Supporting Information

Predictive studies of H-atom abstraction reactions by an iron(IV)-oxo corrole cation radical oxidant

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Methods:

The calculations presented in this work employed extensively tested and benchmarked methods that are based on density functional theory.[1] All structures were fully optimized with the B3LYP density functional method[2] in *Gaussian*–03[3] and followed by a frequency calculation. Vibrational frequencies reported in this work are taken from the *Gaussian–03* frequency calculations of the stationary points and reported without scaling factors. A double–ζ quality LACVP basis set on Fe (with core potential) coupled to 6–31G on the rest of the atoms (C, N, O, H) was used for the geometry optimizations (basis set B1),[4] but followed by single point calculations using an LACV3P+ basis set (with core potential) on Fe and 6–311+G* on the rest of the atoms (basis set B2). All local minima described here had real frequencies only, while the transition states are characterized by a single imaginary frequency for the correct mode, i.e. a C–H–O stretch vibration for the hydrogen abstraction transition states. Energies reported in this work were calculated using an LACV3P+ basis set on Fe and 6-311+G* on the rest of the atoms (basis set B2), whereas zero-point energies were taken from the LACVP (Basis set B1) frequency calculations. Our calculations consider both the doublet and quartet spin state surfaces. Because we deal with open shell doublet spin states with three unpaired electrons the calculations for this spin state contain a minor degree of spin contamination.

Bond dissociation energies (BDE_{CH}) were defined as in Eq 1 and calculated from the energy difference of the substrate (SubH) and the sum of an isolated hydrogen atom and substrate radical rest–group (Sub$^{\bullet}$). Our B3LYP/B2 calculated BDE_{CH} values (with *ZPE* included) match experimental values well.[5]

Following previous studies in the field, we corrected the BDE_{CH} value for the reorganization energy (RE) of the substrate (SubH) by taking the geometry of Sub• in the geometry of SubH as compared to the full relaxed geometry of the radical.[6] The combination of BDE_{CH} and $RE_{Sub\bullet}$ in eq 2 defines the bond strength (D_{CH}), which is a more faithful measure of the interaction strength between the bonded Sub and H moieties in the alkane: [7]

$$SubH \rightarrow Sub^{\bullet} + H^{\bullet} + BDE_{CH} \quad (1)$$

$$D_{CH} = BDE_{CH} + RE_{Sub} \quad (2)$$

References:

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Table S1. Absolute energies, zero–point energies, free energies of isolated reactants and intermediates optimized geometries on UB3LYP/B1. UB3LYP/B2 single points and also solvent single points obtained from UB3LYP/B2//UB3LYP/B1.

Substrate	**E** (B1) (au)	**ZPE** (au)	**G** (au)	**E** (B2) (au)	**E+Esolvent** (B2)
^{2}[Fe^{IV}=O(Corrole$^{+\bullet}$)]	–1148.06160	0.26238	–1147.84299	–1148.58028	–1148.58745
^{4}[Fe^{IV}=O(Corrole$^{+\bullet}$)]	–1148.06270	0.26256	–1147.84453	–1148.58127	–1148.58863
^{1}[Fe^{IV}=O(Corrole)]$^{-}$	–1148.11681	0.26198	–1147.89777	–1148.64694	–1148.71418
^{3}Fe^{IV}=O(Corrole)]$^{-}$	–1148.16072	0.26217	–1147.94248	–1148.69116	–1148.75867
^{1}[Fe^{IV}–OH(Corrole)]	–1148.67085	0.27414	–1148.44012	–1149.19579	–1149.19913
^{1}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	–1148.69145	0.27220	–1148.46338	–1149.21535	–1149.22234
^{3}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	–1148.70978	0.27219	–1148.48328	–1149.23655	–1149.24296
^{5}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	–1148.69754	0.27090	–1148.47285	–1149.22551	–1149.23340

Table S2. Relative energies for isolated reactants and intermediates optimized geometries on UB3LYP/B1. UB3LYP/B2 single points and also solvent single points obtained from UB3LYP/B2//UB3LYP/B1.

Substrate	**Δ(E+ZPE) B1**	**Δ(E+ZPE) B2**	**Δ(E$_{Solvent}$+ZPE) B2**	**ΔG B2**	**ΔG+E$_{Solv}$ B2**
^{2}[Fe^{IV}=O(Corrole$^{+\bullet}$)]	0.58	0.51	0.63	0.90	1.02
^{4}[Fe^{IV}=O(Corrole$^{+\bullet}$)]	0.00	0.00	0.00	0.00	0.00
^{1}[Fe^{IV}=O(Corrole)]$^{-}$	0.00	0.00	0.00	0.00	0.00
^{3}[Fe^{IV}=O(Corrole)]$^{-}$	–27.44	–27.63	–27.80	–28.25	–28.42
^{1}[Fe^{IV}–OH(Corrole)]	0.00	0.00	0.00	0.00	0.00
^{1}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	–14.14	–13.49	–15.78	–13.94	–16.23
^{3}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	–25.65	–26.80	–28.72	–28.24	–30.16
^{5}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	–18.78	–20.68	–23.54	–22.44	–25.29

Table S3. Group spin densities and charges for isolated reactants and intermediates optimized geometries on UB3LYP/B1. UB3LYP/B2 single points and also solvent single points obtained from UB3LYP/B2//UB3LYP/B1.

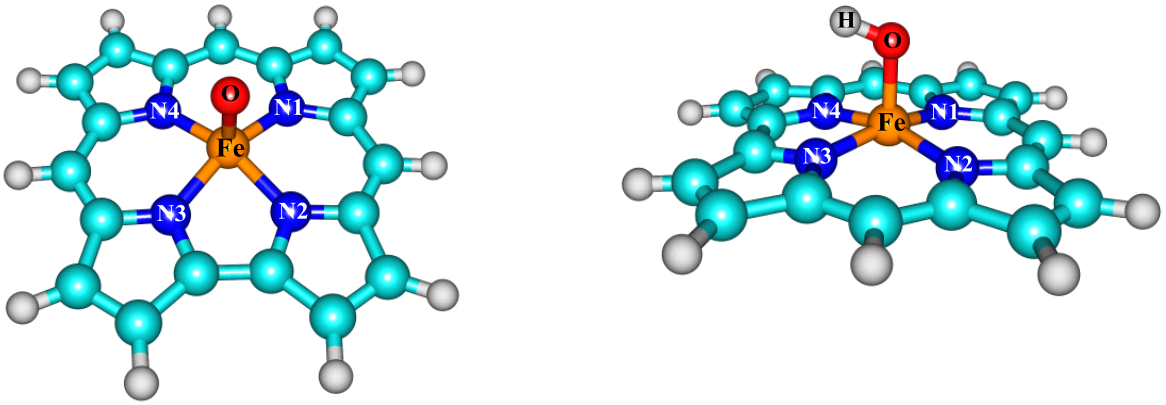
	Basis set	Source file	ρ_{Fe}	ρ_{O}	$\rho_{Corrole}$	ρ_{Total}	Q_{Fe}	Q_{O}	$Q_{Corrole}$	Q_{Total}
^{2}[Fe^{IV}=O(Corrole$^{+\bullet}$)]	LACVP	Freq	1.14	0.78	–0.92	1.00	0.75	–0.33	–0.42	0.00
	LACV3P+*	SPE	1.23	0.77	–0.99	1.00	0.31	–0.24	–0.07	0.00
	LACV3P+*	Solvent	1.32	0.66	–0.98	1.00	0.41	–0.45	0.04	0.00
^{4}[Fe^{IV}=O(Corrole$^{+\bullet}$)]	LACVP	Freq	1.23	0.81	0.97	3.00	0.75	–0.34	–0.41	0.00
	LACV3P+*	SPE	1.27	0.79	0.93	3.00	0.30	–0.25	–0.05	0.00
	LACV3P+*	Solvent	1.39	0.68	0.93	3.00	0.39	–0.47	0.07	0.00
^{1}[Fe^{IV}=O(Corrole)]$^{-}$	LACVP	Freq	0.00	0.00	0.00	0.00	0.67	–0.41	–1.26	–1.00
	LACV3P+*	SPE	0.00	0.00	0.00	0.00	0.30	–0.34	–0.96	–1.00
	LACV3P+*	Solvent	0.00	0.00	0.00	0.00	0.41	–0.58	–0.83	–1.00
^{3}[Fe^{IV}=O(Corrole)]$^{-}$	LACVP	Freq	1.26	0.74	0.01	2.00	0.71	–0.40	–1.31	–1.00
	LACV3P+*	SPE	1.31	0.73	–0.05	2.00	0.31	–0.38	–0.92	–1.00
	LACV3P+*	Solvent	1.47	0.60	–0.06	2.00	0.41	–0.63	–0.78	–1.00
			ρ_{Fe}	ρ_{OH}	$\rho_{Corrole}$	ρ_{Total}	Q_{Fe}	Q_{OH}	$Q_{Corrole}$	Q_{Total}
^{1}Fe^{IV}–OH(Corrole)]	LACVP	Freq	0.05	0.05	–0.10	0.00	0.80	–0.19	–0.61	0.00
	LACV3P+*	SPE	0.03	0.04	–0.07	0.00	0.29	0.12	–0.41	0.00
	LACV3P+*	Solvent	0.02	0.04	–0.06	0.00	0.37	0.06	–0.42	0.00
^{1}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	LACVP	Freq	0.90	0.05	–0.95	0.00	0.76	–0.24	–0.52	0.00
	LACV3P+*	SPE	0.96	0.06	–1.02	0.00	0.20	–0.10	–0.10	0.00
	LACV3P+*	Solvent	0.97	0.05	–1.02	0.00	0.35	–0.21	–0.14	0.00
^{3}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	LACVP	Freq	2.42	0.29	–0.72	2.00	0.88	–0.31	–0.57	0.00
	LACV3P+*	SPE	2.56	0.27	–0.84	2.00	0.03	–0.27	0.24	0.00
	LACV3P+*	Solvent	2.61	0.25	–0.86	2.00	0.13	–0.38	0.25	0.00
^{5}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	LACVP	Freq	2.54	0.40	1.06	4.00	0.89	–0.34	–0.54	0.00
	LACV3P+*	SPE	2.66	0.36	0.98	4.00	0.11	–0.34	0.23	0.00
	LACV3P+*	Solvent	2.71	0.30	0.99	4.00	0.21	–0.46	0.25	0.00

Table S4. Absolute energies, zero–point energies, free energies of UB3LYP/B1 for all substrates discussed in the text. UB3LYP/B2 single points and also solvent single points obtained from UB3LYP/B2//UB3LYP/B1.

Substrate		**E** (B1) (au)	**ZPE** (au)	**G** (au)	**E** (B2) (au)	**Esolvent** (B2)
Ethane	SubH	–79.81274	0.07565	–79.76021	–79.84832	–79.83959
	Sub$^{\bullet}$	–79.14113	0.06000	–79.10537	–79.17734	–79.16991
Propane	SubH	–119.11686	0.10473	–119.03780	–119.17037	–119.16085
(2º carbon atom)	Sub$^{\bullet}$	–118.45181	0.08902	–118.39010	–118.50547	–118.49637
Toluene (aliphatic)	SubH	–271.50698	0.12957	–271.40750	–271.62581	–271.62129
	Sub$^{\bullet}$	–270.85619	0.11613	–270.76970	–270.97479	–270.97190
Propene	SubH	–117.88244	0.08063	–117.82680	–117.93606	–117.92897
	Sub$^{\bullet}$	–117.23638	0.06691	–117.19460	–117.28939	–117.28391
Ethylbenzene (Benzyl hydrogen)	SubH	–310.81080	0.15868	–310.68430	–310.94731	–310.94151
	Sub$^{\bullet}$	–310.16501	0.14454	–310.05290	–310.30081	–310.29591
Indene	SubH	–347.68328	0.14226	–347.57140	–347.83728	–347.83533
	Sub$^{\bullet}$	–347.05017	0.12934	–346.95170	–347.20358	–347.20275
9,10–Dihydroanthracene	SubH	–540.61242	0.21959	–540.42850	–540.84866	–540.84601
	Sub$^{\bullet}$	–539.98391	0.20613	–539.81490	–540.21798	–540.21620
1,4–Cyclohexadiene	SubH	–233.36467	0.12348	–233.26970	–233.47119	–233.46799
	Sub$^{\bullet}$	–232.74133	0.11004	–232.66000	–232.84564	–232.84376
10–methyl–9,10–dihydroacridine	SubH	–595.93840	0.23652	–595.73870	–596.20837	–596.20333
	Sub$^{\bullet}$	–595.31811	0.22388	–595.13150	–595.58568	–595.58196
9,10–dihydroacridine	SubH	–556.64630	0.20784	–556.47260	–556.89630	–556.90008
	Sub$^{\bullet}$	–556.02780	0.19538	–555.86790	–556.27618	–556.28174

Table S5. Bond dissociation energies for different substrates used in the text. UB3LYP/B2 single points and also solvent single points obtained from UB3LYP/B2//UB3LYP/B1.

Substrate	**ΔE (B1) LACVP**	**Δ(E+ZPE) (B1) LACVP**	**ΔE (B2) LACV3P+***	**Δ(E+ZPE) (B2) LACV3P+***	**$\Delta E_{Solvent}$ LACV3P+***	**Δ($E_{Solvent}$+ ZPE) LACV3P+***
Ethane	107.51	97.69	105.94	96.12	105.08	95.26
Propane (2º carbon)	103.40	93.54	102.12	92.26	101.83	91.96
Toluene	94.45	86.02	93.41	84.98	92.35	83.92
Propene	91.48	82.87	90.69	82.08	89.64	81.03
Ethylbenzene	91.31	82.44	90.58	81.70	89.98	81.11
Indene	83.35	75.24	82.54	74.43	81.81	73.70
9,10–Dihydroanthracene	80.47	72.02	80.65	72.20	80.07	71.62
1,4–Cyclohexadiene	77.23	68.79	77.43	69.00	76.57	68.13
10–methyl–9,10–dihydroacridine	75.31	67.38	75.64	67.71	74.78	66.85
9,10–dihydroacridine	74.19	66.37	74.02	66.20	72.87	65.05



	Fe–O	Fe–N1	Fe–N2	Fe–N3	Fe–N4	O–H
^{2}[Fe^{IV}=O(Corrole$^{+\bullet}$)]	1.6337	1.9324	1.9074	1.9075	1.9325	
^{4}[Fe^{IV}=O(Corrole$^{+\bullet}$)]	1.6351	1.9329	1.9075	1.9076	1.9330	
^{1}[Fe^{IV}–OH(Corrole)]	1.7720	1.8958	1.9292	1.8616	1.9332	0.9835
^{1}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	1.8011	1.9358	1.9357	1.8977	1.8974	0.9818
^{3}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	1.8463	1.9425	1.9391	1.9128	1.9113	0.9778
^{5}[Fe^{III}–OH(Corrole$^{+\bullet}$)]	1.8725	1.9571	1.9549	1.9246	1.9216	0.9769

Figure S1. Optimized geometry of [Fe^{IV}=O(Corrole$^{+\bullet}$)], and [Fe^{III}–OH(Corrole$^{+\bullet}$)] as calculated with UB3LYP/B1 in Gaussian. Bond distances are in angstroms.

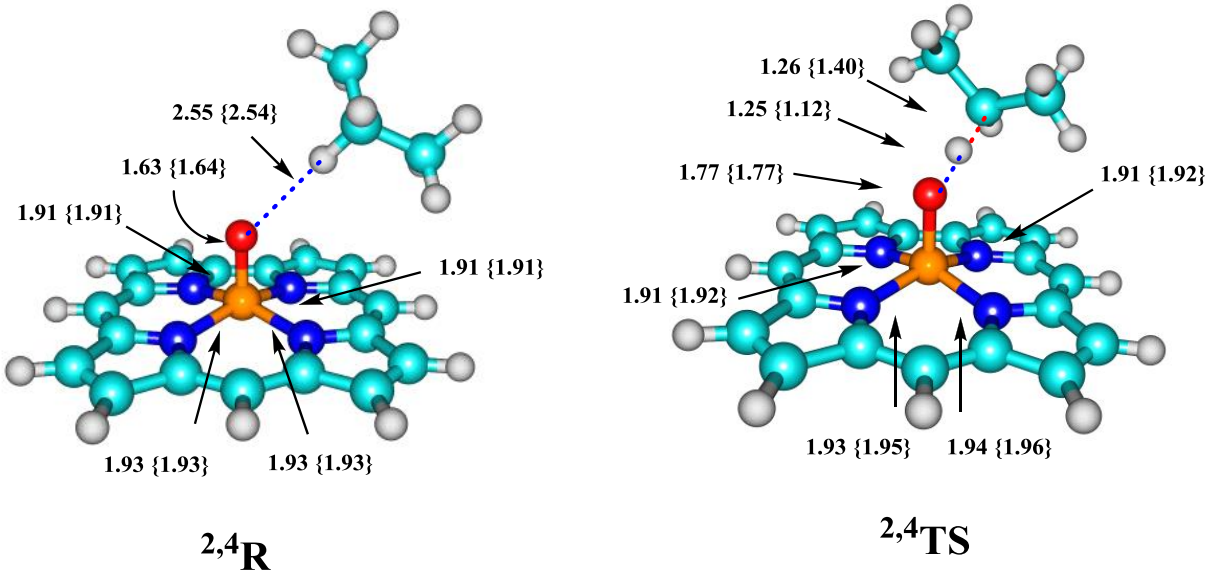


Figure S2. Optimized geometry of ^{2,4}**R**$_2$, and ^{2,4}**TS**$_2$, (quartet data in curly brackets) of hydroxylation of propane (2^{o} carbon atom) as calculated with UB3LYP/B1 in Gaussian. All bond lengths given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

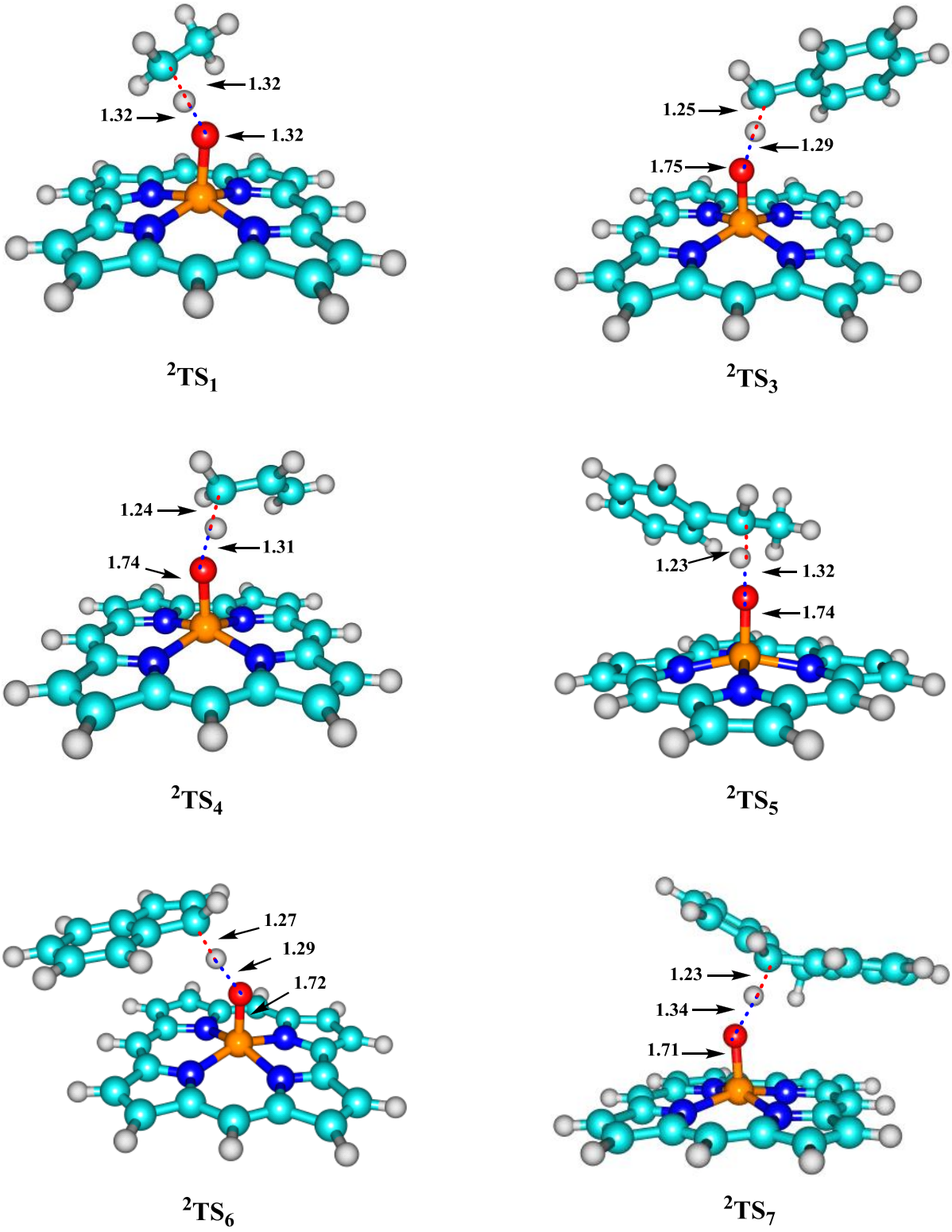


Figure S3. Optimized geometry of Transition States for doublet spin state for substrates **1**, and **3**–**7** as calculated with UB3LYP/B1 in Gaussian. All bond lengths given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

