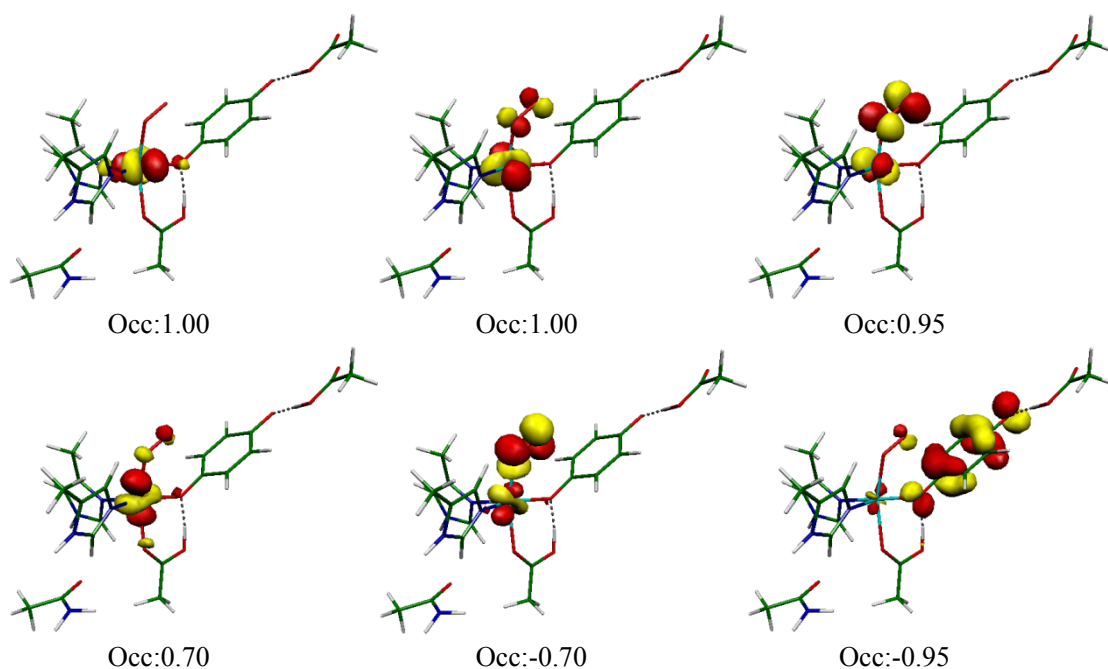


Figure S2. Singly occupied spin natural orbitals and their occupation numbers (Occ) for $^3\text{N-1}$ at the B3LYP(Def2-SVP)/MM level.

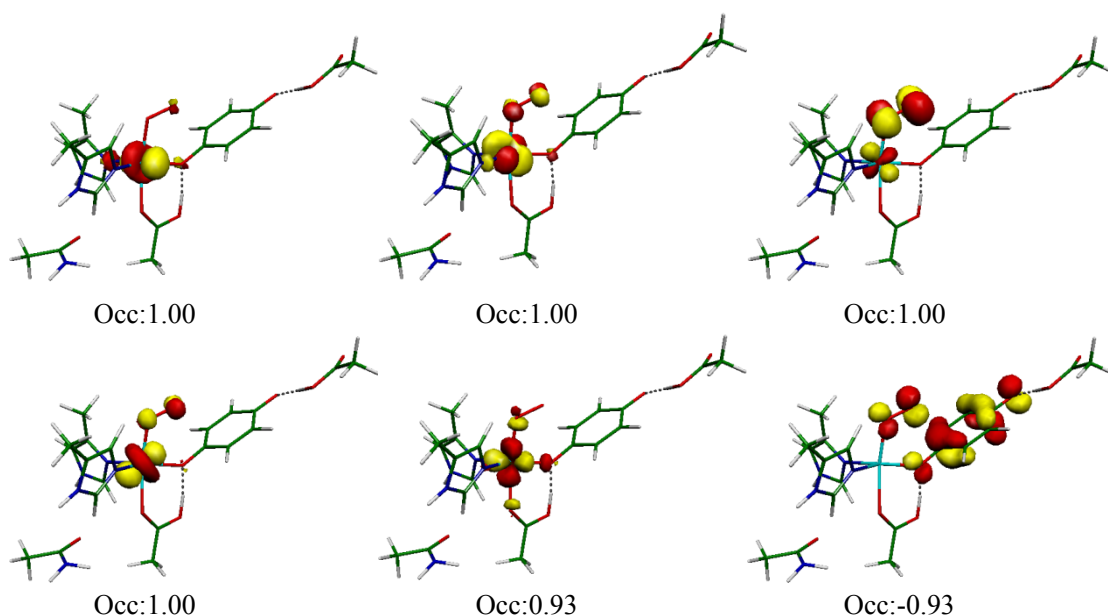


Figure S3. Singly occupied spin natural orbitals and their occupation numbers (Occ) for $^5\text{N-1}$ at the B3LYP(Def2-SVP)/MM level.

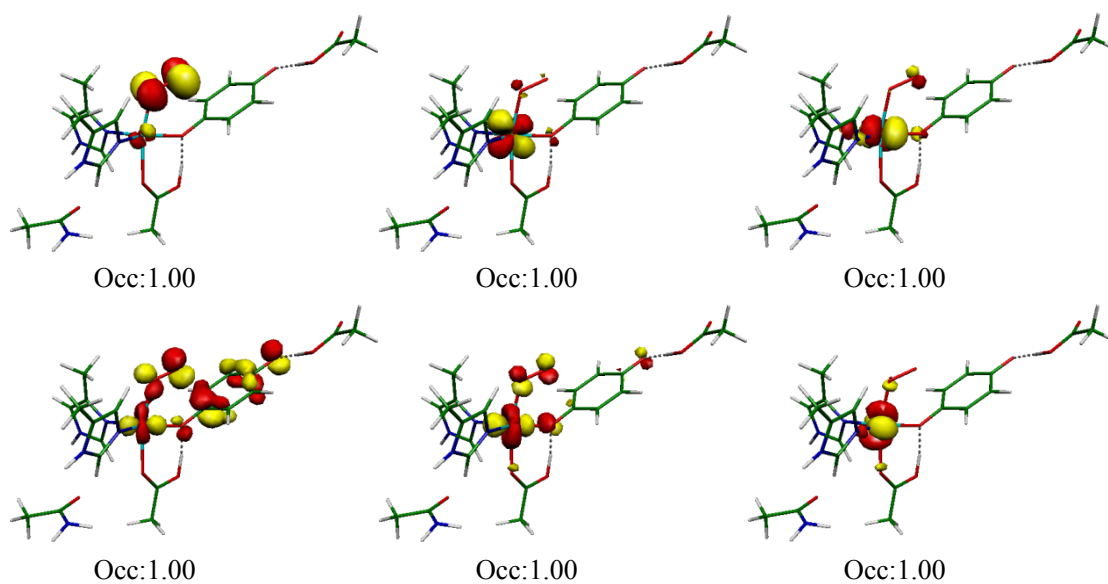


Figure S4. Singly occupied spin natural orbitals and their occupation numbers (Occ) for ${}^7\text{N-1}$ at the B3LYP(Def2-SVP)/MM level.

(2) Model B Using Monoanionic Substrate.

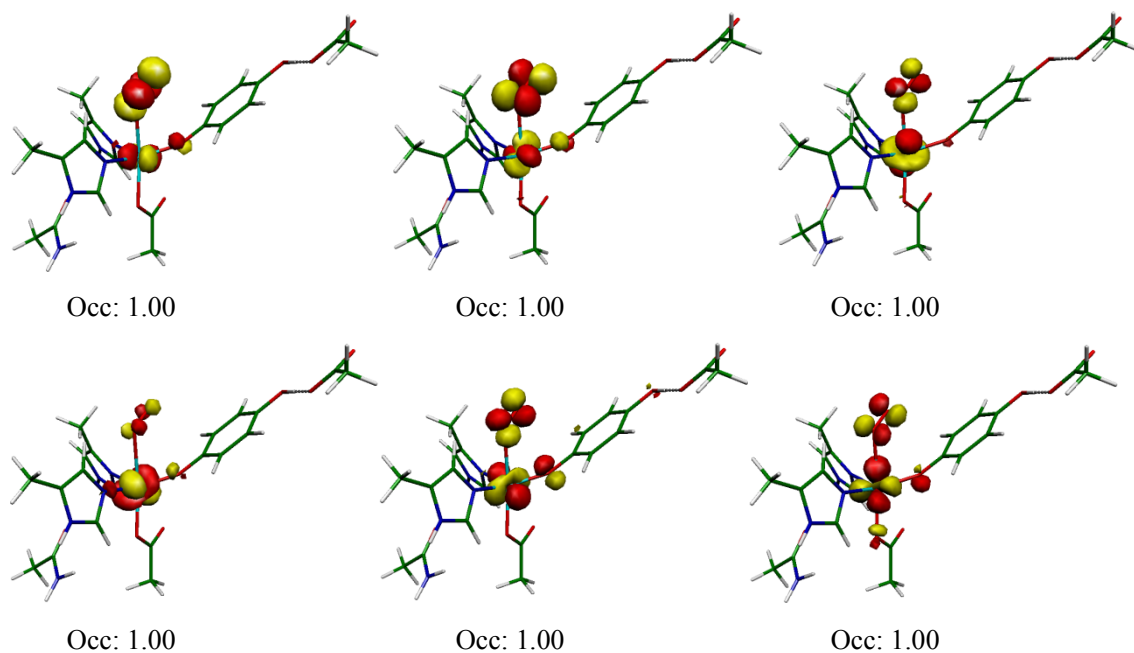


Figure S5. Singly occupied spin natural orbitals and their occupation numbers (Occ) for ${}^7\text{M-1}$ at the B3LYP(Def2-SVP)/MM level.

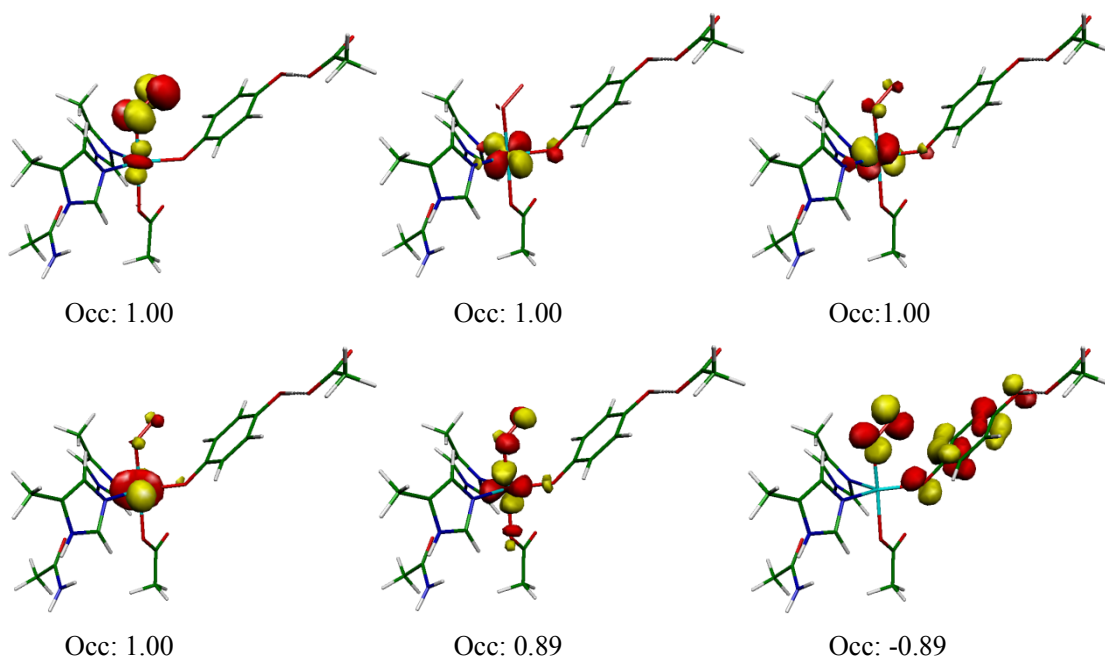


Figure S6. Singly occupied spin natural orbitals and their occupation numbers (Occ) for $^5\mathbf{M-1}$ at the B3LYP(Def2-SVP)/MM level.

