

Comparative oxidative ability of mononuclear and dinuclear high-valent iron-oxo species towards activation of methane: does the axial/bridge atom modulate the reactivity?

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Table S1. B3LYP-D3 computed optimized energy of possible spin states of species **1**, **2**, **3**, **4**, **4a**, **4b**, and **4c**.

Spin states	Energy(kJ/mol)
1	
⁵ 1 _(hs)	43.9
³ 1 _(is)	0.0
¹ 1 _(ls)	114.9
2	
⁶ 2 _(hs)	26.5
⁴ 2 _(hs)	27.9
⁴ 2 _(is)	0.0
² 2 _(is)	6.9
² 2 _(ls)	7.1
3	
¹⁰ 3 _(hs, hs)	101.1
⁸ 3 _(hs, hs)	105.3
² 3 _(hs, hs)	107.8
⁶ 3 _(is, is)	2.9
⁴ 3 _(is, is)	3.3
² 3 _(is, is)	0.0
4	
¹⁰ 4 _(hs, hs)	433.2
⁸ 4 _(hs, hs)	296.7
² 4 _(hs, hs)	0.0
⁶ 4 _(is, is)	88.2
² 4 _(is, is)	55.9
4a	
⁶ 4a _(hs)	0.0
⁴ 4a _(hs)	27.5
⁴ 4a _(is)	9.7
² 4a _(is)	5.6
² 4a _(ls)	46.1
4b	
⁶ 4b _(hs)	130.9
⁴ 4b _(hs)	47.5
⁴ 4b _(is)	0.0
² 4b _(is)	96.1
² 4b _(ls)	44.3
4c	
⁶ 4c _(hs)	58.3
⁴ 4c _(hs)	55.6
⁴ 4c _(is)	4.0
² 4c _(is)	0.0
² 4c _(ls)	36.4

Table S2. Energy computed using DLPNO-CCSD(T) method for species **1**, **2**, **4a**, **4b**, and **4c**.

Spin states	Energy(kJ/mol)
1	
⁵ 1 _(hs)	6.9
³ 1 _(is)	0.0
¹ 1 _(ls)	99.5
2	
⁶ 2 _(hs)	120.6
⁴ 2 _(hs)	37.9
⁴ 2 _(is)	0.0
² 2 _(is)	194.2
² 2 _(ls)	193.5
4a	
⁶ 4a _(hs)	0.0
⁴ 4a _(hs)	197.0
⁴ 4a _(is)	112.0
² 4a _(is)	120.9
² 4a _(ls)	104.4
4b	
⁶ 4b _(hs)	283.7
⁴ 4b _(hs)	61.7
⁴ 4b _(is)	0.0
² 4b _(is)	9.2
² 4b _(ls)	0.9
4c	
⁶ 4c _(hs)	121.0
⁴ 4c _(hs)	5.8
⁴ 4c _(is)	65.4
² 4c _(is)	0.0
² 4c _(ls)	6.9

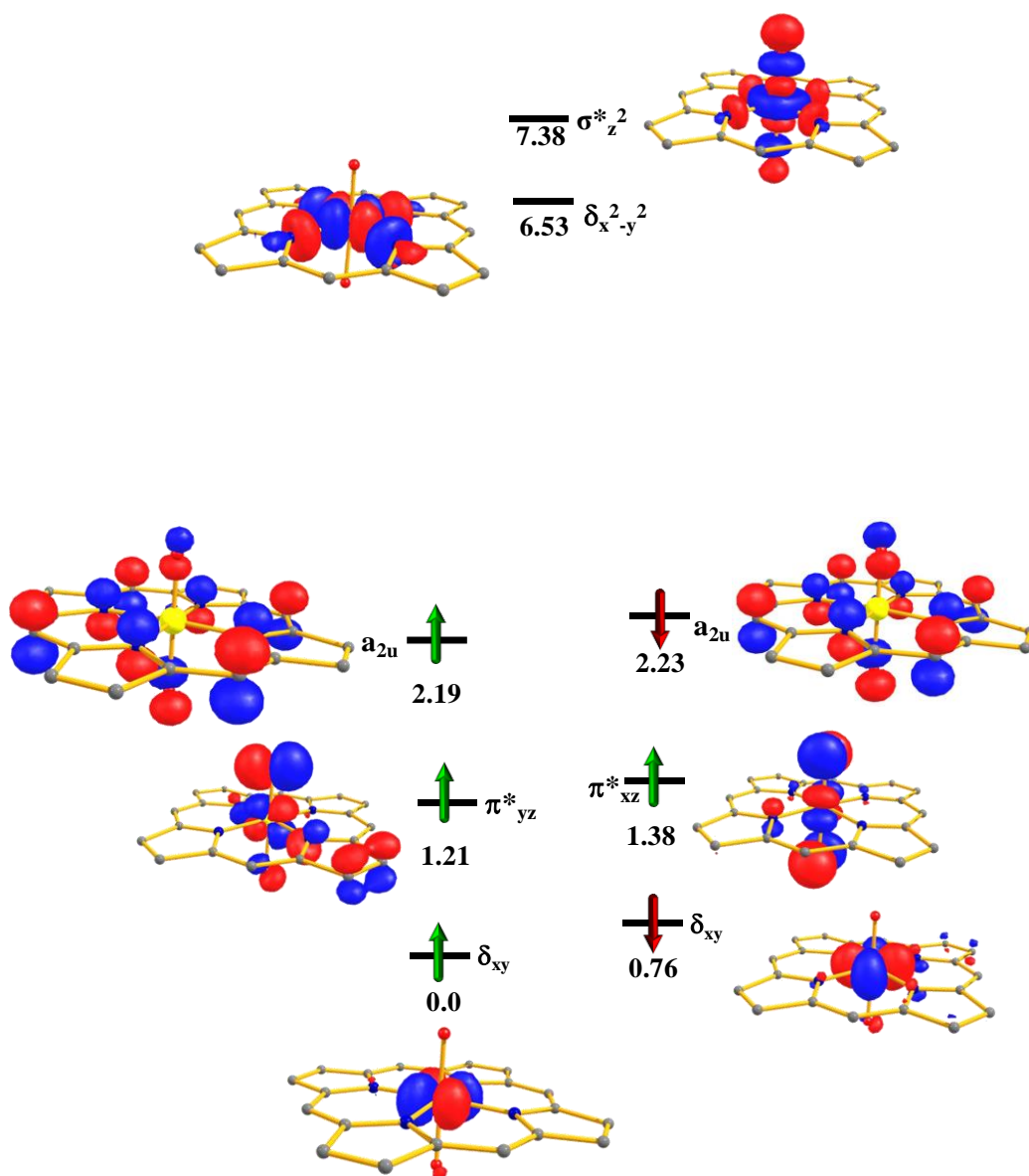


Figure S1. Computed Eigen-value plot incorporating energies computed for d-based orbitals for alpha and beta spin of $^3\mathbf{1}_{(is)}$ species (energies are given in eV).

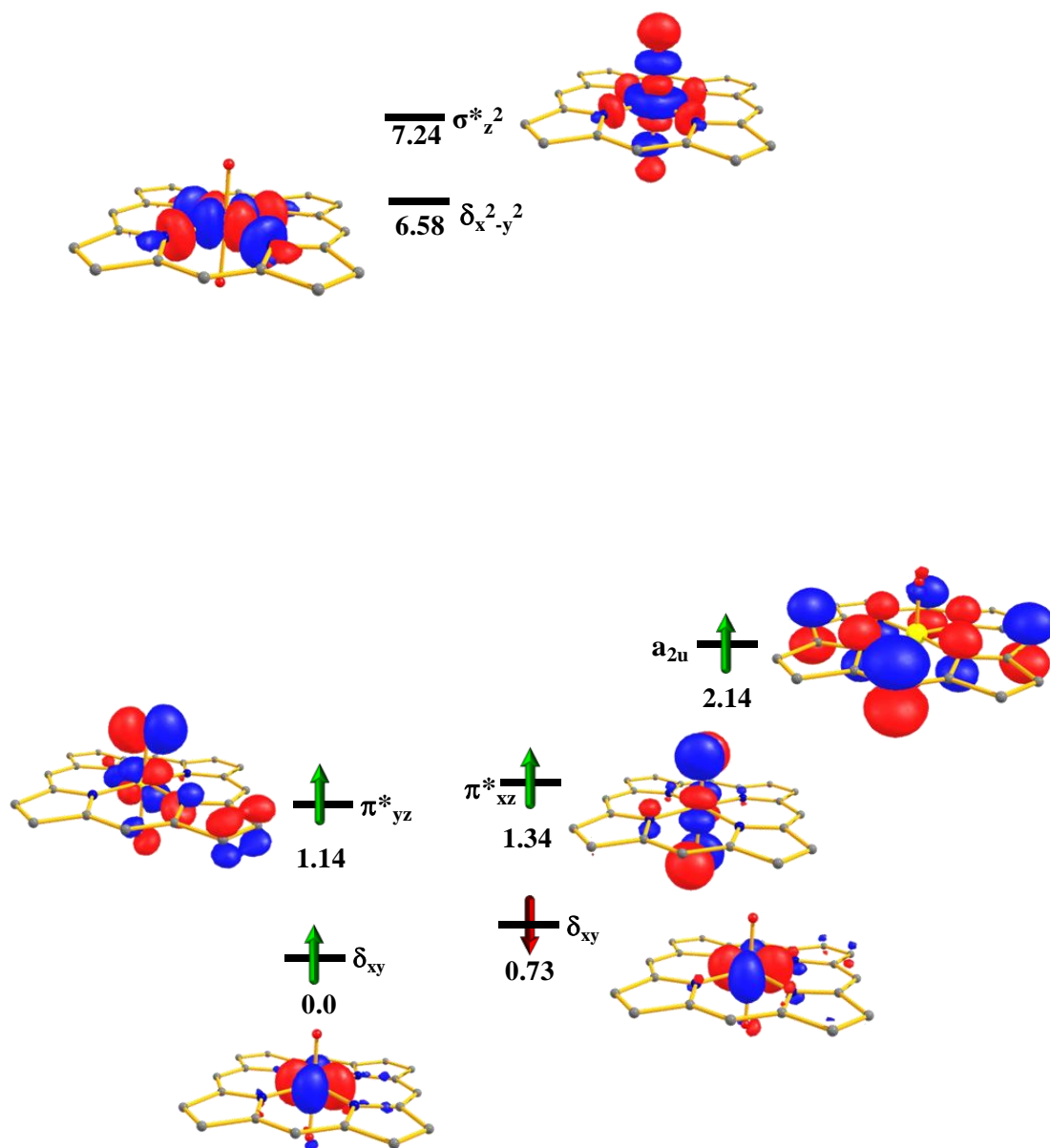


Figure S2. Computed Eigen-value plot incorporating energies computed for d-based orbitals for alpha and beta spin of ${}^42_{(is)}$ species (energies are given in eV).

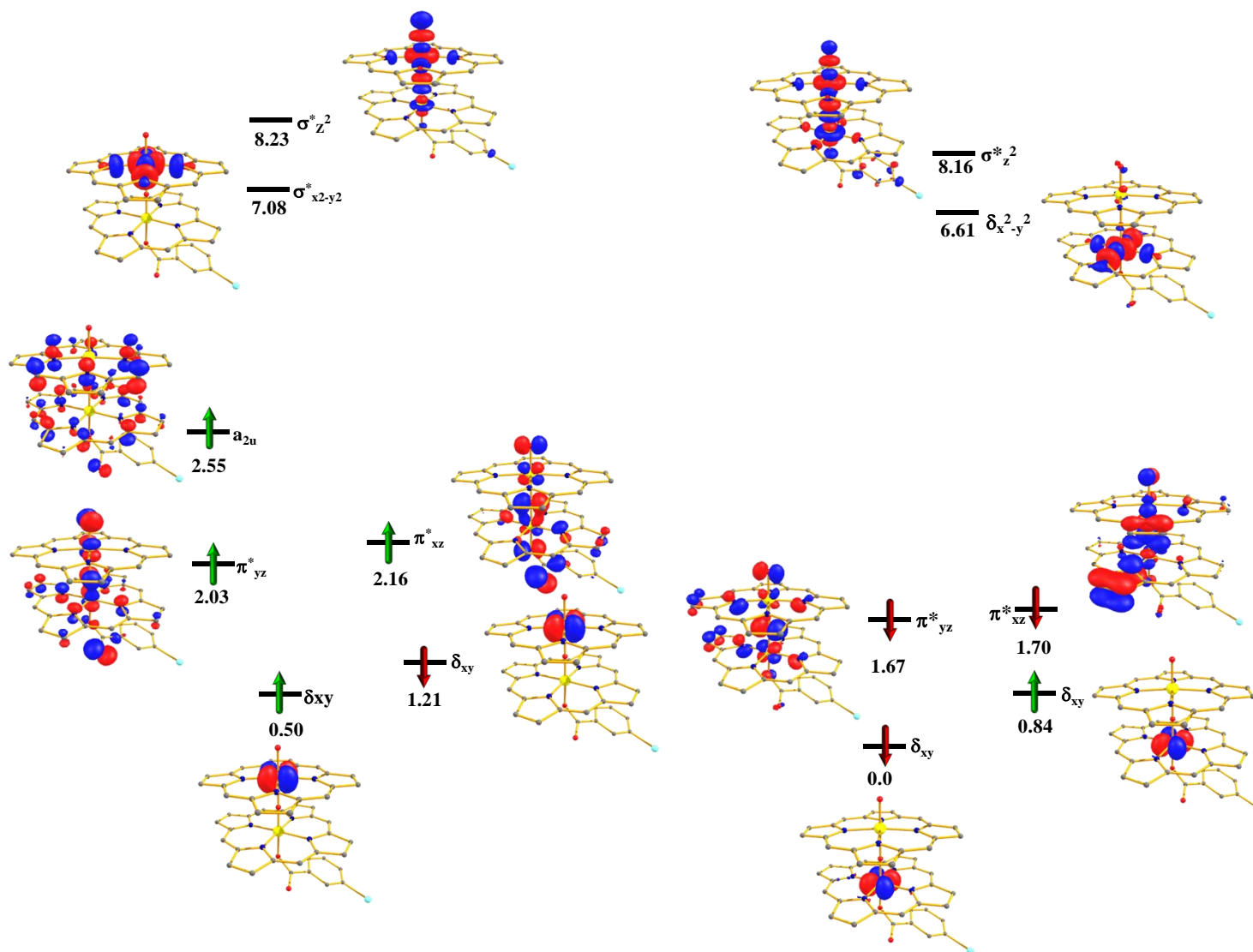
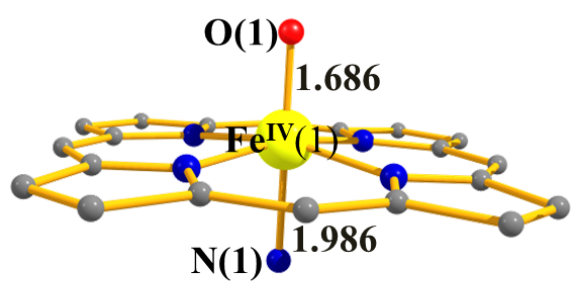


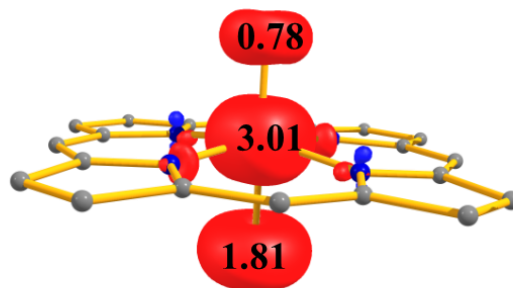
Figure S3. Computed Eigen-value plot incorporating energies computed for d-based orbitals for alpha and beta spin of $^{23}_{(is, is)}$ species (energies are given in eV).



$$\text{Fe}^{\text{IV}}(1)-\text{N}_{\text{avg}} = 2.104$$

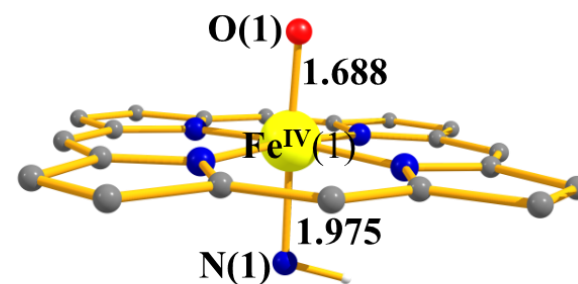
$$\angle \text{N}(1)-\text{Fe}^{\text{IV}}(1)-\text{O}(1) = 179.9^\circ$$

(a)



$$\text{Por}(a_{2u}) = -0.605$$

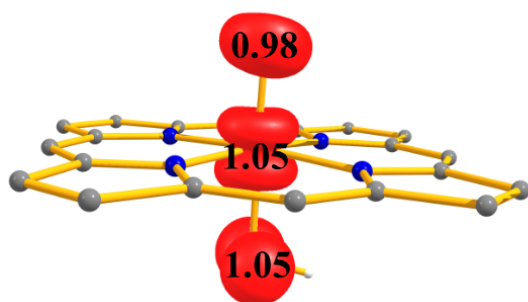
(b)



$$\text{Fe}^{\text{IV}}(1)-\text{N}_{\text{avg}} = 2.028$$

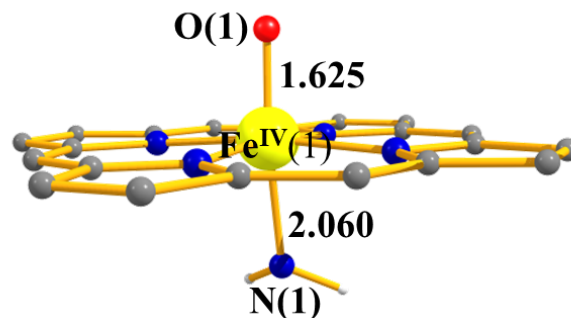
$$\angle \text{N}(1)-\text{Fe}^{\text{IV}}(1)-\text{O}(1) = 177.9^\circ$$

(c)



$$\text{Por}(a_{2u}) = 0.257$$

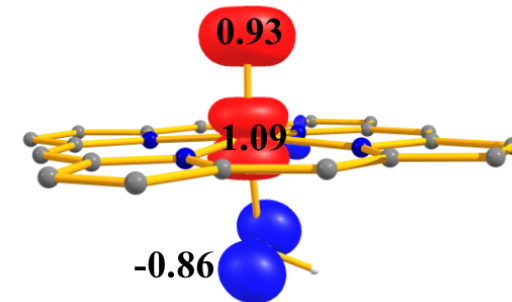
(d)



$$\text{Fe}^{\text{IV}}(1)-\text{N}_{\text{avg}} = 2.020$$

$$\angle \text{N}(1)-\text{Fe}^{\text{IV}}(1)-\text{O}(1) = 168.4^\circ$$

(e)



$$\text{Por}(a_{2u}) = 0.549$$

(f)

Figure S4. a-b) The optimized structure of ${}^6\mathbf{4a}_{(hs)}$ and its corresponding spin density plot, c-d) the optimized structure of ${}^4\mathbf{4b}_{(is)}$ and its corresponding spin density plot, e-f) the optimized structure of ${}^2\mathbf{4c}_{(is)}$ and its corresponding spin density plot. All the distances are given in Å and angles in $^\circ$. All hydrogen atoms are omitted for clarity.