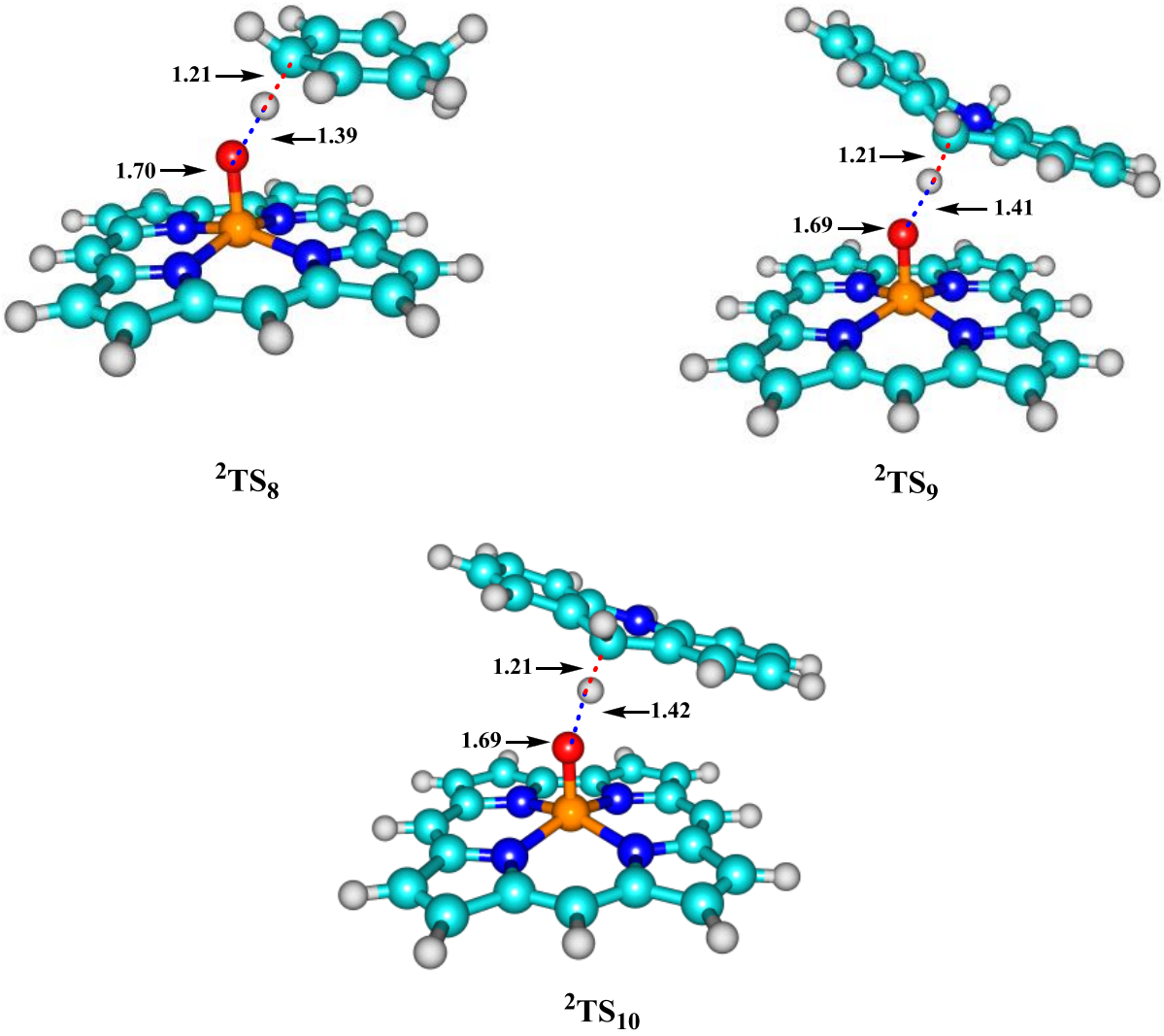


Figure S4. Optimized geometry of Transition States on doublet spin state for substrates **8**–**10** as calculated with UB3LYP/B1 in Gaussian. All bond lengths given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

Table S6. Absolute energies, zero–point energies, free energies of UB3LYP/B1 for hydroxylation of various substrates by [Fe^{IV}(O)(Corrole$^{+\bullet}$)]. UB3LYP/B2 single points and also solvent single points obtained from UB3LYP/B2//UB3LYP/B1.

Substrate		**E** (B1) (au)	**ZPE** (au)	**G** (au)	**E** (B2) (au)	**E+Esolvent** (B2)
Ethane	^{2}**R**	−1227.87601	0.33862	−1227.59347	−1228.42951	−1228.42282
	^{4}**R**	−1227.87714	0.33881	−1227.59500	−1228.43054	−1228.42408
i1204.77	^{2}**TS**	−1227.84834	0.33187	−1227.56894	−1228.40135	−1228.39448
i1152.29	^{4}**TS**	−1227.83700	0.33150	−1227.55844	−1228.38937	−1228.38224
Propane (2º carbon atom)	^{2}**R**	−1267.18035	0.36746	−1266.87063	−1267.75185	−1267.74298
	^{4}**R**	−1267.18148	0.36762	−1266.87228	−1267.75288	−1267.74430
i948.82	^{2}**TS**	−1267.15759	0.36109	−1266.85028	−1267.72812	−1267.71623
i1047.89	^{4}**TS**	−1267.14750	0.35872	−1266.84510	−1267.71882	−1267.70276
Toluene (aliphatic)	^{2}**R**	−1419.57303	0.39260	−1419.23931	−1420.20903	−1420.20397
	^{4}**R**	−1419.57420	0.39279	−1419.24091	−1420.21010	−1420.20522
i1050.69	^{2}**TS**	−1419.55041	0.38682	−1419.22050	−1420.18540	−1420.17850
i1613.77	^{4}**TS**	−1419.54227	0.38635	−1419.21379	−1420.16971	−1420.16320
Propene (aliphatic)	^{2}**R**	−1265.94738	0.34362	−1265.65992	−1266.51849	−1266.51287
	^{4}**R**	−1265.94854	0.34381	−1265.66142	−1266.51955	−1266.51425
i1034.24	^{2}**TS**	−1265.92547	0.33806	−1265.64024	−1266.49467	−1266.48879
i1706.29	^{4}**TS**	−1265.91807	0.33766	−1265.63357	−1266.48624	−1266.47961
Ethylbenzene (benzyl C–H)	^{2}**R**	−1458.87687	0.42158	−1458.51752	−1459.53133	−1459.51939
	^{4}**R**	−1458.87788	0.42154	−1458.51862	−1459.53281	−1459.52033
i957.93	^{2}**TS**	−1458.85547	0.41571	−1458.49887	−1459.50789	−1459.49751
i1637.36	^{4}**TS**	−1458.84780	0.41514	−1458.49182	−1459.49926	−1459.48837
Indene	^{2}**R**	−1495.74979	0.40502	−1495.40370	−1496.42169	−1496.41615
	^{4}**R**	−1495.75097	0.40522	−1495.40535	−1496.42278	−1496.41755
i1431.27	^{2}**TS**	−1495.73118	0.39896	−1495.38909	−1496.40099	−1496.39394
i1735.32	^{4}**TS**	−1495.72687	0.39914	−1495.38435	−1496.39618	−1496.39061
9,10–Dihydroanthracene	^{2}**R**	−1688.67913	0.48242	−1688.26086	−1689.43308	−1689.42603
	^{4}**R**	−1688.68031	0.48261	−1688.26249	−1689.43416	−1689.42740
i1121.39	^{2}**TS**	−1688.66482	0.47672	−1688.25000	−1689.41714	−1689.40478
i1659.51	^{4}**TS**	−1688.65961	0.47648	−1688.24524	−1689.41112	−1689.39847
1,4–Cyclohexadiene	^{2}**R**	−1381.42957	0.38628	−1381.10230	−1382.05403	−1382.04855
	^{4}**R**	−1381.43073	0.38647	−1381.10388	−1382.05508	−1382.05026
i943.62	^{2}**TS**	−1381.41687	0.38135	−1381.09085	−1382.03881	−1382.03255
i1539.16	^{4}**TS**	−1381.41247	0.38074	−1381.08719	−1382.03329	−1382.02765
10–methyl–9,10–dihydroacridine	^{2}**R**	−1744.00628	0.49949	−1743.57107	−1744.79368	−1744.78074
	^{4}**R**	−1744.00743	0.49970	−1743.57265	−1744.79476	−1744.78169
i758.56	^{2}**TS**	−1743.99762	0.49499	−1743.56531	−1744.78303	−1744.77194
i1355.17	^{4}**TS**	−1743.99398	0.49445	−1743.56278	−1744.77873	−1744.76733
9,10–dihydroacridine	^{2}**R**	−1704.71410	0.47094	−1704.30659	−1705.48219	−1705.47783
	^{4}**R**	−1704.71525	0.47115	−1704.30809	−1705.48328	−1705.47903
i778.06	^{2}**TS**	−1704.70577	0.46669	−1704.30012	−1705.47213	−1705.47014
i1391.07	^{4}**TS**	−1704.70194	0.46607	−1704.29752	−1705.46762	−1705.46673

Table S7. Relative energies for hydrogen atom abstraction of various substrates by $^{2,4}[Fe^{IV}(O)(Corrole^{+\bullet})]$. UB3LYP/B2 single points and also solvent single points obtained from UB3LYP/B2//UB3LYP/B1.

Substrate		ΔE (B1) LACVP	Δ(E+ZPE) (B1) LACVP	ΔE (B2) LACV3P+*	Δ(E+ZPE) (B2) LACV3P+*	$\Delta E_{Solvent}$ LACV3P+*	$\Delta(E_{Solvent}+$ ZPE) LACV3P+*	ΔG LACVP	ΔG LACV3P+*	$\Delta G+E_{Solvent}$ LACV3P+*
Ethane	^{2}**R**	0.71	0.59	0.64	0.52	0.79	0.67	0.96	0.90	1.05
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	18.07	13.72	18.31	13.96	18.57	14.22	16.35	16.59	16.85
	^{4}**TS**	25.19	20.60	25.83	21.25	26.26	21.67	22.94	23.59	24.01
Propane	^{2}**R**	0.71	0.61	0.65	0.54	0.83	0.73	1.03	0.97	1.15
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	15.00	10.90	15.54	11.44	17.62	13.52	13.80	14.35	16.43
	^{4}**TS**	21.33	15.74	21.37	15.79	26.07	20.48	17.06	17.10	21.80
Toluene	^{2}**R**	0.74	0.61	0.67	0.55	0.78	0.66	1.00	0.94	1.05
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	14.93	11.18	15.50	11.75	16.76	13.01	12.81	13.38	14.64
	^{4}**TS**	20.04	16.00	25.35	21.30	26.36	22.32	17.02	22.33	23.34
Propene	^{2}**R**	0.72	0.60	0.66	0.54	0.87	0.75	0.94	0.88	1.08
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	14.47	10.86	15.61	12.00	15.97	12.37	13.29	14.43	14.79
	^{4}**TS**	19.12	15.26	20.90	17.04	21.74	17.88	17.47	19.26	20.09
Ethylbenzene	^{2}**R**	0.64	0.66	0.93	0.95	0.59	0.61	0.69	0.98	0.64
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	14.06	10.41	15.64	11.98	14.32	10.66	12.40	13.97	12.65
	^{4}**TS**	18.88	14.86	21.06	17.04	20.06	16.04	16.82	19.00	18.00
Indene	^{2}**R**	0.74	0.62	0.69	0.56	0.88	0.76	1.04	0.98	1.18
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	12.42	8.49	13.68	9.75	14.82	10.89	10.21	11.47	12.61
	^{4}**TS**	15.12	11.31	16.70	12.88	16.91	13.09	13.18	14.75	14.96
9,10–Dihydroanthracene	^{2}**R**	0.74	0.62	0.68	0.56	0.86	0.74	1.03	0.97	1.15
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	9.72	6.03	10.68	6.98	14.20	10.50	7.84	8.80	12.31
	^{4}**TS**	12.99	9.15	14.46	10.61	18.16	14.31	10.82	12.29	15.99
1,4–Cyclohexadiene	^{2}**R**	0.73	0.61	0.66	0.54	1.07	0.95	0.99	0.92	1.33
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	8.70	5.49	10.21	7.00	11.11	7.90	8.17	9.68	10.58
	^{4}**TS**	11.46	7.86	13.67	10.08	14.19	10.59	10.47	12.68	13.20
10–methyl–9,10–dihydroacridine	^{2}**R**	0.72	0.59	0.68	0.55	0.60	0.46	0.99	0.95	0.86
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	6.16	3.20	7.36	4.41	6.11	3.16	4.61	5.82	4.57
	^{4}**TS**	8.44	5.15	10.06	6.77	9.01	5.72	6.19	7.81	6.77
9,10–dihydroacridine	^{2}**R**	0.72	0.59	0.68	0.55	0.76	0.62	0.94	0.91	0.98
	^{4}**R**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	^{2}**TS**	5.95	3.15	7.00	4.20	5.58	2.78	5.00	6.05	4.63
	^{4}**TS**	8.35	5.17	9.83	6.64	7.72	4.54	6.64	8.11	6.00

Table S8. Group spin densities and charges of UB3LYP/B1 optimized geometries of reactant complex for hydroxylation of different substrates by $^{2,4}[Fe^{IV}(O)(Corrole^{+\bullet})]$.

Substrate		ρ_{Fe}	ρ_{O}	ρ_{Ligand}	ρ_{SubH}	ρ_{Total}	Q_{Fe}	Q_{O}	Q_{Ligand}	Q_{SubH}	Q_{Total}
Ethane	^{2}**R**	1.15	0.76	–0.92	0.00	1.00	0.76	–0.34	–0.42	0.00	0.00
	^{4}**R**	1.24	0.79	0.96	0.00	3.00	0.76	–0.35	–0.41	0.00	0.00
Propane	^{2}**R**	1.15	0.76	–0.92	0.00	1.00	0.76	–0.34	–0.41	0.00	0.00
	^{4}**R**	1.24	0.79	0.96	0.00	3.00	0.75	–0.35	–0.40	0.00	0.00
Toluene	^{2}**R**	1.16	0.75	–0.91	0.00	1.00	0.76	–0.35	–0.42	0.01	0.00
	^{4}**R**	1.26	0.78	0.96	0.00	3.00	0.76	–0.36	–0.41	0.01	0.00
Propene	^{2}**R**	1.16	0.75	–0.91	0.00	1.00	0.76	–0.35	–0.41	0.00	0.00
	^{4}**R**	1.25	0.78	0.96	0.00	3.00	0.76	–0.35	–0.40	0.00	0.00
Ethylbenzene	^{2}**R**	1.17	0.74	–0.92	0.00	1.00	0.77	–0.36	–0.40	–0.01	0.00
	^{4}**R**	1.26	0.78	0.96	0.00	3.00	0.76	–0.36	–0.39	–0.01	0.00
Indene	^{2}**R**	1.17	0.74	–0.91	0.00	1.00	0.77	–0.36	–0.41	0.00	0.00
	^{4}**R**	1.27	0.77	0.96	0.01	3.00	0.76	–0.37	–0.40	0.00	0.00
9,10–Dihydroanthracene	^{2}**R**	1.17	0.75	–0.91	0.00	1.00	0.76	–0.35	–0.41	0.00	0.00
	^{4}**R**	1.26	0.77	0.96	0.00	3.00	0.76	–0.36	–0.40	0.00	0.00
1,4–Cyclohexadiene	^{2}**R**	1.16	0.75	–0.91	0.00	1.00	0.76	–0.35	–0.41	0.00	0.00
	^{4}**R**	1.26	0.78	0.96	0.00	3.00	0.76	–0.36	–0.40	0.00	0.00
10–methyl–9,10–dihydroacridine	^{2}**R**	1.19	0.72	–0.88	–0.03	1.00	0.79	–0.37	–0.44	0.02	0.00
	^{4}**R**	1.28	0.76	0.93	0.03	3.00	0.78	–0.37	–0.42	0.01	0.00
9,10–dihydroacridine	^{2}**R**	1.19	0.73	–0.89	–0.03	1.00	0.79	–0.37	–0.44	0.02	0.00
	^{4}**R**	1.28	0.76	0.94	0.03	3.00	0.78	–0.37	–0.42	0.01	0.00

Table S9. Group spin densities and charges of UB3LYP/B1 optimized geometries of transition states for hydrogen abstraction from different substrates by $^{2,4}[Fe^{IV}(O)(Corrole^{+\bullet})]$.

Substrate		ρ_{Fe}	ρ_{OH}	ρ_{Ligand}	$\rho_{Sub.}$	ρ_{Total}	Q_{Fe}	Q_{OH}	Q_{Ligand}	$Q_{Sub.}$	Q_{Total}
Ethane	^{2}**TS**	2.27	–0.05	–0.68	–0.54	1.00	0.87	–0.24	–0.61	–0.03	0.00
	^{4}**TS**	1.10	0.44	0.83	0.64	3.00	0.80	–0.21	–0.56	–0.04	0.00
Propane	^{2}**TS**	2.23	–0.11	–0.66	–0.46	1.00	0.87	–0.23	–0.61	–0.02	0.00
	^{4}**TS**	2.35	0.22	1.02	–0.59	3.00	0.89	–0.29	–0.56	–0.04	0.00
Toluene	^{2}**TS**	2.15	–0.01	–0.71	–0.43	1.00	0.86	–0.21	–0.58	–0.07	0.00
	^{4}**TS**	1.23	0.47	0.76	0.53	3.00	0.82	–0.18	–0.56	–0.08	0.00
Propene	^{2}**TS**	2.13	0.00	–0.72	–0.41	1.00	0.86	–0.21	–0.57	–0.07	0.00
	^{4}**TS**	1.21	0.49	0.78	0.51	3.00	0.82	–0.18	–0.55	–0.09	0.00
Ethylbenzene	^{2}**TS**	2.10	0.05	–0.76	–0.39	1.00	0.86	–0.21	–0.57	–0.08	0.00
	^{4}**TS**	1.29	0.48	0.74	0.49	3.00	0.83	–0.20	–0.57	–0.06	0.00
Indene	^{2}**TS**	1.99	0.16	–0.78	–0.38	1.00	0.86	–0.19	–0.52	–0.15	0.00
	^{4}**TS**	1.49	0.45	0.67	0.39	3.00	0.85	–0.16	–0.51	–0.18	0.00
9,10–Dihydroanthracene	^{2}**TS**	1.95	0.20	–0.79	–0.36	1.00	0.85	–0.18	–0.55	–0.12	0.00
	^{4}**TS**	1.44	0.49	0.67	0.39	3.00	0.84	–0.17	–0.57	–0.09	0.00
1,4–Cyclohexadiene	^{2}**TS**	1.90	0.19	–0.75	–0.34	1.00	0.84	–0.18	–0.57	–0.09	0.00
	^{4}**TS**	1.44	0.54	0.63	0.39	3.00	0.83	–0.17	–0.60	–0.07	0.00
10–methyl–9,10–dihydroacridine	^{2}**TS**	1.80	0.28	–0.64	–0.45	1.00	0.83	–0.16	–0.67	0.00	0.00
	^{4}**TS**	1.53	0.52	0.47	0.48	3.00	0.84	–0.16	–0.71	0.04	0.00
9,10–dihydroacridine	^{2}**TS**	1.80	0.27	–0.63	–0.44	1.00	0.83	–0.17	–0.67	0.01	0.00
	^{4}**TS**	1.51	0.52	0.49	0.48	3.00	0.83	–0.55	–1.69	1.41	0.00

Table S10. Group spin densities and charges (of reactants) of UB3LYP/B2//UB3LYP/B1 single for hydroxylation of different substrates by ^{2,4}[Fe^{IV}(O)(Corrole$^{+\bullet}$)].