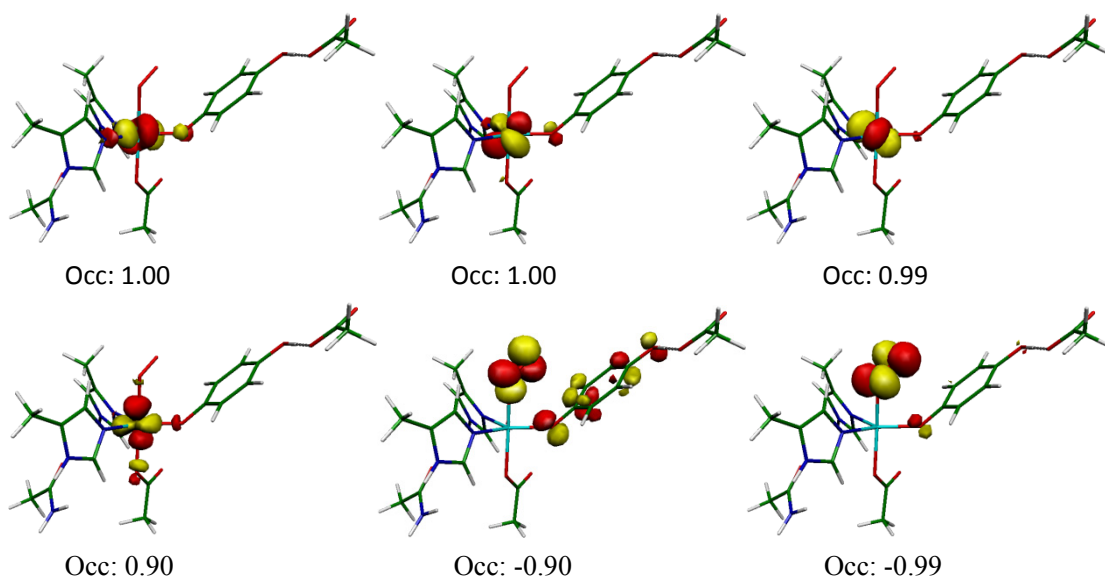


Figure S7. Singly occupied spin natural orbitals and their occupation numbers (Occ) for $^3\mathbf{M-1}$ at the B3LYP(Def2-SVP)/MM level.

Discard Pathways

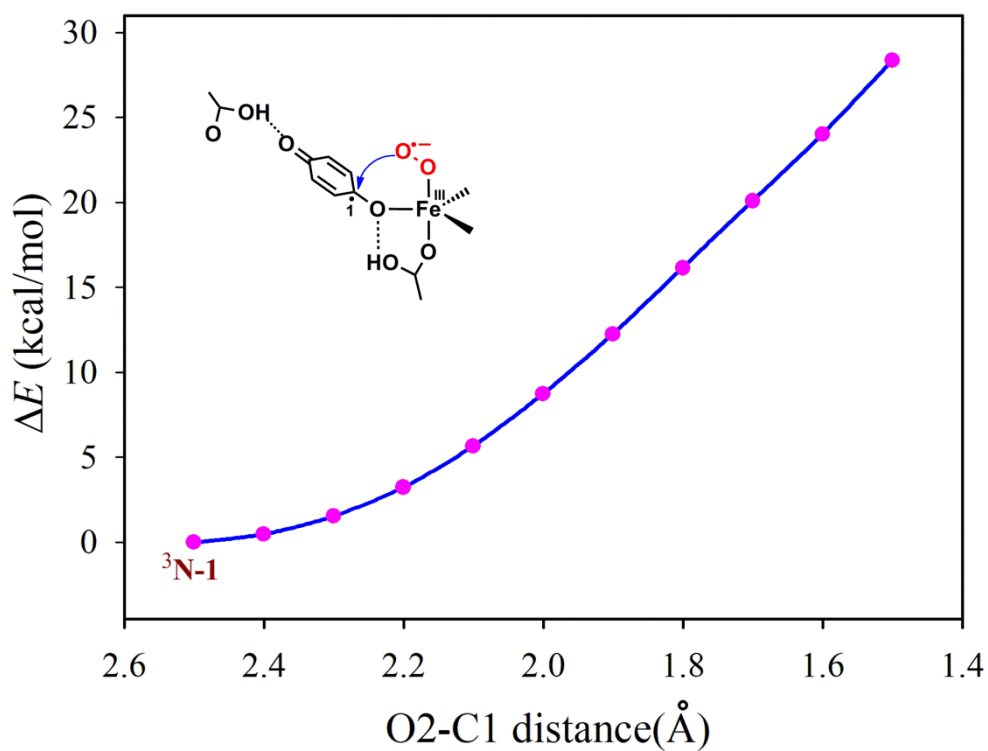


Figure S8. The B3LYP(B1)/MM energy profile along the forming O2-C1 bond starting from ³N-1.

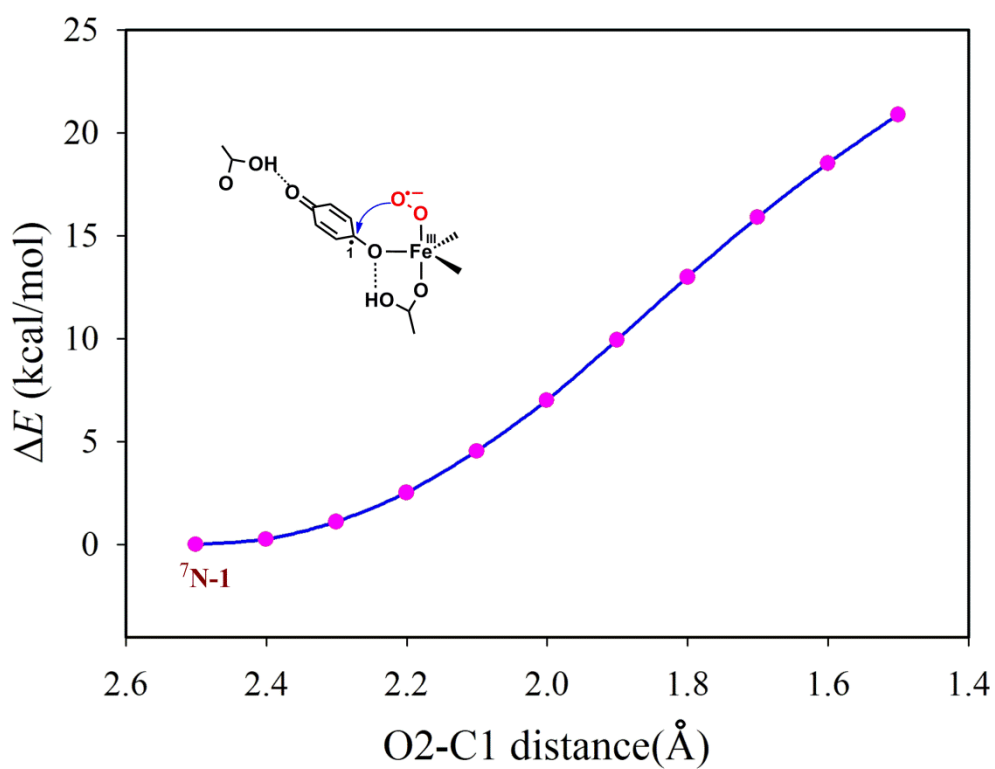


Figure S9. The B3LYP(B1)/MM energy profile along the forming O2-C1 bond starting from ⁷N-1.

QM/MM Energy Scan for Barrier-Free Reactions

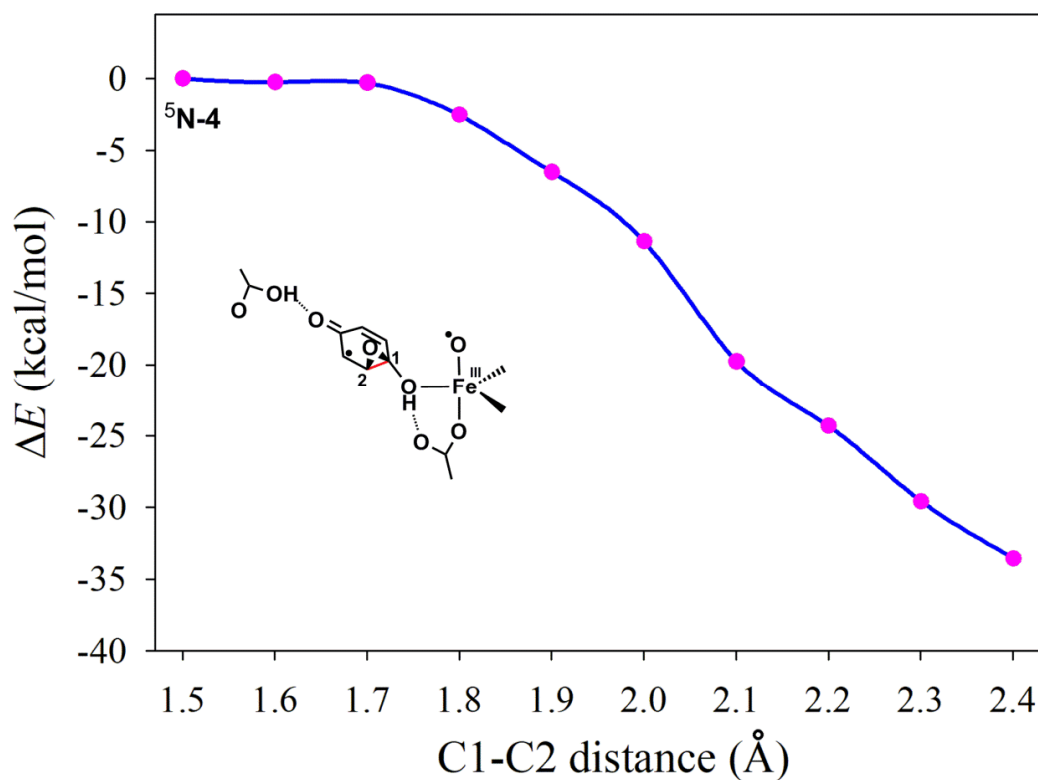


Figure S10. The B3LYP(B1)/MM energy profile along the forming C1-C2 bond starting from ⁵N-4.

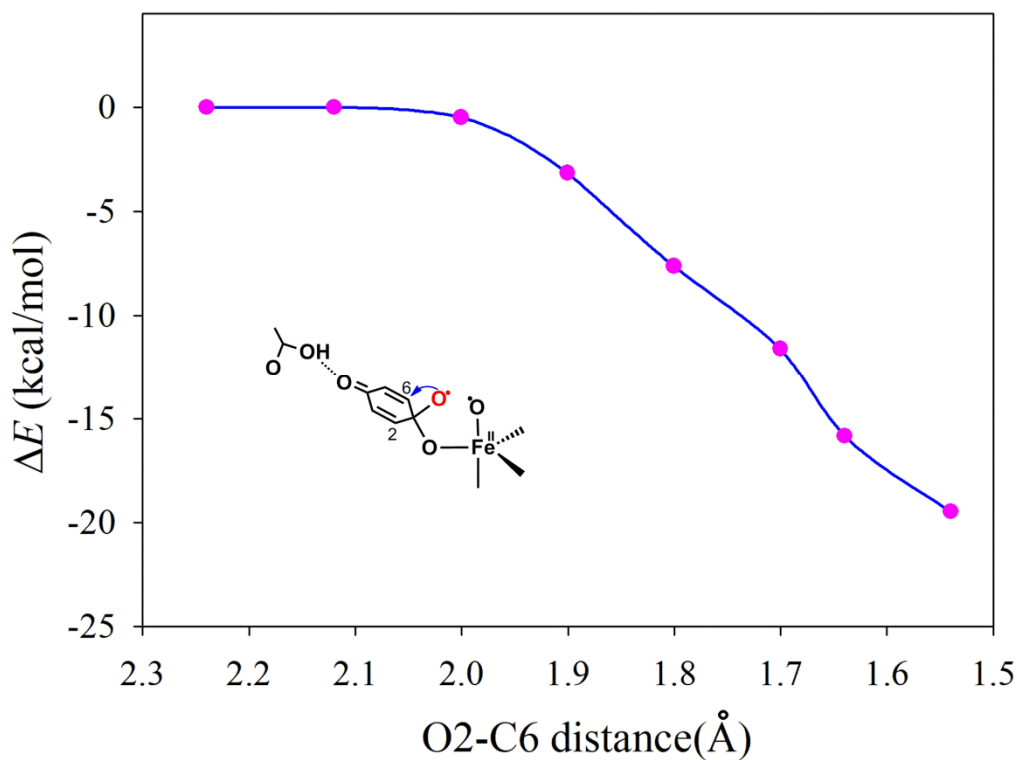


Figure S11. The B3LYP(B1)/MM energy profile along the forming O2-C6 bond starting from ⁵M-3.

Cartesian Coordinates of the QM Region of Key Species

(1) Model A Using Neutral Substrate.