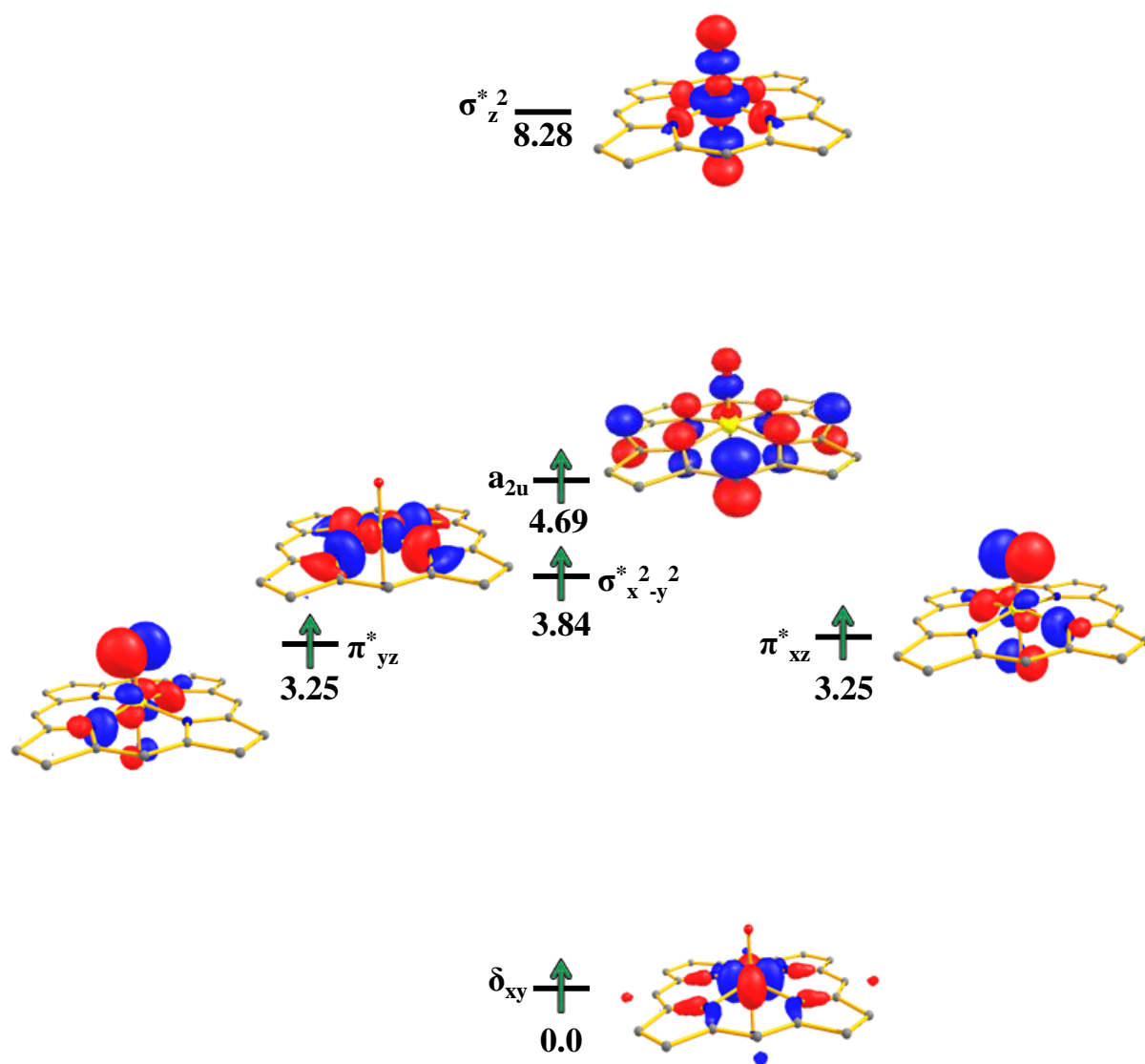


Figure S5. Computed Eigen-value plot incorporating energies computed for d-based orbitals for the alpha spin of ${}^6\mathbf{4a}_{(hs)}$ species (energies are given in eV).

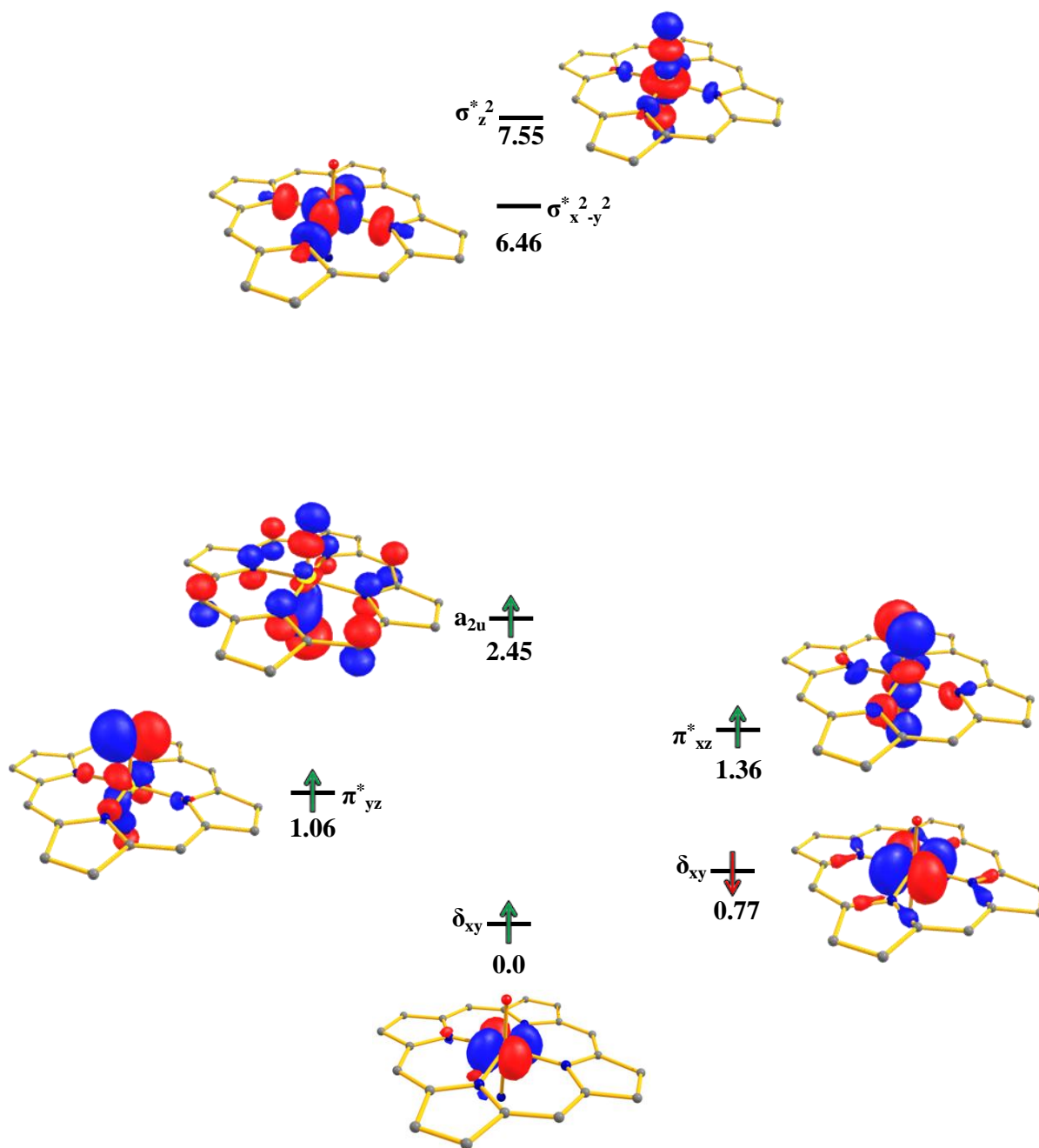


Figure S6. Computed Eigen-value plot incorporating energies computed for d-based orbitals for alpha and beta spins of $4b_{(is)}$ species (energies are given in eV).

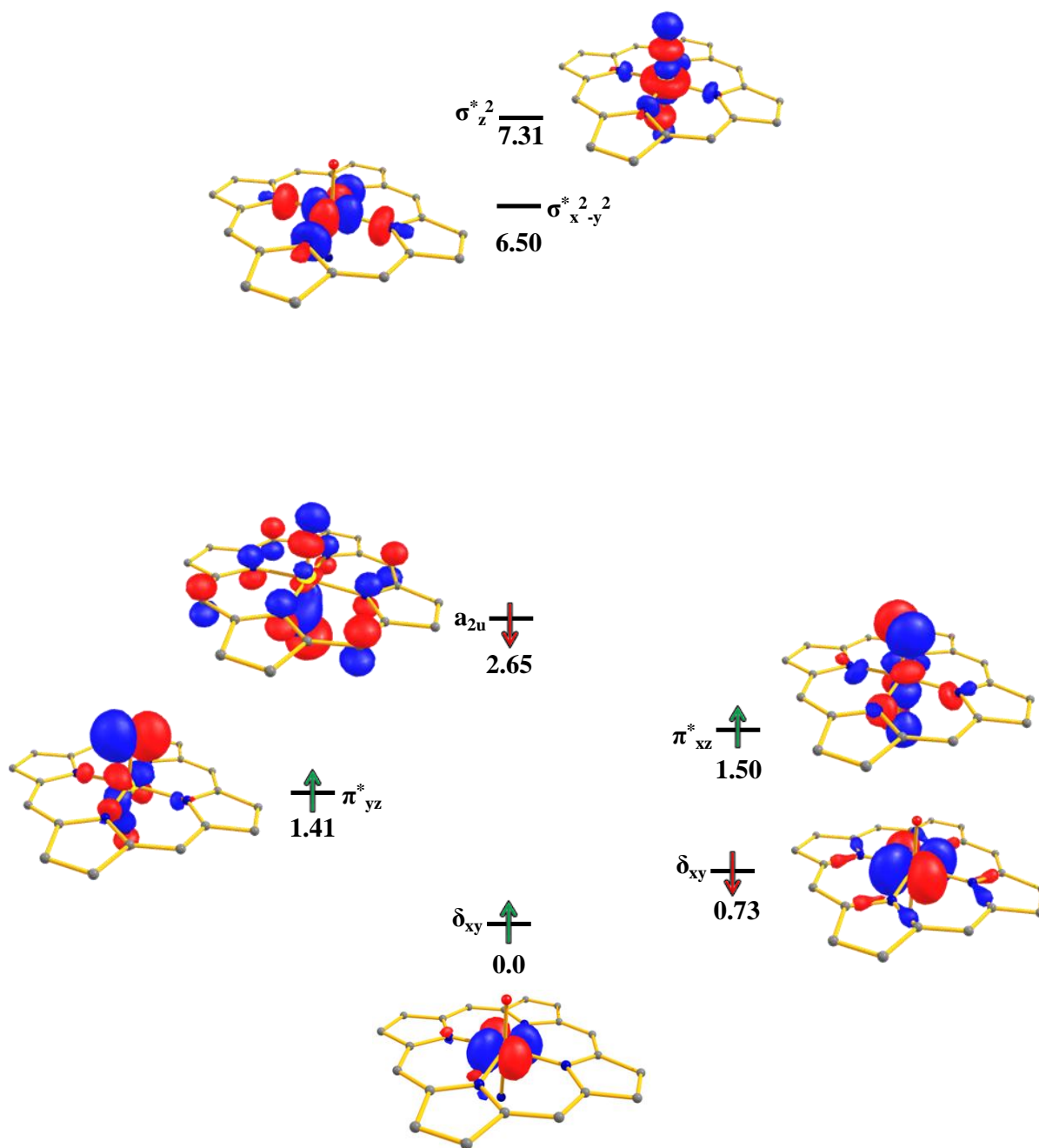


Figure S7. Computed Eigen-value plot incorporating energies computed for d-based orbitals for alpha and beta spins of $24b_{(is)}$ species (energies are given in eV).

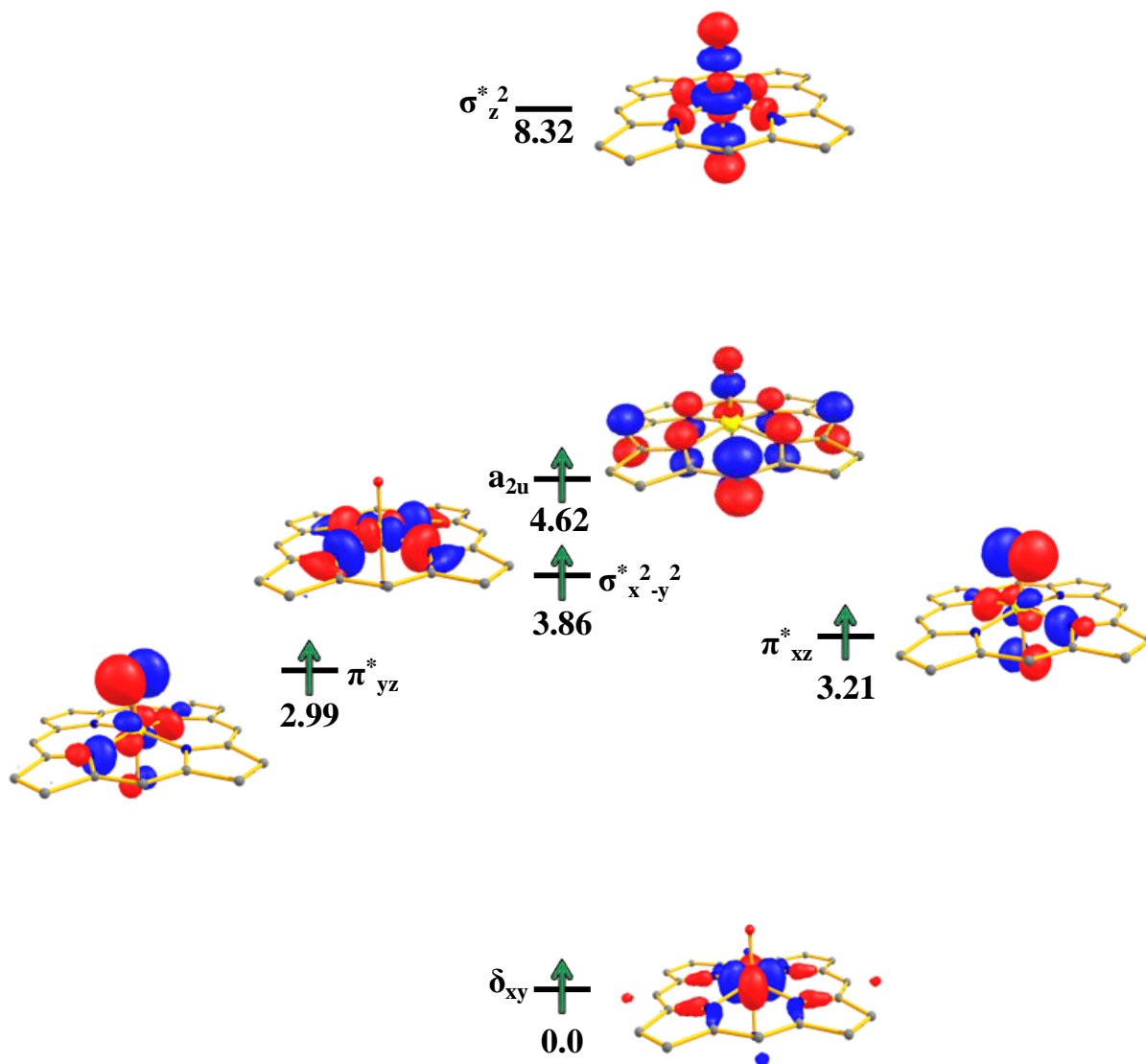


Figure S8. Computed Eigen-value plot incorporating energies computed for d-based orbitals for the alpha spin of ${}^{64}\mathbf{b}_{(\text{ths})}$ species (energies are given in eV).

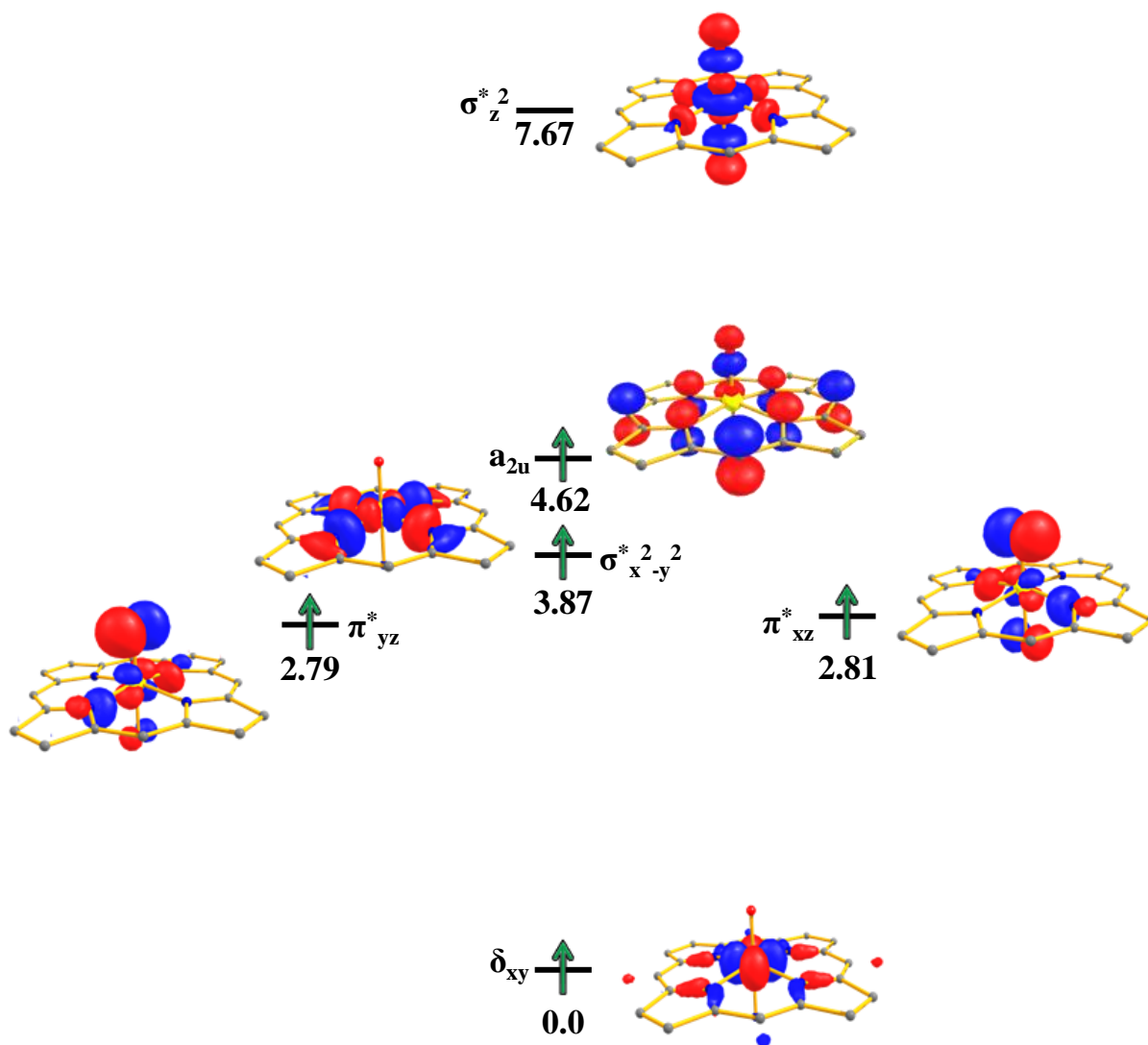


Figure S9. Computed Eigen-value plot incorporating energies computed for d-based orbitals for the alpha spin of ${}^6\mathbf{4c}_{(hs)}$ species (energies are given in eV).

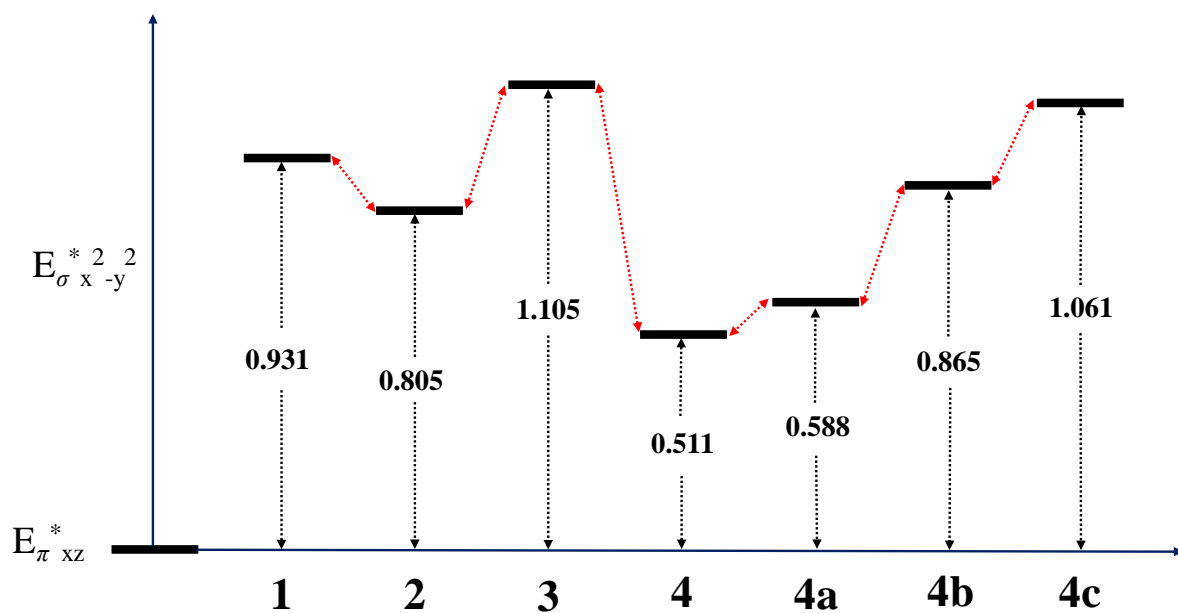


Figure S10. We calculated the relative energy of the $E_{\sigma_{x^2-y^2}}^*$ orbital of all seven species. Here, we have plotted the energy difference between the $\Delta E(E_{\pi_{xz}}^* - E_{\sigma_{x^2-y^2}}^*)$ versus $E_{\pi_{xz}}^*$, and $E_{\pi_{xz}}^*$ is used as a reference for all species. Here, we have used only high-spin structures for our calculating energy differences.