Substrate		ρ_{Fe}	ρ_{O}	ρ_{Ligand}	ρ_{SubH}	ρ_{Total}	Q_{Fe}	Q_{O}	Q_{Ligand}	Q_{SubH}	Q_{Total}
Ethane	^{2}**R**	1.24	0.76	−1.00	0.00	1.00	0.01	−0.17	0.20	−0.03	0.00
	^{4}**R**	1.28	0.78	0.93	0.00	3.00	0.00	−0.18	0.22	−0.03	0.00
Propane	^{2}**R**	1.25	0.76	−1.01	0.00	1.00	−0.25	−0.12	0.40	−0.03	0.00
	^{4}**R**	1.28	0.78	0.93	0.00	3.00	−0.26	−0.13	0.42	−0.03	0.00
Toluene	^{2}**R**	1.25	0.75	−1.00	0.00	1.00	−0.03	−0.16	0.33	−0.14	0.00
	^{4}**R**	1.30	0.77	0.93	0.00	3.00	−0.04	−0.17	0.36	−0.14	0.00
Propene	^{2}**R**	1.25	0.75	−1.00	0.00	1.00	−0.04	−0.16	0.26	−0.06	0.00
	^{4}**R**	1.29	0.77	0.93	0.00	3.00	−0.05	−0.17	0.29	−0.06	0.00
Ethylbenzene	^{2}**R**	1.28	0.75	−1.03	0.00	1.00	−0.77	0.07	0.73	−0.04	0.00
	^{4}**R**	1.29	0.78	0.93	0.00	3.00	−0.81	0.28	0.57	−0.05	0.00
Indene	^{2}**R**	1.26	0.74	−1.00	0.00	1.00	−0.14	−0.07	0.37	−0.15	0.00
	^{4}**R**	1.31	0.76	0.92	0.01	3.00	−0.16	−0.08	0.39	−0.15	0.00
9,10–Dihydroanthracene	^{2}**R**	1.24	0.76	−1.00	0.01	1.00	−0.20	0.05	0.28	−0.12	0.00
	^{4}**R**	1.30	0.77	0.93	0.00	3.00	−0.22	0.04	0.31	−0.13	0.00
1,4–Cyclohexadiene	^{2}**R**	1.25	0.75	−1.00	0.00	1.00	−0.13	−0.06	0.22	−0.03	0.00
	^{4}**R**	1.29	0.78	0.93	0.00	3.00	−0.14	−0.07	0.25	−0.03	0.00
10–methyl–9,10–dihydroacridine	^{2}**R**	1.29	0.73	−0.99	−0.02	1.00	−0.62	−0.06	0.71	−0.03	0.00
	^{4}**R**	1.32	0.75	0.90	0.03	3.00	−0.63	−0.07	0.74	−0.03	0.00
9,10–dihydroacridine	^{2}**R**	1.28	0.73	−0.99	−0.02	1.00	−0.44	−0.06	0.53	−0.04	0.00
	^{4}**R**	1.32	0.76	0.91	0.02	3.00	−0.46	−0.07	0.57	−0.04	0.00

Table S11. Group spin densities and charges (of transition states) of UB3LYP/B2//UB3LYP/B1 single for hydroxylation of different substrates by ^{2,4}[Fe^{IV}(O)(Corrole$^{+\bullet}$)].

Substrate		ρ_{Fe}	ρ_{OH}	ρ_{Ligand}	$\rho_{Sub.}$	ρ_{Total}	Q_{Fe}	Q_{OH}	Q_{Ligand}	$Q_{Sub.}$	Q_{Total}
Ethane	^{2}**TS**	2.40	–0.01	–0.81	–0.58	1.00	–0.46	0.17	0.51	–0.22	0.00
	^{4}**TS**	1.09	0.39	0.84	0.68	3.00	–0.09	0.26	0.07	–0.24	0.00
Propane	^{2}**TS**	2.33	–0.07	–0.78	–0.48	1.00	–0.60	0.32	0.54	–0.26	0.00
	^{4}**TS**	2.20	0.23	1.19	–0.62	3.00	0.44	0.92	–1.14	–0.23	0.00
Toluene	^{2}**TS**	2.24	0.02	–0.81	–0.45	1.00	–0.86	0.36	0.82	–0.32	0.00
	^{4}**TS**	1.07	0.45	–0.93	0.42	1.00	–0.65	0.45	0.55	–0.36	0.00
Propene	^{2}**TS**	2.21	0.02	–0.81	–0.43	1.00	–0.78	0.25	0.84	–0.31	0.00
	^{4}**TS**	1.25	0.46	0.75	0.54	3.00	–0.42	0.34	0.41	–0.33	0.00
Ethylbenzene	^{2}**TS**	2.17	0.06	–0.83	–0.40	1.00	–1.03	0.55	0.84	–0.36	0.00
	^{4}**TS**	1.33	0.46	0.70	0.51	3.00	–0.78	0.61	0.54	–0.36	0.00
Indene	^{2}**TS**	2.05	0.18	–0.84	–0.39	1.00	–0.58	0.63	0.51	–0.57	0.00
	^{4}**TS**	1.56	0.44	0.60	0.41	3.00	–0.52	0.64	0.50	–0.62	0.00
9,10–Dihydroanthracene	^{2}**TS**	1.95	0.20	–0.80	–0.35	1.00	–0.78	1.03	0.28	–0.53	0.00
	^{4}**TS**	1.49	0.49	0.63	0.40	3.00	–0.76	1.03	0.24	–0.51	0.00
1,4–Cyclohexadiene	^{2}**TS**	1.95	0.20	–0.81	–0.34	1.00	–0.63	0.59	0.43	–0.39	0.00
	^{4}**TS**	1.49	0.52	0.58	0.40	3.00	–0.53	0.61	0.32	–0.40	0.00
10–methyl–9,10–dihydroacridine	^{2}**TS**	1.81	0.29	–0.64	–0.46	1.00	–0.92	0.96	0.31	–0.36	0.00
	^{4}**TS**	1.56	0.51	0.44	0.50	3.00	–0.46	1.13	–0.34	–0.34	0.00
9,10–dihydroacridine	^{2}**TS**	1.83	0.28	–0.66	–0.45	1.00	3.00	3.00	44.00	38.00	88.00
	^{4}**TS**	1.54	0.51	0.44	0.51	3.00	–0.78	0.95	0.20	–0.37	0.00

Table S12. Group spin densities and charges (of reactants) of UB3LYP/B2//UB3LYP/B1 for hydroxylation of different substrates by ^{2,4}[Fe^{IV}(O)(Corrole$^{+\bullet}$)] (including solvent effect).

Substrate		ρ_{Fe}	ρ_{O}	ρ_{Ligand}	ρ_{SubH}	ρ_{Total}	Q_{Fe}	Q_{O}	Q_{Ligand}	Q_{SubH}	Q_{Total}
Ethane	^{2}**R**	1.31	0.68	−0.99	0.00	1.00	0.13	−0.33	0.24	−0.04	0.00
	^{4}**R**	1.37	0.70	0.93	0.00	3.00	0.11	−0.34	0.27	−0.04	0.00
Propane	^{2}**R**	1.31	0.68	−1.00	0.00	1.00	−0.14	−0.27	0.44	−0.03	0.00
	^{4}**R**	1.37	0.70	0.92	0.00	3.00	−0.15	−0.28	0.47	−0.03	0.00
Toluene	^{2}**R**	1.32	0.67	−0.99	0.00	1.00	0.09	−0.32	0.35	−0.12	0.00
	^{4}**R**	1.38	0.69	0.93	0.00	3.00	0.07	−0.34	0.39	−0.12	0.00
Propene	^{2}**R**	1.32	0.67	−0.99	0.00	1.00	0.08	−0.32	0.30	−0.06	0.00
	^{4}**R**	1.39	0.69	0.92	0.00	3.00	0.06	−0.34	0.34	−0.06	0.00
Ethylbenzene	^{2}**R**	1.32	0.69	−1.02	0.00	1.00	−0.63	−0.03	0.72	−0.06	0.00
	^{4}**R**	1.34	0.74	0.93	0.00	3.00	−0.67	0.20	0.54	−0.06	0.00
Indene	^{2}**R**	1.32	0.66	−0.99	0.00	1.00	−0.02	−0.23	0.39	−0.13	0.00
	^{4}**R**	1.40	0.69	0.91	0.00	3.00	−0.04	−0.25	0.42	−0.13	0.00
9,10–Dihydroanthracene	^{2}**R**	1.30	0.69	−0.99	0.01	1.00	−0.09	−0.10	0.29	−0.11	0.00
	^{4}**R**	1.37	0.71	0.93	0.00	3.00	−0.10	−0.12	0.33	−0.11	0.00
1,4–Cyclohexadiene	^{2}**R**	1.32	0.67	−0.99	0.00	1.00	−0.02	−0.22	0.27	−0.03	0.00
	^{4}**R**	1.38	0.69	0.92	0.00	3.00	−0.03	−0.24	0.29	−0.03	0.00
10–methyl–9,10–dihydroacridine	^{2}**R**	1.34	0.66	−0.99	−0.01	1.00	−0.48	−0.20	0.72	−0.04	0.00
	^{4}**R**	1.39	0.69	0.90	0.02	3.00	−0.51	−0.21	0.77	−0.04	0.00
9,10–dihydroacridine	^{2}**R**	1.33	0.67	−0.98	−0.02	1.00	−0.31	−0.20	0.55	−0.04	0.00
	^{4}**R**	1.39	0.69	0.91	0.02	3.00	−0.33	−0.21	0.59	−0.05	0.00

Table S13. Group spin densities and charges (of transition states) of UB3LYP/B2//UB3LYP/B1 for hydroxylation of different substrates by ^{2,4}[Fe^{IV}(O)(Corrole$^{+\bullet}$)] (including solvent effect).

Substrate		ρ_{Fe}	ρ_{OH}	ρ_{Ligand}	$\rho_{Sub.}$	ρ_{Total}	Q_{Fe}	Q_{OH}	Q_{Ligand}	$Q_{Sub.}$	Q_{Total}
Ethane	^{2}**TS**	2.47	–0.02	–0.87	–0.58	1.00	–0.37	0.03	0.53	–0.20	0.00
	^{4}**TS**	1.11	0.35	0.86	0.68	3.00	0.00	0.13	0.09	–0.22	0.00
Propane	^{2}**TS**	2.39	–0.07	–0.83	–0.49	1.00	–0.51	0.21	0.55	–0.25	0.00
	^{4}**TS**	2.22	0.21	1.18	–0.62	3.00	0.52	0.90	–1.20	–0.23	0.00
Toluene	^{2}**TS**	2.30	0.01	–0.85	–0.46	1.00	–0.76	0.22	0.83	–0.29	0.00
	^{4}**TS**	1.12	0.40	–0.93	0.41	1.00	–0.54	0.33	0.57	–0.36	0.00
Propene	^{2}**TS**	2.28	0.01	–0.86	–0.43	1.00	–0.68	0.11	0.86	–0.29	0.00
	^{4}**TS**	1.28	0.42	0.78	0.53	3.00	–0.32	0.20	0.43	–0.32	0.00
Ethylbenzene	^{2}**TS**	2.23	0.04	–0.86	–0.41	1.00	–0.94	0.43	0.85	–0.34	0.00
	^{4}**TS**	1.36	0.43	0.70	0.51	3.00	–0.69	0.49	0.53	–0.33	0.00
Indene	^{2}**TS**	2.10	0.15	–0.85	–0.40	1.00	–0.48	0.49	0.51	–0.52	0.00
	^{4}**TS**	1.60	0.40	0.62	0.38	3.00	–0.42	0.51	0.50	–0.60	0.00
9,10–Dihydroanthracene	^{2}**TS**	2.00	0.17	–0.81	–0.36	1.00	–0.70	0.94	0.26	–0.50	0.00
	^{4}**TS**	1.52	0.46	0.62	0.40	3.00	–0.68	0.94	0.19	–0.46	0.00
1,4–Cyclohexadiene	^{2}**TS**	2.01	0.17	–0.81	–0.37	1.00	–0.53	0.45	0.41	–0.34	0.00
	^{4}**TS**	1.55	0.48	0.54	0.43	3.00	–0.43	0.48	0.27	–0.33	0.00
10–methyl–9,10–dihydroacridine	^{2}**TS**	1.85	0.28	–0.55	–0.57	1.00	–0.80	0.86	0.16	–0.21	0.00
	^{4}**TS**	1.72	0.47	0.11	0.70	3.00	–0.37	1.05	–0.59	–0.09	0.00
9,10–dihydroacridine	^{2}**TS**	1.86	0.27	–0.49	–0.64	1.00	–0.98	0.66	0.47	–0.15	0.00
	^{4}**TS**	1.77	0.46	0.02	0.75	3.00	–0.66	0.84	–0.11	–0.07	0.00

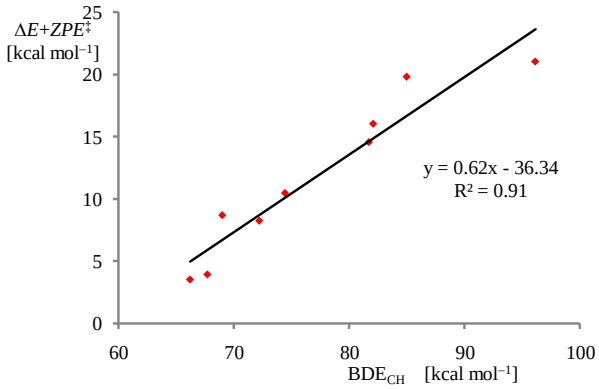


Figure S5. Correlation of BDE_{CH} with barrier height for high-spin barriers of $^{4}[Fe^{IV}(O)(Cor^{+\bullet})]$ with substrates.

Cartesian coordinates of all structures discussed in this work. The value in subscript refers to the substrate: 1 (ethane), 2 (propane), 3 (toluene), 4 (propene), 5 (ethylbenzene), 6 (indene), 7 (9,10-dehydroanthracene), 8 (1,4-cyclohexadiene), 9 (10-methyl-9,10-dehydroacridine) and 10 (9,10-dehydroacridine).

$^{2}R_{1}$:

Fe	0.018635000	0.190869000	0.153644000
N	0.028152000	0.063821000	2.081687000
N	1.925675000	–0.065951000	–0.014738000
N	–0.015306000	0.978419000	–1.582911000
N	–1.661282000	1.090047000	0.236409000
C	–1.056322000	0.251331000	2.922427000
C	–0.674829000	–0.144272000	4.253932000
C	0.636991000	–0.569107000	4.203570000
C	1.076001000	–0.439299000	2.838159000
C	2.751967000	–0.554793000	0.985601000
C	4.053797000	–0.807924000	0.424180000
C	3.995468000	–0.471593000	–0.912822000
C	2.659769000	–0.007580000	–1.187703000
C	0.888014000	0.958298000	–2.630133000
C	0.227815000	1.558422000	–3.767386000
C	–1.052015000	1.928419000	–3.367293000
C	–1.183433000	1.551074000	–1.990813000
C	–2.149537000	1.617736000	–0.922269000
C	–3.477660000	2.100006000	–0.682076000
C	–3.766721000	1.839951000	0.653435000
C	–2.608864000	1.202066000	1.238119000
C	–2.312796000	0.778096000	2.527819000
C	2.341919000	–0.736690000	2.314145000
C	2.171598000	0.463966000	–2.433130000
H	–1.316933000	–0.097611000	5.121598000
H	1.244334000	–0.928717000	5.021441000
H	4.905266000	–1.185784000	0.971301000
H	4.793401000	–0.527026000	–1.639209000
H	0.667219000	1.704210000	–4.743614000
H	–1.804443000	2.413205000	–3.970850000
H	–4.122594000	2.579529000	–1.402864000
H	–4.680824000	2.082258000	1.175964000
O	–0.474697000	–1.325253000	–0.209178000
H	–2.595294000	–2.529230000	0.591413000
C	–3.533132000	–2.951329000	0.969475000
H	–3.297763000	–3.553783000	1.855985000
H	–3.071317000	0.873940000	3.297982000
H	3.080548000	–1.128542000	3.006815000
H	2.863977000	0.456294000	–3.268844000
C	–4.237792000	–3.795094000	–0.102477000
H	–3.604431000	–4.628651000	–0.429205000
H	–5.179082000	–4.218851000	0.270080000
H	–4.471540000	–3.193034000	–0.988922000
H	–4.166732000	–2.116346000	1.294829000

$^{4}R_{1}$:

Fe	0.016092000	0.191650000	0.151719000
N	0.026057000	0.067032000	2.080404000
N	1.924057000	–0.063659000	–0.015315000
N	–0.014583000	0.984601000	–1.582612000
N	–1.660517000	1.096993000	0.235645000
C	–1.058415000	0.253419000	2.920779000
C	–0.678497000	–0.146067000	4.252124000
C	0.632448000	–0.572168000	4.201881000
C	1.072760000	–0.439508000	2.836874000
C	2.749181000	–0.556071000	0.984743000
C	4.050355000	–0.813418000	0.422997000
C	3.992936000	–0.476467000	–0.913421000
C	2.658299000	–0.007581000	–1.187876000
C	0.888847000	0.963121000	–2.630119000
C	0.229119000	1.562746000	–3.767953000
C	–1.050646000	1.932897000	–3.368464000
C	–1.182280000	1.556713000	–1.991366000
C	–2.148685000	1.623931000	–0.923018000
C	–3.477317000	2.106036000	–0.683384000
C	–3.766639000	1.846631000	0.651984000
C	–2.608903000	1.208778000	1.237050000
C	–2.313747000	0.782669000	2.525977000
C	2.337894000	–0.737994000	2.312528000
C	2.171103000	0.466118000	–2.432816000
H	–1.321566000	–0.101114000	5.119167000
H	1.238565000	–0.935236000	5.019126000
H	4.900303000	–1.195156000	0.969783000
H	4.790310000	–0.534671000	–1.640208000
H	0.668392000	1.706848000	–4.744487000
H	–1.802986000	2.417242000	–3.972485000
H	–4.122066000	2.585190000	–1.404582000
H	–4.681276000	2.088132000	1.173947000
O	–0.474089000	–1.327949000	–0.207684000
H	–2.589948000	–2.533178000	0.594720000
C	–3.526851000	–2.956373000	0.973887000
H	–3.289923000	–3.558270000	1.860373000
H	–3.072665000	0.878267000	3.295837000
H	3.075551000	–1.132134000	3.005041000
H	2.863537000	0.457355000	–3.268532000
C	–4.231533000	–3.801378000	–0.097087000
H	–3.597474000	–4.634332000	–0.424002000
H	–5.172055000	–4.226061000	0.276384000
H	–4.466636000	–3.199947000	–0.983605000
H	–4.161303000	–2.122141000	1.299620000

$^{2}R_{2}$:

Fe	–0.085876000	0.296245000	0.111094000
N	–0.120919000	0.158785000	2.038017000
N	1.793765000	–0.128073000	–0.026949000
N	–0.019045000	1.093168000	–1.620170000
N	–1.680740000	1.340635000	0.171159000
C	–1.199319000	0.437335000	2.861163000
C	–0.878448000	0.001446000	4.196254000
C	0.391235000	–0.538521000	4.165123000
C	0.864320000	–0.440214000	2.808655000
C	2.555713000	–0.693805000	0.984137000
C	3.839493000	–1.059094000	0.443158000
C	3.834832000	–0.711832000	–0.892224000
C	2.550608000	–0.129213000	–1.186585000
C	0.897400000	0.998542000	–2.651846000
C	0.313686000	1.662091000	–3.795803000

C	−0.934829000	2.142708000	−3.414998000
C	−1.123819000	1.770332000	−2.043838000
C	−2.098965000	1.917062000	−0.991556000
C	−3.382552000	2.515293000	−0.770458000
C	−3.717375000	2.274144000	0.557924000
C	−2.631752000	1.531479000	1.157464000
C	−2.397068000	1.076024000	2.448936000
C	2.108108000	−0.845860000	2.304040000
C	2.128121000	0.390553000	−2.436874000
H	−1.528834000	0.101353000	5.053204000
H	0.949383000	−0.955439000	4.990791000
H	4.644235000	−1.514082000	1.002167000
H	4.637290000	−0.834206000	−1.605294000
H	0.781542000	1.773619000	−4.763287000
H	−1.630197000	2.696321000	−4.027702000
H	−3.968932000	3.055277000	−1.498463000
H	−4.614943000	2.594727000	1.066786000
O	−0.704079000	−1.168826000	−0.269734000
H	−2.443392000	−2.739014000	0.738554000
C	−3.193065000	−3.412504000	1.173897000
H	−2.641847000	−4.276547000	1.572963000
H	−3.157327000	1.234532000	3.206840000
H	2.796670000	−1.305619000	3.006449000
H	2.831539000	0.326047000	−3.260809000
C	−4.155532000	−3.886947000	0.072902000
H	−3.616725000	−4.395037000	−0.735541000
H	−4.904196000	−4.585283000	0.470911000
H	−4.693620000	−3.037854000	−0.368241000
C	−3.917494000	−2.696599000	2.325936000
H	−4.652849000	−3.356382000	2.805865000
H	−3.209951000	−2.362417000	3.094362000
H	−4.454039000	−1.812075000	1.957841000

$^{4}R_{2}$:

Fe	−0.086129000	0.293675000	0.112516000
N	−0.118532000	0.162743000	2.040430000
N	1.795444000	−0.124651000	−0.024754000
N	−0.019092000	1.092354000	−1.618091000
N	−1.679873000	1.339856000	0.173022000
C	−1.197213000	0.438738000	2.863405000
C	−0.876166000	0.002560000	4.198883000
C	0.394091000	−0.534967000	4.168080000
C	0.867520000	−0.435242000	2.811541000
C	2.558443000	−0.689264000	0.986575000
C	3.841683000	−1.056494000	0.444927000
C	3.835726000	−0.711973000	−0.890715000
C	2.551166000	−0.128722000	−1.184771000
C	0.896352000	0.995955000	−2.650855000
C	0.310196000	1.654470000	−3.796418000
C	−0.939147000	2.132929000	−3.416114000
C	−1.125750000	1.764962000	−2.043184000
C	−2.100566000	1.911926000	−0.990598000
C	−3.386279000	2.506708000	−0.770421000
C	−3.719628000	2.268116000	0.558570000
C	−2.631572000	1.529777000	1.159243000
C	−2.395803000	1.075528000	2.450647000
C	2.111130000	−0.839550000	2.306500000
C	2.127291000	0.388962000	−2.435331000
H	−1.527326000	0.100700000	5.055446000
H	0.952425000	−0.952084000	4.993515000
H	4.646351000	−1.511669000	1.003874000
H	4.637045000	−0.836624000	−1.604676000
H	0.776432000	1.763087000	−4.765008000
H	−1.636539000	2.682667000	−4.030009000
H	−3.974569000	3.043106000	−1.499535000
H	−4.618313000	2.586476000	1.066845000
O	−0.697829000	−1.177583000	−0.261388000
H	−2.440983000	−2.737335000	0.735622000
C	−3.193901000	−3.410069000	1.166510000
H	−2.647457000	−4.281688000	1.555557000
H	−3.156365000	1.233054000	3.208503000
H	2.800363000	−1.298109000	3.009135000
H	2.829991000	0.322948000	−3.259816000
C	−4.162400000	−3.867299000	0.063502000
H	−3.628927000	−4.370564000	−0.751469000
H	−4.914465000	−4.564867000	0.456453000
H	−4.696216000	−3.010422000	−0.367690000
C	−3.910509000	−2.700872000	2.327569000
H	−4.650863000	−3.359638000	2.801220000
H	−3.199053000	−2.381621000	3.098760000
H	−4.439969000	−1.807715000	1.970212000

$^{2}R_{3}$:

Fe	0.023509000	0.225504000	0.141372000
N	−0.004893000	0.140752000	2.070128000
N	1.932744000	−0.043138000	0.015723000
N	0.028884000	0.974325000	−1.612835000
N	−1.650374000	1.136478000	0.170772000
C	−1.110625000	0.335355000	2.880804000
C	−0.760454000	−0.038149000	4.226923000
C	0.554850000	−0.455012000	4.216053000
C	1.026469000	−0.346680000	2.859428000
C	2.738565000	−0.507736000	1.044129000
C	4.050248000	−0.777297000	0.515003000
C	4.018967000	−0.474747000	−0.831110000
C	2.690362000	−0.015020000	−1.143824000
C	0.952160000	0.925613000	−2.641696000
C	0.317311000	1.502680000	−3.804846000
C	−0.968232000	1.888009000	−3.438349000
C	−1.128311000	1.543421000	−2.056547000
C	−2.115884000	1.635720000	−1.009853000
C	−3.453741000	2.108573000	−0.810592000
C	−3.773673000	1.866961000	0.521923000
C	−2.624707000	1.253137000	1.146159000
C	−2.362309000	0.843370000	2.447725000
C	2.302329000	−0.656156000	2.368654000
C	2.229010000	0.429301000	−2.409029000
H	−1.428685000	0.013441000	5.073815000
H	1.144045000	−0.798043000	5.054164000
H	4.889942000	−1.142683000	1.088227000
H	4.831038000	−0.549726000	−1.539891000
H	0.776349000	1.623946000	−4.775411000
H	−1.706020000	2.362857000	−4.067373000
H	−4.085435000	2.568650000	−1.555474000
H	−4.703559000	2.102365000	1.018439000
O	−0.485343000	−1.294643000	−0.186502000
H	−2.614577000	−2.348267000	0.698246000
C	−3.495007000	−2.937849000	0.989206000
C	−4.218906000	−2.315160000	2.161889000
C	−5.347943000	−1.499136000	1.969180000
C	−3.766683000	−2.518427000	3.478888000
C	−4.414809000	−1.920804000	4.565679000
C	−5.534533000	−1.104848000	4.357340000
C	−5.999717000	−0.897916000	3.052841000
H	−3.141851000	−3.947120000	1.229880000
H	−6.874645000	−0.277703000	2.879726000
H	−6.044069000	−0.647574000	5.200110000
H	−4.052290000	−2.098871000	5.574153000

H	−2.899026000	−3.149717000	3.649406000
H	−3.148878000	0.918936000	3.190602000
H	3.026393000	−1.032433000	3.084988000
H	2.937334000	0.399255000	−3.230748000
H	−5.716672000	−1.335685000	0.960348000
H	−4.146575000	−3.008663000	0.111785000

$^{4}R_{3}$:

Fe	0.019039000	0.226290000	0.143671000
N	−0.007090000	0.146709000	2.073380000
N	1.928690000	−0.042533000	0.018052000
N	0.026097000	0.977652000	−1.609479000
N	−1.650705000	1.144921000	0.174959000
C	−1.112096000	0.340728000	2.884145000
C	−0.762900000	−0.036024000	4.230201000
C	0.551498000	−0.454191000	4.219061000
C	1.023710000	−0.343921000	2.862433000
C	2.734244000	−0.509007000	1.045992000
C	4.044611000	−0.784211000	0.515866000
C	4.012927000	−0.483505000	−0.830223000
C	2.685316000	−0.018888000	−1.142062000
C	0.948347000	0.925618000	−2.639449000
C	0.313591000	1.501487000	−3.803025000
C	−0.971241000	1.888670000	−3.436249000
C	−1.130453000	1.547077000	−2.053422000
C	−2.117075000	1.641831000	−1.005889000
C	−3.455601000	2.114364000	−0.806875000
C	−3.774853000	1.874845000	0.525810000
C	−2.625294000	1.261903000	1.150540000
C	−2.363201000	0.851039000	2.451269000
C	2.297993000	−0.655432000	2.370679000
C	2.223860000	0.425928000	−2.406771000
H	−1.431709000	0.014241000	5.076705000
H	1.139865000	−0.800285000	5.056489000
H	4.883259000	−1.152661000	1.088635000
H	4.823722000	−0.562817000	−1.540001000
H	0.771647000	1.619650000	−4.774425000
H	−1.708994000	2.363209000	−4.065556000
H	−4.087698000	2.572942000	−1.552333000
H	−4.705084000	2.109500000	1.022030000
O	−0.487791000	−1.297556000	−0.179231000
H	−2.604707000	−2.352823000	0.693654000
C	−3.485269000	−2.942057000	0.985174000
C	−4.210210000	−2.317564000	2.156216000
C	−5.340165000	−1.503265000	1.961462000
C	−3.758261000	−2.517458000	3.473861000
C	−4.407631000	−1.918498000	4.559176000
C	−5.528342000	−1.104411000	4.348756000
C	−5.993181000	−0.900684000	3.043624000
H	−3.132028000	−3.950803000	1.227999000
H	−6.868882000	−0.282009000	2.868872000
H	−6.038931000	−0.646238000	5.190408000
H	−4.045348000	−2.094150000	5.568167000
H	−2.889877000	−3.147296000	3.646019000
H	−3.149738000	0.926573000	3.194218000
H	3.021723000	−1.033340000	3.086586000
H	2.931374000	0.393082000	−3.229157000
H	−5.708758000	−1.342426000	0.952156000
H	−4.136318000	−3.014762000	0.107505000

$^{2}R_{4}$:

Fe	0.027532000	0.223159000	0.125356000
N	0.058899000	0.055221000	2.049236000
N	1.928343000	−0.058557000	−0.072144000
N	−0.014226000	1.047670000	−1.593418000
N	−1.637085000	1.145292000	0.246949000
C	−1.016210000	0.233172000	2.905141000
C	−0.626171000	−0.198679000	4.222297000
C	0.681015000	−0.634817000	4.148963000
C	1.107794000	−0.477544000	2.782834000
C	2.760186000	−0.578541000	0.908781000
C	4.051396000	−0.838326000	0.325969000
C	3.981596000	−0.474445000	−1.003128000
C	2.649221000	0.013353000	−1.252164000
C	0.876144000	1.035373000	−2.652144000
C	0.210890000	1.668968000	−3.768832000
C	−1.057883000	2.049685000	−3.345479000
C	−1.178514000	1.645998000	−1.975130000
C	−2.131852000	1.703536000	−0.894877000
C	−3.451801000	2.192753000	−0.630138000
C	−3.730241000	1.903833000	0.702651000
C	−2.573844000	1.242375000	1.260022000
C	−2.270972000	0.779890000	2.535836000
C	2.364171000	−0.780850000	2.237686000
C	2.153603000	0.517761000	−2.482218000
H	−1.260633000	−0.168305000	5.096115000
H	1.292481000	−1.020379000	4.951810000
H	4.904154000	−1.238603000	0.854882000
H	4.769737000	−0.526131000	−1.740396000
H	0.640696000	1.828138000	−4.747270000
H	−1.810140000	2.558243000	−3.929367000
H	−4.099144000	2.695607000	−1.332691000
H	−4.636524000	2.142579000	1.240160000
O	−0.501581000	−1.277009000	−0.255862000
H	−2.164890000	−2.630480000	1.009594000
C	−2.916511000	−3.263314000	1.500396000
C	−4.116604000	−2.461787000	1.922234000
C	−4.582659000	−2.357791000	3.174103000
H	−2.445720000	−3.759915000	2.356264000
H	−4.105184000	−2.872703000	4.005134000
H	−3.025340000	0.850574000	3.311693000
H	3.105358000	−1.196488000	2.913562000
H	2.835801000	0.517052000	−3.326248000
H	−3.198970000	−4.036509000	0.771906000
H	−4.632522000	−1.929340000	1.121317000
H	−5.461756000	−1.766045000	3.414585000

$^{4}R_{4}$:

Fe	0.021363000	0.224100000	0.122785000
N	0.054628000	0.055549000	2.047385000
N	1.922298000	−0.059474000	−0.075355000
N	−0.017312000	1.056895000	−1.592177000
N	−1.637678000	1.155759000	0.249343000
C	−1.019241000	0.232344000	2.903971000
C	−0.630820000	−0.207007000	4.219737000
C	0.674626000	−0.646525000	4.144718000
C	1.102205000	−0.484195000	2.779005000
C	2.752870000	−0.585534000	0.903397000
C	4.042403000	−0.850743000	0.318915000
C	3.972964000	−0.484387000	−1.009141000
C	2.642430000	0.010790000	−1.255850000
C	0.871968000	1.043424000	−2.652047000
C	0.207863000	1.679995000	−3.767285000
C	−1.059881000	2.062840000	−3.342550000
C	−1.180217000	1.658092000	−1.972446000
C	−2.132424000	1.716006000	−0.891024000
C	−3.452196000	2.206669000	−0.624892000
C	−3.730272000	1.916476000	0.707238000
C	−2.574320000	1.251984000	1.263103000

C	−2.272583000	0.784643000	2.536661000
C	2.356362000	−0.789541000	2.232061000
C	2.147475000	0.520112000	−2.483696000
H	−1.265760000	−0.179274000	5.093288000
H	1.284605000	−1.038410000	4.945627000
H	4.893393000	−1.256882000	0.846174000
H	4.759853000	−0.539019000	−1.747543000
H	0.636936000	1.838673000	−4.746109000
H	−1.811376000	2.573830000	−3.925311000
H	−4.099129000	2.711275000	−1.326557000
H	−4.636370000	2.154731000	1.245272000
O	−0.507277000	−1.277978000	−0.258926000
H	−2.154025000	−2.632023000	1.004844000
C	−2.899700000	−3.266463000	1.502742000
C	−4.101706000	−2.469270000	1.927169000
C	−4.561209000	−2.360759000	3.181108000
H	−2.421807000	−3.756534000	2.358455000
H	−4.076274000	−2.868555000	4.012201000
H	−3.026535000	0.854883000	3.312984000
H	3.096586000	−1.209954000	2.906140000
H	2.828734000	0.518321000	−3.328567000
H	−3.182062000	−4.044602000	0.779483000
H	−4.625185000	−1.944110000	1.126314000
H	−5.442166000	−1.772479000	3.423325000

$^{2}R_{5}$:

Fe	−0.097301000	0.500768000	0.819387000
N	0.796592000	1.101913000	2.423301000
N	1.486721000	−0.316342000	0.074231000
N	−0.865074000	0.564411000	−0.923832000
N	−1.466795000	1.794288000	1.114072000
C	0.242709000	1.879306000	3.428596000
C	1.163848000	1.916408000	4.534964000
C	2.264002000	1.158864000	4.188036000
C	2.029294000	0.646963000	2.863081000
C	2.640467000	−0.608067000	0.788979000
C	3.507945000	−1.401326000	−0.043367000
C	2.864712000	−1.582076000	−1.250486000
C	1.596692000	−0.902810000	−1.174655000
C	−0.554173000	−0.091863000	−2.102100000
C	−1.614576000	0.204111000	−3.040860000
C	−2.526877000	1.035144000	−2.401652000
C	−2.037025000	1.245885000	−1.070494000
C	−2.390273000	1.969566000	0.125295000
C	−3.409989000	2.854392000	0.603486000
C	−3.067863000	3.197581000	1.909040000
C	−1.829905000	2.526894000	2.229632000
C	−1.004908000	2.545924000	3.349320000
C	2.879940000	−0.163184000	2.094875000
C	0.627425000	−0.811757000	−2.207901000
H	1.002961000	2.456757000	5.456641000
H	3.149356000	0.975061000	4.779144000
H	4.481938000	−1.769190000	0.244949000
H	3.227516000	−2.121186000	−2.113623000
H	−1.667299000	−0.151189000	−4.059791000
H	−3.431396000	1.448715000	−2.821040000
H	−4.271849000	3.194057000	0.049199000
H	−3.611760000	3.860396000	2.566406000
O	−0.827484000	−0.835396000	1.419057000
H	−2.610769000	−3.801645000	2.486476000
C	−3.246569000	−4.021675000	1.618190000
C	−4.408982000	−3.045504000	1.581432000
C	−4.182210000	−1.659811000	1.685921000
C	−5.729558000	−3.498460000	1.424753000
C	−6.800164000	−2.597156000	1.374005000
C	−6.563388000	−1.222512000	1.480101000
C	−5.250483000	−0.757984000	1.635858000
H	−3.633305000	−5.039574000	1.760227000
H	−5.056394000	0.307602000	1.719727000
H	−7.391848000	−0.520952000	1.444299000
H	−7.814115000	−2.968472000	1.254899000
H	−5.919576000	−4.566040000	1.345369000
H	−1.310326000	3.126260000	4.214051000
H	3.820371000	−0.458116000	2.550249000
H	0.851071000	−1.319506000	−3.140495000
C	−2.371501000	−3.975719000	0.346129000
H	−1.569312000	−4.721877000	0.401873000
H	−2.971433000	−4.182990000	−0.548210000
H	−1.908685000	−2.989647000	0.234173000
H	−3.165081000	−1.292931000	1.800093000

$^{4}R_{5}$:

Fe	−0.070944000	0.489140000	0.667501000
N	0.632372000	0.954163000	2.406324000
N	1.590988000	−0.272456000	0.043572000
N	−0.633290000	0.703985000	−1.141837000
N	−1.465635000	1.767824000	0.907311000
C	−0.036378000	1.645955000	3.402883000
C	0.749120000	1.581241000	4.609043000
C	1.883971000	0.848645000	4.329275000
C	1.807335000	0.453777000	2.946338000
C	2.656050000	−0.629271000	0.858658000
C	3.615044000	−1.358660000	0.069337000
C	3.114662000	−1.436590000	−1.213753000
C	1.844391000	−0.756599000	−1.228148000
C	−0.189269000	0.141695000	−2.326156000
C	−1.137461000	0.516513000	−3.351722000
C	−2.119794000	1.298589000	−2.754967000
C	−1.783518000	1.400673000	−1.364770000
C	−2.272714000	2.026775000	−0.161408000
C	−3.345697000	2.873010000	0.269254000
C	−3.155658000	3.107043000	1.628204000
C	−1.957774000	2.407136000	2.031554000
C	−1.268561000	2.326336000	3.235855000
C	2.742058000	−0.294371000	2.216201000
C	0.999238000	−0.575272000	−2.353440000
H	0.479270000	2.040806000	5.548865000
H	2.694313000	0.607474000	5.001739000
H	4.550193000	−1.755981000	0.436348000
H	3.574860000	−1.906655000	−2.070818000
H	−1.073695000	0.243924000	−4.395233000
H	−2.971761000	1.750412000	−3.240016000
H	−4.142066000	3.258763000	−0.349062000
H	−3.773958000	3.716085000	2.271701000
O	−0.853785000	−0.892344000	1.069093000
H	−2.163064000	−3.202742000	1.740779000
C	−3.073247000	−3.765077000	1.502479000
C	−4.286346000	−2.898145000	1.785025000
C	−4.194293000	−1.497084000	1.703531000
C	−5.530973000	−3.471775000	2.099270000
C	−6.656249000	−2.670589000	2.323380000
C	−6.553660000	−1.276858000	2.236256000
C	−5.318772000	−0.693792000	1.926642000
H	−3.092062000	−4.649796000	2.153890000
H	−5.226448000	0.386757000	1.861808000
H	−7.425514000	−0.653447000	2.412319000
H	−7.608606000	−3.132032000	2.568995000
H	−5.615892000	−4.553439000	2.173026000

H	−1.674090000	2.832892000	4.105759000
H	3.624533000	−0.632833000	2.750637000
H	1.329202000	−1.007427000	−3.292664000
C	−2.997612000	−4.223824000	0.028974000
H	−2.118122000	−4.857731000	−0.136969000
H	−3.890496000	−4.794220000	−0.254801000
H	−2.922649000	−3.357528000	−0.637870000
H	−3.232235000	−1.046767000	1.472818000

$^{2}R_{6}$:

Fe	0.069300000	−0.171718000	−0.008378000
N	0.009946000	−0.223401000	1.921713000
N	1.995171000	−0.247431000	−0.092725000
N	0.034966000	0.542695000	−1.775479000
N	−1.690908000	0.564491000	−0.028779000
C	−1.124572000	−0.109178000	2.712146000
C	−0.763342000	−0.416813000	4.071290000
C	0.584277000	−0.716674000	4.088068000
C	1.065031000	−0.596622000	2.737204000
C	2.820892000	−0.627109000	0.957871000
C	4.161580000	−0.785169000	0.454546000
C	4.129126000	−0.500259000	−0.893779000
C	2.770253000	−0.166034000	−1.236772000
C	0.980547000	0.570989000	−2.785100000
C	0.314513000	1.061714000	−3.971524000
C	−1.010157000	1.320631000	−3.637499000
C	−1.164172000	0.984217000	−2.252235000
C	−2.177895000	0.997739000	−1.227275000
C	−3.553713000	1.356310000	−1.059239000
C	−3.872964000	1.120364000	0.275347000
C	−2.686567000	0.621915000	0.929076000
C	−2.405026000	0.277715000	2.247527000
C	2.375933000	−0.799266000	2.272789000
C	2.294914000	0.211233000	−2.519431000
H	−1.442117000	−0.397775000	4.911782000
H	1.188415000	−0.985962000	4.942197000
H	5.015444000	−1.086114000	1.042818000
H	4.955798000	−0.521929000	−1.588504000
H	0.779679000	1.212868000	−4.934952000
H	−1.778986000	1.707408000	−4.289223000
H	−4.210994000	1.742878000	−1.823493000
H	−4.827490000	1.292495000	0.751415000
O	−0.262779000	−1.744908000	−0.314967000
H	−3.201654000	0.330091000	2.982837000
H	3.114444000	−1.106940000	3.005762000
H	3.020378000	0.238938000	−3.325955000
C	3.934775000	−4.678237000	0.957040000
C	2.957183000	−4.557243000	−0.065824000
C	5.294136000	−4.760537000	0.634300000
C	3.239608000	−4.690863000	2.251651000
C	3.338315000	−4.518424000	−1.403919000
C	1.585152000	−4.484519000	0.572922000
C	5.670475000	−4.721828000	−0.715702000
H	6.046707000	−4.858320000	1.411838000
C	1.903966000	−4.582745000	2.051533000
H	3.738298000	−4.780792000	3.209868000
C	4.703996000	−4.601579000	−1.725213000
H	2.595236000	−4.423971000	−2.190543000
H	0.930067000	−5.305638000	0.244008000
H	1.050755000	−3.554546000	0.322981000
H	6.720935000	−4.789017000	−0.983465000
H	1.141576000	−4.565291000	2.820637000
H	5.014216000	−4.576147000	−2.765615000

$^{4}R_{6}$:

Fe	0.066944000	−0.172194000	−0.005127000
N	0.010480000	−0.213118000	1.926086000
N	1.993450000	−0.246017000	−0.090231000
N	0.032414000	0.540533000	−1.773014000
N	−1.690512000	0.570736000	−0.024747000
C	−1.122641000	−0.097397000	2.717070000
C	−0.761237000	−0.404412000	4.076849000
C	0.585608000	−0.705676000	4.093299000
C	1.065990000	−0.587100000	2.741753000
C	2.819840000	−0.624485000	0.960381000
C	4.159563000	−0.787968000	0.456150000
C	4.126077000	−0.508074000	−0.892949000
C	2.767380000	−0.171038000	−1.235237000
C	0.977052000	0.564707000	−2.784101000
C	0.310424000	1.051487000	−3.971494000
C	−1.013893000	1.311638000	−3.637210000
C	−1.166593000	0.980516000	−2.250363000
C	−2.179054000	0.998348000	−1.224053000
C	−3.555689000	1.356576000	−1.056250000
C	−3.873524000	1.126231000	0.279097000
C	−2.685940000	0.630884000	0.934036000
C	−2.403392000	0.290047000	2.252329000
C	2.375229000	−0.792132000	2.276227000
C	2.290922000	0.203454000	−2.518080000
H	−1.439926000	−0.384504000	4.917383000
H	1.189743000	−0.975760000	4.947182000
H	5.013113000	−1.090036000	1.044278000
H	4.951596000	−0.535118000	−1.588855000
H	0.774519000	1.198311000	−4.936096000
H	−1.783215000	1.696346000	−4.289584000
H	−4.213829000	1.739275000	−1.821705000
H	−4.828049000	1.298640000	0.755059000
O	−0.263424000	−1.749507000	−0.301976000
H	−3.199270000	0.344629000	2.988331000
H	3.114264000	−1.098957000	3.009140000
H	3.015600000	0.227495000	−3.325513000
C	3.933969000	−4.679105000	0.952960000
C	2.961797000	−4.559469000	−0.075222000
C	5.294759000	−4.765622000	0.637279000
C	3.232298000	−4.685430000	2.244071000
C	3.349727000	−4.526384000	−1.411525000
C	1.586750000	−4.480500000	0.556346000
C	5.677951000	−4.732556000	−0.710944000
H	6.043257000	−4.862302000	1.418888000
C	1.897906000	−4.574566000	2.036778000
H	3.725923000	−4.773325000	3.205103000
C	4.716811000	−4.613764000	−1.725716000
H	2.610788000	−4.433177000	−2.202203000
H	0.930806000	−5.300697000	0.226829000
H	1.056291000	−3.549628000	0.300724000
H	6.729597000	−4.803065000	−0.973171000
H	1.131715000	−4.552265000	2.801965000
H	5.032297000	−4.592808000	−2.764649000

$^{2}R_{7}$:

Fe	0.347859000	−0.424758000	0.162017000
N	0.349689000	−0.886371000	2.036730000
N	2.136612000	0.303946000	0.193502000
N	−0.006309000	0.556747000	−1.434057000
N	−1.557780000	−0.475574000	0.164230000
C	−0.713153000	−1.419377000	2.748430000
C	−0.234671000	−1.826247000	4.044292000
C	1.112980000	−1.535078000	4.102595000

C	1.478581000	–0.949326000	2.838877000
C	3.058035000	0.103528000	1.211460000
C	4.333155000	0.619546000	0.785189000
C	4.166323000	1.122988000	–0.488655000
C	2.788668000	0.923752000	–0.859050000
C	0.827393000	1.164406000	–2.356001000
C	–0.001143000	1.568861000	–3.470212000
C	–1.309799000	1.197726000	–3.181825000
C	–1.288653000	0.559847000	–1.898008000
C	–2.200039000	–0.048321000	–0.960752000
C	–3.596032000	–0.339349000	–0.828230000
C	–3.764225000	–0.960811000	0.406878000
C	–2.467982000	–1.042277000	1.037860000
C	–2.046005000	–1.515851000	2.275493000
C	2.743452000	–0.492607000	2.439803000
C	2.178356000	1.321507000	–2.076729000
H	–0.846065000	–2.271110000	4.815531000
H	1.787123000	–1.700388000	4.930480000
H	5.237952000	0.609262000	1.375449000
H	4.912720000	1.594784000	–1.111287000
H	0.344902000	2.082690000	–4.355424000
H	–2.180358000	1.361002000	–3.798967000
H	–4.366956000	–0.111159000	–1.548740000
H	–4.692552000	–1.307993000	0.836426000
O	0.667105000	–1.904873000	–0.458685000
H	–0.466503000	–3.993980000	–0.199835000
C	–0.732629000	–5.046793000	0.000951000
C	–1.797721000	–5.097677000	1.081052000
C	–3.154367000	–4.996109000	0.710446000
C	–3.499844000	–4.837655000	–0.759441000
C	–2.548309000	–5.605650000	–1.659793000
C	–1.192665000	–5.703035000	–1.288198000
C	–0.301682000	–6.398290000	–2.118227000
C	–0.741743000	–6.987501000	–3.308093000
C	–2.089197000	–6.893468000	–3.674268000
C	–2.985590000	–6.207625000	–2.847941000
C	–1.466058000	–5.236313000	2.436909000
C	–2.461081000	–5.264842000	3.421033000
C	–3.807900000	–5.162623000	3.052078000
C	–4.147260000	–5.033709000	1.700145000
H	0.189570000	–5.520297000	0.357836000
H	0.742721000	–6.476339000	–1.828539000
H	–0.039444000	–7.521649000	–3.940763000
H	–2.440579000	–7.355210000	–4.591955000
H	–4.034512000	–6.139433000	–3.125399000
H	–3.454008000	–3.765682000	–1.019029000
H	–4.534496000	–5.151204000	–0.943110000
H	–5.192644000	–4.971109000	1.408069000
H	–4.587476000	–5.199938000	3.807165000
H	–2.187822000	–5.382094000	4.465590000
H	–0.420862000	–5.322288000	2.720793000
H	–2.771112000	–1.982448000	2.933357000
H	3.552103000	–0.597047000	3.156787000
H	2.814249000	1.801021000	–2.813884000

C	1.482927000	–0.950397000	2.839575000
C	3.058923000	0.099940000	1.207089000
C	4.334417000	0.612050000	0.776860000
C	4.165493000	1.113934000	–0.496945000
C	2.785871000	0.917981000	–0.863255000
C	0.820368000	1.161601000	–2.354992000
C	–0.009727000	1.565172000	–3.467766000
C	–1.318036000	1.194748000	–3.176317000
C	–1.294625000	0.559070000	–1.891471000
C	–2.204002000	–0.047689000	–0.951047000
C	–3.600058000	–0.340990000	–0.816570000
C	–3.765887000	–0.960654000	0.419163000
C	–2.468245000	–1.039700000	1.048856000
C	–2.043612000	–1.513770000	2.284422000
C	2.746054000	–0.495213000	2.436668000
C	2.172517000	1.315903000	–2.078827000
H	–0.836648000	–2.275018000	4.820258000
H	1.797085000	–1.706590000	4.928858000
H	5.240861000	0.599461000	1.364515000
H	4.911454000	1.582594000	–1.122477000
H	0.334847000	2.076880000	–4.354762000
H	–2.189706000	1.357645000	–3.792003000
H	–4.371965000	–0.115096000	–1.536739000
H	–4.692877000	–1.310192000	0.849661000
O	0.668522000	–1.910955000	–0.454270000
H	–0.463092000	–3.991592000	–0.198646000
C	–0.731908000	–5.043691000	0.002727000
C	–1.801416000	–5.091447000	1.078545000
C	–3.156515000	–4.989446000	0.702417000
C	–3.496069000	–4.833253000	–0.769095000
C	–2.541557000	–5.603458000	–1.664405000
C	–1.187515000	–5.701438000	–1.287186000
C	–0.293846000	–6.398732000	–2.112628000
C	–0.729637000	–6.989349000	–3.303355000
C	–2.075530000	–6.894704000	–3.675098000
C	–2.974609000	–6.206827000	–2.853402000
C	–1.475363000	–5.227891000	2.436017000
C	–2.474340000	–5.253989000	3.416225000
C	–3.819615000	–5.151502000	3.041715000
C	–4.153410000	–5.024683000	1.688196000
H	0.188077000	–5.518043000	0.364214000
H	0.749321000	–6.477191000	–1.818639000
H	–0.025262000	–7.525041000	–3.932404000
H	–2.423636000	–7.357515000	–4.593498000
H	–4.022354000	–6.138122000	–3.135169000
H	–3.448422000	–3.761752000	–1.030283000
H	–4.530226000	–5.146362000	–0.956301000
H	–5.197576000	–4.962012000	1.391778000
H	–4.602256000	–5.187103000	3.793713000
H	–2.205351000	–5.369771000	4.462062000
H	–0.431382000	–5.314238000	2.724221000
H	–2.767050000	–1.981037000	2.943658000
H	3.556838000	–0.600687000	3.151190000
H	2.807236000	1.793573000	–2.818294000

$^{4}R_{7}$:

Fe	0.346116000	–0.428318000	0.163582000
N	0.351069000	–0.884872000	2.040482000
N	2.134884000	0.301320000	0.191765000
N	–0.011776000	0.555985000	–1.429975000
N	–1.559820000	–0.471800000	0.173422000
C	–0.708992000	–1.418518000	2.754253000
C	–0.227078000	–1.828580000	4.048487000
C	1.120436000	–1.538489000	4.103583000

$^{2}R_{8}$:

Fe	–0.313901000	0.199895000	0.263274000
N	–0.464954000	0.167240000	2.188226000
N	1.504800000	–0.450930000	0.253156000
N	–0.060266000	0.894055000	–1.495335000
N	–1.769219000	1.429837000	0.185155000
C	–1.544333000	0.609718000	2.933965000
C	–1.351048000	0.203065000	4.302464000
C	–0.157643000	–0.485592000	4.368718000

C	0.396809000	−0.509301000	3.039789000
C	2.137688000	−1.052437000	1.329528000
C	3.393936000	−1.594214000	0.881289000
C	3.502999000	−1.314545000	−0.466140000
C	2.317046000	−0.598895000	−0.860116000
C	0.892374000	0.643329000	−2.466198000
C	0.456602000	1.315965000	−3.668164000
C	−0.743720000	1.959131000	−3.382010000
C	−1.050113000	1.677777000	−2.011060000
C	−2.053623000	1.991580000	−1.024391000
C	−3.266403000	2.746340000	−0.904967000
C	−3.697423000	2.613189000	0.410634000
C	−2.741769000	1.779535000	1.104834000
C	−2.633141000	1.363869000	2.425730000
C	1.603983000	−1.087701000	2.626992000
C	2.028309000	−0.094227000	−2.152936000
H	−2.030829000	0.418372000	5.114115000
H	0.298862000	−0.929718000	5.241167000
H	4.106335000	−2.112981000	1.506022000
H	4.322092000	−1.565512000	−1.124561000
H	0.986344000	1.325318000	−4.609792000
H	−1.332320000	2.561980000	−4.056991000
H	−3.744791000	3.313620000	−1.689050000
H	−4.576086000	3.061463000	0.851525000
O	−1.088323000	−1.200160000	−0.078304000
H	−3.407774000	1.648171000	3.130577000
H	2.187329000	−1.601970000	3.383914000
H	2.762627000	−0.280241000	−2.930179000
H	0.184452000	−5.351787000	4.722061000
C	−0.030703000	−5.802116000	3.737094000
C	−1.435883000	−5.448137000	3.307293000
C	1.013718000	−5.368472000	2.734294000
H	0.045990000	−6.890361000	3.910117000
C	−1.724952000	−4.848940000	2.143977000
H	−2.235524000	−5.706041000	3.999777000
C	0.719529000	−4.769243000	1.571622000
H	2.051755000	−5.572126000	2.994116000
C	−0.686281000	−4.451794000	1.124129000
H	−2.759762000	−4.620297000	1.895495000
H	1.520554000	−4.483041000	0.892170000
H	−0.893370000	−4.959434000	0.165343000
H	−0.778092000	−3.379251000	0.887438000

$^{4}R_{8}$:

Fe	−0.315442000	0.195221000	0.259886000
N	−0.470181000	0.157666000	2.185044000
N	1.506953000	−0.447379000	0.253701000
N	−0.055514000	0.901454000	−1.493004000
N	−1.770823000	1.425200000	0.183518000
C	−1.553424000	0.592357000	2.929213000
C	−1.364566000	0.177947000	4.296469000
C	−0.169803000	−0.507506000	4.363451000
C	0.389932000	−0.521759000	3.036384000
C	2.137377000	−1.053809000	1.329267000
C	3.395064000	−1.593800000	0.881913000
C	3.507418000	−1.308603000	−0.463625000
C	2.322034000	−0.590966000	−0.857542000
C	0.900207000	0.655837000	−2.462688000
C	0.465241000	1.330318000	−3.664107000
C	−0.737806000	1.968347000	−3.379340000
C	−1.046530000	1.682652000	−2.009371000
C	−2.054010000	1.989808000	−1.024593000
C	−3.270180000	2.739776000	−0.906148000
C	−3.704264000	2.600988000	0.407699000
C	−2.747717000	1.768163000	1.101572000
C	−2.642018000	1.346384000	2.420596000
C	1.599412000	−1.095410000	2.624265000
C	2.036026000	−0.080950000	−2.148967000
H	−2.048518000	0.386172000	5.106467000
H	0.284127000	−0.956391000	5.234792000
H	4.105414000	−2.115930000	1.506167000
H	4.327848000	−1.557175000	−1.121291000
H	0.996779000	1.343095000	−4.604675000
H	−1.326937000	2.570775000	−4.054234000
H	−3.748367000	3.307964000	−1.689700000
H	−4.586204000	3.043994000	0.847349000
O	−1.082480000	−1.209886000	−0.085776000
H	−3.419877000	1.625258000	3.124132000
H	2.181112000	−1.612405000	3.380658000
H	2.772711000	−0.262905000	−2.924986000
H	0.198370000	−5.320153000	4.724417000
C	−0.019479000	−5.779551000	3.744223000
C	−1.427354000	−5.433181000	3.317042000
C	1.019679000	−5.351813000	2.733420000
H	0.060942000	−6.866044000	3.926361000
C	−1.722721000	−4.844450000	2.149956000
H	−2.223525000	−5.687824000	4.014720000
C	0.719087000	−4.763027000	1.567007000
H	2.059285000	−5.551164000	2.990349000
C	−0.689260000	−4.452288000	1.122941000
H	−2.759193000	−4.620994000	1.903680000
H	1.516545000	−4.480833000	0.881711000
H	−0.898940000	−4.967532000	0.168798000
H	−0.784540000	−3.381662000	0.878687000

$^{2}R_{9}$:

Fe	−0.045606000	−0.152750000	0.297082000
N	−0.031779000	−0.045956000	2.224930000
N	1.873081000	−0.008164000	0.134579000
N	−0.227264000	0.405275000	−1.518657000
N	−1.874656000	0.377486000	0.300292000
C	−1.139837000	−0.006747000	3.051476000
C	−0.699126000	−0.159244000	4.415300000
C	0.673659000	−0.291588000	4.398394000
C	1.094482000	−0.222967000	3.021562000
C	2.772870000	−0.185475000	1.170794000
C	4.105209000	−0.213514000	0.627108000
C	3.993005000	−0.056473000	−0.739437000
C	2.592880000	0.071653000	−1.050693000
C	0.669647000	0.462682000	−2.568263000
C	−0.087192000	0.777071000	−3.754591000
C	−1.423813000	0.907785000	−3.382191000
C	−1.488028000	0.668315000	−1.973358000
C	−2.453536000	0.648136000	−0.904897000
C	−3.861345000	0.845464000	−0.704573000
C	−4.104008000	0.675432000	0.650742000
C	−2.838863000	0.382949000	1.294431000
C	−2.480390000	0.180156000	2.616447000
C	2.396344000	−0.297474000	2.521142000
C	2.031080000	0.280479000	−2.330828000
H	−1.348784000	−0.155478000	5.278474000
H	1.333586000	−0.415948000	5.244779000
H	5.010995000	−0.330955000	1.204029000
H	4.793731000	−0.020756000	−1.464102000
H	0.322390000	0.904522000	−4.746258000
H	−2.254412000	1.153223000	−4.026747000
H	−4.587063000	1.072071000	−1.470375000
H	−5.057213000	0.752833000	1.152970000

O	−0.198041000	−1.774679000	0.121659000
H	−1.980301000	−3.241686000	0.933576000
C	−2.896973000	−3.836844000	0.857937000
C	−3.760439000	−3.671114000	2.089648000
C	−5.152490000	−3.906577000	1.982059000
C	−5.045665000	−3.713100000	−0.453964000
C	−3.653471000	−3.469241000	−0.400675000
C	−3.003422000	−2.947665000	−1.522495000
C	−3.703188000	−2.693366000	−2.709488000
C	−5.075379000	−2.955191000	−2.765888000
C	−5.749816000	−3.449835000	−1.644692000
C	−3.217092000	−3.350722000	3.336400000
C	−4.016882000	−3.282243000	4.485243000
C	−5.388406000	−3.528420000	4.376542000
C	−5.958425000	−3.827433000	3.134859000
H	−2.577224000	−4.892216000	0.786973000
H	−1.939260000	−2.742171000	−1.453765000
H	−3.180517000	−2.298164000	−3.574533000
H	−5.633091000	−2.762120000	−3.677624000
H	−6.820746000	−3.605673000	−1.696990000
H	−7.029359000	−3.976278000	3.067563000
H	−6.025254000	−3.477001000	5.254564000
H	−3.572982000	−3.048913000	5.447763000
H	−2.148775000	−3.167029000	3.406044000
H	−3.252845000	0.175047000	3.377479000
H	3.195431000	−0.437964000	3.242608000
H	2.717947000	0.327988000	−3.169927000
N	−5.701135000	−4.190253000	0.709064000
C	−7.057472000	−4.721467000	0.607172000
H	−7.833389000	−3.940437000	0.629207000
H	−7.156714000	−5.280523000	−0.325973000
H	−7.239168000	−5.412858000	1.433193000

$^{4}R_{9}$:

Fe	−0.046401000	−0.149459000	0.296062000
N	−0.030266000	−0.045088000	2.224366000
N	1.873302000	−0.000690000	0.132468000
N	−0.227729000	0.418918000	−1.516500000
N	−1.874461000	0.383961000	0.301844000
C	−1.137532000	−0.010081000	3.051973000
C	−0.695883000	−0.168210000	4.414793000
C	0.677096000	−0.299338000	4.396264000
C	1.096076000	−0.224899000	3.019645000
C	2.774361000	−0.184029000	1.168179000
C	4.106189000	−0.215419000	0.622408000
C	3.992621000	−0.054471000	−0.743182000
C	2.591985000	0.079323000	−1.051793000
C	0.668854000	0.475816000	−2.567675000
C	−0.090415000	0.789249000	−3.754087000
C	−1.425860000	0.918464000	−3.380476000
C	−1.488253000	0.679685000	−1.970293000
C	−2.454250000	0.657035000	−0.901505000
C	−3.861677000	0.853547000	−0.699982000
C	−4.103343000	0.681107000	0.655624000
C	−2.838452000	0.387066000	1.296779000
C	−2.477786000	0.178869000	2.617758000
C	2.398212000	−0.298588000	2.516754000
C	2.028633000	0.292213000	−2.332243000
H	−1.344860000	−0.168750000	5.278493000
H	1.337749000	−0.427592000	5.241466000
H	5.012310000	−0.338349000	1.197673000
H	4.792210000	−0.020609000	−1.469156000
H	0.317871000	0.915330000	−4.746464000
H	−2.257768000	1.161934000	−4.024040000
H	−4.588084000	1.082112000	−1.464567000
H	−5.056285000	0.756945000	1.158531000
O	−0.197098000	−1.773364000	0.121560000
H	−1.980367000	−3.245608000	0.936462000
C	−2.897353000	−3.840269000	0.861742000
C	−3.762796000	−3.669367000	2.091474000
C	−5.154378000	−3.907001000	1.982544000
C	−5.043708000	−3.722973000	−0.454019000
C	−3.652047000	−3.476920000	−0.399315000
C	−3.000881000	−2.957425000	−1.521520000
C	−3.699135000	−2.708055000	−2.710501000
C	−5.070730000	−2.972066000	−2.768223000
C	−5.746323000	−3.464221000	−1.646457000
C	−3.221925000	−3.342403000	3.337613000
C	−4.023769000	−3.269436000	4.484845000
C	−5.394740000	−3.517678000	4.374850000
C	−5.962313000	−3.823229000	3.133512000
H	−2.578799000	−4.896295000	0.795179000
H	−1.937085000	−2.750285000	−1.451552000
H	−3.175674000	−2.315131000	−3.576156000
H	−5.627292000	−2.782867000	−3.681502000
H	−6.816929000	−3.621939000	−1.700084000
H	−7.032939000	−3.973874000	3.065146000
H	−6.033197000	−3.463080000	5.251537000
H	−3.581744000	−3.031540000	5.447138000
H	−2.153850000	−3.157527000	3.408197000
H	−3.249859000	0.170878000	3.379285000
H	3.197332000	−0.442075000	3.237724000
H	2.715067000	0.339997000	−3.171683000
N	−5.700069000	−4.197754000	0.709820000
C	−7.055835000	−4.730014000	0.607838000
H	−7.832472000	−3.949494000	0.625660000
H	−7.153283000	−5.292693000	−0.323346000
H	−7.238476000	−5.418400000	1.436208000

$^{2}R_{10}$:

Fe	0.037230000	−0.087326000	−0.011767000
N	0.002799000	0.102509000	1.909289000
N	1.964878000	−0.056464000	−0.121956000
N	−0.061960000	0.395837000	−1.854650000
N	−1.759476000	0.540005000	−0.088032000
C	−1.125050000	0.236577000	2.698883000
C	−0.732588000	0.118408000	4.080599000
C	0.630953000	−0.088185000	4.111360000
C	1.093695000	−0.101122000	2.746629000
C	2.823961000	−0.236485000	0.948492000
C	4.167216000	−0.362727000	0.447164000
C	4.102194000	−0.261700000	−0.927726000
C	2.720748000	−0.070584000	−1.286497000
C	0.865980000	0.354587000	−2.878089000
C	0.160851000	0.653929000	−4.100240000
C	−1.175777000	0.874819000	−3.775040000
C	−1.292595000	0.705473000	−2.359089000
C	−2.287976000	0.787142000	−1.321112000
C	−3.686873000	1.070736000	−1.172701000
C	−3.977061000	0.974953000	0.181216000
C	−2.749381000	0.642486000	0.874912000
C	−2.439720000	0.477475000	2.215220000
C	2.403854000	−0.267919000	2.289505000
C	2.207242000	0.109505000	−2.591900000
H	−1.405468000	0.193868000	4.922439000
H	1.258495000	−0.211847000	4.982105000
H	5.048467000	−0.504054000	1.055852000
H	4.923537000	−0.303515000	−1.628584000

H	0.604422000	0.712037000	–5.083735000
H	–1.973351000	1.133557000	–4.455052000
H	–4.376637000	1.304735000	–1.969000000
H	–4.937860000	1.129175000	0.650222000
O	–0.204418000	–1.704281000	–0.115270000
H	–2.211971000	–2.774178000	0.867284000
C	–3.110796000	–3.396655000	0.786598000
C	–4.036080000	–3.171420000	1.968959000
C	–5.434503000	–3.278433000	1.793840000
C	–5.191993000	–3.260627000	–0.653551000
C	–3.788548000	–3.148291000	–0.549406000
C	–3.049042000	–2.866793000	–1.703691000
C	–3.673949000	–2.730893000	–2.950248000
C	–5.063596000	–2.875812000	–3.046848000
C	–5.823084000	–3.130210000	–1.903179000
C	–3.542288000	–2.922434000	3.254240000
C	–4.397027000	–2.804573000	4.358466000
C	–5.778829000	–2.936199000	4.174987000
C	–6.297355000	–3.163654000	2.898914000
H	–2.751302000	–4.440796000	0.812825000
H	–1.973017000	–2.749678000	–1.612863000
H	–3.080847000	–2.518894000	–3.833854000
H	–5.559370000	–2.781331000	–4.008326000
H	–6.904593000	–3.220859000	–1.970959000
H	–6.950231000	–3.556533000	0.407606000
H	–7.371235000	–3.247877000	2.751111000
H	–6.454354000	–2.854576000	5.020980000
H	–3.988997000	–2.624216000	5.347737000
H	–2.468053000	–2.832027000	3.390252000
H	–3.232487000	0.547223000	2.951896000
H	3.172769000	–0.420044000	3.040799000
H	2.918908000	0.079970000	–3.410885000
N	–5.950290000	–3.471782000	0.507194000

$^{4}R_{10}$:

Fe	0.036425000	–0.084885000	–0.012362000
N	0.002658000	0.100980000	1.909483000
N	1.965407000	–0.051034000	–0.122171000
N	–0.060238000	0.410536000	–1.852070000
N	–1.758894000	0.546585000	–0.087024000
C	–1.125255000	0.230781000	2.699535000
C	–0.733305000	0.105583000	4.080775000
C	0.630341000	–0.100577000	4.110835000
C	1.092765000	–0.106728000	2.746352000
C	2.824444000	–0.238167000	0.948637000
C	4.167476000	–0.367724000	0.446398000
C	4.102497000	–0.261552000	–0.927707000
C	2.721118000	–0.064051000	–1.285145000
C	0.868214000	0.369392000	–2.876264000
C	0.161823000	0.669675000	–4.098798000
C	–1.173919000	0.889433000	–3.773202000
C	–1.290243000	0.719115000	–2.356197000
C	–2.287087000	0.797640000	–1.318593000
C	–3.685764000	1.080879000	–1.169813000
C	–3.976182000	0.981619000	0.184169000
C	–2.749442000	0.646377000	0.876118000
C	–2.439008000	0.474704000	2.215808000
C	2.403529000	–0.273091000	2.287693000
C	2.207483000	0.121744000	–2.591262000
H	–1.406492000	0.176276000	4.922784000
H	1.257666000	–0.229304000	4.980968000
H	5.048221000	–0.515327000	1.054339000
H	4.923229000	–0.304789000	–1.629160000
H	0.604934000	0.727311000	–5.082528000
H	–1.972209000	1.147566000	–4.452556000
H	–4.375366000	1.317797000	–1.965406000
H	–4.937159000	1.134099000	0.653317000
O	–0.204379000	–1.703615000	–0.116211000
H	–2.211349000	–2.780984000	0.863794000
C	–3.111694000	–3.401625000	0.786658000
C	–4.036223000	–3.168429000	1.968177000
C	–5.434762000	–3.275859000	1.794084000
C	–5.192997000	–3.271895000	–0.653536000
C	–3.789686000	–3.158400000	–0.550285000
C	–3.050411000	–2.881346000	–1.705861000
C	–3.675499000	–2.752112000	–2.953070000
C	–5.064919000	–2.898440000	–3.048678000
C	–5.824211000	–3.147629000	–1.903527000
C	–3.541768000	–2.912163000	3.251808000
C	–4.395987000	–2.786856000	4.355696000
C	–5.777871000	–2.918325000	4.173304000
C	–6.296993000	–3.153328000	2.898730000
H	–2.755085000	–4.446653000	0.817801000
H	–1.974488000	–2.762874000	–1.615247000
H	–3.082689000	–2.544435000	–3.837943000
H	–5.560975000	–2.809167000	–4.010537000
H	–6.905692000	–3.239153000	–1.970838000
H	–6.950918000	–3.562218000	0.410022000
H	–7.371002000	–3.237798000	2.751922000
H	–6.453171000	–2.831025000	5.018942000
H	–3.987444000	–2.601378000	5.343834000
H	–2.467330000	–2.822632000	3.386970000
H	–3.232105000	0.541330000	2.952541000
H	3.171694000	–0.429079000	3.039091000
H	2.919368000	0.092976000	–3.410085000
N	–5.950907000	–3.477740000	0.508817000

$^2TS_1$:

Fe	−0.026351000	0.027830000	−0.183491000
N	−0.127550000	−0.080233000	1.754214000
N	1.904253000	−0.014506000	−0.202096000
N	0.022656000	0.943195000	−1.862544000
N	−1.742968000	0.866852000	−0.171817000
C	−1.282031000	0.000288000	2.527119000
C	−0.960109000	−0.415867000	3.870145000
C	0.377301000	−0.741501000	3.899191000
C	0.899751000	−0.533294000	2.572725000
C	2.697485000	−0.466168000	0.847017000
C	4.052633000	−0.595317000	0.377232000
C	4.065004000	−0.226678000	−0.949418000
C	2.719957000	0.139312000	−1.316622000
C	0.994337000	1.026568000	−2.846022000
C	0.373060000	1.614409000	−4.007801000
C	−0.955730000	1.872251000	−3.694253000
C	−1.159353000	1.443548000	−2.341078000
C	−2.190983000	1.399736000	−1.356076000
C	−3.563968000	1.771226000	−1.193854000
C	−3.922441000	1.454342000	0.112776000
C	−2.767734000	0.888515000	0.762940000
C	−2.534885000	0.450608000	2.063673000
C	2.215417000	−0.720022000	2.134777000
C	2.294579000	0.617133000	−2.574333000
H	−1.661715000	−0.444461000	4.691578000
H	0.953510000	−1.086694000	4.745429000
H	4.888776000	−0.920786000	0.979010000
H	4.915560000	−0.195216000	−1.615083000
H	0.868436000	1.822156000	−4.945273000
H	−1.697516000	2.320916000	−4.338066000
H	−4.193094000	2.226076000	−1.944462000
H	−4.886523000	1.612668000	0.574434000
O	−0.355912000	−1.663493000	−0.653602000
H	−1.418478000	−2.193512000	−0.693026000
C	−2.598522000	−2.782125000	−0.736805000
H	−2.579527000	−3.240863000	−1.728338000
H	−3.350090000	0.479049000	2.779524000
H	2.933184000	−1.074729000	2.868059000
H	3.043061000	0.692573000	−3.356357000
H	−3.284588000	−1.934024000	−0.680813000
C	−2.639500000	−3.740097000	0.431280000
H	−1.840277000	−4.486208000	0.365002000
H	−2.533298000	−3.211489000	1.384900000
H	−3.597324000	−4.283994000	0.458512000

$^4TS_1$:

Fe	0.054277000	0.116980000	0.083641000
N	0.008282000	0.060828000	2.018108000
N	1.988722000	0.062681000	−0.000218000
N	0.023413000	0.922454000	−1.637986000
N	−1.704437000	0.835207000	0.084310000
C	−1.126677000	0.136660000	2.815871000
C	−0.761681000	−0.218871000	4.163231000
C	0.585426000	−0.514071000	4.167300000
C	1.065925000	−0.343335000	2.820679000
C	2.818301000	−0.335841000	1.040159000
C	4.158361000	−0.475922000	0.530389000
C	4.121198000	−0.161065000	−0.812966000
C	2.760607000	0.177299000	−1.142730000
C	0.970429000	0.979824000	−2.651588000
C	0.298256000	1.498384000	−3.826856000
C	−1.023847000	1.736680000	−3.489612000
C	−1.181603000	1.362140000	−2.107782000
C	−2.192894000	1.326301000	−1.097746000
C	−3.567887000	1.690557000	−0.905992000
C	−3.882765000	1.414828000	0.418981000
C	−2.698382000	0.885759000	1.052187000
C	−2.408230000	0.523573000	2.363952000
C	2.375337000	−0.531926000	2.351858000
C	2.280702000	0.603724000	−2.409706000
H	−1.440410000	−0.237274000	5.003928000
H	1.190359000	−0.817641000	5.009493000
H	5.018829000	−0.772319000	1.112880000
H	4.948180000	−0.152255000	−1.508321000
H	0.763255000	1.673002000	−4.786462000
H	−1.795585000	2.133251000	−4.132371000
H	−4.223313000	2.116691000	−1.651085000
H	−4.831096000	1.586689000	0.907395000
O	−0.389621000	−1.534582000	−0.333200000
H	−1.392193000	−1.897583000	−0.656781000
C	−2.628500000	−2.538249000	−1.028996000
H	−2.346488000	−2.981790000	−1.985368000
H	−3.201637000	0.565385000	3.103734000
H	3.116309000	−0.845615000	3.081010000
H	3.000685000	0.656019000	−3.219860000
C	−2.932126000	−3.491368000	0.098039000
H	−2.139934000	−4.238831000	0.215618000
H	−3.042614000	−2.961487000	1.050720000
H	−3.873362000	−4.036868000	−0.084645000
H	−3.279875000	−1.667406000	−1.125447000

$^2TS_2$:

Fe	0.078674000	0.046548000	0.139258000
N	0.020564000	0.146897000	2.076302000
N	2.006022000	0.108147000	0.075180000
N	0.041389000	0.768905000	−1.632536000
N	−1.682881000	0.784173000	0.100607000
C	−1.121290000	0.248206000	2.864628000
C	−0.749552000	0.006407000	4.237271000
C	0.604601000	−0.238074000	4.268298000
C	1.088382000	−0.152513000	2.913616000
C	2.844427000	−0.181283000	1.145915000
C	4.194380000	−0.292430000	0.657213000
C	4.159218000	−0.074687000	−0.701977000
C	2.789055000	0.176689000	−1.071978000
C	0.986633000	0.791838000	−2.644843000
C	0.310334000	1.209655000	−3.848105000
C	−1.024264000	1.432126000	−3.530154000
C	−1.176597000	1.149312000	−2.133006000
C	−2.184056000	1.158779000	−1.122744000
C	−3.573345000	1.466873000	−0.966878000
C	−3.887556000	1.274241000	0.374940000
C	−2.689780000	0.848669000	1.052663000
C	−2.407250000	0.570679000	2.387066000
C	2.403333000	−0.315237000	2.466184000
C	2.313102000	0.485089000	−2.363141000
H	−1.432678000	0.031202000	5.074219000
H	1.216435000	−0.452298000	5.132606000
H	5.059241000	−0.504813000	1.268838000
H	4.992760000	−0.074213000	−1.389577000
H	0.774126000	1.335475000	−4.815854000

H	−1.802172000	1.766612000	−4.200325000
H	−4.242030000	1.802088000	−1.745760000
H	−4.850488000	1.426324000	0.841045000
O	−0.144833000	−1.695631000	−0.119928000
H	−1.233229000	−2.272222000	−0.353375000
C	−2.294759000	−2.909150000	−0.603653000
H	−3.208851000	0.632233000	3.116015000
H	3.154200000	−0.546932000	3.215253000
H	3.040445000	0.510874000	−3.168002000
C	−2.707717000	−3.545035000	0.712431000
H	−1.942995000	−4.245160000	1.068482000
H	−2.868155000	−2.789918000	1.488981000
H	−3.645790000	−4.109646000	0.592014000
H	−2.967730000	−2.103541000	−0.921175000
C	−1.931039000	−3.859823000	−1.730532000
H	−2.810387000	−4.444427000	−2.044145000
H	−1.558813000	−3.318458000	−2.606476000
H	−1.157288000	−4.568323000	−1.413037000

$^{4}TS_{2}$:

Fe	−0.235083000	0.216042000	0.094581000
N	−0.291772000	0.269673000	2.049553000
N	1.689047000	−0.120461000	0.043011000
N	−0.111999000	0.960316000	−1.674926000
N	−1.828237000	1.296506000	0.061510000
C	−1.382440000	0.614553000	2.829674000
C	−1.072931000	0.306407000	4.204122000
C	0.204581000	−0.214343000	4.236538000
C	0.694035000	−0.231623000	2.880479000
C	2.437776000	−0.578764000	1.112299000
C	3.753810000	−0.925959000	0.635766000
C	3.780595000	−0.665423000	−0.718783000
C	2.483363000	−0.155372000	−1.089535000
C	0.843926000	0.846507000	−2.664280000
C	0.295321000	1.459774000	−3.852429000
C	−0.971683000	1.940831000	−3.534557000
C	−1.205253000	1.616268000	−2.158105000
C	−2.209610000	1.815346000	−1.140898000
C	−3.487213000	2.444808000	−0.982261000
C	−3.850714000	2.288022000	0.352611000
C	−2.787959000	1.568083000	1.016177000
C	−2.572987000	1.212843000	2.346280000
C	1.960296000	−0.643447000	2.431603000
C	2.085897000	0.284711000	−2.377064000
H	−1.734478000	0.475657000	5.041691000
H	0.759417000	−0.542243000	5.103841000
H	4.557941000	−1.307229000	1.248570000
H	4.611854000	−0.797440000	−1.396511000
H	0.797490000	1.543662000	−4.805632000
H	−1.648866000	2.465761000	−4.191468000
H	−4.050769000	2.950730000	−1.751767000
H	−4.751434000	2.654743000	0.823844000
O	−0.832600000	−1.425176000	−0.223693000
H	−1.364912000	−2.405213000	−0.265434000
C	−1.943089000	−3.681146000	−0.342579000
H	−3.342278000	1.440502000	3.077517000
H	2.647722000	−1.019722000	3.183338000
H	2.820452000	0.208682000	−3.172606000
C	−1.280368000	−4.442824000	0.782819000
H	−0.195625000	−4.501067000	0.631848000
H	−1.464115000	−3.968419000	1.752708000
H	−1.660714000	−5.476873000	0.839258000
H	−2.989656000	−3.417512000	−0.156811000
C	−1.651451000	−4.126346000	−1.757509000
H	−2.068604000	−5.129186000	−1.951304000
H	−2.083917000	−3.439349000	−2.492547000
H	−0.570968000	−4.181061000	−1.937114000

$^{2}TS_{3}$:

Fe	−0.010641000	0.177038000	0.115287000
N	−0.057903000	0.327874000	2.045813000
N	1.918117000	0.148087000	0.043552000
N	−0.021920000	0.850559000	−1.679218000
N	−1.736272000	1.005009000	0.059522000
C	−1.188841000	0.510365000	2.832663000
C	−0.825510000	0.287718000	4.210615000
C	0.514205000	−0.026713000	4.245502000
C	0.996334000	−0.003239000	2.887785000
C	2.743951000	−0.158037000	1.117492000
C	4.085754000	−0.344815000	0.629462000
C	4.056678000	−0.156219000	−0.734573000
C	2.698671000	0.151166000	−1.106774000
C	0.920567000	0.805702000	−2.693169000
C	0.262465000	1.228749000	−3.904391000
C	−1.058994000	1.524790000	−3.588412000
C	−1.219660000	1.281573000	−2.185325000
C	−2.221640000	1.372548000	−1.170175000
C	−3.590900000	1.763394000	−1.019140000
C	−3.908397000	1.625118000	0.329246000
C	−2.732077000	1.150401000	1.012955000
C	−2.458543000	0.890261000	2.351737000
C	2.299924000	−0.242237000	2.441915000
C	2.232991000	0.447294000	−2.404977000
H	−1.503778000	0.370848000	5.047647000
H	1.117390000	−0.248129000	5.114048000
H	4.941443000	−0.583846000	1.244140000
H	4.887176000	−0.210421000	−1.423737000
H	0.728834000	1.310487000	−4.875631000
H	−1.821102000	1.883628000	−4.264123000
H	−4.242447000	2.117245000	−1.804375000
H	−4.857881000	1.845654000	0.795585000
O	−0.297788000	−1.537695000	−0.072486000
H	−1.313792000	−2.212870000	−0.490943000
C	−2.193033000	−2.914236000	−1.036093000
H	−1.619949000	−3.795401000	−1.333294000
H	−3.252216000	1.009391000	3.081948000
H	3.040420000	−0.494526000	3.194650000
H	2.958830000	0.419969000	−3.211215000
H	−2.473376000	−2.304242000	−1.897839000
C	−3.281717000	−3.174374000	−0.079409000
C	−4.385349000	−2.296004000	0.022280000
C	−3.236557000	−4.291521000	0.786208000
C	−5.407095000	−2.534148000	0.942807000
H	−4.429913000	−1.425087000	−0.624772000
C	−4.258662000	−4.528049000	1.705989000
H	−2.390578000	−4.970085000	0.727527000
C	−5.349738000	−3.651008000	1.788018000
H	−6.249727000	−1.851914000	1.001791000
H	−4.208428000	−5.394262000	2.358475000
H	−6.145869000	−3.836440000	2.502278000

$^{4}TS_{3}$:

Fe	0.016723000	0.164086000	0.114810000
N	−0.020120000	0.240062000	2.047031000
N	1.950032000	0.103955000	0.031370000
N	−0.007595000	0.860724000	−1.655566000
N	−1.721145000	0.930560000	0.079523000
C	−1.148262000	0.387991000	2.843190000

C	−0.783970000	0.110398000	4.208773000
C	0.556943000	−0.209182000	4.227370000
C	1.035289000	−0.131511000	2.871543000
C	2.777154000	−0.249946000	1.089963000
C	4.110845000	−0.447673000	0.586100000
C	4.074207000	−0.216084000	−0.773936000
C	2.720102000	0.127589000	−1.120943000
C	0.936349000	0.847491000	−2.673950000
C	0.271179000	1.311018000	−3.872670000
C	−1.045873000	1.594632000	−3.544914000
C	−1.205206000	1.301892000	−2.146015000
C	−2.206969000	1.355264000	−1.129067000
C	−3.569740000	1.769127000	−0.952713000
C	−3.881317000	1.588272000	0.389211000
C	−2.707427000	1.068542000	1.048685000
C	−2.422875000	0.779858000	2.376658000
C	2.337434000	−0.365709000	2.413039000
C	2.244311000	0.474375000	−2.409949000
H	−1.460067000	0.157727000	5.050338000
H	1.160143000	−0.470154000	5.084945000
H	4.967180000	−0.725157000	1.183726000
H	4.897980000	−0.267388000	−1.471321000
H	0.736324000	1.425377000	−4.841202000
H	−1.811016000	1.973292000	−4.206202000
H	−4.217803000	2.166641000	−1.719844000
H	−4.820359000	1.816871000	0.872210000
O	−0.399465000	−1.486160000	−0.185805000
H	−1.360608000	−2.042973000	−0.562667000
C	−2.323933000	−2.841510000	−1.123593000
H	−1.705430000	−3.698284000	−1.392813000
H	−3.211358000	0.883033000	3.115066000
H	3.077012000	−0.649072000	3.155762000
H	2.963380000	0.467542000	−3.222592000
H	−2.601835000	−2.225296000	−1.979813000
C	−3.362852000	−3.077159000	−0.130004000
C	−4.476548000	−2.206725000	−0.015269000
C	−3.273254000	−4.162178000	0.778904000
C	−5.456579000	−2.420101000	0.953423000
H	−4.556235000	−1.361163000	−0.691580000
C	−4.254791000	−4.371679000	1.745986000
H	−2.422420000	−4.833904000	0.712800000
C	−5.352990000	−3.502940000	1.838854000
H	−6.304426000	−1.744930000	1.020028000
H	−4.168936000	−5.211400000	2.428824000
H	−6.117727000	−3.668690000	2.591160000