³N-1

C	0.854579	0.539714	-7.385720	C	-8.071262	4.793086	1.063357
H	1.889724	0.223220	-7.173959	H	-7.282604	4.836968	1.807113
H	0.781601	1.598826	-7.108054	N	-7.912283	4.944854	-0.246942
C	-0.050898	-0.258010	-6.458743	H	-9.777158	4.533801	2.305808
O	-0.609891	0.492212	-5.547236	C	-9.179868	4.892794	-0.813866
O	-0.167532	-1.478752	-6.521826	C	-10.090922	4.681361	0.197187
C	-8.832040	9.285827	3.221387	H	-11.171355	4.591032	0.199370
H	-8.986976	10.299647	2.829106	C	-9.395432	5.105072	-2.286792
H	-8.546451	9.394880	4.280956	H	-8.608337	5.756047	-2.692881
C	-7.619590	8.620868	2.591179	H	-9.342224	4.157828	-2.850506
O	-7.464161	7.399760	2.517246	N	-6.207873	7.175435	-1.863267
N	-6.663305	9.484456	2.162622	C	-6.433632	8.216329	-1.076957
H	-5.735905	9.089360	2.044832	H	-6.477512	8.194614	0.008104
H	-6.684249	10.479409	2.434346	N	-6.624392	9.328660	-1.820845
O	-6.113644	4.613285	-3.168368	H	-6.842827	10.247684	-1.448954
O	-5.750073	3.475918	-3.604562	C	-6.522340	8.991696	-3.159776
Fe	-6.008569	5.145159	-1.201272	C	-6.264151	7.641440	-3.157542
H	-2.556362	3.904957	-2.387685	H	-6.153027	6.967460	-3.999544
C	-3.005864	2.914134	-2.446124	C	-6.697110	9.971550	-4.278428
C	-2.404139	1.938828	-3.212267	H	-6.681925	11.003682	-3.896658
H	-1.478443	2.153944	-3.752279	H	-5.884483	9.889106	-5.016946
C	-2.968463	0.617695	-3.328981	O	-5.142312	6.004013	0.631723
O	-2.428276	-0.312562	-4.029294	C	-4.492166	5.455419	1.528744
H	-1.326531	0.039883	-4.903325	O	-4.046467	4.229091	1.395093
C	-4.192910	0.391427	-2.602582	C	-4.151463	6.147776	2.827448
H	-4.638748	-0.603860	-2.671696	H	-4.019361	5.406281	3.628342
C	-4.785742	1.372050	-1.834775	H	-4.965035	6.838780	3.083488
H	-5.713549	1.163915	-1.296625	h	0.709438	0.456278	-8.462772
C	-4.214896	2.674660	-1.731071	h	-9.776481	8.750045	3.126341
O	-4.733630	3.607353	-0.924854	h	-10.349165	5.561028	-2.552431
H	-4.281767	3.861774	0.443979	h	-7.663374	9.878213	-4.774097
N	-9.369723	4.625298	1.365030	h	-3.215114	6.698156	2.735810

⁵N-1

C	0.858404	0.543108	-7.389249	C	-8.078095	4.827143	1.047811
H	1.894185	0.228345	-7.177811	H	-7.289560	4.889175	1.789939
H	0.783656	1.602106	-7.112577	N	-7.923436	4.974693	-0.263309
C	-0.044227	-0.253811	-6.460485	H	-9.776974	4.547462	2.296811
O	-0.596240	0.499651	-5.544285	C	-9.191522	4.902032	-0.825767
O	-0.168043	-1.472953	-6.521364	C	-10.097766	4.681780	0.188050
C	-8.826372	9.289799	3.219283	H	-11.176727	4.575106	0.191989
H	-8.979803	10.298765	2.813569	C	-9.416573	5.107792	-2.297756
H	-8.549627	9.413409	4.279860	H	-8.632024	5.755254	-2.711958
C	-7.604288	8.619700	2.613066	H	-9.362008	4.159817	-2.858806
O	-7.440915	7.399178	2.564584	N	-6.133524	7.193881	-1.862346
N	-6.644620	9.481071	2.183076	C	-6.290154	8.255103	-1.085433
H	-5.712004	9.088673	2.104530	H	-6.276759	8.255726	0.000614
H	-6.674527	10.478774	2.443651	N	-6.497135	9.355190	-1.840804
O	-6.371884	4.504716	-3.094310	H	-6.672671	10.286769	-1.477771
O	-5.664886	3.585503	-3.644203	C	-6.481287	8.990569	-3.176882
Fe	-6.003984	5.162764	-1.211708	C	-6.256009	7.633979	-3.161581
H	-2.516227	3.937302	-2.408432	H	-6.218983	6.937701	-3.992426
C	-2.975987	2.951151	-2.459249	C	-6.681172	9.966522	-4.294899
C	-2.381136	1.962624	-3.210084	H	-6.669322	10.997788	-3.910851
H	-1.450123	2.161359	-3.746645	H	-5.876996	9.894365	-5.044062
C	-2.959378	0.645099	-3.316982	O	-5.146036	6.022185	0.656988
O	-2.426202	-0.295195	-4.004334	C	-4.506594	5.472058	1.557731
H	-1.300933	0.048786	-4.904963	O	-4.075357	4.236293	1.429194
C	-4.191128	0.436830	-2.592263	C	-4.156851	6.159744	2.855266
H	-4.646559	-0.554683	-2.656283	H	-4.024622	5.416882	3.654725
C	-4.776999	1.430452	-1.839484	H	-4.966424	6.853825	3.115947
H	-5.709423	1.238654	-1.303524	h	0.711563	0.457880	-8.465930
C	-4.193323	2.730398	-1.747856	h	-9.769525	8.751751	3.124242
O	-4.700303	3.666756	-0.944856	h	-10.371040	5.563576	-2.561043
H	-4.292352	3.883286	0.479906	h	-7.652453	9.871022	-4.780244
N	-9.373452	4.641519	1.354972	h	-3.218221	6.705220	2.757819

⁷N-1

C	0.858062	0.541244	-7.387987	C	-8.092427	4.831971	1.059621
H	1.894102	0.226865	-7.176993	H	-7.306485	4.899030	1.804522
H	0.783486	1.600334	-7.111097	N	-7.934040	4.982932	-0.250674
C	-0.045397	-0.256647	-6.459071	H	-9.793281	4.542484	2.301527
O	-0.599098	0.494415	-5.544477	C	-9.198962	4.903697	-0.819202
O	-0.165408	-1.476849	-6.522958	C	-10.107469	4.676250	0.190824
C	-8.825864	9.289508	3.219665	H	-11.185655	4.563549	0.191631
H	-8.978880	10.298774	2.814663	C	-9.418288	5.108989	-2.292541
H	-8.549537	9.412295	4.280430	H	-8.633304	5.758719	-2.703266
C	-7.603927	8.619378	2.613158	H	-9.362195	4.160859	-2.853161
O	-7.441895	7.398762	2.561357	N	-6.148380	7.209309	-1.850393
N	-6.643145	9.480364	2.185377	C	-6.307258	8.274692	-1.079041
H	-5.710665	9.087132	2.107236	H	-6.298439	8.284036	0.007074
H	-6.672326	10.477999	2.447099	N	-6.508857	9.370517	-1.841373
O	-6.329077	4.466674	-3.103147	H	-6.683647	10.304825	-1.484222
O	-5.619072	3.560585	-3.650945	C	-6.487765	8.999064	-3.175279
Fe	-6.020192	5.201274	-1.164923	C	-6.264984	7.642128	-3.152793
H	-2.508840	3.926045	-2.401185	H	-6.220369	6.941159	-3.979404
C	-2.969269	2.940143	-2.452670	C	-6.682121	9.970041	-4.297876
C	-2.372832	1.952431	-3.206804	H	-6.668768	11.002866	-3.918268
H	-1.442785	2.154407	-3.743958	H	-5.876620	9.891664	-5.044805
C	-2.949571	0.637170	-3.319285	O	-5.141065	6.033147	0.655911
O	-2.416784	-0.302710	-4.014337	C	-4.498460	5.465395	1.546794
H	-1.312796	0.043889	-4.898146	O	-4.076309	4.232279	1.399868
C	-4.178501	0.426998	-2.594882	C	-4.147347	6.145763	2.848286
H	-4.634583	-0.564199	-2.659968	H	-4.014067	5.400716	3.645241
C	-4.766051	1.419245	-1.837227	H	-4.959175	6.836981	3.109907
H	-5.698665	1.223050	-1.302805	h	0.711478	0.457110	-8.464788
C	-4.192581	2.722694	-1.753032	h	-9.769106	8.751671	3.124304
O	-4.717266	3.670008	-0.964618	h	-10.372156	5.564318	-2.558770
H	-4.303529	3.882173	0.439393	h	-7.653572	9.872951	-4.782565
N	-9.387427	4.639141	1.360475	h	-3.211730	6.696886	2.753677

⁵N-TS1

C	0.883696	0.550108	-7.397148	C	-8.129926	4.835324	1.102807
H	1.920133	0.233960	-7.191754	H	-7.352298	4.915891	1.855205
H	0.812210	1.609085	-7.120716	N	-7.962079	4.984673	-0.205542
C	-0.013613	-0.242437	-6.463859	H	-9.839254	4.539442	2.32879
O	-0.556439	0.518695	-5.542680	C	-9.218087	4.891236	-0.787785
O	-0.149132	-1.458851	-6.516387	C	-10.135233	4.657251	0.213011
C	-8.831347	9.289289	3.228422	H	-11.211813	4.533268	0.201774
H	-8.985445	10.299063	2.825505	C	-9.413352	5.099978	-2.26372
H	-8.551884	9.409072	4.288442	H	-8.618718	5.752284	-2.651567
C	-7.613584	8.619832	2.612724	H	-9.342851	4.154577	-2.826841
O	-7.451219	7.398849	2.564047	N	-6.230659	7.182982	-1.883338
N	-6.660876	9.480138	2.169619	C	-6.414254	8.238729	-1.107271
H	-5.733016	9.084377	2.057925	H	-6.435582	8.234356	-0.02142
H	-6.683490	10.477750	2.430652	N	-6.595263	9.345995	-1.862703
O	-6.175560	4.349404	-2.962151	H	-6.788099	10.274516	-1.501271
O	-5.313545	3.463258	-3.437717	C	-6.527837	8.98852	-3.198029
Fe	-6.079307	5.163630	-1.196224	C	-6.301507	7.63115	-3.18184
H	-2.546394	3.903158	-2.355774	H	-6.217441	6.940016	-4.014014
C	-3.011737	2.924420	-2.464320	C	-6.704558	9.96796	-4.316498
C	-2.381486	1.944226	-3.168841	H	-6.68341	10.99931	-3.932982
H	-1.405596	2.121785	-3.627403	H	-5.897994	9.885112	-5.061855
C	-2.979613	0.626234	-3.331851	O	-5.161016	6.021116	0.610888
O	-2.416294	-0.295728	-3.991369	C	-4.482879	5.464998	1.483166
H	-1.238143	0.058666	-4.915193	O	-4.003797	4.256657	1.31824
C	-4.265279	0.416747	-2.693647	C	-4.146389	6.140185	2.793988
H	-4.704883	-0.578767	-2.786418	H	-4.007523	5.387483	3.58322
C	-4.901318	1.412953	-2.005875	H	-4.965756	6.820095	3.061296
H	-5.869807	1.236110	-1.531335	h	0.728861	0.463058	-8.472562
C	-4.333441	2.745229	-1.886096	h	-9.774901	8.751898	3.133644
O	-4.759135	3.572385	-0.939094	h	-10.363812	5.55646	-2.539974
H	-4.242058	3.877293	0.362452	h	-7.675687	9.879160	-4.803417
N	-9.426835	4.630398	1.390097	h	-3.214907	6.700155	2.711272

⁵N-2

C	0.888939	0.573786	-7.400578	C	-8.175958	4.926378	1.078365
H	1.922054	0.249004	-7.192733	H	-7.408187	5.083102	1.828877
H	0.831709	1.636704	-7.138165	N	-8.014860	5.065554	-0.230441
C	-0.009140	-0.189946	-6.450104	H	-9.865992	4.536225	2.305038
O	-0.527419	0.602688	-5.529764	C	-9.255090	4.870275	-0.814970
O	-0.172685	-1.400504	-6.475560	C	-10.160553	4.587890	0.184873
C	-8.825557	9.286474	3.251663	H	-11.225356	4.386089	0.168553
H	-8.972701	10.292162	2.835802	C	-9.454611	5.046344	-2.294880
H	-8.561428	9.418401	4.313993	H	-8.632033	5.644291	-2.711754
C	-7.599387	8.607292	2.662813	H	-9.440360	4.082770	-2.831757
O	-7.435948	7.386136	2.640526	N	-6.287420	7.346155	-1.846594
N	-6.642816	9.458420	2.213077	C	-6.510322	8.420136	-1.110697
H	-5.717949	9.055727	2.100792	H	-6.566384	8.456229	-0.026047
H	-6.665514	10.460726	2.453710	N	-6.675242	9.503263	-1.905946
O	-5.881025	4.715412	-3.058960	H	-6.887887	10.441155	-1.582536
O	-5.775015	3.270077	-3.090100	C	-6.553300	9.104447	-3.226343
Fe	-6.130151	5.296931	-1.216031	C	-6.309662	7.752204	-3.160287
H	-3.169107	4.160674	-2.767485	H	-6.175115	7.029520	-3.959711
C	-3.445799	3.108781	-2.698377	C	-6.726192	10.040755	-4.380433
C	-2.650155	2.154071	-3.227479	H	-6.704281	11.085602	-4.035543
H	-1.699860	2.397718	-3.710417	H	-5.923006	9.929158	-5.125287
C	-3.062456	0.748895	-3.228115	O	-5.148443	6.044838	0.594018
O	-2.413921	-0.142616	-3.812461	C	-4.485958	5.433044	1.440297
H	-1.166407	0.159576	-4.886899	O	-4.054044	4.213993	1.238428
C	-4.308749	0.418336	-2.515222	C	-4.125506	6.070737	2.767910
H	-4.571750	-0.641181	-2.458803	H	-3.958194	5.300230	3.533204
C	-5.095480	1.369121	-1.976266	H	-4.952822	6.726975	3.070120
H	-6.022796	1.108167	-1.459334	h	0.730757	0.475067	-8.474496
C	-4.811670	2.851334	-2.095983	h	-9.768623	8.749411	3.150390
O	-5.014958	3.534989	-0.923553	h	-10.389393	5.535286	-2.569078
H	-4.361353	3.832105	0.283568	h	-7.700757	9.928818	-4.855575
N	-9.457841	4.633773	1.365621	h	-3.212639	6.660574	2.685244