Table S3. B3LYP-D2 computed structural parameters (\AA) of species **4-4c** for a high spin state.

Species	$\text{Fe}^{\text{IV}}\text{-O(1)}$	$\text{Fe}^{\text{IV}}\text{-N}_{\text{ax}}$
4	1.695	1.920
4a	1.687	1.986
4b	1.680	1.991
4c	1.623	2.097

Table S4. B3LYP-D2 computed spin density and Mulliken charges on the a_{2u} , O(2)H, N(1) and O(1) atoms for a high spin with the radical up state. The ρ and σ represent spin density and Mulliken charges, respectively.

$\rho_{a_{2u}}$	$\sigma_{a_{2u}}$	$\rho_{O(2)H}$	$\sigma_{O(2)H}$	$\rho_{O(1)}$	$\sigma_{O(1)}$
1					
0.224	-0.927	0.009	-0.481	0.787	-0.376
2					
1.143	-0.005	0.117	-0.447	0.829	-0.292
3					
0.675	-0.217	-0.002	-0.321	0.681	-0.311
0.866	-0.012			0.035 (<i>m</i> -CBA)	-1.255 (<i>m</i> -CBA)
$\rho_{a_{2u}}$	$\sigma_{a_{2u}}$	$\rho_{N(1)}$	$\sigma_{N(1)}$	$\rho_{O(1)}$	$\sigma_{O(1)}$
4					
0.271	-0.570	0.074	-0.222	0.968	-0.535
0.484	-0.775			0.163 (<i>m</i> -CBA)	-1.255 (<i>m</i> -CBA)
4a					
-0.605	-1.738	1.812	-0.191	0.783	-0.499
4b					
0.257	-0.866	0.861	-0.256	0.861	-0.463
4c					
0.549	-0.350	0.828	-0.176	0.716	-0.229

Table S5. B3LYP-D2 computed optimized energy with zero-point energy corrections (ZPE) of possible spin states of species **1**.

Spin states	Energy(kJ/mol)
1	
$^5\mathbf{1}_{(hs)}$	38.6
$^3\mathbf{1}_{(is)}$	0.0
$^1\mathbf{1}_{(ls)}$	121.4
1-ts1	
$\mathbf{1-}^5\mathbf{ts1}_{(hs)}$	46.8
$\mathbf{1-}^3\mathbf{ts1}_{(is)}$	0.0
$\mathbf{1-}^1\mathbf{ts1}_{(ls)}$	125.4
1-int1	
$\mathbf{1-}^7\mathbf{int1}_{(hs)}$	21.9
$\mathbf{1-}^5\mathbf{int1}_{(hs)}$	22.6
$\mathbf{1-}^5\mathbf{int1}_{(is)}$	42.1
$\mathbf{1-}^3\mathbf{int1}_{(is)}$	43.2
$\mathbf{1-}^3\mathbf{int1}_{(ls)}$	0.0
$\mathbf{1-}^1\mathbf{int1}_{(ls)}$	2.5
1-ts2	
$\mathbf{1-}^7\mathbf{ts2}_{(hs)}$	30.7
$\mathbf{1-}^5\mathbf{ts2}_{(hs)}$	7.1
$\mathbf{1-}^5\mathbf{ts2}_{(is)}$	32.4
$\mathbf{1-}^3\mathbf{ts2}_{(is)}$	36.9
$\mathbf{1-}^3\mathbf{ts2}_{(ls)}$	12.2
$\mathbf{1-}^1\mathbf{ts2}_{(ls)}$	0.0
1-P	
$\mathbf{1-}^5\mathbf{P}_{(hs)}$	0.0
$\mathbf{1-}^3\mathbf{P}_{(is)}$	54.3
$\mathbf{1-}^1\mathbf{P}_{(ls)}$	21.9

Table S6. B3LYP-D2 computed structural parameters (Å) of species **1**.

Spin state	Fe ^{IV} (1)- O(1)	Fe ^{IV} (1)- N _{avg}	Fe ^{IV} (1)- O(2)	O(1)- H	H-C	O(1)- C	∠Fe ^{IV} (1)- O(1)-H	∠Fe ^{IV} (1)- O(1)-C
1								
⁵ 1 _(hs)	1.689	2.086	1.911	-	-	-	-	-
³ 1 _(is)	1.699	2.026	1.911	-	-	-	-	-
¹ 1 _(ls)	1.700	2.028	1.886	-	-	-	-	-
1-ts1								
1 ⁻⁵ ts1 _(hs)	1.837	2.084	1.876	1.077	1.525	2.602	114.6	114.7
1 ⁻³ ts1 _(is)	1.845	2.024	1.879	1.072	1.529	2.601	114.2	113.7
1 ⁻¹ ts1 _(ls)	1.847	2.022	1.888	1.041	1.575	2.296	115.9	115.5
1-int1								
1 ⁻⁷ int1 _(hs)	1.969	2.099	1.941	0.980	3.198	3.169	112.8	117.5
1 ⁻⁵ int1 _(hs)	1.969	2.099	1.941	0.980	3.198	3.173	112.8	117.4
1 ⁻⁵ int1 _(is)	1.866	2.086	1.848	0.980	3.216	3.228	109.0	114.3
1 ⁻³ int1 _(is)	1.866	2.086	1.848	0.980	3.215	3.231	109.0	114.2
1 ⁻³ int1 _(ls)	1.890	2.024	1.873	0.981	3.034	3.214	107.3	115.1
1 ⁻¹ int1 _(ls)	1.891	2.024	1.873	0.981	3.030	3.218	107.3	115.0
1-ts2								
1 ⁻⁷ ts2 _(hs)	2.044	2.097	1.913	0.980	2.568	2.254	110.3	119.8
1 ⁻⁵ ts2 _(hs)	1.995	2.098	1.949	0.980	2.541	2.378	111.1	120.3
1 ⁻⁵ ts2 _(is)	1.910	2.094	1.864	0.982	2.654	2.253	109.4	133.1
1 ⁻³ ts2 _(is)	1.914	2.075	1.871	0.981	2.498	2.251	107.0	120.5
1 ⁻³ ts2 _(ls)	1.944	2.025	1.857	0.982	2.506	2.164	107.0	121.6
1 ⁻¹ ts2 _(ls)	1.913	2.021	1.876	0.982	2.479	2.230	107.3	118.6
1-P								
1 ⁻⁵ P _(hs)	3.586	2.163	1.904	0.986	2.011	1.449	29.8	84.2
1 ⁻³ P _(is)	3.382	2.027	1.924	0.984	2.013	1.453	37.3	81.6
1 ⁻¹ P _(ls)	2.175	2.016	1.915	0.979	2.036	1.462	95.6	115.6

Table S7. B3LYP-D2 computed spin densities of the complex **1**.

Spin states	Fe ^{IV} (1)	O(1)	O(2)	H	C
1					
⁵ 1 _(hs)	2.98	0.79	0.01	-	-
³ 1 _(is)	1.05	0.97	0.08	-	-
¹ 1 _(ls)	0.00	0.00	0.00	-	-
1-ts1					
1-⁵ts1 _(hs)	2.81	0.37	0.04	-0.08	0.79
1-³ts1 _(is)	0.88	0.46	0.12	-0.08	0.80
1-¹ts1 _(ls)	0.00	0.00	0.00	0.00	0.00
1-int1					
1-⁷int1 _(hs)	4.06	0.28	0.32	0.00	1.17
1-⁵int1 _(hs)	4.05	0.28	0.32	0.00	-1.16
1-⁵int1 _(is)	2.74	0.05	0.08	0.00	1.17
1-³int1 _(is)	2.73	0.05	0.08	0.00	-1.16
1-³int1 _(ls)	0.88	0.09	0.11	0.00	1.16
1-¹int1 _(ls)	0.87	0.09	0.11	0.00	-1.16
1-ts2					
1-⁷ts2 _(hs)	4.09	0.21	0.35	0.00	0.81
1-⁵ts2 _(hs)	4.00	0.24	0.29	0.00	-0.95
1-⁵ts2 _(is)	3.01	-0.06	0.09	0.00	0.93
1-³ts2 _(is)	2.56	0.10	0.10	0.00	-0.88
1-³ts2 _(ls)	0.99	0.05	0.12	0.00	0.77
1-¹ts2 _(ls)	0.75	0.07	0.09	0.00	-0.86
1-P					
1-⁵P _(hs)	3.46	0.00	0.17	0.00	0.00
1-³P _(is)	2.30	0.00	0.30	0.00	0.00
1-¹P _(ls)	0.00	0.00	0.00	0.00	0.00

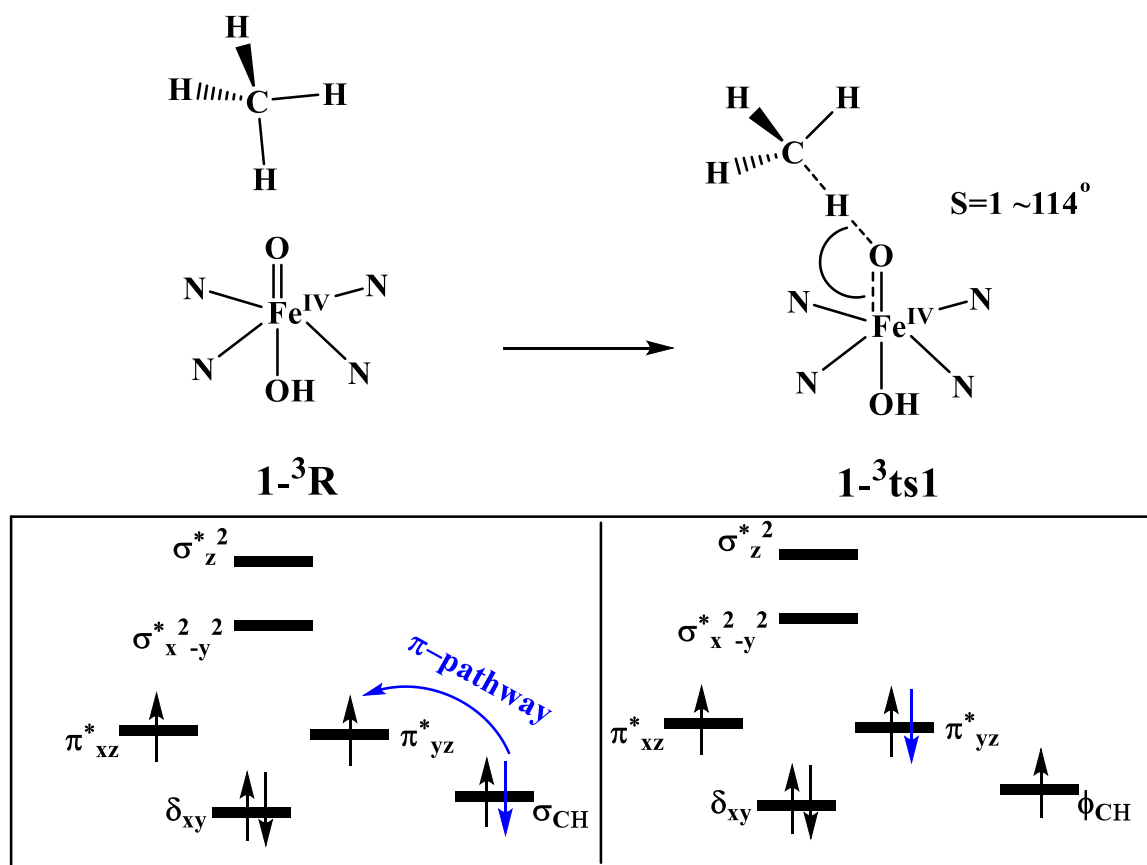


Figure S11. Orbitals and their occupancy changes during the hydrogen atom abstraction from methane.

Table S8. B3LYP-D2 computed optimized energy with zero-point energy corrections (ZPE) of possible spin states of complex **2**.

Spin states	Energy(kJ/mol)
2	
${}^6\mathbf{2}_{(hs)}$	26.1
${}^4\mathbf{2}_{(hs)}$	27.3
${}^4\mathbf{2}_{(is)}$	0.0
${}^2\mathbf{2}_{(is)}$	6.8
${}^2\mathbf{2}_{(ls)}$	7.8
2-ts1	
${}^2\text{-}{}^6\mathbf{ts1}_{(hs)}$	70.8
${}^2\text{-}{}^4\mathbf{ts1}_{(hs)}$	64.2
${}^2\text{-}{}^4\mathbf{ts1}_{(is)}$	24.6
${}^2\text{-}{}^2\mathbf{ts1}_{(is)}$	0.0
${}^2\text{-}{}^2\mathbf{ts1}_{(ls)}$	39.5
2-int1	
${}^2\text{-}{}^6\mathbf{int1}_{(hs)}$	57.2
${}^2\text{-}{}^4\mathbf{int1}_{(hs)}$	82.4
${}^2\text{-}{}^4\mathbf{int1}_{(is)}$	0.0
${}^2\text{-}{}^2\mathbf{int1}_{(is)}$	0.6
${}^2\text{-}{}^2\mathbf{int1}_{(ls)}$	49.7
2-ts2	
${}^2\text{-}{}^6\mathbf{ts2}_{(hs)}$	61.6
${}^2\text{-}{}^4\mathbf{ts2}_{(hs)}$	128.3
${}^2\text{-}{}^4\mathbf{ts2}_{(is)}$	6.5
${}^2\text{-}{}^2\mathbf{ts2}_{(is)}$	0.0
${}^2\text{-}{}^2\mathbf{ts2}_{(ls)}$	38.5
2-P	
${}^2\text{-}{}^6\mathbf{P}_{(hs)}$	0.0
${}^2\text{-}{}^4\mathbf{P}_{(is)}$	70.5
${}^2\text{-}{}^2\mathbf{P}_{(ls)}$	6.4

Table S9. B3LYP-D2 computed structural parameters (Å) of the complex **2**.

Spin state	Fe ^{IV} (1)- O(1)	Fe ^{IV} (1)- N _{avg}	Fe ^{IV} (1)- O(2)	O(1)- H	H-C	O(1)- C	∠Fe ^{IV} (1)- O(1)-H	∠Fe ^{IV} (1)- O(1)-C
2								
⁶ 2 _(hs)	1.684	2.083	1.905	-	-	-	-	-
⁴ 2 _(hs)	1.682	2.083	1.926	-	-	-	-	-
⁴ 2 _(is)	1.687	2.019	1.933	-	-	-	-	-
² 2 _(is)	1.661	2.019	1.971					
² 2 _(ls)	1.661	2.019	1.972					
2-ts1								
2-⁶ts1 _(hs)	1.788	2.072	1.827	1.165	1.368	2.532	116.9	118.5
2-⁴ts1 _(hs)	1.785	2.071	1.824	1.169	1.347	2.514	115.1	114.5
2-⁴ts1 _(is)	1.799	2.008	1.817	1.178	1.349	2.526	115.4	115.7
2-²ts1 _(is)	1.776	2.009	1.818	1.156	1.362	2.518	114.9	114.0
2-²ts1 _(ls)	1.776	2.012	1.819	1.157	1.361	2.516	115.3	114.3
2-int1								
2-⁶int1 _(hs)	1.803	2.072	1.817	0.994	2.042	3.024	113.8	118.0
2-⁴int1 _(hs)	1.799	2.072	1.819	0.997	1.994	2.979	114.3	116.5
2-⁴int1 _(is)	1.799	2.014	1.811	0.990	2.077	3.060	114.2	116.9
2-²int1 _(is)	1.795	2.014	1.813	0.993	2.028	3.017	114.4	116.0
2-²int1 _(ls)	1.796	2.014	1.808	1.000	1.951	2.948	114.4	116.8
2-ts2								
2-⁶ts2 _(hs)	1.849	2.074	1.826	0.983	2.523	2.738	109.7	124.6
2-⁴ts2 _(hs)	1.814	2.071	1.813	0.983	2.368	2.842	112.8	115.6
2-⁴ts2 _(is)	1.849	2.019	1.824	0.982	2.714	2.457	111.2	131.8
2-²ts2 _(is)	1.813	2.014	1.810	0.981	2.593	2.780	113.3	118.9
2-²ts2 _(ls)	1.851	2.019	1.826	0.982	2.718	2.450	111.2	131.9
2-P								
2-⁶P _(hs)	2.369	2.091	1.841	0.978	2.041	1.459	97.4	120.8
2-⁴P _(is)	2.380	2.029	1.885	0.978	2.037	1.461	97.4	117.1
2-²P _(ls)	2.062	2.017	1.804	0.976	2.056	1.465	107.6	121.6

Table S10. B3LYP-D2 computed spin densities of the complex **2**.

Spin states	Fe ^{IV} (1)	O(1)	O(2)	H	C	a _{2u}
2						
⁶ 2 _(hs)	2.91	0.83	0.12	-	-	1.14
⁴ 2 _(hs)	3.02	0.77	-0.14	-	-	-0.66
⁴ 2 _(is)	0.99	1.07	0.38	-	-	0.56
² 2 _(is)	1.06	0.97	-0.46			-0.59
² 2 _(ls)	1.06	0.97	-0.46			-0.59
2-ts1						
²⁻⁶ ts1 _(hs)	3.19	0.57	0.22	-0.04	0.65	0.48
²⁻⁴ ts1 _(hs)	3.29	-0.25	0.15	0.04	-0.62	0.33
²⁻⁴ ts1 _(is)	1.50	0.73	0.28	-0.05	0.65	-0.02
²⁻² ts1 _(is)	1.62	-0.15	0.22	0.04	-0.65	-0.15
²⁻² ts1 _(ls)	1.62	-0.15	0.22	0.04	-0.65	-0.15
2-int1						
²⁻⁶ int1 _(hs)	3.28	0.17	0.23	0.01	1.08	0.38
²⁻⁴ int1 _(hs)	3.29	0.14	0.14	-0.00	-1.07	0.36
²⁻⁴ int1 _(is)	1.61	0.32	0.25	-0.00	1.09	-0.06
²⁻² int1 _(is)	1.62	0.22	0.23	-0.00	-1.08	-0.07
²⁻² int1 _(ls)	-0.07	0.41	-0.28	-0.01	1.06	0.03
2-ts2						
²⁻⁶ ts2 _(hs)	3.49	-0.02	0.25	0.02	1.05	0.37
²⁻⁴ ts2 _(hs)	3.22	0.21	0.12	-0.00	-1.08	0.37
²⁻⁴ ts2 _(is)	1.94	0.06	0.29	-0.02	0.99	-0.13
²⁻² ts2 _(is)	1.51	0.28	0.24	-0.00	-1.08	-0.14
²⁻² ts2 _(ls)	1.53	0.29	0.22	-0.00	-1.08	-0.12
2-P						
²⁻⁶ P _(hs)	4.07	0.03	0.42	0.00	0.03	0.48
²⁻⁴ P _(is)	2.61	0.03	0.40	0.00	0.03	-0.05
²⁻² P _(ls)	0.91	0.00	0.14	0.00	0.00	-0.05

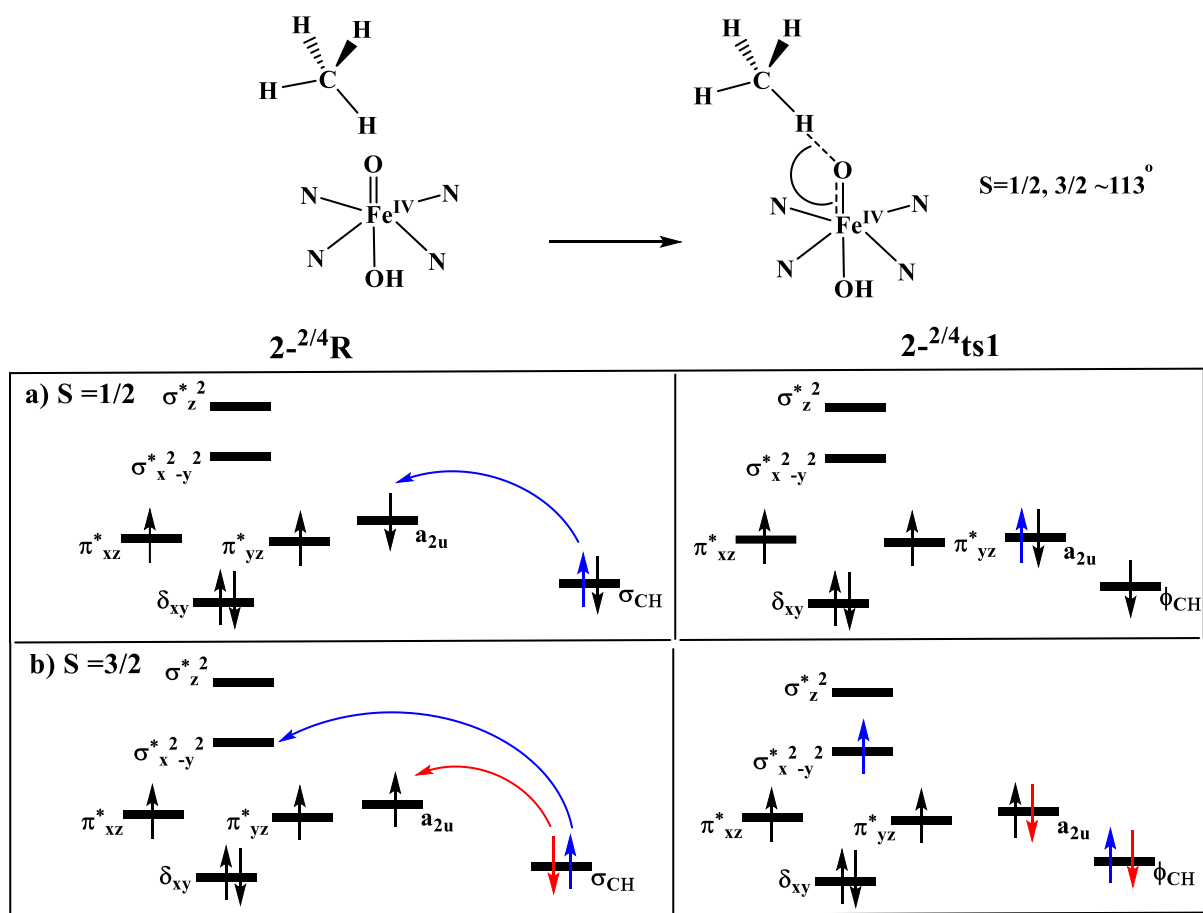


Figure S12. Orbitals and their occupancy changes during the hydrogen atom abstraction from methane.