$^{2}TS_{4}$:

Fe	0.041768000	0.070974000	0.114165000
N	0.033098000	0.051281000	2.050820000
N	1.967740000	0.069084000	0.001188000
N	−0.014728000	0.896165000	−1.614878000
N	−1.692038000	0.880236000	0.166038000
C	−1.082075000	0.152873000	2.873279000
C	−0.686774000	−0.179909000	4.219822000
C	0.656760000	−0.479711000	4.200556000
C	1.109220000	−0.336407000	2.840146000
C	2.819506000	−0.317548000	1.027490000
C	4.152550000	−0.443883000	0.498220000
C	4.092283000	−0.139040000	−0.843704000
C	2.723509000	0.181477000	−1.160476000
C	0.905249000	0.947921000	−2.648551000
C	0.215904000	1.461306000	−3.806071000
C	−1.101947000	1.711691000	−3.438814000
C	−1.228580000	1.350595000	−2.058112000
C	−2.209569000	1.339372000	−1.018495000
C	−3.583908000	1.683775000	−0.810640000
C	−3.872223000	1.422864000	0.525532000
C	−2.672050000	0.920067000	1.145998000
C	−2.367483000	0.552586000	2.451520000
C	2.404869000	−0.520456000	2.349070000
C	2.227366000	0.581914000	−2.418631000
H	−1.347242000	−0.174795000	5.075034000
H	1.281018000	−0.765351000	5.034791000
H	5.023864000	−0.723529000	1.072470000
H	4.908522000	−0.122549000	−1.551569000
H	0.659743000	1.629850000	−4.776685000
H	−1.883060000	2.114576000	−4.066263000
H	−4.258621000	2.086452000	−1.551494000
H	−4.817547000	1.578991000	1.025060000
O	−0.231151000	−1.617432000	−0.224687000
H	−1.270582000	−2.267581000	−0.686439000
C	−2.161813000	−2.910989000	−1.260543000
C	−3.269136000	−3.134563000	−0.325573000
C	−4.406391000	−2.405511000	−0.288082000
H	−1.617211000	−3.811178000	−1.557425000
H	−3.147503000	0.595867000	3.204612000
H	3.164352000	−0.826592000	3.061843000
H	2.936040000	0.631630000	−3.238961000
H	−3.134344000	−3.933859000	0.403313000
H	−5.190079000	−2.605406000	0.436183000
H	−4.581589000	−1.588671000	−0.983045000
H	−2.407615000	−2.282207000	−2.120368000

$^{4}TS_{4}$:

Fe	0.054424000	0.078740000	0.163233000
N	0.069438000	0.080306000	2.098161000
N	1.985692000	0.073166000	0.025647000
N	−0.040931000	0.825146000	−1.583393000
N	−1.701857000	0.800202000	0.202534000
C	−1.039034000	0.167818000	2.927428000
C	−0.630176000	−0.142931000	4.272834000
C	0.720213000	−0.422195000	4.245372000
C	1.158448000	−0.285757000	2.880844000
C	2.851740000	−0.291561000	1.048146000
C	4.176176000	−0.430630000	0.502785000
C	4.095257000	−0.152813000	−0.846862000
C	2.722597000	0.160505000	−1.145490000
C	0.874812000	0.877021000	−2.626157000
C	0.165506000	1.366165000	−3.787742000
C	−1.149399000	1.602346000	−3.414042000
C	−1.261863000	1.254590000	−2.024007000
C	−2.234294000	1.246320000	−0.976165000
C	−3.608084000	1.600320000	−0.752151000
C	−3.878716000	1.357427000	0.587679000
C	−2.667567000	0.861575000	1.200324000
C	−2.339723000	0.535093000	2.507467000
C	2.452611000	−0.465011000	2.379232000
C	2.200740000	0.535597000	−2.408077000
H	−1.283564000	−0.143018000	5.133467000
H	1.353866000	−0.692654000	5.077690000
H	5.056725000	−0.701712000	1.067200000
H	4.900771000	−0.154386000	−1.567098000
H	0.600649000	1.530253000	−4.763033000
H	−1.941627000	1.985882000	−4.039680000
H	−4.290772000	1.997140000	−1.489022000
H	−4.813993000	1.529107000	1.100609000
O	−0.332373000	−1.562980000	−0.191863000
H	−1.266166000	−2.096431000	−0.714509000

C	−2.182997000	−2.819812000	−1.392724000
C	−3.296825000	−3.066844000	−0.497555000
C	−4.440617000	−2.336303000	−0.450936000
H	−1.561931000	−3.680195000	−1.646375000
H	−3.110599000	0.585778000	3.269664000
H	3.221467000	−0.750424000	3.090794000
H	2.897537000	0.579990000	−3.238865000
H	−3.176429000	−3.885994000	0.211813000
H	−5.230975000	−2.557787000	0.259195000
H	−4.607927000	−1.500180000	−1.123954000
H	−2.382130000	−2.166485000	−2.244772000

$^{2}TS_{5}$:

Fe	0.067321000	0.032390000	−0.006184000
N	−0.067511000	0.012259000	1.931040000
N	1.995642000	0.115757000	0.007533000
N	0.086943000	0.857490000	−1.734923000
N	−1.702865000	0.767453000	−0.067175000
C	−1.237565000	0.065492000	2.678558000
C	−0.917301000	−0.249741000	4.048956000
C	0.437359000	−0.489023000	4.118016000
C	0.969909000	−0.325521000	2.789204000
C	2.794133000	−0.229458000	1.090612000
C	4.163945000	−0.293030000	0.650947000
C	4.177972000	0.008395000	−0.693385000
C	2.819020000	0.263461000	−1.099861000
C	1.070397000	0.953718000	−2.705248000
C	0.436939000	1.448591000	−3.904227000
C	−0.909316000	1.644475000	−3.622219000
C	−1.110553000	1.267088000	−2.253453000
C	−2.158052000	1.212133000	−1.280855000
C	−3.555374000	1.502903000	−1.163769000
C	−3.921098000	1.225313000	0.150087000
C	−2.744785000	0.766238000	0.846955000
C	−2.508833000	0.410225000	2.171495000
C	2.303553000	−0.449625000	2.382308000
C	2.387628000	0.644208000	−2.390568000
H	−1.631407000	−0.273472000	4.859672000
H	1.017752000	−0.745778000	4.992377000
H	5.007926000	−0.529664000	1.282571000
H	5.037544000	0.063750000	−1.345797000
H	0.935918000	1.641000000	−4.843065000
H	−1.664949000	2.017411000	−4.297268000
H	−4.195112000	1.880167000	−1.947610000
H	−4.902261000	1.345021000	0.586905000
O	−0.096064000	−1.658841000	−0.361993000
H	−1.022245000	−2.518223000	−0.731029000
C	−1.831072000	−3.430495000	−0.930072000
H	−1.163978000	−4.299875000	−0.910043000
H	−3.336984000	0.422444000	2.872876000
H	3.028259000	−0.718744000	3.144651000
H	3.145904000	0.727491000	−3.162378000
C	−2.758230000	−3.395765000	0.280639000
H	−2.182579000	−3.547207000	1.198805000
H	−3.275492000	−2.434991000	0.373523000
H	−3.519884000	−4.185560000	0.217498000
C	−2.409425000	−3.223505000	−2.283730000
C	−1.771525000	−3.791415000	−3.410037000
C	−3.567565000	−2.445604000	−2.501982000
C	−2.275049000	−3.602869000	−4.697756000
H	−0.874165000	−4.385416000	−3.261151000
C	−4.072155000	−2.257847000	−3.791011000
H	−4.071487000	−1.982417000	−1.660960000
C	−3.431121000	−2.835671000	−4.894752000
H	−1.770290000	−4.053949000	−5.546596000
H	−4.967165000	−1.660180000	−3.935893000
H	−3.826252000	−2.689195000	−5.895163000

$^{4}TS_{5}$:

Fe	0.112612000	0.024874000	−0.040389000
N	−0.084590000	0.016375000	1.884051000
N	2.043546000	0.133771000	0.035540000
N	0.172977000	0.807516000	−1.773744000
N	−1.676280000	0.652603000	−0.188072000
C	−1.282542000	0.040725000	2.591442000
C	−1.002686000	−0.259252000	3.972759000
C	0.354677000	−0.466638000	4.089468000
C	0.929157000	−0.296726000	2.779853000
C	2.811502000	−0.193022000	1.147869000
C	4.194367000	−0.254056000	0.749340000
C	4.246146000	0.030858000	−0.599144000
C	2.898200000	0.272756000	−1.045806000
C	1.190933000	0.915199000	−2.710499000
C	0.583192000	1.372874000	−3.943997000
C	−0.773853000	1.530172000	−3.715776000
C	−1.016957000	1.165422000	−2.345164000
C	−2.098608000	1.088550000	−1.418259000
C	−3.501494000	1.370140000	−1.344328000
C	−3.904976000	1.102144000	−0.041157000
C	−2.746721000	0.660316000	0.695915000
C	−2.542740000	0.341583000	2.035311000
C	2.280932000	−0.401146000	2.422633000
C	2.500088000	0.637569000	−2.356825000
H	−1.743557000	−0.298319000	4.758542000
H	0.909749000	−0.707666000	4.984567000
H	5.021385000	−0.481767000	1.406438000
H	5.124273000	0.081345000	−1.226734000
H	1.111469000	1.563989000	−4.867000000
H	−1.516329000	1.865942000	−4.424094000
H	−4.119440000	1.737253000	−2.150222000
H	−4.897658000	1.226262000	0.367284000
O	−0.123783000	−1.643296000	−0.406415000
H	−0.991035000	−2.403654000	−0.715024000
C	−1.810162000	−3.444427000	−0.940363000
H	−1.046983000	−4.224321000	−1.022464000
H	−3.393271000	0.351198000	2.709791000
H	2.980509000	−0.650073000	3.214788000
H	3.279444000	0.725570000	−3.106512000
C	−2.615940000	−3.525426000	0.345330000
H	−1.950805000	−3.688348000	1.198627000
H	−3.176776000	−2.604521000	0.538144000
H	−3.337014000	−4.356054000	0.311968000
C	−2.477119000	−3.164445000	−2.220552000
C	−1.835142000	−3.510539000	−3.436120000
C	−3.736838000	−2.523694000	−2.299566000
C	−2.426942000	−3.239692000	−4.668492000
H	−0.863587000	−3.994820000	−3.395350000
C	−4.328460000	−2.255850000	−3.535270000
H	−4.249971000	−2.233913000	−1.389745000
C	−3.679827000	−2.611311000	−4.725679000
H	−1.916844000	−3.518716000	−5.585388000
H	−5.298488000	−1.769124000	−3.571715000
H	−4.143385000	−2.402392000	−5.684721000

$^{2}TS_{6}$:

Fe	−0.627460000	0.245498000	−0.261058000
N	−0.707539000	0.015763000	1.662660000
N	1.064796000	−0.690095000	−0.416480000

N	−0.232283000	1.148658000	−1.894539000
N	−1.770382000	1.759357000	−0.091145000
C	−1.668066000	0.547116000	2.512418000
C	−1.538943000	−0.085832000	3.800331000
C	−0.505980000	−0.994817000	3.718453000
C	0.015860000	−0.932040000	2.378008000
C	1.580717000	−1.556941000	0.539299000
C	2.687695000	−2.273387000	−0.036679000
C	2.832165000	−1.832157000	−1.335375000
C	1.816538000	−0.840584000	−1.576399000
C	0.643376000	0.866261000	−2.928697000
C	0.329762000	1.771801000	−4.007427000
C	−0.722736000	2.579910000	−3.591284000
C	−1.063023000	2.171274000	−2.261108000
C	−1.962452000	2.528901000	−1.205271000
C	−2.993209000	3.484321000	−0.926148000
C	−3.411275000	3.260583000	0.380692000
C	−2.631960000	2.168126000	0.912486000
C	−2.587056000	1.562551000	2.162347000
C	1.076434000	−1.669154000	1.841051000
C	1.620062000	−0.110539000	−2.769535000
H	−2.150355000	0.138424000	4.662639000
H	−0.135989000	−1.644769000	4.497668000
H	3.283958000	−3.012568000	0.478254000
H	3.570551000	−2.148245000	−2.058295000
H	0.841448000	1.815089000	−4.958119000
H	−1.192194000	3.372741000	−4.154164000
H	−3.362925000	4.238511000	−1.604550000
H	−4.169454000	3.809744000	0.920165000
O	−1.745786000	−0.946437000	−0.790215000
H	−1.894041000	−2.224666000	−0.799298000
H	−3.274755000	1.897063000	2.932298000
H	1.556656000	−2.389380000	2.495324000
H	2.293692000	−0.317538000	−3.594889000
H	−0.528654000	−5.846788000	3.629148000
C	−0.906447000	−5.341051000	2.745527000
C	−0.250844000	−5.512732000	1.512961000
C	−2.045860000	−4.532738000	2.842837000
C	−0.758150000	−4.865515000	0.383957000
H	0.625320000	−6.151298000	1.443160000
C	−2.555975000	−3.869726000	1.709401000
H	−2.541773000	−4.413931000	3.801116000
C	−1.916449000	−4.039866000	0.485346000
C	−0.329220000	−4.864214000	−1.017015000
H	−3.430212000	−3.231808000	1.796684000
C	−2.187093000	−3.455757000	−0.861924000
C	−1.179806000	−4.079811000	−1.746361000
H	0.521598000	−5.413545000	−1.400596000
H	−3.220511000	−3.385739000	−1.209388000
H	−1.119772000	−3.893705000	−2.810704000

$^{4}TS_{6}$:

Fe	−0.641680000	0.253078000	−0.264156000
N	−0.745495000	−0.016554000	1.639632000
N	0.995283000	−0.740406000	−0.439955000
N	−0.226937000	1.165931000	−1.886099000
N	−1.754727000	1.786602000	−0.075123000
C	−1.701469000	0.521123000	2.494374000
C	−1.590393000	−0.134063000	3.773547000
C	−0.576263000	−1.061198000	3.684516000
C	−0.045562000	−0.990951000	2.347575000
C	1.502335000	−1.623678000	0.506065000
C	2.599045000	−2.350399000	−0.077363000
C	2.750210000	−1.899756000	−1.370238000
C	1.750200000	−0.889897000	−1.604642000
C	0.626333000	0.865717000	−2.932060000
C	0.321088000	1.775040000	−4.005192000
C	−0.715327000	2.603372000	−3.577761000
C	−1.046507000	2.202925000	−2.247107000
C	−1.940229000	2.564923000	−1.186916000
C	−2.968150000	3.520596000	−0.908087000
C	−3.393794000	3.289490000	0.396594000
C	−2.623273000	2.188683000	0.923392000
C	−2.599541000	1.558192000	2.161154000
C	0.998142000	−1.742353000	1.806263000
C	1.574774000	−0.144491000	−2.784984000
H	−2.201850000	0.090958000	4.635631000
H	−0.223086000	−1.730135000	4.455144000
H	3.185172000	−3.100859000	0.432588000
H	3.485986000	−2.217193000	−2.095270000
H	0.820071000	1.806745000	−4.963049000
H	−1.176624000	3.403279000	−4.137400000
H	−3.332369000	4.280359000	−1.583156000
H	−4.157227000	3.834166000	0.933322000
O	−1.736897000	−0.945773000	−0.776490000
H	−1.809255000	−2.149195000	−0.773505000
H	−3.288117000	1.886648000	2.932804000
H	1.462547000	−2.480330000	2.451422000
H	2.239764000	−0.363203000	−3.614402000
H	−0.448471000	−5.754519000	3.671600000
C	−0.834287000	−5.270837000	2.779169000
C	−0.152849000	−5.418708000	1.558035000
C	−2.012005000	−4.515359000	2.852758000
C	−0.672402000	−4.804740000	0.413457000
H	0.751935000	−6.018201000	1.505580000
C	−2.534448000	−3.881362000	1.707970000
H	−2.529208000	−4.416040000	3.802030000
C	−1.870575000	−4.027038000	0.492710000
C	−0.227765000	−4.794503000	−0.974755000
H	−3.438838000	−3.284699000	1.779889000
C	−2.136760000	−3.466046000	−0.854880000
C	−1.112328000	−4.046442000	−1.720403000
H	0.651664000	−5.303605000	−1.348186000
H	−3.157714000	−3.331502000	−1.212151000
H	−1.050127000	−3.869472000	−2.786323000

$^{2}TS_{7}$:

Fe	−0.017694000	0.150384000	0.022498000
N	−0.043959000	−0.036680000	1.954297000
N	1.907537000	0.063948000	−0.084392000
N	−0.032027000	1.104172000	−1.635881000
N	−1.725152000	1.015323000	0.133364000
C	−1.159983000	0.041784000	2.775800000
C	−0.791621000	−0.420664000	4.090985000
C	0.539741000	−0.773130000	4.053355000
C	1.008861000	−0.533096000	2.712263000
C	2.734090000	−0.436216000	0.911792000
C	4.065842000	−0.572021000	0.380756000
C	4.027902000	−0.157141000	−0.933041000
C	2.674594000	0.240863000	−1.227725000
C	0.898534000	1.205633000	−2.655074000
C	0.243343000	1.853751000	−3.765250000
C	−1.063903000	2.132664000	−3.381385000
C	−1.217595000	1.652374000	−2.040084000
C	−2.209038000	1.598855000	−1.005979000
C	−3.564535000	2.003730000	−0.769927000
C	−3.873592000	1.645479000	0.538125000
C	−2.704969000	1.024018000	1.112819000

C	−2.425523000	0.532798000	2.382685000
C	2.300870000	−0.727163000	2.211924000
C	2.201682000	0.764986000	−2.451774000
H	−1.458681000	−0.461256000	4.940108000
H	1.144363000	−1.153144000	4.864177000
H	4.921993000	−0.928877000	0.934793000
H	4.850025000	−0.114639000	−1.633016000
H	0.702923000	2.089547000	−4.714257000
H	−1.820547000	2.626722000	−3.972455000
H	−4.211227000	2.506083000	−1.473934000
H	−4.811853000	1.807720000	1.048615000
O	−0.371936000	−1.446207000	−0.470107000
H	−1.287781000	−2.403592000	−0.669236000
C	−2.040409000	−3.366101000	−0.840892000
C	−3.221850000	−3.127641000	0.030360000
C	−4.333710000	−2.419824000	−0.483412000
C	−4.280297000	−1.889349000	−1.902375000
C	−3.422991000	−2.726574000	−2.830762000
C	−2.317042000	−3.430466000	−2.300534000
C	−1.489746000	−4.166296000	−3.170304000
C	−1.754832000	−4.215358000	−4.539253000
C	−2.859426000	−3.527268000	−5.060145000
C	−3.686089000	−2.790822000	−4.204942000
C	−3.248707000	−3.575367000	1.364862000
C	−4.358438000	−3.338372000	2.176901000
C	−5.465301000	−2.649424000	1.660761000
C	−5.447291000	−2.197116000	0.337193000
H	−1.409887000	−4.188971000	−0.489455000
H	−0.637025000	−4.700479000	−2.761053000
H	−1.109760000	−4.789317000	−5.197029000
H	−3.076303000	−3.567181000	−6.123072000
H	−4.544584000	−2.259526000	−4.607648000
H	−3.864628000	−0.866098000	−1.870886000
H	−5.294192000	−1.788013000	−2.308852000
H	−6.306116000	−1.666130000	−0.064906000
H	−6.337365000	−2.472809000	2.282965000
H	−4.367431000	−3.695886000	3.201892000
H	−2.391170000	−4.114149000	1.757698000
H	−3.208816000	0.544397000	3.133219000
H	3.042802000	−1.119264000	2.900934000
H	2.917633000	0.853579000	−3.262552000

$^{4}TS_{7}$:

Fe	−0.008405000	0.132497000	0.011971000
N	−0.042584000	−0.051159000	1.935072000
N	1.921372000	0.066431000	−0.082699000
N	−0.016524000	1.077564000	−1.642670000
N	−1.727811000	0.946303000	0.097434000
C	−1.166727000	0.014135000	2.752596000
C	−0.800638000	−0.445290000	4.068827000
C	0.533570000	−0.785528000	4.038583000
C	1.009346000	−0.540749000	2.701113000
C	2.745076000	−0.438948000	0.916835000
C	4.076182000	−0.583310000	0.387320000
C	4.042061000	−0.170770000	−0.928055000
C	2.692127000	0.234453000	−1.224168000
C	0.921376000	1.185171000	−2.657520000
C	0.260923000	1.816793000	−3.779055000
C	−1.051169000	2.074717000	−3.408933000
C	−1.209848000	1.599234000	−2.063289000
C	−2.208974000	1.533587000	−1.044283000
C	−3.564064000	1.938797000	−0.810787000
C	−3.877418000	1.582847000	0.496714000
C	−2.712352000	0.963552000	1.075738000
C	−2.431929000	0.487929000	2.351925000
C	2.307002000	−0.728316000	2.211966000
C	2.223979000	0.757857000	−2.452778000
H	−1.472328000	−0.492519000	4.914011000
H	1.137114000	−1.160949000	4.852370000
H	4.929283000	−0.947495000	0.941494000
H	4.864911000	−0.136206000	−1.627609000
H	0.724235000	2.050857000	−4.726721000
H	−1.812187000	2.550417000	−4.009368000
H	−4.207360000	2.444530000	−1.515739000
H	−4.814765000	1.751721000	1.006480000
O	−0.420630000	−1.448286000	−0.466171000
H	−1.292966000	−2.302150000	−0.637519000
C	−2.075069000	−3.343432000	−0.829107000
C	−3.237951000	−3.108098000	0.047612000
C	−4.371680000	−2.426823000	−0.461579000
C	−4.347938000	−1.910280000	−1.885981000
C	−3.453284000	−2.706067000	−2.814736000
C	−2.328083000	−3.382147000	−2.282123000
C	−1.463139000	−4.070163000	−3.158443000
C	−1.710281000	−4.100970000	−4.530041000
C	−2.833591000	−3.442945000	−5.051699000
C	−3.696353000	−2.753423000	−4.192669000
C	−3.238394000	−3.531831000	1.392857000
C	−4.339077000	−3.298687000	2.215869000
C	−5.466295000	−2.638476000	1.703826000
C	−5.475880000	−2.210183000	0.371970000
H	−1.399450000	−4.125970000	−0.473526000
H	−0.596517000	−4.581037000	−2.748816000
H	−1.037011000	−4.637594000	−5.191011000
H	−3.036054000	−3.469448000	−6.117804000
H	−4.568131000	−2.245015000	−4.596406000
H	−3.984786000	−0.866700000	−1.863533000
H	−5.367214000	−1.861465000	−2.289391000
H	−6.349703000	−1.700860000	−0.025747000
H	−6.331753000	−2.465369000	2.335985000
H	−4.326988000	−3.637009000	3.247277000
H	−2.365739000	−4.048365000	1.782074000
H	−3.218252000	0.500830000	3.099321000
H	3.044436000	−1.117394000	2.907437000
H	2.942010000	0.848388000	−3.261146000

$^{2}TS_{8}$:

Fe	0.240144000	−0.260202000	0.362340000
N	0.409572000	−0.270396000	2.298412000
N	2.152919000	−0.191663000	0.078726000
N	−0.009754000	0.526561000	−1.353063000
N	−1.522710000	0.455524000	0.571035000
C	−0.631074000	−0.214082000	3.217514000
C	−0.104221000	−0.525549000	4.522213000
C	1.246527000	−0.764106000	4.383105000
C	1.569275000	−0.603353000	2.989232000
C	3.110171000	−0.524211000	1.028745000
C	4.395140000	−0.599429000	0.381623000
C	4.199887000	−0.316818000	−0.952754000
C	2.794233000	−0.061039000	−1.144978000
C	0.812615000	0.612065000	−2.462631000
C	0.000343000	1.091427000	−3.555123000
C	−1.288555000	1.286646000	−3.071897000
C	−1.276017000	0.922781000	−1.685932000
C	−2.161194000	0.879531000	−0.561445000
C	−3.523471000	1.180233000	−0.231296000
C	−3.678355000	0.924315000	1.126273000
C	−2.406845000	0.468996000	1.636669000
C	−1.967360000	0.129505000	2.910984000

C	2.825289000	–0.726451000	2.384133000
C	2.164150000	0.304894000	–2.355332000
H	–0.684135000	–0.545134000	5.433984000
H	1.954009000	–1.017177000	5.159619000
H	5.327297000	–0.829997000	0.876911000
H	4.947402000	–0.274316000	–1.731915000
H	0.349629000	1.278523000	–4.560362000
H	–2.139757000	1.652073000	–3.626752000
H	–4.277835000	1.547181000	–0.911196000
H	–4.578325000	1.053822000	1.710163000
O	–0.052749000	–1.893781000	–0.010491000
H	–2.674933000	0.154080000	3.733664000
H	3.659756000	–0.983996000	3.029372000
H	2.790024000	0.377750000	–3.238887000
H	–2.616668000	–3.156783000	3.901153000
C	–2.380496000	–4.128809000	3.426995000
C	–3.003482000	–4.183521000	2.055216000
C	–0.886118000	–4.326242000	3.409282000
H	–2.853469000	–4.875584000	4.087916000
C	–2.271949000	–4.237822000	0.924238000
H	–4.090111000	–4.181977000	2.005866000
C	–0.171905000	–4.379779000	2.267005000
H	–0.390019000	–4.429463000	4.371528000
C	–0.789097000	–4.209035000	0.929570000
H	–2.766758000	–4.273073000	–0.043124000
H	0.905500000	–4.520325000	2.305175000
H	–0.335141000	–4.837414000	0.152915000
H	–0.459489000	–3.110400000	0.531411000

$^{4}TS_{8}$:

Fe	0.320821000	–0.305714000	0.402779000
N	0.533403000	–0.348450000	2.316699000
N	2.214203000	–0.138721000	0.068735000
N	–0.007575000	0.467635000	–1.303254000
N	–1.472859000	0.291219000	0.650141000
C	–0.489484000	–0.333955000	3.270643000
C	0.092287000	–0.613537000	4.560332000
C	1.446248000	–0.786815000	4.383299000
C	1.723028000	–0.618249000	2.979293000
C	3.211162000	–0.445781000	0.991393000
C	4.479893000	–0.466915000	0.306025000
C	4.236670000	–0.183910000	–1.019047000
C	2.816430000	0.019604000	–1.171373000
C	0.778665000	0.597100000	–2.432068000
C	–0.093872000	1.019650000	–3.509254000
C	–1.378243000	1.132584000	–2.997622000
C	–1.309549000	0.778405000	–1.607740000
C	–2.164392000	0.685971000	–0.470847000
C	–3.525552000	0.918548000	–0.104227000
C	–3.631152000	0.659313000	1.260574000
C	–2.330418000	0.267603000	1.733918000
C	–1.837176000	–0.050233000	3.002638000
C	2.972089000	–0.676355000	2.344726000
C	2.143654000	0.361360000	–2.366696000
H	–0.459399000	–0.652602000	5.488912000
H	2.188330000	–0.997784000	5.139815000
H	5.433388000	–0.668108000	0.772878000
H	4.959276000	–0.109152000	–1.818995000
H	0.217658000	1.215656000	–4.525283000
H	–2.265037000	1.437460000	–3.532808000
H	–4.315518000	1.249824000	–0.761944000
H	–4.519856000	0.749525000	1.868533000
O	0.094509000	–1.959509000	0.099648000
H	–2.522500000	–0.044687000	3.844596000
H	3.831654000	–0.899730000	2.969210000
H	2.742663000	0.465403000	–3.265095000
H	–2.939058000	–2.774809000	3.485894000
C	–2.713869000	–3.816642000	3.177850000
C	–3.119778000	–4.004648000	1.739521000
C	–1.255757000	–4.100293000	3.428193000
H	–3.344058000	–4.436138000	3.838616000
C	–2.217223000	–4.197296000	0.752251000
H	–4.183210000	–3.975201000	1.515102000
C	–0.372898000	–4.291442000	2.422523000
H	–0.927088000	–4.142052000	4.463549000
C	–0.765911000	–4.202217000	1.006111000
H	–2.550520000	–4.318023000	–0.275169000
H	0.673520000	–4.482646000	2.645692000
H	–0.180548000	–4.827352000	0.324261000
H	–0.355162000	–3.053909000	0.612879000

$^{2}TS_{9}$:

Fe	–0.010757000	0.333237000	0.090338000
N	–0.020222000	–0.145815000	1.968671000
N	1.903620000	0.163224000	–0.069272000
N	0.005993000	1.527265000	–1.400524000
N	–1.666690000	1.253003000	0.367732000
C	–1.120433000	–0.135253000	2.819281000
C	–0.756788000	–0.811110000	4.041075000
C	0.551856000	–1.221796000	3.920492000
C	1.014996000	–0.805989000	2.619970000
C	2.714784000	–0.529162000	0.819416000
C	4.028071000	–0.658791000	0.240367000
C	3.994443000	–0.049832000	–0.994500000
C	2.662814000	0.466285000	–1.193947000
C	0.925304000	1.731397000	–2.413861000
C	0.292486000	2.573877000	–3.398345000
C	–0.992197000	2.860843000	–2.947862000
C	–1.155266000	2.192558000	–1.691471000
C	–2.131701000	2.033638000	–0.659052000
C	–3.455751000	2.470252000	–0.332819000
C	–3.768466000	1.929788000	0.912671000
C	–2.630078000	1.164465000	1.358250000
C	–2.360275000	0.473106000	2.535733000
C	2.286723000	–0.990381000	2.069643000
C	2.204966000	1.193679000	–2.311296000
H	–1.411666000	–0.943087000	4.890678000
H	1.147469000	–1.749809000	4.651380000
H	4.869581000	–1.143865000	0.713788000
H	4.806541000	0.050681000	–1.700475000
H	0.752100000	2.926890000	–4.310429000
H	–1.726657000	3.480756000	–3.440637000
H	–4.077700000	3.120089000	–0.931164000
H	–4.684168000	2.071504000	1.468767000
O	–0.465305000	–1.126975000	–0.631122000
H	–1.504558000	–2.045994000	–0.874985000
C	–2.312835000	–2.922606000	–1.083812000
C	–3.430294000	–2.689754000	–0.140299000
C	–4.534209000	–1.896990000	–0.556059000
C	–3.808276000	–2.047513000	–2.891405000
C	–2.687525000	–2.834607000	–2.513895000
C	–1.920476000	–3.447779000	–3.518079000
C	–2.237474000	–3.298916000	–4.866760000
C	–3.350486000	–2.526675000	–5.231589000
C	–4.133860000	–1.910817000	–4.257149000
C	–3.389650000	–3.153703000	1.183731000
C	–4.405027000	–2.852191000	2.090288000
C	–5.495770000	–2.074842000	1.671142000

C	−5.565442000	−1.603000000	0.361875000
H	−1.731193000	−3.819525000	−0.847765000
H	−1.058206000	−4.036887000	−3.221306000
H	−1.629988000	−3.777514000	−5.627279000
H	−3.616099000	−2.413205000	−6.277664000
H	−5.008465000	−1.349621000	−4.560780000
H	−6.429754000	−1.030624000	0.050643000
H	−6.300287000	−1.846167000	2.362942000
H	−4.354887000	−3.221664000	3.108992000
H	−2.536444000	−3.746911000	1.497837000
H	−3.130070000	0.414528000	3.297781000
H	3.015150000	−1.521161000	2.675045000
H	2.911979000	1.365086000	−3.116686000
N	−4.587274000	−1.439335000	−1.885556000
C	−5.525869000	−0.368363000	−2.236577000
H	−6.532128000	−0.746968000	−2.461571000
H	−5.583747000	0.339665000	−1.407895000
H	−5.147821000	0.170096000	−3.105780000

$^{4}TS_{9}$:

Fe	−0.040670000	0.353841000	0.074090000
N	−0.051417000	−0.149089000	1.937306000
N	1.873221000	0.158280000	−0.092273000
N	−0.003062000	1.560912000	−1.400147000
N	−1.681831000	1.279975000	0.356236000
C	−1.151437000	−0.131250000	2.794528000
C	−0.792091000	−0.825330000	4.007286000
C	0.508951000	−1.254208000	3.877680000
C	0.975226000	−0.832637000	2.580071000
C	2.673734000	−0.568090000	0.782445000
C	3.977895000	−0.726073000	0.189935000
C	3.950357000	−0.102615000	−1.038016000
C	2.632109000	0.451917000	−1.219936000
C	0.917165000	1.760855000	−2.414300000
C	0.288851000	2.617111000	−3.394232000
C	−0.991441000	2.911561000	−2.942875000
C	−1.161460000	2.236340000	−1.688906000
C	−2.139241000	2.079862000	−0.663372000
C	−3.454732000	2.530449000	−0.328320000
C	−3.771562000	1.983265000	0.914047000
C	−2.645005000	1.199090000	1.348767000
C	−2.379859000	0.494143000	2.521503000
C	2.243054000	−1.034168000	2.026484000
C	2.186298000	1.203326000	−2.327214000
H	−1.445644000	−0.955343000	4.858307000
H	1.099637000	−1.797968000	4.601031000
H	4.809368000	−1.241427000	0.649109000
H	4.758602000	−0.017137000	−1.750398000
H	0.750857000	2.968971000	−4.305628000
H	−1.721175000	3.540249000	−3.431558000
H	−4.068950000	3.196275000	−0.917284000
H	−4.681423000	2.137395000	1.476424000
O	−0.582939000	−1.078900000	−0.640778000
H	−1.492272000	−1.994436000	−0.834646000
C	−2.302842000	−2.943309000	−1.054747000
C	−3.411605000	−2.709900000	−0.116336000
C	−4.519717000	−1.922478000	−0.537886000
C	−3.776570000	−2.067410000	−2.868836000
C	−2.652615000	−2.848580000	−2.480794000
C	−1.864541000	−3.444846000	−3.481531000
C	−2.165903000	−3.287375000	−4.831675000
C	−3.283147000	−2.524135000	−5.205870000
C	−4.085463000	−1.923785000	−4.237581000
C	−3.368138000	−3.159828000	1.214621000
C	−4.383429000	−2.851848000	2.116966000
C	−5.478788000	−2.082977000	1.690679000
C	−5.551656000	−1.624550000	0.377211000
H	−1.677630000	−3.804660000	−0.804331000
H	−1.000521000	−4.027823000	−3.178211000
H	−1.543636000	−3.752990000	−5.588273000
H	−3.535829000	−2.405787000	−6.254490000
H	−4.961600000	−1.369192000	−4.548579000
H	−6.417496000	−1.057037000	0.061674000
H	−6.283097000	−1.850600000	2.381272000
H	−4.331284000	−3.209433000	3.139746000
H	−2.512562000	−3.746387000	1.534249000
H	−3.148073000	0.441413000	3.285679000
H	2.961914000	−1.585675000	2.624652000
H	2.891995000	1.370089000	−3.134404000
N	−4.570627000	−1.471252000	−1.868898000
C	−5.506934000	−0.397856000	−2.223390000
H	−6.512485000	−0.776264000	−2.450148000
H	−5.564756000	0.311067000	−1.395508000
H	−5.125442000	0.138982000	−3.091765000

$^{2}TS_{10}$:

Fe	0.035276000	0.062122000	0.060573000
N	−0.014742000	−0.085882000	1.990582000
N	1.960617000	0.039467000	−0.016609000
N	0.014096000	0.977115000	−1.617662000
N	−1.702074000	0.863007000	0.125289000
C	−1.147243000	−0.029688000	2.794723000
C	−0.781033000	−0.449947000	4.125407000
C	0.561381000	−0.756156000	4.114936000
C	1.043503000	−0.530014000	2.775287000
C	2.788636000	−0.413671000	1.001101000
C	4.132078000	−0.517653000	0.491097000
C	4.100615000	−0.132526000	−0.831012000
C	2.739884000	0.216537000	−1.155207000
C	0.955213000	1.088691000	−2.625426000
C	0.295236000	1.686103000	−3.759496000
C	−1.028256000	1.924779000	−3.402434000
C	−1.187197000	1.471495000	−2.053494000
C	−2.189744000	1.402779000	−1.036835000
C	−3.562962000	1.754879000	−0.831793000
C	−3.880904000	1.412615000	0.478930000
C	−2.698683000	0.853121000	1.087476000
C	−2.422281000	0.402963000	2.374057000
C	2.347583000	−0.692075000	2.300453000
C	2.271128000	0.697447000	−2.394188000
H	−1.458525000	−0.492493000	4.966444000
H	1.167206000	−1.095492000	4.942910000
H	4.990569000	−0.835119000	1.065343000
H	4.931604000	−0.077693000	−1.519835000
H	0.761407000	1.917304000	−4.706597000
H	−1.792248000	2.377617000	−4.016994000
H	−4.216236000	2.217931000	−1.556811000
H	−4.832614000	1.551032000	0.971602000
O	−0.265883000	−1.539312000	−0.391556000
H	−1.301521000	−2.456244000	−0.697651000
C	−2.081990000	−3.351357000	−0.913600000
C	−3.234132000	−3.128923000	−0.000481000
C	−4.430709000	−2.553901000	−0.501126000
C	−3.612610000	−2.743820000	−2.812949000
C	−2.394570000	−3.316046000	−2.366982000
C	−1.480658000	−3.764095000	−3.336143000
C	−1.751925000	−3.648311000	−4.698917000
C	−2.960646000	−3.070523000	−5.123835000

C	−3.888584000	−2.623511000	−4.187807000
C	−3.151815000	−3.390074000	1.377095000
C	−4.207267000	−3.089615000	2.238170000
C	−5.383199000	−2.512473000	1.727484000
C	−5.497235000	−2.247282000	0.366307000
H	−1.477196000	−4.220526000	−0.630808000
H	−0.541006000	−4.193286000	−3.002410000
H	−1.029571000	−3.997510000	−5.428759000
H	−3.176163000	−2.973702000	−6.182848000
H	−4.828674000	−2.183836000	−4.510467000
H	−6.406997000	−1.810010000	−0.036164000
H	−6.208281000	−2.276940000	2.391917000
H	−4.120240000	−3.300934000	3.298522000
H	−2.235252000	−3.819324000	1.769511000
H	−3.216868000	0.404190000	3.112596000
H	3.091485000	−1.044700000	3.008359000
H	2.995636000	0.793841000	−3.196517000
N	−4.549123000	−2.324916000	−1.868705000
H	−5.397088000	−1.891833000	−2.204227000
C	−3.128902000	−3.379245000	1.428742000
C	−4.182950000	−3.060859000	2.283444000
C	−5.360077000	−2.491988000	1.763875000
C	−5.476576000	−2.252671000	0.398226000
H	−1.412067000	−4.188580000	−0.553459000
H	−0.512291000	−4.245544000	−2.930643000
H	−0.992220000	−4.077296000	−5.359920000
H	−3.135325000	−3.063738000	−6.135687000
H	−4.797111000	−2.256376000	−4.480154000
H	−6.386102000	−1.821265000	−0.010808000
H	−6.183283000	−2.243103000	2.425558000
H	−4.095230000	−3.251785000	3.347574000
H	−2.212663000	−3.802151000	1.828405000
H	−3.238648000	0.434515000	3.074364000
H	3.050668000	−1.089587000	2.968836000
H	2.991358000	0.816926000	−3.218254000
N	−4.527039000	−2.367988000	−1.834618000
H	−5.372226000	−1.934478000	−2.177356000

$^{4}TS_{10}$:

Fe	0.012195000	0.088965000	0.026818000
N	−0.040755000	−0.078388000	1.949860000
N	1.941509000	0.049734000	−0.044744000
N	0.010561000	1.018726000	−1.636153000
N	−1.716400000	0.884031000	0.087975000
C	−1.176193000	−0.020090000	2.754761000
C	−0.815880000	−0.458992000	4.080527000
C	0.522837000	−0.779576000	4.068709000
C	1.010720000	−0.543976000	2.733131000
C	2.760987000	−0.435412000	0.968338000
C	4.100168000	−0.566637000	0.454287000
C	4.075856000	−0.167295000	−0.864429000
C	2.724115000	0.218048000	−1.181679000
C	0.957515000	1.131157000	−2.640566000
C	0.302603000	1.743391000	−3.773983000
C	−1.018562000	1.985533000	−3.421582000
C	−1.187819000	1.520393000	−2.075020000
C	−2.195144000	1.447995000	−1.069392000
C	−3.561411000	1.819849000	−0.859334000
C	−3.885644000	1.469803000	0.447950000
C	−2.714911000	0.885747000	1.050903000
C	−2.443394000	0.426784000	2.336501000
C	2.314912000	−0.718626000	2.261820000
C	2.265572000	0.722753000	−2.417132000
H	−1.495211000	−0.503467000	4.920063000
H	1.123625000	−1.134881000	4.893698000
H	4.951478000	−0.913609000	1.022313000
H	4.906560000	−0.127363000	−1.554629000
H	0.774505000	1.978085000	−4.717425000
H	−1.777978000	2.447285000	−4.035214000
H	−4.206391000	2.303713000	−1.578392000
H	−4.833138000	1.624882000	0.943765000
O	−0.376654000	−1.487959000	−0.445656000
H	−1.295594000	−2.392345000	−0.665681000
C	−2.071566000	−3.372665000	−0.864598000
C	−3.212116000	−3.142839000	0.045027000
C	−4.411163000	−2.574793000	−0.463765000
C	−3.588028000	−2.795915000	−2.771450000
C	−2.369939000	−3.362179000	−2.311285000
C	−1.450837000	−3.820918000	−3.272834000
C	−1.717646000	−3.720418000	−4.636871000
C	−2.925296000	−3.148265000	−5.074633000
C	−3.858152000	−2.691427000	−4.148291000