⁵N-TS2

C	0.893038	0.581100	-7.401980	C	-8.202044	4.965056	1.074162
H	1.924462	0.250932	-7.194207	H	-7.436595	5.140779	1.822987
H	0.842727	1.645232	-7.143630	N	-8.042794	5.103759	-0.235113
C	-0.007460	-0.172445	-6.446127	H	-9.883709	4.537925	2.298581
O	-0.518393	0.628571	-5.526831	C	-9.275840	4.875222	-0.821940
O	-0.179718	-1.381318	-6.465478	C	-10.175907	4.573245	0.176865
C	-8.824312	9.290938	3.248689	H	-11.235034	4.343281	0.158268
H	-8.967395	10.292217	2.820534	C	-9.475085	5.043995	-2.302586
H	-8.565834	9.435761	4.310731	H	-8.650259	5.637606	-2.721335
C	-7.595737	8.602057	2.675439	H	-9.466121	4.078127	-2.835568
O	-7.439016	7.380285	2.662775	N	-6.278539	7.394019	-1.855272
N	-6.629063	9.444708	2.230311	C	-6.464417	8.480109	-1.126605
H	-5.705822	9.033724	2.134253	H	-6.494574	8.530476	-0.040983
H	-6.648621	10.447998	2.466568	N	-6.629153	9.556869	-1.930243
O	-5.859044	4.739182	-3.017372	H	-6.817405	10.502290	-1.613401
O	-5.810779	3.286776	-3.027378	C	-6.546061	9.141328	-3.248307
Fe	-6.151654	5.354873	-1.187759	C	-6.325079	7.785731	-3.173207
H	-3.214961	4.187011	-2.690222	H	-6.221584	7.053514	-3.968501
C	-3.480110	3.131464	-2.631467	C	-6.731672	10.067653	-4.408455
C	-2.674115	2.189145	-3.164353	H	-6.715732	11.115041	-4.071166
H	-1.722167	2.447506	-3.637129	H	-5.932163	9.957613	-5.157678
C	-3.075584	0.778788	-3.191113	O	-5.131876	6.058580	0.561989
O	-2.413768	-0.096660	-3.781630	C	-4.466617	5.415091	1.399131
H	-1.152070	0.191536	-4.879854	O	-4.047705	4.212177	1.179775
C	-4.325994	0.429138	-2.495006	C	-4.117319	6.055683	2.734100
H	-4.581840	-0.632697	-2.450337	H	-3.945829	5.283949	3.497257
C	-5.125973	1.367138	-1.954530	H	-4.951782	6.702327	3.038531
H	-6.056958	1.095526	-1.450230	h	0.732714	0.479231	-8.475286
C	-4.851654	2.850825	-2.054084	h	-9.767582	8.753944	3.148959
O	-5.091821	3.513128	-0.863244	h	-10.407488	5.536362	-2.578751
H	-4.430120	3.777744	0.138535	h	-7.708912	9.946159	-4.875689
N	-9.476951	4.641666	1.359023	h	-3.210383	6.655607	2.659090

⁵N-3

C	0.908179	0.582566	-7.411633	C	-8.162270	4.904878	1.083069
H	1.941662	0.256078	-7.208423	H	-7.388737	5.028806	1.834432
H	0.853661	1.645731	-7.150593	N	-7.995501	5.056745	-0.223389
C	0.013689	-0.178099	-6.457807	H	-9.864066	4.546166	2.304907
O	-0.500151	0.617324	-5.533844	C	-9.240742	4.904042	-0.808998
O	-0.156045	-1.387066	-6.477798	C	-10.155308	4.633195	0.186454
C	-8.835158	9.292826	3.234574	H	-11.225153	4.459908	0.167056
H	-8.977881	10.295415	2.809407	C	-9.433976	5.101656	-2.286920
H	-8.570146	9.434679	4.295407	H	-8.629206	5.741518	-2.676742
C	-7.612612	8.601436	2.651039	H	-9.383198	4.150160	-2.844007
O	-7.467349	7.379351	2.618789	N	-6.337509	7.376243	-1.850229
N	-6.638617	9.443348	2.217924	C	-6.508451	8.464518	-1.121778
H	-5.717980	9.026315	2.120876	H	-6.539512	8.513352	-0.036298
H	-6.652101	10.443609	2.466057	N	-6.648773	9.546373	-1.924793
O	-5.581667	4.735574	-2.912276	H	-6.819505	10.494446	-1.606230
O	-5.734483	3.294135	-2.976052	C	-6.568990	9.131380	-3.242101
Fe	-6.075612	5.364871	-1.118105	C	-6.372631	7.771644	-3.166882
H	-3.132843	4.026258	-2.374955	H	-6.277462	7.041570	-3.965040
C	-3.437476	2.984208	-2.448977	C	-6.739027	10.059747	-4.403281
C	-2.632086	2.063762	-3.014571	H	-6.719283	11.106862	-4.065420
H	-1.639172	2.326987	-3.390975	H	-5.935461	9.945170	-5.147584
C	-3.076386	0.675358	-3.201189	O	-5.102956	6.019144	0.543162
O	-2.405820	-0.165309	-3.824280	C	-4.396676	5.387025	1.394513
H	-1.123301	0.161404	-4.895238	O	-3.930516	4.234479	1.189341
C	-4.379260	0.307399	-2.620160	C	-4.106278	6.091024	2.719041
H	-4.652137	-0.749727	-2.655950	H	-3.958557	5.342459	3.510622
C	-5.196648	1.227269	-2.080344	H	-4.948581	6.746001	2.979075
H	-6.164215	0.953364	-1.651871	h	0.743607	0.480873	-8.484312
C	-4.863090	2.699737	-2.027203	h	-9.779534	8.757269	3.137630
O	-5.199005	3.207794	-0.766748	h	-10.380233	5.565798	-2.564833
H	-4.485945	3.491147	-0.096415	h	-7.714799	9.943406	-4.874876
N	-9.453026	4.643898	1.367068	h	-3.192858	6.682137	2.653350

⁵N-TS3

C	0.888399	0.576295	-7.400930	C	-8.105140	4.949894	0.992374
H	1.918485	0.244363	-7.189980	H	-7.322900	5.107365	1.727893
H	0.835785	1.639445	-7.138690	N	-7.966200	5.077626	-0.322090
C	-0.019860	-0.183960	-6.457970	H	-9.778800	4.561504	2.245278
O	-0.555520	0.610854	-5.548500	C	-9.216310	4.883010	-0.885220
O	-0.178880	-1.395010	-6.479830	C	-10.104200	4.608532	0.132182
C	-8.834010	9.284766	3.249560	H	-11.170000	4.408820	0.134985
H	-8.975940	10.289490	2.829151	C	-9.443190	5.057240	-2.360220
H	-8.574540	9.422077	4.312263	H	-8.629530	5.656975	-2.791810
C	-7.606960	8.600760	2.668482	H	-9.435140	4.092607	-2.895650
O	-7.461490	7.378246	2.614762	N	-6.354870	7.492358	-1.740430
N	-6.630030	9.448297	2.258737	C	-6.615200	8.581660	-1.039990
H	-5.707750	9.038132	2.150937	H	-6.697860	8.653969	0.041357
H	-6.649300	10.449450	2.503967	N	-6.759620	9.640654	-1.870020
O	-5.798820	4.970951	-2.888540	H	-6.984070	10.586740	-1.578520
O	-5.856910	2.488478	-2.774180	C	-6.586710	9.207971	-3.175830
Fe	-6.059970	5.395777	-1.252470	C	-6.331260	7.863350	-3.065070
H	-3.209790	3.979633	-2.319820	H	-6.152220	7.114966	-3.830430
C	-3.519500	2.939754	-2.411040	C	-6.737910	10.099090	-4.367850
C	-2.761370	2.045143	-3.075670	H	-6.722150	11.156690	-4.063520
H	-1.804710	2.335155	-3.519520	H	-5.921230	9.958493	-5.092430
C	-3.174260	0.639547	-3.245720	O	-5.013250	5.999959	0.422350
O	-2.491580	-0.178390	-3.905270	C	-4.382720	5.384114	1.342174
H	-1.210310	0.165038	-4.926680	O	-3.967640	4.198748	1.221567
C	-4.395240	0.225288	-2.582300	C	-4.120230	6.123932	2.652897
H	-4.649140	-0.836320	-2.615470	H	-4.009060	5.391964	3.465828
C	-5.192910	1.118019	-1.871280	H	-4.961390	6.795039	2.872899
H	-6.037170	0.780759	-1.270470	h	0.732436	0.477665	-8.475180
C	-4.871920	2.590389	-1.842020	h	-9.777370	8.748756	3.145435
O	-5.254770	3.321954	-0.731330	h	-10.383700	5.543967	-2.618300
H	-4.565160	3.519335	0.011417	h	-7.705190	9.966899	-4.852580
N	-9.382260	4.661640	1.301691	h	-3.195430	6.698929	2.606103

⁵N-4

C	0.872166	0.571874	-7.392691	C	-8.094002	4.989070	0.980752
H	1.900692	0.238812	-7.176393	H	-7.319206	5.156306	1.721773
H	0.817426	1.634648	-7.128499	N	-7.951502	5.131927	-0.331718
C	-0.043051	-0.193126	-6.459172	H	-9.764619	4.559087	2.224889
O	-0.597107	0.596232	-5.557192	C	-9.194987	4.913808	-0.900104
O	-0.190092	-1.405975	-6.484383	C	-10.082230	4.613005	0.110788
C	-8.831508	9.284983	3.255202	H	-11.144023	4.391753	0.106427
H	-8.972159	10.288476	2.831494	C	-9.422968	5.091534	-2.374560
H	-8.576237	9.425089	4.318497	H	-8.619041	5.706859	-2.803372
C	-7.602774	8.599528	2.679370	H	-9.404261	4.129588	-2.914728
O	-7.454150	7.376904	2.635694	N	-6.353254	7.587260	-1.722384
N	-6.629724	9.445454	2.259168	C	-6.696159	8.667400	-1.043009
H	-5.709815	9.033912	2.136655	H	-6.822958	8.745354	0.033948
H	-6.646872	10.447824	2.499534	N	-6.847393	9.713478	-1.887186
O	-5.640306	5.116072	-2.837763	H	-7.122350	10.651656	-1.613819
O	-5.893318	2.177758	-2.670791	C	-6.595894	9.280659	-3.180376
Fe	-6.026143	5.512409	-1.236353	C	-6.282761	7.951207	-3.047619
H	-3.265068	3.962425	-2.356796	H	-6.028383	7.206835	-3.794859
C	-3.596744	2.930946	-2.459697	C	-6.750341	10.147731	-4.388602
C	-2.882595	2.036376	-3.178718	H	-6.739881	11.211158	-4.105210
H	-1.949564	2.335499	-3.664595	H	-5.932261	9.995495	-5.108736
C	-3.262520	0.619627	-3.304713	O	-4.994684	6.027698	0.449284
O	-2.560776	-0.203367	-3.957027	C	-4.403809	5.373089	1.366894
H	-1.269455	0.150611	-4.949593	O	-4.051886	4.167863	1.230529
C	-4.414027	0.184363	-2.563061	C	-4.115627	6.088206	2.683548
H	-4.557380	-0.889871	-2.430681	H	-3.981681	5.346562	3.483457
C	-5.310186	1.095995	-1.901979	H	-4.957779	6.750000	2.929119
H	-5.983888	0.699485	-1.136581	h	0.723163	0.475407	-8.468125
C	-4.892915	2.585776	-1.808984	h	-9.774616	8.749037	3.148553
O	-5.315231	3.340522	-0.761438	h	-10.370339	5.566768	-2.628938
H	-4.646405	3.538902	0.012883	h	-7.717103	9.998921	-4.869530
N	-9.366542	4.671887	1.283623	h	-3.201117	6.678245	2.623624

⁵N-5

C	0.912985	0.556399	-7.411106	C	-8.126852	4.954305	0.996501
H	1.948738	0.235900	-7.209778	H	-7.342925	5.156221	1.717964
H	0.845822	1.615111	-7.133802	N	-8.008323	5.044886	-0.323500
C	0.014067	-0.232425	-6.478874	H	-9.773581	4.573643	2.288101
O	-0.536607	0.531656	-5.562885	C	-9.269434	4.810590	-0.860006
O	-0.122643	-1.448511	-6.523864	C	-10.132610	4.552145	0.181676
C	-8.816337	9.291390	3.262579	H	-11.194788	4.335971	0.207555
H	-8.962313	10.295167	2.841706	C	-9.541069	4.933065	-2.332430
H	-8.551297	9.427058	4.324448	H	-8.685303	5.415974	-2.823796
C	-7.592408	8.606159	2.677205	H	-9.633499	3.943375	-2.812201
O	-7.433437	7.384441	2.665117	N	-6.142090	7.404553	-1.895991
N	-6.630182	9.453018	2.229444	C	-6.243717	8.492523	-1.150607
H	-5.703940	9.050315	2.133191	H	-6.201455	8.531260	-0.066041
H	-6.655397	10.456357	2.464923	N	-6.443591	9.572507	-1.939221
O	-6.515213	4.800353	-3.051565	H	-6.590947	10.519832	-1.606375
O	-5.213314	1.876239	-1.448281	C	-6.477806	9.159064	-3.262142
Fe	-6.199684	5.318046	-1.456426	C	-6.289577	7.799866	-3.206169
H	-2.665754	3.802802	-2.485946	H	-6.305585	7.053946	-3.994276
C	-3.193308	2.849176	-2.466681	C	-6.710600	10.092503	-4.408175
C	-2.598865	1.812613	-3.212566	H	-6.716906	11.135992	-4.058797
H	-1.661456	2.055994	-3.718854	H	-5.920227	10.013633	-5.171468
C	-3.059619	0.479975	-3.397587	O	-5.184308	6.245398	0.668635
O	-2.416202	-0.372395	-4.078138	C	-4.581631	5.673529	1.569297
H	-1.218231	0.056674	-4.956287	O	-4.173098	4.416714	1.437024
C	-4.320787	0.016827	-2.789780	C	-4.204930	6.308587	2.886193
H	-4.568646	-1.018065	-3.033357	H	-4.118860	5.541599	3.669273
C	-5.185789	0.630113	-1.958369	H	-4.970264	7.041909	3.166611
H	-6.049098	0.079612	-1.577928	h	0.752498	0.468593	-8.485629
C	-4.336833	2.915926	-1.675359	h	-9.759464	8.754116	3.163001
O	-4.681140	3.962062	-1.016853	h	-10.448677	5.476754	-2.594570
H	-4.335026	4.127893	0.480099	h	-7.689970	9.954696	-4.866333
N	-9.393029	4.653731	1.336209	h	-3.232044	6.791458	2.794568