Table S11. B3LYP-D2 computed optimized energy with zero-point energy corrections (ZPE) of possible spin states of complex **3**.

Spin states	Energy(kJ/mol)
3	
$^{10}\mathbf{3}_{(hs, hs)}$	109.3
$^8\mathbf{3}_{(hs, hs)}$	112.4
$^2\mathbf{3}_{(hs, hs)}$	114.5
$^6\mathbf{3}_{(is, is)}$	6.7
$^4\mathbf{3}_{(is, is)}$	6.1
$^2\mathbf{3}_{(is, is)}$	0.0
3-ts1	
$\mathbf{3}^{-10}\mathbf{ts1}_{(hs, hs)}$	119.3
$\mathbf{3}^{-8}\mathbf{ts1}_{(hs, hs)}$	113.7
$\mathbf{3}^{-2}\mathbf{ts1}_{(hs, hs)}$	125.8
$\mathbf{3}^{-6}\mathbf{ts1}_{(is, is)}$	3.8
$\mathbf{3}^{-4}\mathbf{ts1}_{(is, is)}$	2.8
$\mathbf{3}^{-2}\mathbf{ts1}_{(is, is)}$	0.0
3-int1	
$\mathbf{3}^{-12}\mathbf{int1}_{(hs, hs)}$	59.4
$\mathbf{3}^{-10}\mathbf{int1}_{(hs, hs)}$	48.8
$\mathbf{3}^{-4}\mathbf{int1}_{(hs, hs)}$	79.0
$\mathbf{3}^{-2}\mathbf{int1}_{(hs, hs)}$	65.7
$\mathbf{3}^{-8}\mathbf{int1}_{(is, is)}$	17.9
$\mathbf{3}^{-6}\mathbf{int1}_{(is, is)}$	25.3
$\mathbf{3}^{-4}\mathbf{int1}_{(is, is)}$	13.6
$\mathbf{3}^{-2}\mathbf{int1}_{(is, is)}$	0.0
3-ts2	
$\mathbf{3}^{-12}\mathbf{ts1}_{(hs, hs)}$	29.2
$\mathbf{3}^{-10}\mathbf{ts1}_{(hs, hs)}$	35.9
$\mathbf{3}^{-4}\mathbf{ts1}_{(hs, hs)}$	30.5
$\mathbf{3}^{-2}\mathbf{ts1}_{(hs, hs)}$	51.5
$\mathbf{3}^{-8}\mathbf{ts1}_{(is, is)}$	25.4
$\mathbf{3}^{-6}\mathbf{ts1}_{(is, is)}$	0.3
$\mathbf{3}^{-4}\mathbf{ts1}_{(is, is)}$	27.1
$\mathbf{3}^{-2}\mathbf{ts1}_{(is, is)}$	0.0
3-P	
$\mathbf{3}^{-10}\mathbf{P}_{(hs, hs)}$	62.9
$\mathbf{3}^{-2}\mathbf{P}_{(hs, hs)}$	30.6
$\mathbf{3}^{-6}\mathbf{P}_{(is, is)}$	7.3
$\mathbf{3}^{-2}\mathbf{P}_{(is, is)}$	0.0

Table S12a. B3LYP-D2 computed structural parameters (Å) of the complex **3**.

Spin states	Fe ^{IV} (1)-O(1)	Fe ^{IV} (1)-N _(porp)	Fe ^{IV} (2)-O(2)	Fe ^{IV} (1)-O(1)	Fe ^{IV} (2)-O(3)	O(1)-H	H-C	O(1)-C	∠Fe ^{III} (1)-O(1)-C	∠Fe ^{III} (1)-O(1)-H	∠O(1)-H-C	∠Fe ^{IV} (1)-O(2)-Fe ^{IV} (2)
3												
¹⁰ 3 _(hs, hs)	1.650	2.079	1.992	1.667	1.926	-	-	-	-	-	-	178.3
⁸ 3 _(hs, hs)	1.650	2.079	1.989	1.666	1.924	-	-	-	-	-	-	177.4
² 3 _(hs, hs)	1.645	2.080	1.968	1.662	1.928	-	-	-	-	-	-	179.8
⁶ 3 _(is, is)	1.658	2.019	1.952	1.666	1.929	-	-	-	-	-	-	178.8
⁴ 3 _(is, is)	1.657	2.019	1.952	1.664	1.930	-	-	-	-	-	-	178.8
² 3 _(is, is)	1.656	2.019	1.917	1.662	1.927	-	-	-	-	-	-	179.2
3-ts1												
³⁻¹⁰ ts1 _(hs, hs)	1.791	2.076	1.902	1.682	1.912	1.107	1.461	2.568	116.2	114.9	177.5	176.1
³⁻⁸ ts1 _(hs, hs)	1.792	2.076	1.894	1.686	1.908	1.108	1.458	2.566	116.0	114.7	177.4	176.0
³⁻² ts1 _(hs, hs)	1.785	2.078	1.925	1.664	1.916	1.102	1.473	2.574	116.5	115.3	176.5	178.1
³⁻⁶ ts1 _(is, is)	1.787	2.018	1.883	1.682	1.914	1.104	1.468	2.573	114.6	114.7	178.5	176.7
³⁻⁴ ts1 _(is, is)	1.791	2.017	1.860	1.699	1.914	1.106	1.456	2.563	113.3	114.0	178.6	176.8
³⁻² ts1 _(is, is)	1.790	2.018	1.874	1.670	1.922	1.100	1.472	2.572	114.3	114.2	179.5	178.7
3-int1												
³⁻¹² int1 _(hs, hs)	1.843	2.087	2.083	1.665	1.944	0.979	2.265	3.175	111.4	128.9	153.9	177.1
³⁻¹⁰ int1 _(hs, hs)	1.835	2.087	2.083	1.665	1.945	0.984	2.110	3.044	114.1	129.0	157.5	177.6
³⁻⁴ int1 _(hs, hs)	1.847	2.089	2.144	1.654	1.940	0.980	2.243	3.165	110.7	127.3	156.1	179.3
³⁻² int1 _(hs, hs)	1.838	2.087	2.119	1.655	1.936	0.984	2.113	3.048	113.7	128.4	157.8	177.4
³⁻⁸ int1 _(is, is)	1.883	2.027	2.092	1.659	1.958	0.981	2.280	3.228	110.9	122.5	162.0	178.9
³⁻⁶ int1 _(is, is)	1.872	2.029	2.091	1.659	1.954	0.985	2.139	3.095	113.4	123.1	163.1	179.9
³⁻⁴ int1 _(is, is)	1.813	2.017	1.823	1.723	1.906	0.990	2.064	3.054	112.4	111.2	177.7	179.8
³⁻² int1 _(is, is)	1.826	2.018	1.713	1.801	1.899	0.9891	2.081	3.070	112.8	112.5	179.5	179.9

Table S12b. B3LYP-D2 computed structural parameters (Å) of the complex **3**.

Spin states	Fe ^{IV} (1)-O(1)	Fe ^{IV} (1)-N _(porp)	Fe ^{IV} (2)-O(2)	Fe ^{IV} (1)-O(1)	Fe ^{IV} (2)-O(3)	O(1)-H	H-C	O(1)-C	∠Fe ^{III} (1)-O(1)-C	∠Fe ^{III} (1)-O(1)-H	∠O(1)-H-C	∠Fe ^{IV} (1)-O(2)-Fe ^{IV} (2)
3-ts2												
3-¹²ts2 _(hs, hs)	1.879	2.082	1.715	1.946	1.957	0.981	2.798	2.577	127.6	112.1	92.5	178.5
3-¹⁰ts2 _(hs, hs)	1.868	2.085	2.059	1.667	1.945	0.975	2.611	2.614	114.4	126.3	79.0	178.2
3-⁴ts2 _(hs, hs)	1.885	2.055	1.938	1.693	2.021	0.981	2.646	2.643	131.2	110.5	79.4	176.8
3-²ts2 _(hs, hs)	1.871	2.085	2.092	1.657	1.935	0.975	2.593	2.604	126.3	113.4	78.5	174.0
3-⁸ts2 _(is, is)	1.887	2.040	2.023	1.663	1.943	0.979	2.801	2.427	118.8	117.0	102.0	177.7
3-⁶ts2 _(is, is)	1.905	2.025	2.074	1.661	1.951	0.977	2.637	2.779	112.4	121.3	71.5	177.5
3-⁴ts2 _(is, is)	1.855	2.047	1.876	1.665	1.918	0.980	2.804	2.479	131.8	113.8	98.9	178.6
3-²ts2 _(is, is)	1.911	2.026	2.021	1.656	1.947	0.978	2.660	2.797	113.4	119.6	87.6	176.5
3-P												
3-¹⁰P _(hs, hs)	2.178	2.076	1.663	2.062	1.910	0.978	2.053	1.466	121.1	102.6	112.7	179.2
3-²P _(hs, hs)	2.320	2.092	1.768	1.812	2.051	0.978	2.044	1.462	118.9	99.3	112.2	175.9
3-⁶P _(is, is)	2.263	2.019	1.898	1.697	1.906	0.977	2.046	1.465	118.4	103.3	112.2	179.5
3-²P _(is, is)	2.281	2.020	1.846	1.675	1.901	0.977	2.045	1.465	118.6	102.3	112.1	179.4

Table S13. B3LYP-D2 computed spin densities of the complex **3**.

Spin states	Fe ^{IV} (1)	Fe ^{IV} (2)	O(1)	O(2)	O(3)	C	H	a _{2u}
3								
¹⁰ 3 _(hs, hs)	3.08	3.06	0.68	0.60	0.04	--	--	0.68
⁸ 3 _(hs, hs)	3.08	3.06	0.62	0.69	-0.01	--	--	-0.42
² 3 _(hs, hs)	3.02	-3.08	0.70	-0.65	-0.02	--	--	0.74
⁶ 3 _(is, is)	1.02	1.21	0.99	0.83	0.07	--	--	0.45
⁴ 3 _(is, is)	1.05	1.24	0.99	0.81	0.03	--	--	-0.49
² 3 _(is, is)	1.03	-1.25	1.00	-0.76	-0.04	--	--	0.42
3-ts1								
3 ⁻¹⁰ ts1 _(hs, hs)	2.83	3.00	0.38	0.71	0.04	0.74	-0.05	0.63
3 ⁻⁸ ts1 _(hs, hs)	2.85	3.00	0.38	0.71	-0.00	0.73	-0.06	-0.52
3 ⁻² ts1 _(hs, hs)	2.78	-3.08	0.42	-0.66	-0.01	0.76	-0.06	0.73
3 ⁻⁶ ts1 _(is, is)	0.90	1.16	0.55	0.84	0.06	0.76	-0.06	0.47
3 ⁻⁴ ts1 _(is, is)	0.96	1.14	0.53	0.84	0.04	0.74	-0.06	-0.42
3 ⁻² ts1 _(is, is)	0.84	-1.21	0.55	-0.76	-0.04	0.77	-0.07	0.44
3-int1								
3 ⁻¹² int1 _(hs, hs)	4.04	3.13	0.46	0.63	0.06	1.12	0.02	0.82
3 ⁻¹⁰ int1 _(hs, hs)	4.02	3.13	0.39	0.63	0.07	-1.09	-0.00	0.81
3 ⁻⁴ int1 _(hs, hs)	4.09	-3.06	0.47	-0.66	-0.00	1.12	0.02	0.77
3 ⁻² int1 _(hs, hs)	4.08	-3.02	0.39	-0.67	0.02	-1.09	-0.00	0.82
3 ⁻⁸ int1 _(is, is)	2.57	1.29	0.43	0.82	0.08	1.13	0.01	0.35
3 ⁻⁶ int1 _(is, is)	2.55	1.29	0.36	0.81	0.08	-1.11	0.01	0.35
3 ⁻⁴ int1 _(is, is)	1.00	1.08	0.21	0.85	0.06	1.09	-0.01	-0.55
3 ⁻² int1 _(is, is)	1.12	-0.95	0.11	0.62	-0.07	-1.09	0.00	0.29
3-ts2								
3 ⁻¹² ts2 _(hs, hs)	3.32	4.09	0.20	0.71	0.02	1.04	0.01	0.75
3 ⁻¹⁰ ts2 _(hs, hs)	3.99	3.16	0.39	0.61	0.06	-1.04	0.00	0.79
3 ⁻⁴ ts2 _(hs, hs)	3.23	-2.72	-0.09	0.52	-0.14	1.06	0.01	0.81
3 ⁻² ts2 _(hs, hs)	4.06	-3.03	0.39	-0.65	0.02	-1.02	0.00	0.82
3 ⁻⁸ ts2 _(is, is)	3.13	1.33	0.07	0.77	-0.01	0.83	0.02	0.54
3 ⁻⁶ ts2 _(is, is)	2.57	1.30	0.36	0.80	0.08	-1.04	0.00	0.31
3 ⁻⁴ ts2 _(is, is)	2.91	-1.31	0.02	-0.62	-0.05	1.01	0.02	0.72
3 ⁻² ts2 _(is, is)	2.59	-1.23	0.36	-0.71	-0.02	-1.04	0.00	0.29
3-P								
3 ⁻¹⁰ P _(hs, hs)	3.37	4.08	0.00	0.62	0.25	0.00	0.00	0.22
3 ⁻² P _(hs, hs)	4.00	-4.06	0.03	0.12	-0.09	0.00	0.00	0.49
3 ⁻⁶ P _(is, is)	2.72	1.62	0.04	0.66	0.11	0.00	0.00	-0.05
3 ⁻² P _(is, is)	2.69	-1.45	0.04	-0.27	-0.06	0.00	0.00	-0.08

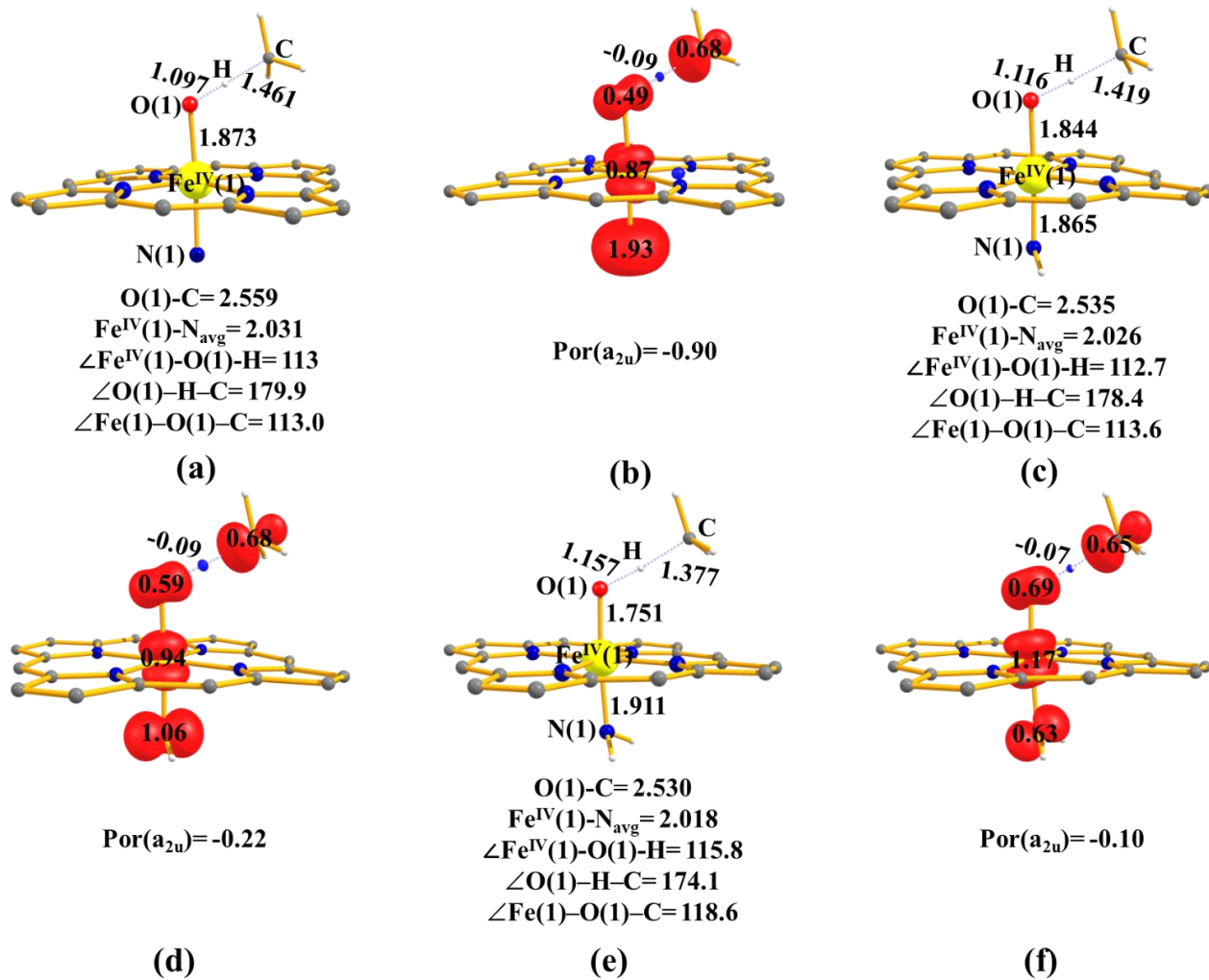


Figure S13. The optimized structures and its corresponding spin density plots for a-b) $4\mathbf{a}\text{-}^4\mathbf{ts1}_{(\text{is})}$, c-d) $4\mathbf{b}\text{-}^4\mathbf{ts1}_{(\text{is})}$ e-f), and $4\mathbf{c}\text{-}^4\mathbf{ts1}_{(\text{is})}$. All the distances are given in Å and angles in °. All hydrogen atoms (except CH_4) are omitted for clarity.

Table S14. B3LYP-D2 computed optimized energy with Gibb's free energy corrections (GFE) of possible spin states of complexes **4a/4b/4c**.