⁵N-TS4

C	0.915950	0.560691	-7.410655	C	-7.986459	4.620403	1.040394
H	1.945935	0.226003	-7.203415	H	-7.179049	4.507432	1.757827
H	0.862255	1.621158	-7.137404	N	-7.841606	4.831493	-0.261814
C	-0.001509	-0.211077	-6.480220	H	-9.689683	4.446597	2.308336
O	-0.562135	0.567487	-5.586089	C	-9.119404	4.909433	-0.799204
O	-0.139210	-1.428250	-6.516231	C	-10.026418	4.728470	0.221629
C	-8.850192	9.258072	3.232078	H	-11.110749	4.728384	0.247263
H	-9.004694	10.301530	2.932031	C	-9.336003	5.165600	-2.264368
H	-8.509213	9.266325	4.280223	H	-8.572081	5.858015	-2.647176
C	-7.697799	8.627052	2.470474	H	-9.234438	4.236267	-2.850139
O	-7.574483	7.410687	2.306215	N	-6.185980	7.085041	-1.919475
N	-6.765230	9.504861	2.022199	C	-6.632726	8.039129	-1.115993
H	-5.869090	9.104862	1.762139	H	-6.818153	7.925808	-0.050698
H	-6.744250	10.481662	2.351922	N	-6.844219	9.172078	-1.819462
O	-5.816022	3.981523	-2.728553	H	-7.209077	10.035589	-1.429993
O	-5.149027	1.824123	-1.309156	C	-6.530053	8.938746	-3.149558
Fe	-5.980096	5.060250	-1.344825	C	-6.118710	7.627840	-3.181397
H	-2.811396	3.889501	-2.584740	H	-5.802755	7.032581	-4.029636
C	-3.306886	2.919270	-2.556550	C	-6.694727	9.950907	-4.239640
C	-2.743886	1.921584	-3.344924	H	-6.677715	10.974389	-3.834567
H	-1.855370	2.197825	-3.919565	H	-5.874929	9.878327	-4.970436
C	-3.132478	0.552788	-3.460729	O	-5.113355	6.168894	0.700827
O	-2.460479	-0.291499	-4.128384	C	-4.685293	5.612712	1.705761
H	-1.272922	0.116991	-4.980044	O	-4.518694	4.295442	1.752335
C	-4.343085	0.045308	-2.801805	C	-4.284791	6.333614	2.970532
H	-4.581850	-0.988986	-3.058139	H	-4.243636	5.632918	3.815679
C	-5.158116	0.615217	-1.890147	H	-5.010855	7.129495	3.181139
H	-5.980131	0.027137	-1.471725	h	0.757867	0.472182	-8.485477
C	-4.399597	2.941109	-1.644394	h	-9.804718	8.740334	3.137766
O	-4.448356	3.832390	-0.705399	h	-10.304238	5.591694	-2.527106
H	-4.539842	3.919921	0.803325	h	-7.654982	9.870213	-4.749019
N	-9.289552	4.546769	1.366710	h	-3.293433	6.770247	2.849590

⁵N-6

C	0.914295	0.560146	-7.410392	C	-8.049746	4.616328	1.189683
H	1.948316	0.235907	-7.206710	H	-7.260619	4.504481	1.929130
H	0.852321	1.619676	-7.135251	N	-7.850743	4.885829	-0.095676
C	0.013191	-0.222461	-6.475841	H	-9.794242	4.388171	2.378650
O	-0.531188	0.548231	-5.558898	C	-9.106415	4.945708	-0.690039
O	-0.131166	-1.436703	-6.517463	C	-10.051662	4.702838	0.281320
C	-8.847123	9.234313	3.283208	H	-11.135197	4.666949	0.255248
H	-8.966814	10.280940	2.975759	C	-9.285076	5.216438	-2.159131
H	-8.507752	9.242512	4.331547	H	-8.520411	5.923962	-2.511210
C	-7.719509	8.554773	2.521823	H	-9.163729	4.291371	-2.750053
O	-7.689803	7.339022	2.302070	N	-6.393749	7.276137	-1.716319
N	-6.715796	9.371763	2.131836	C	-6.999091	8.244360	-1.048416
H	-5.870558	8.912254	1.800148	H	-7.330923	8.182819	-0.016211
H	-6.647776	10.347746	2.450061	N	-7.149463	9.330514	-1.834086
O	-4.870029	4.310435	-1.837992	H	-7.609325	10.191352	-1.556804
O	-5.339282	2.089158	-1.740977	C	-6.638747	9.045140	-3.089788
Fe	-5.887275	5.482657	-0.672591	C	-6.156500	7.761156	-2.982461
H	-2.599559	3.943154	-2.816836	H	-5.660264	7.158893	-3.736034
C	-3.127000	2.994672	-2.680047	C	-6.737274	9.983665	-4.250918
C	-2.664123	1.944868	-3.380401	H	-6.702257	11.031061	-3.911955
H	-1.802804	2.124497	-4.031429	H	-5.899472	9.841312	-4.949327
C	-3.108156	0.537854	-3.390769	O	-5.037467	6.641738	0.794346
O	-2.415666	-0.303532	-4.022268	C	-4.732477	5.809671	1.710102
H	-1.206256	0.085624	-4.942553	O	-4.880394	4.565955	1.518937
C	-4.306563	0.106333	-2.730647	C	-4.215124	6.346780	3.029348
H	-4.528528	-0.956927	-2.840532	H	-4.163610	5.550410	3.783076
C	-5.244989	0.830865	-2.036854	H	-4.897177	7.136330	3.377528
H	-6.119496	0.270630	-1.675087	h	0.755237	0.470796	-8.485000
C	-4.218073	3.189343	-1.642848	h	-9.814929	8.741745	3.189438
O	-3.654241	2.987456	-0.414438	h	-10.256544	5.620130	-2.444346
H	-4.131539	3.530194	0.257140	h	-7.688759	9.893691	-4.774987
N	-9.361782	4.498871	1.451740	h	-3.223234	6.782081	2.907965

⁵N-TS5

C	0.905842	0.560834	-7.405712	C	-8.057499	4.576030	1.195162
H	1.939397	0.235405	-7.200582	H	-7.271028	4.462827	1.937454
H	0.846798	1.621408	-7.133345	N	-7.855724	4.853226	-0.088961
C	0.002777	-0.216852	-6.465381	H	-9.804220	4.346088	2.377528
O	-0.533102	0.555284	-5.548872	C	-9.110159	4.916669	-0.687757
O	-0.141985	-1.432002	-6.510698	C	-10.056251	4.667678	0.280483
C	-8.845705	9.221319	3.285049	H	-11.139451	4.630444	0.251113
H	-8.965022	10.274590	3.000996	C	-9.287036	5.195084	-2.155732
H	-8.494037	9.206194	4.329116	H	-8.521387	5.902464	-2.505922
C	-7.730785	8.555404	2.493997	H	-9.168118	4.271868	-2.749743
O	-7.718907	7.347456	2.226907	N	-6.426775	7.272933	-1.686326
N	-6.717667	9.371115	2.131045	C	-7.069586	8.229939	-1.036330
H	-5.880371	8.915899	1.774941	H	-7.437495	8.155605	-0.016623
H	-6.644010	10.342108	2.463127	N	-7.210024	9.313658	-1.824948
O	-4.784267	4.385595	-1.820888	H	-7.694578	10.165675	-1.562596
O	-5.398939	2.021360	-1.807283	C	-6.657473	9.037417	-3.065887
Fe	-5.921528	5.498606	-0.636426	C	-6.155661	7.762611	-2.944368
H	-2.498784	3.971596	-2.928511	H	-5.622872	7.169457	-3.680046
C	-3.058738	3.054643	-2.709273	C	-6.741106	9.973043	-4.230647
C	-2.682980	1.962357	-3.395076	H	-6.703335	11.021469	-3.894884
H	-1.853730	2.116949	-4.093289	H	-5.897458	9.823066	-4.920025
C	-3.126706	0.541168	-3.392112	O	-5.022855	6.638166	0.800516
O	-2.381970	-0.277404	-4.014412	C	-4.713071	5.801884	1.710991
H	-1.222444	0.107782	-4.914607	O	-4.859029	4.558382	1.507111
C	-4.314546	0.081566	-2.769250	C	-4.198306	6.335048	3.031487
H	-4.505192	-0.986811	-2.893130	H	-4.144823	5.537844	3.783891
C	-5.304964	0.792731	-2.087708	H	-4.882772	7.122721	3.379526
H	-6.163610	0.178729	-1.750642	h	0.747676	0.470223	-8.480346
C	-4.060700	3.356626	-1.631873	h	-9.816043	8.733337	3.193490
O	-3.618275	3.040391	-0.418984	h	-10.256646	5.603674	-2.440295
H	-4.128376	3.540575	0.269119	h	-7.688037	9.886154	-4.763412
N	-9.369294	4.456185	1.451353	h	-3.208433	6.775629	2.912721

⁵N-7

C	0.897096	0.558949	-7.401045	C	-8.056176	4.587977	1.192733
H	1.930230	0.232901	-7.194359	H	-7.269704	4.475878	1.935133
H	0.839047	1.619728	-7.128934	N	-7.854740	4.864020	-0.092131
C	-0.006723	-0.218650	-6.460066	H	-9.801532	4.355691	2.375615
O	-0.543354	0.553421	-5.545862	C	-9.109591	4.924915	-0.690979
O	-0.148677	-1.434648	-6.506995	C	-10.055002	4.676017	0.277909
C	-8.843893	9.225036	3.282143	H	-11.138270	4.638067	0.248855
H	-8.964002	10.276886	2.993181	C	-9.286914	5.200815	-2.159294
H	-8.496800	9.215978	4.327954	H	-8.521755	5.908033	-2.511147
C	-7.722908	8.558522	2.500843	H	-9.168686	4.276714	-2.751956
O	-7.701655	7.348355	2.246271	N	-6.421854	7.290834	-1.688730
N	-6.714882	9.378323	2.131074	C	-7.052231	8.256041	-1.038273
H	-5.871941	8.925272	1.785993	H	-7.411312	8.191878	-0.015048
H	-6.645272	10.350528	2.460925	N	-7.192418	9.335657	-1.831695
O	-4.753227	4.413939	-1.820268	H	-7.667739	10.193198	-1.569787
O	-5.416482	1.999835	-1.808711	C	-6.652894	9.048913	-3.075880
Fe	-5.927650	5.518217	-0.638584	C	-6.158809	7.771346	-2.952323
H	-2.446354	3.974307	-2.931004	H	-5.637768	7.170340	-3.690248
C	-3.024458	3.071933	-2.695951	C	-6.740309	9.980823	-4.243150
C	-2.676408	1.968089	-3.379448	H	-6.703082	11.030049	-3.910116
H	-1.851369	2.112322	-4.085257	H	-5.899063	9.829866	-4.935264
C	-3.131175	0.546403	-3.386550	O	-5.015278	6.638933	0.797784
O	-2.377415	-0.267745	-4.011267	C	-4.709030	5.802674	1.709915
H	-1.238495	0.111939	-4.903623	O	-4.855669	4.559215	1.506331
C	-4.318596	0.079301	-2.778399	C	-4.196986	6.335782	3.030901
H	-4.500086	-0.990035	-2.909732	H	-4.145683	5.538890	3.783706
C	-5.317498	0.778817	-2.083128	H	-4.882015	7.124009	3.376498
H	-6.159034	0.143355	-1.735291	h	0.741292	0.468496	-8.476038
C	-4.007738	3.412873	-1.617801	h	-9.813118	8.735102	3.189223
O	-3.607705	3.073737	-0.406255	h	-10.256713	5.609346	-2.443300
H	-4.130116	3.568974	0.280070	h	-7.689196	9.890540	-4.771855
N	-9.367527	4.467740	1.449158	h	-3.206803	6.775993	2.913348

(2) Model A Using Monoanionized Substrate.