Spin states	Energy(kJ/mol)
4a	
4a-⁶R _(hs)	0.0
4a-⁴R _(hs)	26.9
4a-⁴R _(is)	12.2
4a-²R _(is)	4.9
4a-²R _(ls)	52.6
4a-ts1	
4a-⁶ts1 _(hs)	90.2
4a-⁴ts1 _(hs)	96.1
4a-⁴ts1 _(is)	58.4
4a-²ts1 _(is)	65.9
4a-²ts1 _(ls)	79.3
4b	
4b-⁶R _(hs)	122.3
4b-⁴R _(hs)	38.3
4b-⁴R _(is)	0.0
4b-²R _(is)	99.3
4b-²R _(ls)	44.1
4b-ts1	
4b-⁶ts1 _(hs)	126.9
4b-⁴ts1 _(hs)	144.7
4b-⁴ts1 _(is)	88.3
4b-²ts1 _(is)	94.9
4b-²ts1 _(ls)	95.6
4c	
4c-⁶R _(hs)	48.1
4c-⁴R _(hs)	46.1
4c-⁴R _(is)	1.9
4c-²R _(is)	0.0
4c-²R _(ls)	35.9
4c-ts1	
4c-⁶ts1 _(hs)	198.4
4c-⁴ts1 _(hs)	163.8
4c-⁴ts1 _(is)	90.6
4c-²ts1 _(is)	104.9
4c-²ts1 _(ls)	139.8

Table S15. Computed relative deformation energies in each fragment with respect to the catalyst and interaction energy in the reorganization HATs (**ts1s**) are values for the **1-³ts1_(is)**, **2-²ts1_(is)**, **3-²ts1_(is, is)**, **4-²ts1_(is, is)**, **4a-⁴ts1_(is)**, **4b-⁴ts1_(is)**, and **4c-⁴ts1_(is)**. Note:- All energies (in kJ/mol) have been calculated using hydrogen atom abstraction transition state and reactant from the ground spin state energetics.

ts1s	ΔE_{def}	ΔE_{int}	ΔE_{act}	ΔE^\ddagger
1-³ts1_(is)	147.6	-40.7	106.9	108.4
2-²ts1_(is)	81.2	-16.7	64.5	67.8
3-²ts1_(is, is)	124.1	-12.7	111.4	113.4
4-²ts1_(is, is)	67.1	-23.7	43.4	26.6
4a-⁴ts1_(is)	77.5	-7.6	69.9	58.4
4b-⁴ts1_(is)	147.1	-51.8	95.3	88.3
4c-⁴ts1_(is)	112.1	-20.9	91.2	90.6

Where, ΔE_{def} , ΔE_{int} , ΔE_{act} , and ΔE^\ddagger are a deformation, interaction, activation strain energy, and barrier height of the hydrogen atom abstraction, respectively.

$$\Delta E_{\text{act}} = \Delta E_{\text{def}} + \Delta E_{\text{int}}$$

$$\Delta E_{\text{dis}} = [\{E_{f1(\text{TS})} + E_{f2(\text{TS})}\} - \{E_{f1} + E_{f2}\}]$$

$$\Delta E_{\text{int}} = [E_{(\text{TS})} - \{E_{f1} + E_{f2}\}]$$

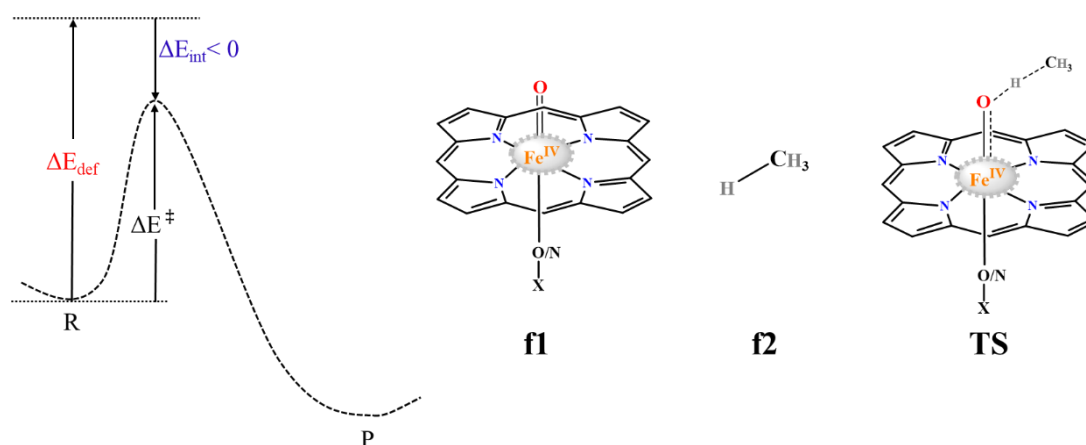


Figure S14. Illustration of interaction and distortion energies in the activation strain analysis for hydrogen atom abstraction transition state. Relationship between the barrier ΔE^\ddagger , the deformation energy of reactants, ΔE_{def} , and their interaction energy, ΔE_{int} , at the TS: $\Delta E_{\text{int}} < 0$.

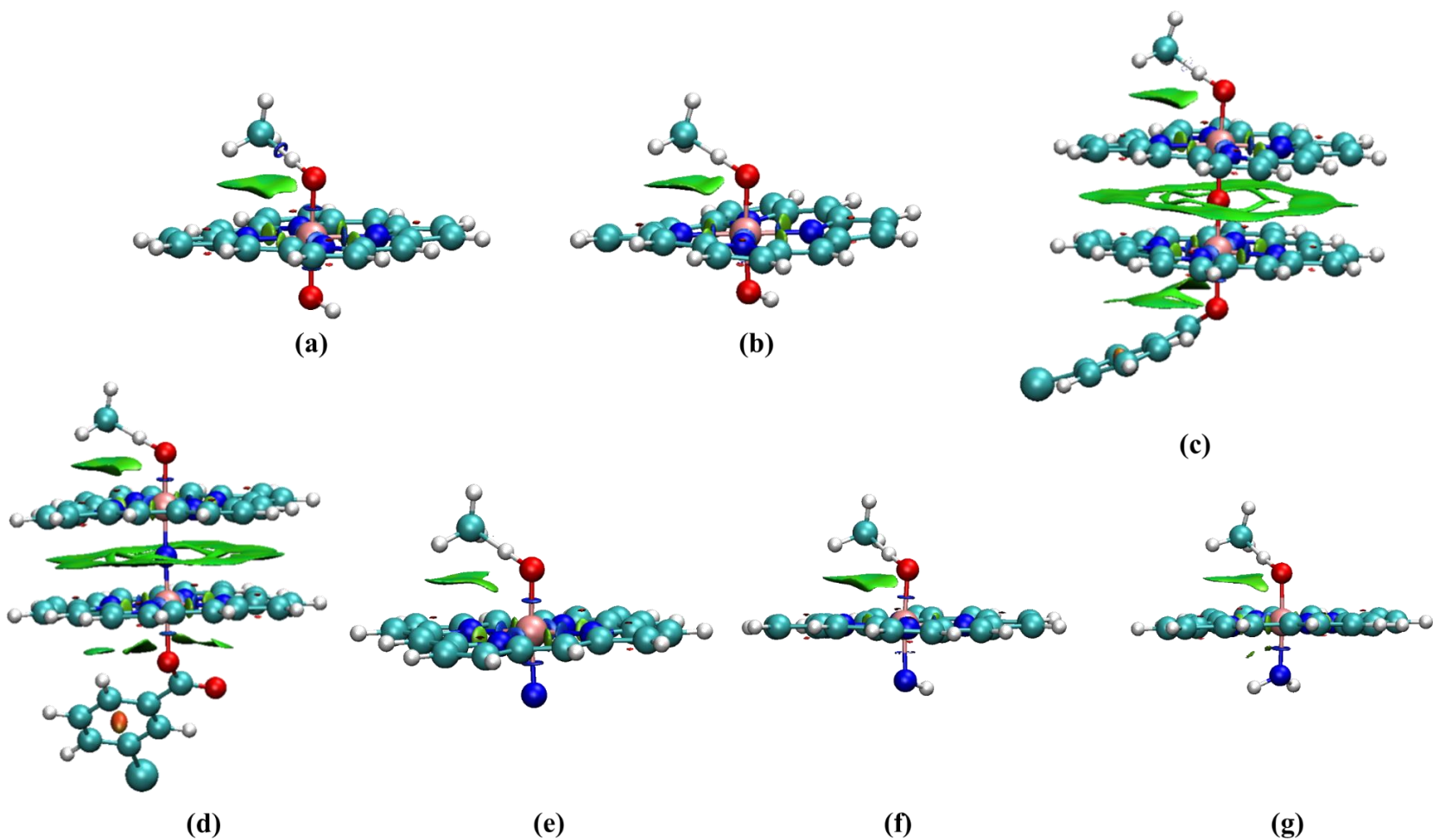


Figure S15. Non-covalent interaction (NCI) plots showing the comparison among C–H bond activation transition states (HAT) of a) ${}^3\mathbf{1}_{(is)}$, b) ${}^2\mathbf{2}_{(is)}$, c) ${}^2\mathbf{3}_{(is, is)}$, d) ${}^2\mathbf{4}_{(is, is)}$, e) ${}^4\mathbf{4a}_{(is)}$, f) ${}^4\mathbf{4b}_{(is)}$, and g) ${}^4\mathbf{4c}_{(is)}$. Only the non-covalent stabilization interaction between the methyl group and the π -cloud of the porphyrin ring are shown, with the strongest stabilizing interaction between the methyl group and the porphyrin in the NCI plots of the HAT transition states, as indicated by the green colour between hydrogen atom of the methyl and the porphyrin groups.

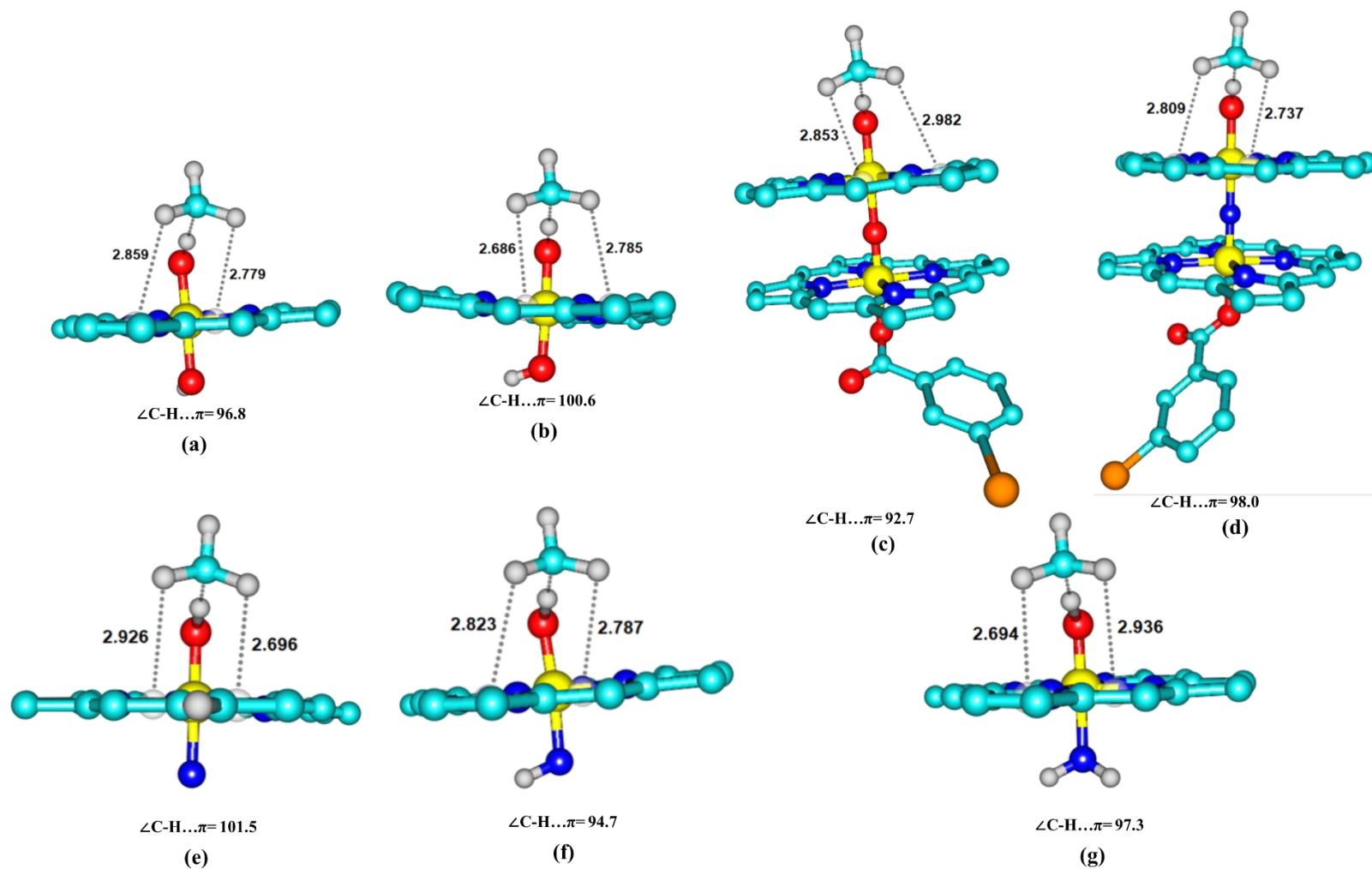


Figure S16. Optimized structures of hydrogen abstraction transition states; a) ${}^3\mathbf{1}_{(is)}$, b) ${}^2\mathbf{2}_{(is)}$, c) ${}^2\mathbf{3}_{(is, is)}$, d) ${}^2\mathbf{4}_{(is, is)}$, e) ${}^4\mathbf{4a}_{(is)}$, f) ${}^4\mathbf{4b}_{(is)}$, g) ${}^4\mathbf{4c}_{(is)}$, showing the shortest distance between the H atoms of the methyl group and the π -cloud of the porphyrin ring (CH... π interactions). (Colour code: Yellow= Fe, Orange= Cl, Red= O, Blue= N, and Cyan= C, Silver= H). All the distances are given in Å angles in $^\circ$.

The source of stabilizing energy between methane and porphyrin ring

The amount of stabilization by methane is analogous in the porphyrin ring and solvent phase with Gibb's free energy corrections. Here, we have used solvent-phase values for calculating the bond distances, Mulliken charge densities, and electrostatic interaction. These Mulliken charge densities are entirely dependent on the theory level. Here, the calculation is not a completely accurate approach for the calculation of interactions energy, however, it gives some insight into electrostatic and other types of interactions between methane and catalyst.

a) UB3LYP Data for species 1

Distances (Å)

O(1)-H1	1.072
O(1)-H2	2.999
O(1)-H3	3.012
O(1)-H4	3.009
O(1)-C	2.601
Fe(1)-O(1)	1.689

Mulliken Charge Densities

O(1)	-0.545
C	-0.476
H1	0.199
H2	0.143
H3	0.134
H4	0.133

b) Stabilization Energy by methane

Evaluated as $E_{ts1} - (E_R + E_{CH_4})$ neglecting counterpoise corrections.

For $\mathbf{1}^{-3}\mathbf{ts1}_{(is)}$: $-2444.012075 - (-2403.531227 - 40.46535673) = -0.0154908$ Hartree = - **40.67** kJ/mol

c) Electrostatic Interaction

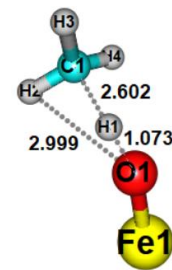
Evaluated (general equation) in kcal/mol from $E_{el} = 332 \cdot \sum_{A,B} q_A \cdot q_B / R_{AB}$

where the distance between two-point charges R_{AB} is in Å.

In our case, we include the interactions between C1, H1, and one shorted distance H2 atom from the O1 atom and the oxo ligand.

Evaluated in kJ/mol from

$$E_{el} = 1388 \cdot q_O \left(\frac{q_C}{R_{Oc}} + \sum_n \frac{q_H}{R_{OH}} \right)$$



For 1-³ts1_(is):-

$$E_{el} = 1388 \cdot (-0.545) \left[\left(\frac{-0.476}{2.601} \right) + \left\{ \left(\frac{0.199}{1.072} \right) + \left(\frac{0.143}{2.999} \right) \right\} \right] = 1388 \cdot (-0.16806) \cdot [0.047682084] = -37.93 \text{ kJ/mol}$$

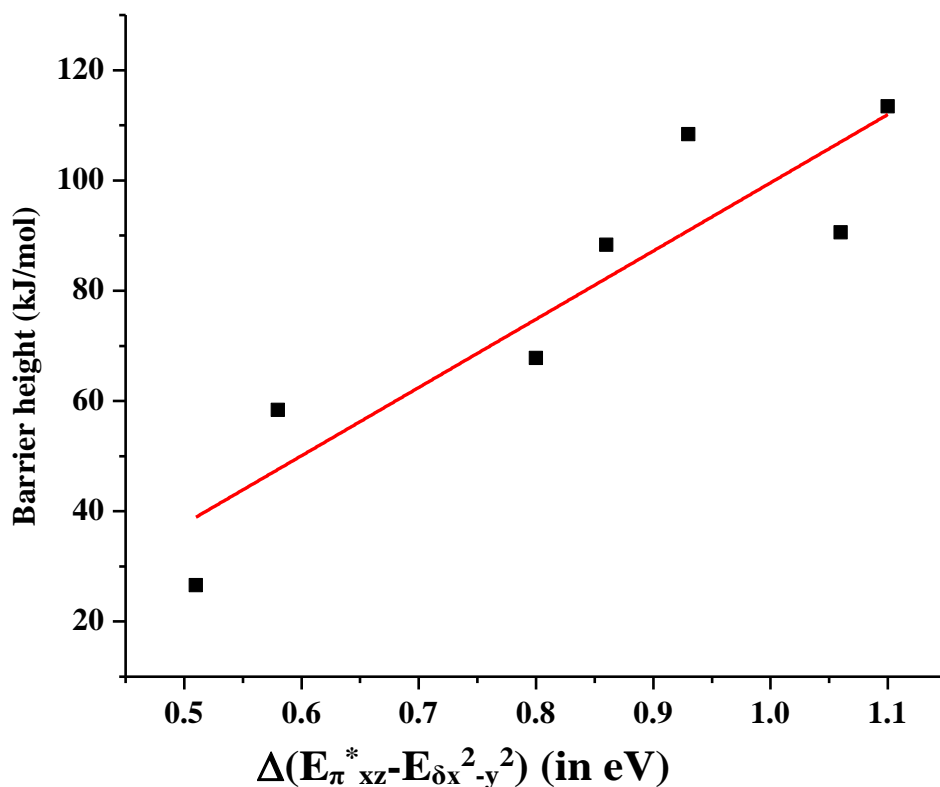


Figure S17. Correlation between methane hydroxylation barrier height and $\Delta E(E_{\pi^*_{xz}} - E_{\delta_{x^2-y^2}})$ gap for the high-spin reactions by all seven species.

Table S16. Summary of EDA performed for species **1**, **2**, and **3**. The ΔE is given in kJ/mol.

Species	EDA [{OH}/[(Por)(<i>m</i> -CBA)Fe ^{IV} (μ -O) + {Fe} + {O}]		
	ΔE_{int} (kJ/mol)	ΔE_{steric} (kJ/mol)	ΔE_{orb} (kJ/mol)
[(HO)Fe ^{IV} (O)(Por)] ⁻ (1)	-305.2	45.5	-350.7
[(HO)Fe ^{IV} (O)(Por ^{•+})] (2)	-658.7	261.6	-397.1
[(Por)(<i>m</i> -CBA)Fe ^{IV} (μ -O)Fe ^{IV} (O)(Por ^{•+})] ⁻ (3)	-338.5	42.1	-296.4

Coordinates

The coordinates are given in xyz-format, and the specific multiplicity/species/spin state pair for each of the calculations is given in parenthesis in the comment line of the structure.