⁵M-1

C	0.842470	0.432132	-7.340546	H	-7.442441	4.730483	2.033673
H	1.847243	0.049907	-7.086898	N	-8.027660	4.942692	-0.010065
H	0.819282	1.491607	-7.059362	H	-9.996113	4.453282	2.450301
C	-0.167625	-0.332117	-6.467153	C	-9.278857	4.927843	-0.611765
O	-0.773490	0.361536	-5.593827	C	-10.227875	4.719749	0.362404
O	-0.269757	-1.571862	-6.604227	H	-11.307587	4.640941	0.323164
C	-8.885630	9.459930	3.060618	C	-9.462331	5.134211	-2.084293
H	-9.036480	10.545965	2.953820	H	-8.672605	5.792786	-2.464930
H	-8.369220	9.298368	4.020219	H	-9.368397	4.188900	-2.643162
C	-7.923384	8.947990	1.974337	N	-5.910537	6.999481	-1.882008
O	-8.122827	7.991188	1.246569	C	-5.378201	8.053073	-1.294315
N	-6.756139	9.651221	1.942044	H	-4.895347	8.013505	-0.319492
H	-6.050432	9.324601	1.295969	N	-5.532517	9.148114	-2.073036
H	-6.610964	10.529759	2.448280	H	-5.188742	10.077962	-1.862111
O	-6.715274	4.305831	-2.635930	C	-6.206327	8.786762	-3.227483
O	-6.747131	3.080338	-2.950185	C	-6.421855	7.431400	-3.086273
Fe	-5.991510	5.076876	-0.834802	H	-6.913747	6.733825	-3.759368
H	-2.571735	3.973494	-2.711829	C	-6.500221	9.812360	-4.280949
C	-3.051495	2.994002	-2.678061	H	-6.484766	10.819616	-3.835173
C	-2.565566	1.959892	-3.459545	H	-5.747184	9.828898	-5.086249
H	-1.708952	2.098928	-4.123644	O	-5.044414	6.127397	0.738027
C	-3.165016	0.671803	-3.404730	C	-4.971874	5.611859	1.904340
O	-2.707931	-0.362280	-4.109016	O	-5.387517	4.469084	2.181657
H	-1.891382	-0.117577	-4.707499	C	-4.378180	6.460224	3.032598
C	-4.278143	0.493227	-2.551228	H	-4.407333	5.881332	3.966591
H	-4.739434	-0.495359	-2.506565	H	-4.990848	7.368474	3.162537
C	-4.763635	1.527917	-1.763721	h	0.750088	0.387873	-8.425707
H	-5.607775	1.365699	-1.091878	h	-9.865323	8.982290	3.049324
C	-4.157123	2.821817	-1.786829	h	-10.408596	5.575358	-2.397402
O	-4.550222	3.787833	-1.007531	h	-7.495541	9.747252	-4.720454
N	-9.547732	4.629665	1.550339	h	-3.350064	6.774775	2.853429
C	-8.235151	4.774981	1.291146				

⁷M-1

C	0.847068 0.425053 -7.338524	H	-7.519698 4.714756 2.057420
H	1.854754 0.046615 -7.089690	N	-8.073653 4.946676 0.006848
H	0.821343 1.483962 -7.054521	H	-10.068637 4.372328 2.430569
C	-0.156492 -0.345723 -6.459195	C	-9.317469 4.926484 -0.611631
O	-0.754220 0.339282 -5.578794	C	-10.275199 4.681103 0.344558
O	-0.254352 -1.586946 -6.605598	H	-11.352010 4.582388 0.286847
C	-8.884320 9.449865 3.069326	C	-9.486394 5.153845 -2.080864
H	-9.024146 10.534742 2.939439	H	-8.686472 5.812836 -2.439914
H	-8.379195 9.304269 4.037615	H	-9.401141 4.213464 -2.648271
C	-7.913873 8.900051 2.009002	N	-5.917860 7.040579 -1.887520
O	-8.106918 7.907998 1.327254	C	-5.309835 8.087904 -1.361666
N	-6.751023 9.606616 1.947507	H	-4.776134 8.068701 -0.413316
H	-6.029627 9.233109 1.344226	N	-5.462833 9.170389 -2.157477
H	-6.600292 10.491100 2.440633	H	-5.072536 10.089997 -1.985200
O	-6.758705 4.375377 -3.023156	C	-6.212554 8.810441 -3.262570
O	-7.139198 3.206047 -3.055916	C	-6.473862 7.468444 -3.074082
Fe	-6.004260 5.190724 -0.669917	H	-7.021534 6.779988 -3.711367
H	-2.634916 3.989111 -2.785634	C	-6.518856 9.827725 -4.319443
C	-3.115457 3.010698 -2.733973	H	-6.502971 10.837513 -3.879189
C	-2.590168 1.943808 -3.456760	H	-5.772910 9.842862 -5.131625
H	-1.705644 2.067895 -4.086407	O	-5.090335 6.357705 0.796384
C	-3.192605 0.666590 -3.394188	C	-4.996778 5.736834 1.909896
O	-2.718506 -0.396742 -4.065555	O	-5.419947 4.571703 2.062723
H	-1.913690 -0.153787 -4.650707	C	-4.378169 6.471745 3.093836
C	-4.331950 0.518522 -2.577280	H	-4.393420 5.821617 3.979583
H	-4.790482 -0.470299 -2.504619	H	-4.976424 7.374215 3.303161
C	-4.861941 1.589080 -1.858156	h	0.751518 0.383713 -8.423526
H	-5.739346 1.445822 -1.223537	h	-9.867337 8.979161 3.055864
C	-4.272525 2.877885 -1.921337	h	-10.429267 5.598870 -2.398683
O	-4.762212 3.908663 -1.263761	h	-7.517723 9.757060 -4.749950
N	-9.610953 4.577007 1.539295	h	-3.351477 6.786227 2.906564
C	-8.299133 4.747079 1.302074		

³M-1

C	0.839325 0.426363 -7.337831	H	-7.444116 4.720059 2.027095
H	1.844612 0.044641 -7.085303	N	-8.026354 4.943201 -0.016164
H	0.815065 1.485334 -7.054320	H	-9.998130 4.433225 2.437794
C	-0.169776 -0.342394 -6.465546	C	-9.276976 4.926749 -0.620796
O	-0.777492 0.345688 -5.591449	C	-10.226777 4.709811 0.350383
O	-0.266418 -1.582986 -6.607211	H	-11.305942 4.626104 0.308967
C	-8.885371 9.455593 3.060793	C	-9.457170 5.138064 -2.092379
H	-9.034261 10.542008 2.955252	H	-8.665301 5.798165 -2.467350
H	-8.368799 9.292287 4.020032	H	-9.364121 4.193798 -2.653851
C	-7.924457 8.942308 1.973733	N	-5.911672 7.000685 -1.906961
O	-8.125048 7.983895 1.248076	C	-5.382398 8.051786 -1.311352
N	-6.757748 9.645787 1.938686	H	-4.905080 8.005544 -0.333432
H	-6.051257 9.316108 1.294872	N	-5.538616 9.152530 -2.082265
H	-6.611506 10.523766 2.445404	H	-5.201643 10.082962 -1.862834
O	-6.665073 4.320149 -2.703681	C	-6.207850 8.797395 -3.241060
O	-6.917740 3.108803 -2.882308	C	-6.420871 7.440940 -3.108653
Fe	-5.993286 5.102999 -0.823758	H	-6.907957 6.748743 -3.790549
H	-2.547101 3.976229 -2.738817	C	-6.502860 9.824998 -4.292189
C	-3.039499 3.003310 -2.695128	H	-6.488797 10.831864 -3.845520
C	-2.565702 1.952403 -3.465819	H	-5.751554 9.843583 -5.099019
H	-1.707385 2.074439 -4.130971	O	-5.072756 6.156470 0.754202
C	-3.180955 0.675423 -3.400381	C	-4.981800 5.621696 1.910417
O	-2.734883 -0.374270 -4.098837	O	-5.395340 4.474879 2.174708
H	-1.922574 -0.136330 -4.690827	C	-4.378482 6.455402 3.043423
C	-4.293390 0.520101 -2.545475	H	-4.402389 5.866290 3.971026
H	-4.765580 -0.462918 -2.482779	H	-4.989457 7.362802 3.186216
C	-4.768162 1.573464 -1.770331	h	0.748035 0.384762 -8.423189
H	-5.609325 1.427333 -1.090755	h	-9.865839 8.979556 3.049072
C	-4.149561 2.857172 -1.810573	h	-10.403794 5.578616 -2.405242
O	-4.541446 3.847512 -1.050738	h	-7.498624 9.756631 -4.730192
N	-9.548735 4.615444 1.538780	h	-3.351248 6.771131 2.861293
C	-8.236567 4.768390 1.284563		

⁵M-TS1

C	0.946499 0.468601 -7.364682	H	-7.570154 4.736579 2.204306
H	1.935805 0.045559 -7.120921	N	-8.052572 4.972810 0.140148
H	0.969028 1.527042 -7.087391	H	-10.126904 4.305186 2.471407
C	-0.070827 -0.242364 -6.492907	C	-9.259581 4.901369 -0.531894
O	-0.632456 0.543820 -5.614582	C	-10.252006 4.612368 0.378696
O	-0.273532 -1.452635 -6.563747	H	-11.319923 4.464546 0.273420
C	-8.900974 9.481530 3.046291	C	-9.359614 5.133525 -2.007783
H	-9.070649 10.567582 2.967388	H	-8.567064 5.827974 -2.312584
H	-8.365185 9.304362 3.992196	H	-9.172050 4.204621 -2.568687
C	-7.957205 9.021722 1.918988	N	-5.907087 6.952047 -1.811647
O	-8.206555 8.167210 1.089097	C	-5.430393 8.025228 -1.215236
N	-6.744372 9.648893 1.972642	H	-4.977273 8.009277 -0.225952
H	-6.092746 9.405256 1.238456	N	-5.595470 9.116785 -2.000688
H	-6.597755 10.520952 2.489651	H	-5.300801 10.059966 -1.778337
O	-6.644747 3.921600 -2.222970	C	-6.216108 8.729217 -3.175084
O	-5.697407 3.255274 -2.967389	C	-6.391192 7.365304 -3.032699
Fe	-5.970415 4.982449 -0.672828	H	-6.837976 6.649641 -3.719134
H	-2.821930 4.065233 -2.720879	C	-6.486553 9.754049 -4.236875
C	-3.219264 3.048999 -2.743762	H	-6.463724 10.761300 -3.790740
C	-2.594334 2.073464 -3.446277	H	-5.722957 9.764263 -5.032313
H	-1.685497 2.275081 -4.019061	O	-5.025011 6.151858 0.815454
C	-3.100680 0.699262 -3.450019	C	-4.965959 5.622135 1.973830
O	-2.528676 -0.217962 -4.121737	O	-5.411597 4.485845 2.231097
H	-1.385384 0.127247 -5.000146	C	-4.359001 6.446282 3.112011
C	-4.274359 0.433760 -2.655081	H	-4.369526 5.850062 4.035698
H	-4.664078 -0.586577 -2.672910	H	-4.976336 7.347718 3.267103
C	-4.878117 1.412611 -1.911564	h	0.822894 0.414712 -8.446294
H	-5.763016 1.205028 -1.304410	h	-9.874549 8.991437 3.041058
C	-4.438786 2.828872 -1.923410	h	-10.310657 5.538871 -2.353152
O	-4.529853 3.555972 -0.839966	h	-7.476147 9.707762 -4.691440
N	-9.638780 4.536340 1.604131	h	-3.337636 6.773160 2.916995
C	-8.321083 4.759323 1.419552		

⁵M-2

C	0.972178 0.467644 -7.359463	H	-7.528330 4.656845 2.174924
H	1.960160 0.038894 -7.119675	N	-8.034393 4.912212 0.120394
H	1.003480 1.525260 -7.080031	H	-10.095709 4.292261 2.475740
C	-0.042521 -0.236217 -6.481949	C	-9.252602 4.880240 -0.535351
O	-0.581879 0.556679 -5.588935	C	-10.240483 4.616476 0.387704
O	-0.268685 -1.440352 -6.552841	H	-11.314081 4.502995 0.297762
C	-8.901667 9.469397 3.059524	C	-9.361564 5.121848 -2.008954
H	-9.058481 10.554843 2.952754	H	-8.562962 5.807081 -2.317545
H	-8.380928 9.310459 4.017240	H	-9.182652 4.196189 -2.578607
C	-7.944043 8.962617 1.964605	N	-5.865062 6.988692 -1.770300
O	-8.166620 8.038145 1.205180	C	-5.387017 8.069268 -1.191595
N	-6.756179 9.633798 1.963296	H	-4.921841 8.065262 -0.208060
H	-6.060718 9.311295 1.304111	N	-5.558181 9.149729 -1.991866
H	-6.602399 10.506485 2.475566	H	-5.263385 10.096593 -1.785744
O	-6.628968 4.098240 -2.346016	C	-6.184298 8.741910 -3.157645
O	-5.407783 3.804446 -3.065737	C	-6.355282 7.379837 -2.995344
Fe	-5.949189 4.999833 -0.697307	H	-6.797227 6.645139 -3.664965
H	-2.728305 4.147395 -2.791105	C	-6.461190 9.750318 -4.233400
C	-3.169545 3.150154 -2.820030	H	-6.435207 10.764301 -3.802584
C	-2.497536 2.114612 -3.373692	H	-5.701195 9.747696 -5.032881
H	-1.500955 2.243544 -3.801691	O	-5.024022 6.146232 0.832206
C	-3.084137 0.778503 -3.433229	C	-4.952805 5.613641 1.987119
O	-2.515955 -0.172796 -4.042232	O	-5.370624 4.466901 2.247548
H	-1.307861 0.141904 -4.975796	C	-4.353163 6.447089 3.124356
C	-4.367452 0.590201 -2.768910	H	-4.359873 5.854344 4.050490
H	-4.772389 -0.425424 -2.778989	H	-4.973812 7.346397 3.277373
C	-5.034877 1.627831 -2.201251	h	0.843735 0.415536 -8.440599
H	-6.021338 1.494621 -1.749213	h	-9.878817 8.986529 3.050429
C	-4.528369 3.054472 -2.173146	h	-10.310994 5.534333 -2.350284
O	-4.497097 3.586246 -0.937701	h	-7.453005 9.699159 -4.682569
N	-9.612184 4.513751 1.604100	h	-3.333045 6.776216 2.926616
C	-8.290962 4.699451 1.401904		

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C	0.950582	0.473109	-7.361544	H	-7.404438	4.597510	2.127161
H	1.942011	0.053263	-7.120454	N	-7.953887	4.860257	0.085658
H	0.970313	1.531593	-7.083520	H	-9.982259	4.368470	2.495241
C	-0.059448	-0.239645	-6.485384	C	-9.189949	4.883894	-0.542965
O	-0.606303	0.548014	-5.594166	C	-10.163288	4.681358	0.409251
O	-0.273513	-1.446432	-6.557445	H	-11.243913	4.628328	0.350140
C	-8.913812	9.471384	3.056211	C	-9.330265	5.116623	-2.015925
H	-9.078594	10.557914	2.976393	H	-8.542438	5.800235	-2.355394
H	-8.379569	9.292247	4.002732	H	-9.167862	4.186573	-2.584256
C	-7.969594	9.002021	1.934281	N	-5.799102	7.031380	-1.750659
O	-8.197418	8.103175	1.145638	C	-5.443385	8.128653	-1.119849
N	-6.783648	9.677780	1.944072	H	-5.048305	8.132683	-0.106877
H	-6.116193	9.414932	1.232489	N	-5.644904	9.208164	-1.912638
H	-6.640926	10.551211	2.459747	H	-5.447089	10.171459	-1.670323
O	-6.529636	4.401492	-2.449246	C	-6.162086	8.778458	-3.125449
O	-4.779195	4.063828	-3.105803	C	-6.241537	7.406328	-2.997861
Fe	-5.936496	4.982534	-0.866713	H	-6.586172	6.643898	-3.692914
H	-2.281499	4.026232	-2.442920	C	-6.441050	9.772649	-4.213250
C	-2.853923	3.109502	-2.578359	H	-6.420372	10.792573	-3.797109
C	-2.293997	2.041646	-3.202241	H	-5.678982	9.761189	-5.009932
H	-1.268884	2.076206	-3.572809	O	-5.123007	6.078114	0.800889
C	-3.035013	0.811917	-3.416837	C	-4.978276	5.571888	1.959015
O	-2.547534	-0.162546	-4.062611	O	-5.320824	4.411278	2.268151
H	-1.332129	0.129630	-4.978389	C	-4.383469	6.459751	3.060604
C	-4.386418	0.751678	-2.868227	H	-4.401427	5.906060	4.010544
H	-4.909640	-0.201491	-2.982247	H	-4.997332	7.369817	3.169851
C	-4.972219	1.834953	-2.300363	h	0.824233	0.417290	-8.442741
H	-6.006038	1.803605	-1.947667	h	-9.888736	8.984015	3.048392
C	-4.300424	3.193144	-2.140532	h	-10.286024	5.523758	-2.345824
O	-4.457402	3.679203	-0.863074	h	-7.431826	9.706396	-4.662738
N	-9.509812	4.555128	1.609979	h	-3.357595	6.772142	2.865516
C	-8.187812	4.674619	1.377267				

⁵M-3

C	0.914415 0.474258 -7.379952	H	-7.357390 4.031735 1.985898
H	1.912203 0.074288 -7.131848	N	-7.951278 4.614182 0.021001
H	0.907245 1.532137 -7.099026	H	-9.964608 3.939514 2.399270
C	-0.089794 -0.264065 -6.519782	C	-9.195453 4.797369 -0.564151
O	-0.659929 0.506105 -5.629958	C	-10.156812 4.545214 0.385781
O	-0.282912 -1.474640 -6.594792	H	-11.239226 4.581554 0.359028
C	-8.910284 9.490276 3.031073	C	-9.331097 5.171721 -2.006516
H	-9.088491 10.574435 2.943819	H	-8.576181 5.923720 -2.268114
H	-8.370410 9.325387 3.976643	H	-9.095871 4.306291 -2.645711
C	-7.966343 9.033244 1.902129	N	-5.838360 6.862054 -1.803844
O	-8.222892 8.201490 1.052124	C	-5.476029 7.926900 -1.121019
N	-6.744416 9.642944 1.979154	H	-5.106100 7.882516 -0.099161
H	-6.095569 9.419704 1.236833	N	-5.660609 9.040745 -1.867667
H	-6.596486 10.508777 2.506252	H	-5.462095 9.991120 -1.579849
O	-6.691330 4.242780 -2.532900	C	-6.179646 8.672107 -3.100711
O	-4.784463 3.879473 -3.356765	C	-6.274996 7.296865 -3.034710
Fe	-5.986243 4.799850 -1.011063	H	-6.630398 6.571122 -3.762906
H	-2.279935 3.877238 -2.556781	C	-6.435000 9.719387 -4.145087
C	-2.850109 2.959486 -2.703039	H	-6.402180 10.718289 -3.681037
C	-2.272044 1.864573 -3.248962	H	-5.662658 9.732401 -4.931669
H	-1.227183 1.865163 -3.559291	O	-5.255181 5.816652 0.753888
C	-3.034763 0.647539 -3.483298	C	-5.017124 5.286710 1.888620
O	-2.537763 -0.332765 -4.107009	O	-5.284388 4.104613 2.188346
H	-1.358014 0.039090 -5.019666	C	-4.423458 6.192720 2.985343
C	-4.410125 0.613155 -3.008425	H	-4.355982 5.614646 3.918548
H	-4.940944 -0.330746 -3.148322	H	-5.099045 7.049727 3.149247
C	-5.003753 1.719212 -2.497273	h	0.797784 0.416788 -8.462154
H	-6.062389 1.731958 -2.225711	h	-9.881112 8.994743 3.033704
C	-4.319403 3.070358 -2.355169	h	-10.298862 5.552148 -2.333277
O	-4.481427 3.585128 -1.078296	h	-7.419039 9.695628 -4.613241
N	-9.484782 4.213628 1.538587	h	-3.435592 6.596664 2.763947
C	-8.160409 4.266903 1.283771		

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C	0.843874	0.420404	-7.337083	H	-7.353891	4.617628	2.078692
H	1.853947	0.046374	-7.090879	N	-7.926541	4.923753	0.039155
H	0.811431	1.478078	-7.046954	H	-9.913818	4.422994	2.480077
C	-0.157602	-0.359185	-6.463302	C	-9.176305	4.958646	-0.569875
O	-0.750265	0.320178	-5.575819	C	-10.129194	4.759351	0.401821
O	-0.261282	-1.598687	-6.619065	H	-11.211348	4.718851	0.362251
C	-8.897508	9.479968	3.058175	C	-9.357964	5.183920	-2.039690
H	-9.065396	10.564159	2.958376	H	-8.594459	5.879193	-2.407268
H	-8.377745	9.320100	4.016046	H	-9.208541	4.250371	-2.604692
C	-7.927797	8.996412	1.967152	N	-5.901226	6.951077	-1.801158
O	-8.118499	8.061771	1.208376	C	-5.590354	8.038629	-1.124014
N	-6.759607	9.700550	1.971357	H	-5.253352	8.021975	-0.092117
H	-6.059465	9.427552	1.297016	N	-5.759459	9.127632	-1.902481
H	-6.636659	10.584844	2.475550	H	-5.597843	10.087667	-1.622186
O	-6.645804	4.386629	-2.267282	C	-6.205592	8.724820	-3.151400
O	-4.043050	3.712051	-3.266990	C	-6.279691	7.350679	-3.063698
Fe	-5.986370	5.000207	-0.916400	H	-6.582295	6.617228	-3.807010
H	-2.143987	3.831565	-2.322968	C	-6.449942	9.735975	-4.231142
C	-2.865732	3.097190	-2.690404	H	-6.395853	10.751817	-3.809941
C	-2.337316	1.894129	-3.328492	H	-5.688442	9.697368	-5.026991
H	-1.327880	1.886089	-3.738604	O	-5.182386	5.977081	0.677468
C	-3.113165	0.773230	-3.442847	C	-4.969188	5.456392	1.832020
O	-2.742549	-0.343877	-4.088036	O	-5.239220	4.279031	2.116410
H	-1.908571	-0.163597	-4.662223	C	-4.405639	6.368389	2.925809
C	-4.397835	0.711742	-2.750229	H	-4.414890	5.812391	3.873881
H	-4.903029	-0.257242	-2.759622	H	-5.043644	7.261481	3.031691
C	-4.917992	1.752730	-2.058598	h	0.746654	0.382017	-8.422044
H	-5.821604	1.633451	-1.457293	h	-9.870912	8.989664	3.045799
C	-4.238053	3.071499	-2.022982	h	-10.324329	5.578460	-2.353604
O	-4.509380	3.883614	-0.968201	h	-7.444162	9.695075	-4.676025
N	-9.454588	4.615169	1.587701	h	-3.385406	6.707323	2.746041
C	-8.138467	4.726304	1.336720				

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C	0.891463	0.465212	-7.371967	H	-7.338712	4.047992	1.976824
H	1.890779	0.069517	-7.121668	N	-7.932321	4.633257	0.011538
H	0.880223	1.523645	-7.091590	H	-9.942672	3.953678	2.391912
C	-0.117342	-0.276213	-6.508199	C	-9.178635	4.810076	-0.573436
O	-0.692787	0.479324	-5.627050	C	-10.137686	4.555171	0.377630
O	-0.289783	-1.495089	-6.599513	H	-11.220332	4.587118	0.350898
C	-8.907010	9.488051	3.031141	C	-9.321123	5.178693	-2.016553
H	-9.084576	10.572307	2.944251	H	-8.571066	5.933713	-2.284606
H	-8.368810	9.322727	3.977605	H	-9.093665	4.309345	-2.653288
C	-7.960120	9.031579	1.905003	N	-5.851020	6.888593	-1.815356
O	-8.210456	8.194378	1.057842	C	-5.468733	7.953358	-1.141131
N	-6.741597	9.647543	1.981363	H	-5.080528	7.909960	-0.126212
H	-6.090260	9.426155	1.240787	N	-5.656654	9.064271	-1.888953
H	-6.598053	10.515642	2.506496	H	-5.442751	10.013613	-1.607885
O	-6.690611	4.248882	-2.515274	C	-6.197640	8.697689	-3.112438
O	-4.931967	3.398914	-3.390765	C	-6.304254	7.323874	-3.041025
Fe	-5.962744	4.849409	-1.000495	H	-6.682107	6.603505	-3.762851
H	-2.091629	3.719043	-2.287841	C	-6.456873	9.743354	-4.157259
C	-2.731683	2.881203	-2.567870	H	-6.431745	10.742178	-3.692965
C	-2.219518	1.797428	-3.178355	H	-5.682962	9.761256	-4.941745
H	-1.156323	1.733386	-3.414370	O	-5.247586	5.850159	0.740993
C	-3.043449	0.629083	-3.546271	C	-5.002454	5.302767	1.869990
O	-2.506083	-0.342034	-4.197577	O	-5.256028	4.112848	2.141743
H	-1.463608	0.016058	-4.975061	C	-4.417709	6.197204	2.977169
C	-4.396090	0.642605	-3.164714	H	-4.353464	5.609973	3.904604
H	-5.013583	-0.207776	-3.454956	H	-5.093864	7.052771	3.144778
C	-4.952906	1.756955	-2.521459	h	0.780497	0.410274	-8.454896
H	-5.992602	1.772491	-2.193793	h	-9.878170	8.993165	3.032703
C	-4.201705	3.015835	-2.249217	h	-10.290784	5.557898	-2.339087
O	-4.410023	3.747687	-1.116056	h	-7.440151	9.711688	-4.626542
N	-9.463925	4.227001	1.529810	h	-3.428741	6.601555	2.761514
C	-8.140635	4.285138	1.275249				