$[(\text{HO})\text{Fe}^{\text{IV}}(\text{O})(\text{Por})]^-$ (1)

$^5\mathbf{1}_{(\text{hs})}$ or $\mathbf{1}^{-5}\mathbf{R}_{(\text{hs})}$

Fe	-0.011464000	0.003398000	-0.098650000	C	3.487044000	-2.513667000	0.000245000
N	-1.621284000	-1.317757000	-0.034122000	C	-2.511559000	3.477003000	0.000176000
N	-1.330622000	1.607471000	-0.031649000	C	-2.507902000	-3.479616000	0.000203000
N	1.326072000	-1.602197000	0.017996000	C	-3.482203000	2.514663000	-0.015392000
N	1.618251000	1.312695000	-0.001101000	C	-3.479555000	-2.518289000	-0.015381000
C	-1.531036000	-2.686256000	-0.000192000	H	2.629337000	4.554721000	0.035084000
C	-0.973514000	2.931594000	0.001995000	H	2.634121000	-4.551970000	0.035269000
C	-2.948112000	-0.968967000	-0.019655000	H	4.559290000	2.640716000	0.008104000
C	-2.700171000	1.525278000	-0.016505000	H	4.562067000	-2.635954000	0.007781000
C	0.967574000	-2.930377000	0.015102000	H	-2.627457000	4.552771000	0.006445000
C	1.525019000	2.683948000	0.006957000	H	-2.622681000	-4.555504000	0.006453000
C	2.700095000	-1.524664000	-0.003034000	H	-4.556994000	2.639284000	-0.024296000
C	2.948957000	0.968976000	-0.010321000	H	-4.554214000	-2.644035000	-0.024317000
C	-2.880202000	-3.243689000	0.027030000	C	0.001565000	3.423212000	0.010573000
C	-2.187188000	3.742141000	0.031092000	C	0.005162000	-3.423211000	0.010560000
C	-3.751604000	-2.187306000	0.015435000	C	-3.442104000	-0.001796000	-0.027179000
C	-3.248993000	2.877158000	0.019959000	C	3.443443000	0.001802000	-0.026674000
C	2.179602000	-3.740012000	0.004255000	H	0.001505000	4.509543000	0.022905000
C	2.872315000	3.243060000	0.007217000	H	0.006232000	-4.509541000	0.022901000
C	3.244083000	-2.876541000	-0.007293000	H	-4.528272000	-0.002369000	-0.037271000
C	3.747792000	2.189063000	-0.003987000	H	4.529683000	0.002376000	-0.021366000
H	-3.111846000	-4.300564000	0.056703000	O	-0.016849000	-0.000033000	-1.767197000
H	-2.207361000	4.823872000	0.060888000	H	-0.881133000	-0.001573000	2.160387000
H	-4.833483000	-2.214024000	0.033121000	O	0.046968000	0.000116000	1.842386000
H	-4.304673000	3.115196000	0.038736000				
H	2.198792000	-4.822197000	0.002286000	$^1\mathbf{1}_{(\text{ls})}$ or $\mathbf{1}^{-1}\mathbf{R}_{(\text{ls})}$			
H	3.101481000	4.300885000	0.014018000	Fe	0.008683000	0.000115000	-0.056581000
H	4.299144000	-3.117864000	-0.019863000	N	1.451146000	1.419640000	-0.018309000
H	4.829724000	2.220019000	-0.007201000	N	1.443064000	-1.427698000	-0.018412000
C	-0.341982000	-3.422894000	0.014246000	N	-1.439476000	1.426174000	0.001485000
C	0.336576000	3.421815000	0.011831000	N	-1.447719000	-1.417877000	0.001302000
C	3.444487000	-0.339629000	-0.012116000	C	1.246818000	2.780820000	0.005756000
C	-3.442270000	0.339435000	-0.020054000	C	1.230775000	-2.787673000	0.005968000
H	-0.446813000	-4.505153000	0.026217000	C	2.812437000	1.223809000	-0.025741000
H	0.444158000	4.503768000	0.028034000	C	2.805456000	-1.239760000	-0.025685000
H	4.526196000	-0.448015000	-0.021130000	C	-1.226539000	2.789132000	0.010459000
H	-4.524118000	0.447020000	-0.005007000	C	-1.242609000	-2.782018000	0.010122000
O	0.016799000	-0.004835000	-1.787654000	C	-2.805709000	1.240469000	-0.025518000
H	0.844121000	-0.236214000	2.133743000	C	-2.812913000	-1.224365000	-0.025701000
O	-0.045891000	0.021165000	1.811994000	C	2.527337000	3.470596000	0.011886000

$^3\mathbf{1}_{(\text{is})}$ or $\mathbf{1}^{-3}\mathbf{R}_{(\text{is})}$

Fe	0.009950000	0.000019000	-0.067911000	C	3.481096000	-2.527194000	-0.008651000
N	1.440526000	1.426831000	-0.025641000	C	-2.501489000	3.485002000	-0.001822000
N	1.442034000	-1.425327000	-0.025680000	C	-2.521479000	-3.470623000	-0.002306000
N	-1.436711000	1.424629000	-0.002976000	C	-3.477457000	2.527962000	-0.025100000
N	-1.435200000	-1.426119000	-0.002885000	C	-3.491962000	-2.508015000	-0.025664000
C	1.235586000	2.788263000	-0.000181000	H	2.643983000	4.546169000	0.029928000
C	1.238522000	-2.786975000	-0.000238000	H	2.617758000	-4.561048000	0.030467000
C	2.803731000	1.233306000	-0.021769000	H	4.570614000	2.629729000	-0.010387000
C	2.805032000	-1.230374000	-0.021808000	H	4.555450000	-2.655803000	-0.009544000
C	-1.232949000	2.788695000	0.005235000	H	-2.611798000	4.561397000	0.003232000
C	-1.230014000	-2.789980000	0.005275000	H	-2.637951000	-4.546371000	0.002520000
C	-2.803404000	1.231280000	-0.019301000	H	-4.551414000	2.659179000	-0.041686000
C	-2.802108000	-1.234201000	-0.019252000	H	-4.566642000	-2.633162000	-0.042523000
C	2.514690000	3.479016000	0.014387000	C	0.012266000	3.417182000	0.019109000
C	2.518348000	-3.476388000	0.014465000	C	-0.007333000	-3.417041000	0.019037000
C	3.484395000	2.517307000	0.000450000	C	-3.449724000	0.009910000	-0.039497000

C	3.448643000	-0.009787000	-0.035732000
H	0.015550000	4.503631000	0.030485000
H	-0.010114000	-4.503491000	0.030485000
H	-4.535803000	0.013117000	-0.058215000
H	4.534958000	-0.012851000	-0.039592000
O	0.002528000	-0.000502000	-1.757046000
H	-0.882711000	-0.003494000	2.144720000
O	0.047527000	-0.000394000	1.828899000

1⁻⁵ts1_(hs)

Fe	-0.090729000	0.023624000	-0.122025000
N	-1.829591000	1.136915000	-0.055671000
N	-1.247207000	-1.744692000	-0.119222000
N	1.052534000	1.796463000	-0.140610000
N	1.631624000	-1.082243000	-0.237408000
C	-1.895703000	2.510882000	0.023758000
C	-0.743013000	-3.018785000	-0.136333000
C	-3.110796000	0.638363000	0.039910000
C	-2.612374000	-1.819482000	-0.026588000
C	0.550331000	3.070209000	-0.087384000
C	1.701108000	-2.456572000	-0.261521000
C	2.416532000	1.871550000	-0.248757000
C	2.910497000	-0.585198000	-0.341034000
C	-3.292905000	2.904288000	0.153713000
C	-1.853388000	-3.965059000	-0.060818000
C	-4.038721000	1.755068000	0.163219000
C	-3.005529000	-3.226062000	0.006063000
C	1.661457000	4.016573000	-0.152915000
C	3.099906000	-2.852250000	-0.368237000
C	2.811355000	3.277984000	-0.253771000
C	3.842300000	-1.701963000	-0.420092000
H	-3.640362000	3.926214000	0.234157000
H	-1.751421000	-5.042772000	-0.056232000
H	-5.112988000	1.656826000	0.251896000
H	-4.024585000	-3.584845000	0.074471000
H	1.561225000	5.094218000	-0.130097000
H	3.450153000	-3.875624000	-0.406094000
H	3.830016000	3.636973000	-0.326555000
H	4.916895000	-1.603567000	-0.503210000
C	-0.808426000	3.392726000	-0.002825000
C	0.616564000	-3.340143000	-0.203611000
C	3.270503000	0.767656000	-0.341697000
C	-3.469106000	-0.715319000	0.038695000
H	-1.051681000	4.451363000	0.050231000
H	0.863060000	-4.399261000	-0.218662000
H	4.333538000	0.980850000	-0.424351000
H	-4.532301000	-0.929408000	0.117495000
O	-0.104084000	0.022181000	1.714944000
H	-1.026647000	0.358947000	-2.276357000
H	0.830420000	-0.259900000	2.170515000
H	2.774465000	0.231902000	2.453188000
H	1.903132000	-0.575853000	3.875443000
H	2.393807000	-1.569981000	2.389127000
C	2.170163000	-0.595825000	2.818680000
O	-0.137644000	0.049415000	-1.997779000

1⁻³ts1_(is)

Fe	-0.096193000	0.003872000	-0.117632000
N	-1.345576000	-1.594189000	-0.077090000
N	1.514788000	-1.206223000	-0.217002000
N	-1.719132000	1.219512000	-0.041409000
N	1.143133000	1.600133000	-0.177044000
C	-2.722715000	-1.589234000	-0.014301000
C	2.834871000	-0.841580000	-0.372622000
C	-0.955642000	-2.915728000	-0.045477000
C	1.491537000	-2.583722000	-0.172945000
C	-3.047570000	0.853255000	0.018810000
C	2.511814000	1.597500000	-0.338429000
C	-1.689066000	2.596701000	0.024345000
C	0.758742000	2.921772000	-0.109666000

C	-3.219716000	-2.953430000	0.042779000
C	3.674449000	-2.025666000	-0.411520000
C	-2.126675000	-3.773548000	0.028361000
C	2.844262000	-3.103675000	-0.281016000
C	-3.883534000	2.037837000	0.109737000
C	3.010502000	2.961716000	-0.359208000
C	-3.043189000	3.115668000	0.117522000
C	1.926581000	3.780883000	-0.212289000
H	-4.266250000	-3.223427000	0.095599000
H	4.750685000	-2.011352000	-0.521883000
H	-2.093189000	-4.854517000	0.064109000
H	3.099451000	-4.155130000	-0.268283000
H	-4.963982000	2.023440000	0.167364000
H	4.051978000	3.232590000	-0.472027000
H	-3.293624000	4.166496000	0.180576000
H	1.896219000	4.862122000	-0.183365000
C	-3.520660000	-0.452783000	0.015934000
C	3.304152000	0.462564000	-0.441849000
C	-0.546192000	3.384779000	-0.001332000
C	0.353920000	-3.375402000	-0.080471000
H	-4.596167000	-0.596390000	0.068296000
H	4.374188000	0.605725000	-0.561618000
H	-0.686250000	4.461208000	0.048233000
H	0.501361000	-4.451617000	-0.052603000
O	-0.098665000	-0.012302000	1.727397000
H	-1.100578000	0.015764000	-2.266721000
H	0.878719000	-0.047164000	2.168250000
H	2.734045000	0.779194000	2.313494000
H	2.049355000	-0.020836000	3.839315000
H	2.636272000	-1.058629000	2.419881000
C	2.280892000	-0.094181000	2.776659000
O	-0.156872000	0.014162000	-1.996209000

1⁻¹ts1_(ls)

Fe	-0.075503000	-0.010560000	-0.129739000
N	-1.935718000	-0.807196000	0.004145000
N	0.703304000	-1.862066000	-0.165463000
N	-0.859086000	1.873068000	-0.106326000
N	1.763834000	0.795500000	-0.231599000
C	-3.121283000	-0.107576000	0.021161000
C	2.035190000	-2.189953000	-0.307476000
C	-2.267313000	-2.139234000	0.061207000
C	0.016713000	-3.056774000	-0.087911000
C	-2.202767000	2.188628000	-0.065599000
C	2.954712000	0.100459000	-0.342965000
C	-0.176807000	3.071426000	-0.085109000
C	2.105037000	2.138495000	-0.172691000
C	-4.242420000	-1.033164000	0.100011000
C	2.195221000	-3.635316000	-0.314154000
C	-3.713007000	-2.291656000	0.128940000
C	0.946677000	-4.170905000	-0.174206000
C	-2.369800000	3.631653000	-0.034826000
C	4.070487000	1.026002000	-0.345051000
C	-1.116271000	4.178378000	-0.041477000
C	3.546285000	2.284981000	-0.233543000
H	-5.282683000	-0.736222000	0.128680000
H	3.143545000	-4.147204000	-0.412414000
H	-4.229321000	-3.241160000	0.183342000
H	0.659193000	-5.213519000	-0.137105000
H	-3.325861000	4.137699000	-0.002940000
H	5.109451000	0.732521000	-0.418325000
H	-0.835466000	5.223329000	-0.020240000
H	4.068044000	3.232564000	-0.203195000
C	-3.247684000	1.274780000	-0.020699000

C	3.081173000	-1.280981000	-0.398941000
C	1.207794000	3.196286000	-0.102328000
C	-1.359063000	-3.189902000	0.030835000
H	-4.256078000	1.679483000	0.006556000
H	4.085765000	-1.684417000	-0.491352000
H	1.621348000	4.200561000	-0.072218000
H	-1.759735000	-4.198848000	0.079987000
O	-0.109969000	0.054623000	1.716404000
H	-0.089735000	0.855154000	-2.332353000
H	0.654090000	0.600195000	2.168146000
H	2.631092000	0.680614000	2.470217000
H	1.668840000	-0.184743000	3.804845000
H	2.053922000	-1.045554000	2.219573000
C	1.933819000	-0.110484000	2.751327000
O	-0.305013000	-0.044860000	-2.004194000

1-⁷int1_(hs)

Fe	-0.158147000	0.023544000	-0.149298000
N	-2.216979000	0.267151000	0.021556000
N	-0.386707000	-2.079751000	-0.038621000
N	0.113015000	2.086466000	-0.137957000
N	1.932059000	-0.256291000	-0.364199000
C	-2.871888000	1.470908000	0.085232000
C	0.617406000	-3.012520000	-0.146945000
C	-3.139309000	-0.745577000	0.115493000
C	-1.591746000	-2.734860000	0.035882000
C	-0.890243000	3.018182000	-0.050469000
C	2.592044000	-1.462349000	-0.378217000
C	1.316902000	2.739289000	-0.239898000
C	2.859783000	0.754323000	-0.420346000
C	-4.302630000	1.211449000	0.215418000
C	0.017367000	-4.342347000	-0.114928000
C	-4.466951000	-0.149555000	0.233363000
C	-1.339397000	-4.171731000	-0.003573000
C	-0.289894000	4.348227000	-0.091680000
C	4.024250000	-1.203612000	-0.481256000
C	1.065329000	4.176961000	-0.207071000
C	4.188437000	0.158481000	-0.507527000
H	-5.066943000	1.974561000	0.286564000
H	0.567345000	-5.272559000	-0.178598000
H	-5.390531000	-0.706895000	0.322835000
H	-2.103730000	-4.936947000	0.041393000
H	-0.840793000	5.278434000	-0.038973000
H	4.791482000	-1.966412000	-0.514418000
H	1.829767000	4.940871000	-0.266843000
H	5.114703000	0.715443000	-0.564242000
C	-2.259208000	2.731596000	0.049656000
C	1.982575000	-2.722953000	-0.289991000
C	2.570171000	2.126043000	-0.370315000
C	-2.849143000	-2.116983000	0.116731000
H	-2.924716000	3.589391000	0.111021000
H	2.650194000	-3.580136000	-0.337888000
H	3.424836000	2.795792000	-0.428258000
H	-3.704623000	-2.785096000	0.185006000
O	0.086190000	0.004311000	1.804920000
H	0.500642000	-0.356328000	-2.545510000
H	0.098720000	-0.902046000	2.177861000
O	-0.317136000	-0.082983000	-2.081350000
H	2.027086000	0.189568000	2.558621000
H	3.328728000	0.291147000	3.941333000
H	3.828950000	-0.249034000	2.218236000
C	3.055906000	0.072772000	2.910372000

1-⁵int1_(hs)

Fe	-0.158526000	0.023692000	-0.149262000
N	-2.215830000	0.279124000	0.021341000
N	-0.398540000	-2.078406000	-0.037409000
N	0.123934000	2.084999000	-0.139658000
N	1.930300000	-0.268280000	-0.363772000
C	-2.864130000	1.486454000	0.084702000
C	0.600307000	-3.016886000	-0.144998000
C	-3.143611000	-0.728539000	0.116327000
C	-1.607224000	-2.726592000	0.037593000
C	-0.873939000	3.022479000	-0.052329000
C	2.583636000	-1.477928000	-0.377065000
C	1.331574000	2.730880000	-0.241945000
C	2.863450000	0.737206000	-0.421281000
C	-4.296210000	1.234869000	0.215627000
C	-0.007244000	-4.343308000	-0.112118000
C	-4.467923000	-0.125210000	0.234468000
C	-1.363015000	-4.164935000	-0.000907000
C	-0.265996000	4.349033000	-0.094109000
C	4.017242000	-1.227097000	-0.480659000
C	1.088219000	4.169968000	-0.209620000
C	4.188814000	0.134068000	-0.508211000
H	-5.056323000	2.002164000	0.286747000
H	0.537453000	-5.276665000	-0.175175000
H	-5.394468000	-0.677485000	0.324725000
H	-2.131646000	-4.925805000	0.044591000
H	-0.811553000	5.282397000	-0.041632000
H	4.780314000	-1.994077000	-0.513500000
H	1.856992000	4.929485000	-0.269731000
H	5.118080000	0.685941000	-0.565592000
C	-2.244485000	2.743706000	0.048294000
C	1.967109000	-2.735080000	-0.287983000
C	2.581359000	2.110519000	-0.372173000
C	-2.861087000	-2.101521000	0.118271000
H	-2.905152000	3.605244000	0.109467000
H	2.629928000	-3.596018000	-0.335271000
H	3.439710000	2.775485000	-0.430647000
H	-3.720290000	-2.764771000	0.187242000
O	0.086845000	0.003447000	1.804713000
H	0.498963000	-0.365355000	-2.544655000
H	0.105910000	-0.903012000	2.176987000
O	-0.316738000	-0.084843000	-2.081151000
H	2.034257000	0.200252000	2.556081000
H	3.337007000	0.302300000	3.937276000
H	3.830441000	-0.263183000	2.220237000
C	3.061844000	0.077284000	2.908392000

1-⁵int1_(is)

Fe	0.118525000	-0.004388000	-0.143213000
N	0.203949000	2.031251000	-0.058507000
N	-2.001786000	0.090935000	-0.302594000
N	2.267919000	-0.080206000	-0.055510000
N	0.052645000	-2.029096000	-0.139264000
C	1.352376000	2.798222000	0.000219000
C	-2.836490000	-0.987491000	-0.381392000
C	-0.877159000	2.885628000	-0.168578000
C	-2.754838000	1.229095000	-0.360834000
C	3.103138000	0.997632000	0.081790000
C	-1.093135000	-2.789384000	-0.220955000
C	3.014499000	-1.223498000	0.064278000
C	1.130581000	-2.881431000	-0.050522000
C	0.976363000	4.203106000	-0.048892000
C	-4.214182000	-0.511563000	-0.504219000
C	-0.389173000	4.256349000	-0.153806000
C	-4.163948000	0.859032000	-0.492207000

C	4.470597000	0.516339000	0.263408000
C	-0.721413000	-4.198131000	-0.178871000
C	4.415460000	-0.854866000	0.253380000
C	0.642557000	-4.254950000	-0.072632000
H	1.676217000	5.028225000	-0.016284000
H	-5.088955000	-1.144254000	-0.584457000
H	-1.019478000	5.133646000	-0.221884000
H	-4.989784000	1.555747000	-0.561019000
H	5.341996000	1.145168000	0.396213000
H	-1.423275000	-5.020878000	-0.223442000
H	5.233776000	-1.553456000	0.374901000
H	1.272586000	-5.133238000	-0.015370000
C	2.671000000	2.329092000	0.081420000
C	-2.407303000	-2.318196000	-0.335579000
C	2.480864000	-2.516799000	0.043121000
C	-2.224641000	2.522290000	-0.294112000
H	3.441906000	3.092263000	0.161094000
H	-3.180622000	-3.080757000	-0.393492000
H	3.189514000	-3.337506000	0.128757000
H	-2.933289000	3.344899000	-0.357246000
O	0.025993000	-0.057412000	1.720206000
H	1.162462000	-0.059864000	-2.243717000
H	-0.026649000	0.859103000	2.064002000
O	0.220111000	0.032800000	-1.988368000
H	-1.964759000	-0.236945000	2.520293000
H	-3.199425000	-0.211569000	3.961766000
H	-3.785341000	0.115534000	2.210235000
C	-2.977893000	-0.106361000	2.901585000

1-³int1_(is)

Fe	0.118677000	-0.004276000	-0.142959000
N	0.204540000	2.031297000	-0.058697000
N	-2.001765000	0.091636000	-0.301884000
N	2.268025000	-0.080855000	-0.055777000
N	0.052257000	-2.028967000	-0.138970000
C	1.353189000	2.797864000	0.000077000
C	-2.836643000	-0.986557000	-0.381909000
C	-0.876325000	2.886008000	-0.168372000
C	-2.754491000	1.230019000	-0.360537000
C	3.103490000	0.996790000	0.081420000
C	-1.093751000	-2.788905000	-0.221258000
C	3.014292000	-1.224312000	0.064355000
C	1.129888000	-2.881678000	-0.050186000
C	0.977616000	4.202902000	-0.048692000
C	-4.214120000	-0.510283000	-0.505530000
C	-0.387914000	4.256597000	-0.153361000
C	-4.163576000	0.860315000	-0.493029000
C	4.470825000	0.515177000	0.263225000
C	-0.722479000	-4.197762000	-0.179362000
C	4.415350000	-0.856007000	0.253412000
C	0.641443000	-4.255030000	-0.072702000
H	1.677762000	5.027774000	-0.016027000
H	-5.088990000	-1.142721000	-0.586666000
H	-1.017976000	5.134091000	-0.221134000
H	-4.989217000	1.557217000	-0.562359000
H	5.342367000	1.143810000	0.395988000
H	-1.424576000	-5.020283000	-0.224378000
H	5.233469000	-1.554792000	0.375162000
H	1.271175000	-5.133534000	-0.015459000
C	2.671692000	2.328349000	0.081027000
C	-2.407752000	-2.317367000	-0.336343000
C	2.480291000	-2.517465000	0.043493000
C	-2.223927000	2.523069000	-0.293749000
H	3.442803000	3.091309000	0.160687000