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C	0.833513 0.434006 -7.349394	H	-7.381335 4.527226 2.055963
H	1.841378 0.058095 -7.097390	N	-7.971507 4.886886 0.032139
H	0.803302 1.492894 -7.066372	H	-9.946289 4.324155 2.473650
C	-0.170471 -0.335197 -6.473586	C	-9.227628 4.946402 -0.561034
O	-0.758528 0.355869 -5.588718	C	-10.175120 4.727436 0.411011
O	-0.282373 -1.574301 -6.616859	H	-11.257554 4.693768 0.379724
C	-8.893978 9.461052 3.046047	C	-9.410095 5.193647 -2.026186
H	-9.048703 10.547870 2.952785	H	-8.646373 5.899020 -2.379836
H	-8.364435 9.290455 3.996678	H	-9.250221 4.270164 -2.603237
C	-7.948515 8.968402 1.935017	N	-5.804816 7.078818 -1.939957
O	-8.173493 8.049580 1.167584	C	-5.277462 8.137661 -1.358711
N	-6.763199 9.644804 1.928232	H	-4.771796 8.109893 -0.396852
H	-6.092967 9.361673 1.225853	N	-5.479218 9.232001 -2.126351
H	-6.615401 10.521707 2.436911	H	-5.148289 10.167648 -1.919788
O	-6.858247 4.525188 -2.528920	C	-6.179930 8.862785 -3.263022
O	-5.268581 2.808602 -3.139132	C	-6.363910 7.502785 -3.124795
Fe	-5.978079 5.083838 -1.040200	H	-6.861070 6.787673 -3.775443
H	-2.224130 3.835293 -2.595846	C	-6.515688 9.890209 -4.301432
C	-2.871428 2.968385 -2.737066	H	-6.523538 10.892356 -3.843638
C	-2.426040 1.874458 -3.397976	H	-5.772156 9.939200 -5.113890
H	-1.438338 1.862689 -3.863335	O	-5.159587 6.129279 0.579180
C	-3.183362 0.620909 -3.457650	C	-4.976228 5.557107 1.711820
O	-2.639428 -0.436093 -4.068874	O	-5.258622 4.365020 1.924915
H	-1.838366 -0.174241 -4.667624	C	-4.421949 6.404192 2.861821
C	-4.371212 0.519990 -2.780408	H	-4.451080 5.806604 3.784018
H	-4.837434 -0.457474 -2.650250	H	-5.049290 7.300868 2.996710
C	-5.005164 1.709117 -2.222194	h	0.739135 0.388842 -8.434345
H	-5.806054 1.580269 -1.484314	h	-9.873366 8.982668 3.042379
C	-4.243390 3.026415 -2.173894	h	-10.369962 5.593362 -2.353219
O	-4.482012 3.962599 -1.229173	h	-7.512383 9.804734 -4.734281
N	-9.490556 4.544953 1.585764	h	-3.395376 6.736423 2.707425
C	-8.174161 4.652221 1.323392		

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C	0.833516	0.415692	-7.333125	H	-7.386418	4.679289	2.064276
H	1.844745	0.045759	-7.085602	N	-7.952144	4.957165	0.018983
H	0.794342	1.472622	-7.041317	H	-9.942007	4.426638	2.451931
C	-0.165538	-0.369285	-6.461050	C	-9.198342	4.956761	-0.597901
O	-0.765965	0.307539	-5.576518	C	-10.152853	4.738743	0.368302
O	-0.259765	-1.609339	-6.616231	H	-11.233111	4.668432	0.320351
C	-8.897984	9.467823	3.055409	C	-9.380668	5.175663	-2.068613
H	-9.059377	10.554059	2.967811	H	-8.611406	5.861979	-2.439210
H	-8.371482	9.294499	4.007308	H	-9.241845	4.238972	-2.631558
C	-7.943321	8.988878	1.948442	N	-5.870444	7.015583	-1.821690
O	-8.146926	8.059370	1.187130	C	-5.448806	8.096948	-1.196445
N	-6.773639	9.690635	1.937847	H	-5.032103	8.085179	-0.193060
H	-6.094580	9.422063	1.239721	N	-5.621882	9.179464	-1.985126
H	-6.640643	10.571369	2.445283	H	-5.364730	10.131144	-1.750122
O	-6.627409	4.465225	-2.297573	C	-6.188103	8.778373	-3.184668
O	-3.980352	3.555496	-3.141550	C	-6.325113	7.411863	-3.059326
Fe	-6.001688	5.074140	-0.922680	H	-6.720382	6.679684	-3.758809
H	-2.032192	3.796156	-2.382365	C	-6.466106	9.784480	-4.261005
C	-2.739547	3.042731	-2.737136	H	-6.434740	10.800733	-3.837800
C	-2.276308	1.821344	-3.271600	H	-5.711255	9.768565	-5.064255
H	-1.216113	1.690265	-3.491300	O	-5.194109	6.053476	0.674303
C	-3.128930	0.731091	-3.437100	C	-5.000017	5.538589	1.834778
O	-2.757629	-0.376255	-4.100211	O	-5.292534	4.368193	2.126584
H	-1.928667	-0.185172	-4.677600	C	-4.425514	6.446584	2.924947
C	-4.350136	0.673902	-2.691113	H	-4.464245	5.903861	3.879862
H	-4.829384	-0.307769	-2.649318	H	-5.035888	7.360957	3.009718
C	-4.815165	1.680031	-1.873854	h	0.738813	0.378359	-8.418346
H	-5.563093	1.455749	-1.109091	h	-9.874323	8.983346	3.044927
C	-4.297958	3.022782	-1.898168	h	-10.343943	5.579437	-2.380277
O	-4.546959	3.880232	-0.918444	h	-7.462335	9.723421	-4.699032
N	-9.483315	4.621255	1.559844	h	-3.392434	6.748547	2.752811
C	-8.168764	4.763995	1.316248				

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C	0.884947 0.426055 -7.352419	H	-7.603597 4.910937 2.075827
H	1.890697 0.040893 -7.108692	N	-8.146960 5.000149 0.012410
H	0.863774 1.483457 -7.063612	H	-10.127997 4.384790 2.429654
C	-0.119679 -0.343049 -6.486222	C	-9.362921 4.823251 -0.628163
O	-0.726337 0.351618 -5.608875	C	-10.316806 4.543955 0.324059
O	-0.235928 -1.578216 -6.618484	H	-11.377699 4.336790 0.252800
C	-8.891216 9.468221 3.074677	C	-9.516554 4.977002 -2.109893
H	-9.049127 10.554841 2.985197	H	-8.641705 5.500497 -2.513112
H	-8.367297 9.293650 4.027702	H	-9.530615 3.999250 -2.620603
C	-7.937334 8.981922 1.969548	N	-5.907618 7.219720 -1.794747
O	-8.143814 8.044618 1.219587	C	-5.408905 8.299559 -1.236152
N	-6.767963 9.683204 1.947078	H	-4.930828 8.305580 -0.259423
H	-6.097771 9.407921 1.242194	N	-5.563369 9.363710 -2.062083
H	-6.635381 10.570261 2.442539	H	-5.240610 10.307565 -1.883375
O	-6.466535 4.594057 -2.492510	C	-6.200922 8.938526 -3.217341
O	-3.293427 3.419614 -1.892217	C	-6.394166 7.586621 -3.025527
Fe	-6.170167 5.201956 -0.919589	H	-6.841048 6.833113 -3.669723
H	-1.692967 3.851283 -2.998587	C	-6.498694 9.905158 -4.322060
C	-2.396703 3.032054 -2.826310	H	-6.497823 10.934475 -3.929147
C	-2.245734 1.881491 -3.514003	H	-5.747068 9.891790 -5.128744
H	-1.413831 1.856439 -4.220139	O	-5.080897 6.157968 0.653978
C	-3.029119 0.661348 -3.439270	C	-5.056826 5.710838 1.849642
O	-2.628564 -0.381739 -4.155844	O	-5.552903 4.621400 2.196924
H	-1.797106 -0.154416 -4.769944	C	-4.429564 6.581863 2.944317
C	-4.174864 0.523419 -2.652082	H	-4.510008 6.048222 3.902000
H	-4.659556 -0.452807 -2.734312	H	-4.998570 7.524031 3.024800
C	-4.776100 1.435349 -1.773945	h	0.778446 0.386949 -8.436483
H	-5.684310 1.112030 -1.262237	h	-9.868577 8.985914 3.060106
C	-4.398338 2.750806 -1.373146	h	-10.420003 5.494911 -2.431787
O	-4.995538 3.398590 -0.517297	h	-7.495057 9.799731 -4.751260
N	-9.672154 4.578141 1.536401	h	-3.382206 6.836744 2.782629
C	-8.374521 4.857801 1.311814		

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C	0.856055	0.426573	-7.349090	H	-7.516946	4.560933	2.047392
H	1.859756	0.040765	-7.097265	N	-8.009453	4.760541	-0.015163
H	0.834240	1.485197	-7.063678	H	-10.096826	4.236174	2.338624
C	-0.158636	-0.340750	-6.484534	C	-9.224834	4.750428	-0.682539
O	-0.777460	0.352189	-5.621355	C	-10.222536	4.521089	0.238276
O	-0.254843	-1.581050	-6.617349	H	-11.297801	4.431168	0.139317
C	-8.869988	9.519597	3.158402	C	-9.340685	5.014818	-2.153325
H	-9.022473	10.582298	2.916886	H	-8.505040	5.642850	-2.491189
H	-8.459567	9.477240	4.180387	H	-9.291363	4.083467	-2.743086
C	-7.777097	8.891681	2.293457	N	-6.268543	6.888432	-1.639513
O	-7.772414	7.719886	1.945967	C	-6.674828	7.913029	-0.917781
N	-6.756403	9.738595	1.975628	H	-6.931137	7.860710	0.140049
H	-5.891108	9.300332	1.677647	N	-6.767551	9.016283	-1.692778
H	-6.684418	10.675012	2.393458	H	-7.081778	9.924494	-1.370669
O	-5.602246	4.100654	-2.274705	C	-6.414267	8.679671	-2.992998
O	-3.196441	3.351129	-1.682131	C	-6.100491	7.339532	-2.926842
Fe	-5.930292	4.913504	-0.741628	H	-5.778353	6.655755	-3.706397
H	-1.798662	3.934166	-2.994135	C	-6.474299	9.665775	-4.118907
C	-2.472633	3.095794	-2.794680	H	-6.352795	10.693765	-3.741576
C	-2.399563	1.990107	-3.571522	H	-5.662883	9.504260	-4.842782
H	-1.647130	2.004903	-4.363908	O	-4.982005	6.054244	0.726634
C	-3.163357	0.770209	-3.456275	C	-5.010049	5.663389	1.944053
O	-2.769481	-0.302458	-4.156860	O	-5.584037	4.626531	2.324156
H	-1.937582	-0.106782	-4.736522	C	-4.360702	6.534442	3.019281
C	-4.319678	0.647202	-2.671213	H	-4.399140	5.986631	3.971476
H	-4.811508	-0.326346	-2.756780	H	-4.964113	7.450259	3.139637
C	-4.913695	1.559671	-1.805127	h	0.761630	0.386159	-8.434225
H	-5.837265	1.257893	-1.308363	h	-9.834519	9.015526	3.097916
C	-4.441150	2.841521	-1.302383	h	-10.267492	5.508785	-2.445028
O	-4.786560	3.240314	-0.154671	h	-7.437471	9.671647	-4.629135
N	-9.605284	4.423823	1.460400	h	-3.327998	6.829136	2.832879
C	-8.282284	4.575906	1.273234				

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C	0.833910 0.407903 -7.337026	H	-7.681358 4.858328 2.163721
H	1.839868 0.029792 -7.082345	N	-8.123515 4.991261 0.083020
H	0.797750 1.463626 -7.041746	H	-10.217219 4.311144 2.388666
C	-0.179087 -0.379550 -6.488504	C	-9.309485 4.848290 -0.616032
O	-0.813534 0.298789 -5.625763	C	-10.309646 4.540934 0.279249
O	-0.260977 -1.619317 -6.632089	H	-11.365874 4.339625 0.149749
C	-8.879996 9.458708 3.064311	C	-9.395605 5.069961 -2.095812
H	-9.032104 10.544375 2.957688	H	-8.578052 5.731101 -2.412261
H	-8.369398 9.296555 4.027146	H	-9.286591 4.132030 -2.666125
C	-7.907768 8.946197 1.988234	N	-5.955608 6.987383 -1.853616
O	-8.080455 7.959190 1.293879	C	-5.441072 8.053801 -1.270257
N	-6.764101 9.683238 1.924516	H	-4.973645 8.034019 -0.287776
H	-6.041658 9.345129 1.303466	N	-5.582353 9.139218 -2.063393
H	-6.627987 10.565977 2.426573	H	-5.254962 10.074159 -1.849758
O	-5.943904 3.785951 -2.389407	C	-6.225651 8.761440 -3.228294
O	-3.105911 3.601695 -1.979301	C	-6.437461 7.405548 -3.075081
Fe	-6.075151 5.163277 -0.614567	H	-6.906012 6.703922 -3.760613
H	-1.367863 3.870339 -2.973810	C	-6.495675 9.779422 -4.295359
C	-2.268991 3.227812 -2.788213	H	-6.465881 10.790138 -3.858431
C	-2.265276 2.015329 -3.558316	H	-5.738155 9.775952 -5.096055
H	-1.420165 1.874419 -4.234450	O	-5.044570 6.249571 0.824787
C	-3.126730 0.940274 -3.473994	C	-5.061536 5.810731 2.028896
O	-2.844647 -0.174041 -4.156222	O	-5.636513 4.759894 2.359349
H	-1.993585 -0.065051 -4.740148	C	-4.389970 6.643426 3.114978
C	-4.369518 0.748826 -2.698316	H	-4.464501 6.104908 4.069833
H	-4.631681 -0.314451 -2.738188	H	-4.935259 7.597880 3.214141
C	-5.246145 1.498521 -1.993778	h	0.746371 0.375126 -8.422995
H	-6.054112 0.906857 -1.540554	h	-9.858184 8.978191 3.046460
C	-5.445500 2.935076 -1.596622	h	-10.329602 5.525502 -2.424745
O	-5.315118 3.192530 -0.371404	h	-7.490541 9.725469 -4.737397
N	-9.723903 4.532572 1.519722	h	-3.341358 6.871854 2.924452
C	-8.415594 4.807858 1.364538		