H	-3.181195000	-3.079750000	-0.394981000
H	3.188680000	-3.338379000	0.129278000
H	-2.932324000	3.345889000	-0.356959000
O	0.026716000	-0.056588000	1.720554000
H	1.161927000	-0.061431000	-2.243695000
H	-0.030057000	0.859618000	2.064452000
O	0.219768000	0.032571000	-1.988177000
H	-1.967192000	-0.244474000	2.522633000
H	-3.201959000	-0.203625000	3.963421000
H	-3.785835000	0.113650000	2.209299000
C	-2.980054000	-0.108861000	2.902346000

1-³int1_(ls)

Fe	-0.138618000	-0.001761000	-0.134854000
N	-2.070454000	-0.572365000	0.032071000
N	0.407736000	-1.942819000	-0.185686000
N	-0.673571000	1.955065000	-0.066796000
N	1.797266000	0.589522000	-0.295189000
C	-3.158272000	0.266376000	0.118183000
C	1.692927000	-2.417836000	-0.312811000
C	-2.560054000	-1.857109000	0.079691000
C	-0.410844000	-3.045120000	-0.103064000
C	-1.967493000	2.432367000	0.036071000
C	2.882516000	-0.253666000	-0.423178000
C	0.150018000	3.066872000	-0.105167000
C	2.298972000	1.876914000	-0.302929000
C	-4.379761000	-0.517069000	0.221881000
C	1.686361000	-3.872824000	-0.307904000
C	-4.009023000	-1.831246000	0.199479000
C	0.384082000	-4.261075000	-0.176933000
C	-1.955926000	3.882858000	0.059232000
C	4.102653000	0.525721000	-0.517454000
C	-0.648069000	4.275013000	-0.025890000
C	3.742906000	1.843156000	-0.439068000
H	-5.373341000	-0.096113000	0.302201000
H	2.571057000	-4.489941000	-0.392455000
H	-4.635625000	-2.711490000	0.256826000
H	-0.021839000	-5.263087000	-0.133453000
H	-2.841062000	4.500756000	0.134272000
H	5.092708000	0.101844000	-0.620687000
H	-0.244003000	5.278751000	-0.035840000
H	4.377031000	2.719288000	-0.470298000
C	-3.115248000	1.654516000	0.116300000
C	2.837234000	-1.641007000	-0.429622000
C	1.535250000	3.034066000	-0.210214000
C	-1.792802000	-3.011839000	0.021701000
H	-4.063310000	2.179817000	0.193344000
H	3.784280000	-2.164937000	-0.522638000
H	2.059934000	3.984910000	-0.228413000
H	-2.314528000	-3.963343000	0.073122000
O	0.012795000	-0.058781000	1.749195000
H	-0.016764000	0.844473000	-2.332038000
H	0.300666000	0.831525000	2.046508000
O	-0.309136000	-0.031999000	-2.000421000
H	3.739391000	0.304821000	2.264507000
H	3.317972000	-0.590498000	3.857340000
H	2.009980000	-0.401347000	2.495604000
C	3.018809000	-0.232273000	2.874583000

1-¹int1_(ls)

Fe	-0.138812000	-0.001520000	-0.134633000
N	-2.078746000	-0.544185000	0.032380000
N	0.379810000	-1.950219000	-0.182801000

N	-0.645541000	1.962822000	-0.069242000
N	1.805525000	0.561664000	-0.295718000
C	-3.154372000	0.310196000	0.117247000
C	1.657959000	-2.443832000	-0.310179000
C	-2.586607000	-1.821698000	0.082320000
C	-0.454529000	-3.040546000	-0.098715000
C	-1.932496000	2.458780000	0.032911000
C	2.878513000	-0.297143000	-0.423286000
C	0.193997000	3.062606000	-0.108414000
C	2.325621000	1.841694000	-0.305042000
C	-4.386958000	-0.455520000	0.222239000
C	1.630451000	-3.898568000	-0.303758000
C	-4.035046000	-1.774908000	0.202098000
C	0.322796000	-4.267899000	-0.171678000
C	-1.900028000	3.908973000	0.054928000
C	4.109648000	0.464587000	-0.519272000
C	-0.586656000	4.282179000	-0.030270000
C	3.768856000	1.787118000	-0.441967000
H	-5.374419000	-0.020297000	0.301952000
H	2.506134000	-4.528427000	-0.388181000
H	-4.674158000	-2.646007000	0.260995000
H	-0.097452000	-5.263931000	-0.126981000
H	-2.776201000	4.539597000	0.129266000
H	5.093445000	0.026494000	-0.622909000
H	-0.168228000	5.279999000	-0.040941000
H	4.415343000	2.654101000	-0.474980000
C	-3.091333000	1.697597000	0.113624000
C	2.813276000	-1.683684000	-0.428391000
C	1.578627000	3.009791000	-0.213377000
C	-1.835857000	-2.987322000	0.026241000
H	-4.031773000	2.236521000	0.189958000
H	3.752688000	-2.221206000	-0.521274000
H	2.116868000	3.953004000	-0.232429000
H	-2.371026000	-3.931249000	0.079084000
O	0.010435000	-0.057260000	1.749693000
H	-0.006722000	0.839430000	-2.333442000
H	0.307936000	0.830204000	2.045933000
O	-0.310255000	-0.032602000	-2.000144000
H	3.741713000	0.289738000	2.255570000
H	3.316703000	-0.574070000	3.864987000
H	2.011807000	-0.410606000	2.497355000
C	3.020417000	-0.236643000	2.874037000

1⁻⁷ts₂(_{hs})

Fe	-0.091485000	0.046103000	-0.253202000
N	0.635292000	-1.951929000	-0.197203000
N	-2.045362000	-0.707951000	-0.014802000
N	-0.802781000	1.982593000	-0.148721000
N	1.878438000	0.744525000	-0.245190000
C	-0.136048000	-3.096193000	-0.122085000
C	0.748203000	-4.248419000	-0.128289000
H	0.422812000	-5.279767000	-0.077546000
C	2.037103000	-3.772739000	-0.199030000
H	2.955992000	-4.344515000	-0.219906000
C	1.958842000	-2.319520000	-0.236730000
C	3.048181000	-1.431285000	-0.278487000
H	4.035753000	-1.885597000	-0.294034000
C	3.012789000	-0.028688000	-0.271989000
C	4.173558000	0.852752000	-0.259331000
H	5.203111000	0.519079000	-0.271742000
C	3.704307000	2.142806000	-0.225613000
H	4.279485000	3.059484000	-0.203223000
C	2.251283000	2.070808000	-0.215043000
C	1.369631000	3.157511000	-0.168181000

H	1.825666000	4.144392000	-0.141719000
C	-0.030389000	3.123693000	-0.127331000
C	-0.911311000	4.274638000	-0.017521000
H	-0.581075000	5.304884000	0.018359000
C	-2.198334000	3.798636000	0.038624000
H	-3.114567000	4.366900000	0.133118000
C	-2.124244000	2.346135000	-0.032448000
C	-3.212781000	1.464749000	0.041136000
H	-4.195493000	1.923281000	0.118951000
C	-3.179817000	0.063853000	0.061013000
C	-4.336567000	-0.819993000	0.163581000
H	-5.363523000	-0.487629000	0.243925000
C	-3.865471000	-2.108426000	0.141251000
H	-4.436921000	-3.026290000	0.196902000
C	-2.415664000	-2.036167000	0.023927000
C	-1.535490000	-3.123893000	-0.029260000
H	-1.990823000	-4.110478000	0.020588000
O	-0.040257000	-0.030409000	1.788807000
H	-0.384491000	-0.892229000	2.105953000
O	-0.187075000	-0.090696000	-2.159369000
H	0.161123000	-0.912572000	-2.559573000
C	1.942068000	-0.105671000	2.859065000
H	2.143654000	0.874453000	2.452584000
H	1.495289000	-0.200931000	3.841795000
H	2.283051000	-0.980483000	2.321181000

1⁻⁵ts₂(_{hs})

Fe	-0.104318000	0.023738000	-0.189888000
N	-0.529014000	-2.046210000	-0.045732000
N	-2.139438000	0.451441000	-0.012102000
N	0.352717000	2.057067000	-0.144532000
N	1.943295000	-0.433379000	-0.354025000
C	-1.790597000	-2.590909000	0.003717000
C	-1.667465000	-4.043864000	-0.018860000
H	-2.498392000	-4.737019000	0.011460000
C	-0.328242000	-4.336359000	-0.092029000
H	0.137179000	-5.312818000	-0.134919000
C	0.387914000	-3.066618000	-0.119361000
C	1.778033000	-2.897153000	-0.216856000
H	2.371931000	-3.808343000	-0.220794000
C	2.494524000	-1.695501000	-0.301271000
C	3.946917000	-1.566921000	-0.304986000
H	4.641937000	-2.396146000	-0.271606000
C	4.235478000	-0.226478000	-0.334523000
H	5.210244000	0.243895000	-0.328252000
C	2.964899000	0.488202000	-0.350688000
C	2.806034000	1.880496000	-0.310674000
H	3.721463000	2.467052000	-0.330525000
C	1.608424000	2.605722000	-0.216160000
C	1.482532000	4.058454000	-0.176034000
H	2.310997000	4.754023000	-0.214759000
C	0.144036000	4.345209000	-0.084826000
H	-0.325268000	5.319324000	-0.034462000
C	-0.569011000	3.073196000	-0.065454000
C	-1.958955000	2.908331000	0.013120000
H	-2.545261000	3.822914000	0.065129000
C	-2.684035000	1.709229000	0.037588000
C	-4.136071000	1.582540000	0.137439000
H	-4.828118000	2.412993000	0.193769000
C	-4.424903000	0.243201000	0.146721000
H	-5.397225000	-0.227782000	0.213149000
C	-3.153323000	-0.471375000	0.054873000
C	-2.988774000	-1.862803000	0.055762000
H	-3.902168000	-2.451386000	0.103771000

O	0.037668000	-0.001630000	1.799928000
H	-0.105434000	-0.904813000	2.153312000
O	-0.336079000	-0.053426000	-2.124154000
H	0.498519000	-0.248267000	-2.599789000
C	2.169929000	-0.015124000	2.853759000
H	2.303126000	0.944332000	2.376267000
H	1.728542000	-0.072888000	3.841703000
H	2.480491000	-0.913094000	2.334639000

1⁻⁵ts_(is)

Fe	0.087865000	0.017979000	-0.217739000
N	1.236299000	-1.748682000	-0.170056000
N	-1.649535000	-1.129826000	-0.282144000
N	-1.062141000	1.784998000	-0.189868000
N	1.808137000	1.152365000	0.053421000
C	2.600059000	-1.809382000	-0.019501000
C	3.001501000	-3.210767000	0.061494000
H	4.019266000	-3.560827000	0.179798000
C	1.855937000	-3.961932000	-0.016858000
H	1.764225000	-5.040150000	0.022333000
C	0.740287000	-3.029997000	-0.151168000
C	-0.618434000	-3.369723000	-0.208750000
C	-1.717841000	-2.500173000	-0.256308000
C	-3.123006000	-2.900511000	-0.270623000
H	-3.477731000	-3.923372000	-0.256932000
C	-3.867305000	-1.749945000	-0.300585000
H	-4.945665000	-1.654222000	-0.3111211000
C	-2.928079000	-0.631011000	-0.302186000
C	-3.280702000	0.725888000	-0.301506000
C	-2.429839000	1.838951000	-0.253835000
C	-2.844972000	3.241141000	-0.245186000
H	-3.869976000	3.587352000	-0.289423000
C	-1.702968000	3.997114000	-0.174998000
H	-1.620245000	5.076423000	-0.148202000
C	-0.577480000	3.065071000	-0.134639000
C	0.780224000	3.401421000	-0.035996000
C	1.874931000	2.528324000	0.035111000
C	3.276467000	2.927955000	0.089104000
H	3.628693000	3.951763000	0.090869000
C	4.024508000	1.779104000	0.123862000
H	5.102803000	1.687453000	0.156748000
C	3.092440000	0.657562000	0.089430000
C	3.449631000	-0.698139000	0.074197000
H	4.513692000	-0.911804000	0.150123000
H	1.014802000	4.463581000	-0.019636000
H	-0.849308000	-4.432639000	-0.185992000
H	-4.347124000	0.939763000	-0.330741000
O	0.204641000	0.097089000	-2.076717000
O	-0.102774000	-0.055261000	1.681468000
H	0.365195000	0.707514000	2.087032000
H	0.589257000	-0.741463000	-2.408319000
C	-1.875231000	-0.350090000	3.040919000
H	-2.000117000	-1.312395000	2.565018000
H	-2.358369000	0.516923000	2.610117000
H	-1.338928000	-0.273125000	3.980285000

1⁻³ts_(is)

Fe	-0.006138000	0.070203000	-0.165643000
N	2.118032000	0.367270000	-0.128187000
N	0.253509000	-1.887963000	-0.281628000
N	-2.158799000	-0.216559000	-0.005617000
N	-0.294552000	2.046810000	-0.054310000
C	2.758629000	1.572129000	-0.058221000

C	4.202183000	1.348045000	-0.078723000
H	4.957678000	2.122552000	-0.035785000
C	4.389686000	-0.009018000	-0.166106000
H	5.326811000	-0.549917000	-0.207087000
C	3.060748000	-0.615954000	-0.199811000
C	2.746546000	-1.976231000	-0.294599000
C	1.469941000	-2.545276000	-0.327463000
C	1.227010000	-3.979106000	-0.370519000
H	2.005256000	-4.729975000	-0.411099000
C	-0.127569000	-4.164278000	-0.341390000
H	-0.677207000	-5.096500000	-0.353909000
C	-0.744290000	-2.847699000	-0.278328000
C	-2.125804000	-2.643976000	-0.205872000
C	-2.798726000	-1.420930000	-0.107252000
C	-4.239831000	-1.194939000	-0.134471000
H	-4.993818000	-1.968571000	-0.209078000
C	-4.431048000	0.164410000	-0.070987000
H	-5.369221000	0.704947000	-0.083426000
C	-3.106648000	0.772365000	-0.002683000
C	-2.791532000	2.134599000	0.026162000
C	-1.514182000	2.706295000	0.019353000
C	-1.268009000	4.136336000	0.114891000
H	-2.045122000	4.886380000	0.185171000
C	0.088122000	4.319174000	0.111285000
H	0.638656000	5.248714000	0.177115000
C	0.705070000	3.006735000	0.010198000
C	2.088142000	2.796888000	0.002706000
H	2.702480000	3.692787000	0.057553000
H	-3.623881000	2.833905000	0.057125000
H	3.579365000	-2.674091000	-0.338579000
H	-2.739550000	-3.540911000	-0.247070000
O	-0.095308000	0.163242000	-2.032283000
O	0.035823000	0.030785000	1.747919000
H	-0.896062000	0.009053000	2.056028000
H	-0.240478000	1.089213000	-2.319082000
C	0.555634000	-1.866195000	2.843384000
H	1.524090000	-1.833828000	2.365813000
H	-0.231444000	-2.460278000	2.396062000
H	0.426159000	-1.438140000	3.830753000

1⁻³ts_(is)

Fe	-0.087868000	0.024684000	-0.165720000
N	1.926894000	0.251727000	-0.272682000
N	0.112035000	-1.996956000	-0.152666000
N	-2.088382000	-0.209410000	0.005308000
N	-0.275434000	2.033484000	-0.107948000
C	2.853512000	-0.766754000	-0.330458000
C	4.194160000	-0.213220000	-0.322533000
H	5.100153000	-0.803753000	-0.357624000
C	4.065469000	1.148802000	-0.251490000
H	4.844189000	1.899593000	-0.221991000
C	2.647419000	1.434281000	-0.216330000
C	2.092920000	2.704939000	-0.147450000
H	2.776357000	3.549210000	-0.124067000
C	0.733054000	2.981181000	-0.105542000
C	0.160020000	4.310527000	-0.049821000
H	0.736496000	5.226291000	-0.036282000
C	-1.199248000	4.157217000	-0.016816000
H	-1.963943000	4.921330000	0.029852000
C	-1.465340000	2.730574000	-0.046833000
C	-2.735309000	2.169333000	0.004443000
H	-3.578439000	2.853410000	0.042658000
C	-3.019290000	0.809894000	0.035472000
C	-4.358569000	0.252932000	0.097338000

H	-5.265519000	0.841924000	0.132892000
C	-4.223956000	-1.108933000	0.093190000
H	-4.998936000	-1.863563000	0.126977000
C	-2.805387000	-1.392931000	0.027770000
C	-2.251589000	-2.666268000	-0.003319000
H	-2.935412000	-3.509953000	0.029738000
C	-0.895402000	-2.945298000	-0.089596000
C	-0.323555000	-4.274671000	-0.146177000
H	-0.897583000	-5.191546000	-0.115515000
C	1.032478000	-4.119455000	-0.252232000
H	1.795555000	-4.883467000	-0.322744000
C	1.296943000	-2.691668000	-0.257270000
C	2.567064000	-2.128892000	-0.340942000
H	3.409712000	-2.812162000	-0.396246000
O	0.022738000	0.018747000	1.775680000
H	-0.508928000	-0.744705000	2.091559000
O	-0.220569000	0.002081000	-2.018814000
H	0.378587000	0.697351000	-2.368007000
C	1.873002000	-0.428875000	2.806830000
H	2.308727000	0.481938000	2.421685000
H	1.460756000	-0.441971000	3.809680000
H	2.049280000	-1.356565000	2.277719000

1-¹ts_(1s)

Fe	-0.079100000	0.012794000	-0.143911000
N	1.822511000	0.678849000	-0.245711000
N	0.558557000	-1.905721000	-0.154611000
N	-1.985610000	-0.659461000	-0.002811000
N	-0.715457000	1.931509000	-0.102911000
C	2.952816000	-0.105700000	-0.343811000
C	4.138204000	0.732059000	-0.342211000
H	5.151754000	0.358595000	-0.405011000
C	3.711130000	2.027002000	-0.235611000
H	4.302909000	2.932281000	-0.199511000
C	2.262536000	1.988708000	-0.178711000
C	1.443486000	3.106198000	-0.096111000
H	1.925456000	4.079163000	-0.058011000
C	0.054890000	3.076612000	-0.070411000
C	-0.799567000	4.248298000	-0.011311000
H	-0.440504000	5.268646000	0.021889000
C	-2.090207000	3.797325000	-0.006811000
H	-3.006284000	4.371902000	0.033989000
C	-2.030812000	2.346433000	-0.054911000
C	-3.143001000	1.515284000	-0.022111000
H	-4.117865000	1.994553000	0.004989000
C	-3.119315000	0.127587000	0.009489000
C	-4.303903000	-0.712272000	0.066789000
H	-5.319253000	-0.338808000	0.088289000
C	-3.870629000	-2.008714000	0.083989000
H	-4.458508000	-2.916592000	0.120489000
C	-2.420635000	-1.968619000	0.031089000
C	-1.595285000	-3.086009000	0.007389000
H	-2.071854000	-4.061673000	0.043889000
C	-0.211389000	-3.053024000	-0.090011000
C	0.639268000	-4.225710000	-0.170211000
H	0.281004000	-5.246358000	-0.140711000
C	1.923807000	-3.775838000	-0.299211000
H	2.834985000	-4.351816000	-0.393011000
C	1.865713000	-2.324245000	-0.291011000
C	2.975502000	-1.493897000	-0.387211000
H	3.947466000	-1.971967000	-0.471711000
O	-0.029407000	0.067601000	1.768089000
H	-0.405294000	-0.778650000	2.095789000
O	-0.232495000	-0.020826000	-2.013711000

H	0.042686000	0.862110000	-2.343211000
C	1.918339000	-0.275638000	2.798589000
H	2.265011000	0.677308000	2.426089000
H	1.506548000	-0.343794000	3.799489000
H	2.147859000	-1.173008000	2.239289000

1-⁵P_(hs)

Fe	0.100195000	0.046035000	-0.755775000
N	-1.398667000	-1.421408000	-0.224078000
N	-1.391390000	1.480989000	-0.072781000
N	1.526132000	1.471039000	-0.010320000
N	1.519515000	-1.443229000	-0.089731000
C	-1.196433000	-2.784920000	-0.156009000
C	-2.482782000	-3.463583000	-0.087942000
H	-2.615003000	-4.536152000	-0.024343000
C	-3.448992000	-2.491499000	-0.104664000
H	-4.523141000	-2.615781000	-0.054655000
C	-2.761015000	-1.210634000	-0.180847000
C	-3.386274000	0.040585000	-0.177033000
C	-2.758920000	1.287049000	-0.137476000
C	-3.431131000	2.576108000	-0.127200000
H	-4.503859000	2.715709000	-0.163561000
C	-2.455628000	3.536739000	-0.059057000
H	-2.578861000	4.611701000	-0.030544000
C	-1.176500000	2.845472000	-0.025968000
C	0.074616000	3.460808000	0.050883000
C	1.321518000	2.829149000	0.079287000
C	2.604127000	3.506424000	0.227340000
H	2.732366000	4.577021000	0.322059000
C	3.568628000	2.534593000	0.235171000
H	4.639644000	2.655869000	0.334856000
C	2.883122000	1.255885000	0.090206000
C	3.504444000	0.004420000	0.086138000
C	2.877919000	-1.243704000	0.021158000
C	3.553405000	-2.532459000	0.098662000
H	4.623440000	-2.667339000	0.191955000
C	2.581057000	-3.496741000	0.044313000
H	2.702886000	-4.571692000	0.084469000
C	1.304092000	-2.804330000	-0.069997000
C	0.048900000	-3.418362000	-0.111129000
H	0.038100000	-4.505057000	-0.068607000
H	4.588454000	-0.00008000	0.172978000
H	-4.473477000	0.041413000	-0.176425000
H	0.078454000	4.546636000	0.106930000
O	0.180950000	0.156020000	-2.655485000
O	-0.929992000	0.446382000	2.656250000
H	-1.002833000	0.698631000	1.705009000
C	-0.596723000	-0.959339000	2.769741000
H	0.231093000	-1.238988000	2.106283000
H	-0.300758000	-1.126796000	3.812014000
H	-1.454779000	-1.607103000	2.533028000
H	-0.348182000	-0.435892000	-3.222522000

1-³P_(is)

Fe	0.069042000	0.084324000	-0.410934000
N	-0.379293000	-1.855361000	-0.338828000
N	-1.933068000	0.507727000	-0.081017000
N	0.495133000	1.996978000	-0.104813000
N	2.037875000	-0.387579000	-0.031473000
C	0.518215000	-2.929346000	-0.294313000
C	-0.209454000	-4.184420000	-0.330701000
H	0.262104000	-5.158021000	-0.307943000
C	-1.537528000	-3.883280000	-0.370456000

H	-2.383571000	-4.557535000	-0.385647000
C	-1.653494000	-2.436282000	-0.357122000
C	-2.856196000	-1.766125000	-0.303121000
C	-2.997962000	-0.382681000	-0.179827000
C	-4.239824000	0.329843000	-0.157369000
H	-5.216276000	-0.133017000	-0.209880000
C	-3.931575000	1.673078000	-0.070845000
H	-4.608734000	2.516334000	-0.042165000
C	-2.503227000	1.774888000	-0.041909000
C	-1.778096000	2.968009000	-0.020395000
C	-0.404565000	3.061630000	-0.045770000
C	0.320542000	4.319164000	0.036493000
H	-0.154941000	5.289376000	0.092246000
C	1.647862000	4.019622000	0.047953000
H	2.492954000	4.691829000	0.115341000
C	1.763649000	2.572167000	-0.024575000
C	2.960276000	1.894713000	0.040884000
C	3.094118000	0.504008000	0.052616000
C	4.338379000	-0.208048000	0.128275000
H	5.311330000	0.258994000	0.205031000
C	4.034811000	-1.552648000	0.072464000
H	4.711516000	-2.396727000	0.093937000
C	2.607564000	-1.651779000	-0.039917000
C	1.886783000	-2.841486000	-0.166364000
H	2.448631000	-3.770939000	-0.147684000
H	3.869555000	2.484955000	0.107355000
H	-3.764155000	-2.360886000	-0.338177000
H	-2.343498000	3.894209000	0.022740000
O	0.118568000	0.234882000	-2.329218000
O	-1.075140000	-0.139047000	2.763845000
H	-1.355870000	0.068461000	1.843200000
C	-0.212517000	-1.308711000	2.766331000
H	-0.736648000	-2.207695000	2.410359000
H	0.094684000	-1.457509000	3.806631000
H	0.679095000	-1.164173000	2.143033000
H	-0.079781000	-0.623020000	-2.762202000

1-¹P_(ls)

Fe	-0.054701000	0.016561000	-0.185698000
N	1.140518000	-1.616473000	-0.151296000
N	1.562631000	1.207807000	-0.147228000
N	-1.671390000	-1.191796000	-0.036725000
N	-1.245306000	1.633360000	-0.099036000
C	0.749880000	-2.945259000	-0.128438000
C	1.584105000	2.593546000	-0.101907000
C	2.521360000	-1.630605000	-0.257320000
C	2.887083000	0.811727000	-0.230893000
C	-1.689221000	-2.578839000	-0.023812000
C	-0.854964000	2.962862000	-0.062323000
C	-2.998933000	-0.796339000	-0.035600000
C	-2.629632000	1.645078000	-0.074047000
C	1.911901000	-3.811101000	-0.203031000
C	2.953515000	3.074538000	-0.132307000
C	3.008352000	-2.997425000	-0.286690000
C	3.759171000	1.972754000	-0.215412000
C	-3.057879000	-3.061086000	0.009866000
C	-2.020212000	3.826552000	-0.021723000
C	-3.867487000	-1.959083000	-0.002225000
C	-3.118463000	3.011357000	-0.032053000
H	1.872504000	-4.892860000	-0.203874000
H	3.238270000	4.118587000	-0.104995000
H	4.051228000	-3.276227000	-0.366565000
H	4.839574000	1.928821000	-0.266552000
H	-3.340392000	-4.105934000	0.027153000

H	-1.982217000	4.907931000	0.009169000
H	-4.949103000	-1.916746000	0.005742000
H	-4.164710000	3.287996000	-0.008884000
C	-0.563898000	-3.392036000	-0.054886000
C	0.460870000	3.408238000	-0.059866000
C	-3.442408000	0.518377000	-0.061196000
C	3.330671000	-0.502337000	-0.295673000
H	-0.724922000	-4.466988000	-0.043224000
H	0.624020000	4.482646000	-0.031142000
H	-4.517233000	0.681134000	-0.050940000
H	4.403600000	-0.661699000	-0.368179000
O	-0.074183000	-0.096101000	1.986642000
H	-0.339318000	0.857382000	-2.387944000
H	-0.469105000	-0.990960000	2.032434000
O	-0.081183000	-0.045512000	-2.100133000
C	1.236019000	-0.054037000	2.634772000
H	1.135468000	-0.262328000	3.708811000
H	1.922189000	-0.759600000	2.157747000
H	1.601130000	0.959600000	2.475915000

[(OH)(Por^{•+})Fe^{IV}=O] (2)

⁶2_(hs) or 2-⁶R_(hs)

Fe	0.009194000	-0.007580000	-0.103324000
N	1.955014000	0.735383000	-0.015622000
N	0.741319000	-1.943229000	-0.041669000
N	-0.735663000	1.938044000	0.027562000
N	-1.953079000	-0.726816000	-0.040813000
C	2.319876000	2.060622000	0.002269000
C	-0.014829000	-3.089057000	-0.012843000
C	3.102646000	-0.015744000	-0.004687000
C	2.063714000	-2.309914000	-0.006779000
C	0.019931000	3.088328000	0.025441000
C	-2.311981000	-2.051345000	-0.013531000
C	-2.061556000	2.310288000	0.002337000
C	-3.107497000	0.021570000	-0.022404000
C	3.773072000	2.154731000	0.017564000
C	0.872481000	-4.243273000	0.030139000
C	4.255821000	0.874158000	0.014772000
C	2.153783000	-3.762971000	0.034517000
C	-0.865477000	4.239855000	0.013926000
C	-3.764472000	-2.151099000	0.017439000
C	-2.149385000	3.759956000	-0.000992000
C	-4.255081000	-0.873117000	0.010129000
H	4.333846000	3.078506000	0.032983000
H	0.546275000	-5.273236000	0.058379000
H	5.286917000	0.550386000	0.026291000
H	3.076300000	-4.324995000	0.067203000
H	-0.539506000	5.270324000	0.013113000
H	-4.320222000	-3.077708000	0.042946000
H	-3.071134000	4.324070000	-0.016181000
H	-5.287899000	-0.555274000	0.030170000
C	1.421848000	3.132032000	0.019127000
C	-1.413793000	-3.127150000	-0.008681000
C	-3.144432000	1.419527000	-0.018905000
C	3.141539000	-1.416508000	0.002318000
H	1.863955000	4.124629000	0.025825000
H	-1.861103000	-4.117191000	0.014639000
H	-4.132096000	1.872371000	-0.023972000
H	4.130992000	-1.864894000	0.026273000
O	0.033627000	0.031218000	-1.787189000
H	-0.586185000	0.606498000	2.181643000
O	-0.027323000	-0.101896000	1.798935000

⁴2_(hs) or 2-⁴R_(hs)

Fe	-0.014977000	0.006651000	-0.119273000
N	-1.677666000	-1.239952000	-0.034554000

N	-1.247981000	1.668345000	-0.030500000
N	1.241651000	-1.659506000	0.025460000
N	1.675803000	-1.230464000	-0.017816000
C	-1.663593000	-2.612327000	0.006453000
C	-0.835636000	2.976280000	-0.004591000
C	-2.987348000	-0.832755000	-0.007058000
C	-2.620055000	1.658382000	-0.016613000
C	0.829092000	-2.972864000	0.014294000
C	1.656984000	2.604505000	0.010501000
C	2.619425000	-1.656076000	-0.002883000
C	2.991581000	0.830300000	-0.006843000
C	-3.034111000	-3.102629000	0.049644000
C	-2.004847000	3.844119000	0.018744000
C	-3.850829000	-2.004443000	0.041992000
C	-3.105864000	3.030888000	0.011435000
C	1.995972000	-3.839040000	-0.005699000
C	3.025576000	3.099362000	0.038346000
C	3.099531000	-3.027369000	-0.017008000
C	3.848610000	2.005422000	0.026026000
H	-3.318333000	-4.144675000	0.086421000
H	-1.973434000	4.924148000	0.042050000
H	-4.930850000	-1.976673000	0.070942000
H	-4.147499000	3.318479000	0.027860000
H	1.963281000	-4.919310000	-0.013512000
H	3.305049000	4.143066000	0.064082000
H	4.140362000	-3.317937000	-0.035499000
H	4.929065000	1.983733000	0.040675000
C	-0.506051000	-3.398081000	0.015147000
C	0.500516000	3.394654000	0.011588000
C	3.415133000	-0.503594000	-0.013861000
C	-3.410844000	0.502699000	-0.009003000
H	-0.660420000	-4.473555000	0.025902000
H	0.661337000	4.469031000	0.033911000
H	4.489433000	-0.665102000	-0.021930000
H	-4.485561000	0.660983000	0.011874000
O	0.012637000	-0.011925000	-1.801326000
H	0.784126000	-0.387066000	2.161856000
O	-0.023795000	0.040914000	1.806911000

$42_{(is)}$ or $2\text{-}^4\mathbf{R}_{(is)}$

Fe	-0.017789000	0.004226000	-0.083052000
N	-1.251200000	-1.584320000	-0.026557000
N	-1.600991000	1.238949000	0.009878000
N	1.591828000	-1.232738000	-0.044557000
N	1.236326000	1.593362000	0.022365000
C	-0.885925000	-2.913987000	-0.000263000
C	-1.575607000	2.621182000	0.040315000
C	-2.630155000	-1.565624000	-0.018679000
C	-2.933998000	0.882243000	-0.020493000
C	1.565128000	-2.613065000	-0.003394000
C	0.874908000	2.926077000	0.057196000
C	2.928514000	-0.874229000	-0.058817000
C	2.617877000	1.575074000	-0.041766000
C	-2.067255000	-3.754172000	0.020002000
C	-2.927274000	3.142913000	0.025186000
C	-3.147172000	-2.919464000	0.007942000
C	-3.767190000	2.067604000	-0.015300000
C	2.916741000	-3.134418000	0.012247000
C	2.054692000	3.763101000	0.031569000
C	3.759235000	-2.060324000	-0.024939000
C	3.133976000	2.926538000	-0.034477000
H	-2.049657000	-4.834297000	0.042399000
H	-3.177362000	4.193945000	0.042519000
H	-4.197195000	-3.174006000	0.019402000
H	-4.847423000	2.056101000	-0.035830000
H	3.166211000	-4.185193000	0.046541000
H	2.040190000	4.843302000	0.053930000
H	4.839737000	-2.050924000	-0.025032000
H	4.183140000	3.182028000	-0.074525000
C	0.416936000	-3.390819000	0.004197000
C	-0.430441000	3.400806000	0.079122000
C	3.402135000	0.428603000	-0.084795000
C	-3.412616000	-0.420224000	-0.027016000
H	0.549252000	-4.467839000	0.021869000

H	-0.564698000	4.477379000	0.106614000
H	4.478128000	0.565348000	-0.119492000
H	-4.489560000	-0.553448000	-0.030447000
O	-0.060067000	0.089899000	-1.767647000
H	0.946755000	0.180031000	2.167959000
O	0.109842000	-0.211896000	1.833711000

$22_{(is)}$ or $2\text{-}^2\mathbf{R}_{(is)}$

Fe	0.025274000	0.013000000	-0.108233000
N	1.500081000	1.364765000	0.015495000
N	1.376687000	-1.474863000	-0.031624000
N	-1.352151000	1.495473000	0.011726000
N	-1.481554000	-1.348591000	-0.012985000
C	1.366149000	2.740055000	0.043185000
C	1.118285000	-2.827325000	-0.010864000
C	2.856463000	1.114849000	0.006008000
C	2.752743000	-1.347067000	-0.026919000
C	-1.098240000	2.855648000	0.024762000
C	-1.345678000	-2.727290000	0.011786000
C	-2.727201000	1.365824000	-0.035716000
C	-2.846886000	-1.097474000	-0.025601000
C	2.670707000	3.366703000	0.056021000
C	2.362093000	-3.572397000	-0.001611000
C	3.593934000	2.359874000	0.031479000
C	3.373607000	-2.656193000	-0.012361000
C	-2.341699000	3.593546000	-0.002851000
C	-2.652837000	-3.351187000	0.025090000
C	-3.350177000	2.671325000	-0.042542000
C	-3.577663000	-2.347496000	0.000332000
H	2.836783000	4.434126000	0.079566000
H	2.428481000	-4.650739000	0.014859000
H	4.671958000	2.432913000	0.032113000
H	4.440350000	-2.827865000	-0.005219000
H	-2.414615000	4.671611000	0.004379000
H	-2.819041000	-4.418647000	0.047332000
H	-4.417018000	2.840233000	-0.073225000
H	-4.655460000	-2.425005000	-0.000475000
C	0.163136000	3.431416000	0.049828000
C	-0.142670000	-3.409958000	0.004492000
C	-3.421531000	0.160599000	-0.054090000
C	3.440608000	-0.145733000	-0.016688000
H	0.214161000	4.515289000	0.064564000
H	-0.186882000	-4.494104000	0.016159000
H	-4.505008000	0.213171000	-0.079659000
H	4.524727000	-0.191081000	-0.016328000
O	-0.015221000	0.013470000	-1.769247000
H	-0.983998000	0.146227000	2.154683000
O	-0.141258000	-0.251959000	1.838569000

$22_{(ls)}$ or $2\text{-}^2\mathbf{R}_{(ls)}$

Fe	-0.017789000	0.004226000	-0.083052000
N	-1.251200000	-1.584320000	-0.026557000
N	-1.600991000	1.238949000	0.009878000
N	1.591828000	-1.232738000	-0.044557000
N	1.236326000	1.593362000	0.022365000
C	-0.885925000	-2.913987000	-0.000263000
C	-1.575607000	2.621182000	0.040315000
C	-2.630155000	-1.565624000	-0.018679000
C	-2.933998000	0.882243000	-0.020493000
C	1.565128000	-2.613065000	-0.003394000
C	0.874908000	2.926077000	0.057196000
C	2.928514000	-0.874229000	-0.058817000
C	2.617877000	1.575074000	-0.041766000
C	-2.067255000	-3.754172000	0.020002000
C	-2.927274000	3.142913000	0.025186000
C	-3.147172000	-2.919464000	0.007942000
C	-3.767190000	2.067604000	-0.015300000
C	2.916741000	-3.134418000	0.012247000
C	2.054692000	3.763101000	0.031569000
C	3.759235000	-2.060324000	-0.024939000
C	3.133976000	2.926538000	-0.034477000
H	-2.049657000	-4.834297000	0.042399000
H	-3.177362000	4.193945000	0.042519000
H	-4.197195000	-3.174006000	0.019402000
H	-4.847423000	2.056101000	-0.035830000
H	3.166211000	-4.185193000	0.046541000
H	2.040190000	4.843302000	0.053930000
H	4.839737000	-2.050924000	-0.025032000
H	4.183140000	3.182028000	-0.074525000
C	0.416936000	-3.390819000	0.004197000
C	-0.430441000	3.400806000	0.079122000
C	3.402135000	0.428603000	-0.084795000
C	-3.412616000	-0.420224000	-0.027016000
H	0.549252000	-4.467839000	0.021869000

H	-3.177362000	4.193945000	0.042519000
H	-4.197195000	-3.174006000	0.019402000
H	-4.847423000	2.056101000	-0.035830000
H	3.166211000	-4.185193000	0.046541000
H	2.040190000	4.843302000	0.053930000
H	4.839737000	-2.050924000	-0.025032000
H	4.183140000	3.182028000	-0.074525000
C	0.416936000	-3.390819000	0.004197000
C	-0.430441000	3.400806000	0.079122000
C	3.402135000	0.428603000	-0.084795000
C	-3.412616000	-0.420224000	-0.027016000
H	0.549252000	-4.467839000	0.021869000
H	-0.564698000	4.477379000	0.106614000
H	4.478128000	0.565348000	-0.119492000
H	-4.489560000	-0.553448000	-0.030447000
O	-0.060067000	0.089899000	-1.767647000
H	0.946755000	0.180031000	2.167959000
O	0.109842000	-0.211896000	1.833711000

2-⁶ts1_(hs)

Fe	-0.131938000	0.019425000	-0.131155000
N	-0.792243000	-1.953405000	-0.179442000
N	1.845187000	-0.681928000	-0.201604000
N	-2.049305000	0.684710000	-0.000144000
N	0.580982000	1.969061000	-0.166708000
C	-2.111043000	-2.348885000	-0.092756000
C	2.971622000	0.104516000	-0.330595000
C	-0.004586000	-3.089555000	-0.129197000
C	2.244497000	-2.002421000	-0.197083000
C	-3.185925000	-0.098582000	0.035509000
C	1.896345000	2.361208000	-0.288629000
C	-2.439602000	2.009035000	0.076278000
C	-0.196849000	3.098549000	-0.088488000
C	-2.161451000	-3.798770000	-0.027407000
C	4.136972000	-0.758383000	-0.384802000
C	-0.869333000	-4.252870000	-0.046183000
C	3.691752000	-2.051984000	-0.297720000
C	-4.34597000	0.769718000	0.145478000
C	1.950786000	3.814805000	-0.290798000
C	-3.888464000	2.059356000	0.172641000
C	0.664903000	4.267831000	-0.165553000
H	-3.070788000	-4.379270000	0.039406000
H	5.155680000	-0.409457000	-0.479260000
H	-0.521260000	-5.275212000	0.000233000
H	4.276671000	-2.960862000	-0.313824000
H	-5.368492000	0.423751000	0.192973000
H	2.857647000	4.396871000	-0.375961000
H	-4.466440000	2.969751000	0.245981000
H	0.318669000	5.291163000	-0.130371000
C	-3.211056000	-1.490997000	-0.019742000
C	2.991379000	1.500982000	-0.368423000
C	-1.589270000	3.111860000	0.035354000
C	1.389703000	-3.106920000	-0.143862000
H	-4.188348000	-1.960537000	0.032600000
H	3.967616000	1.966584000	-0.463099000
H	-2.061326000	4.087789000	0.091788000
H	1.862600000	-4.083918000	-0.123751000
O	-0.080558000	-0.010877000	1.656184000
H	0.971767000	-0.072224000	2.153092000
O	-0.071733000	0.043349000	-1.957783000
H	-0.016262000	-0.863569000	-2.330991000
H	2.621879000	0.852887000	2.431171000
H	1.881074000	-0.061180000	3.851907000
H	2.665257000	-0.982815000	2.459935000
C	2.176955000	-0.070767000	2.802024000

2-⁴ts1_(hs)

Fe	-0.082084000	0.022755000	-0.123765000
N	-1.101273000	-1.807246000	-0.174107000
N	1.719206000	-0.980561000	-0.185629000
N	-1.906929000	1.004874000	0.004242000
N	0.920839000	1.812629000	-0.160123000

C	-2.469348000	-1.975258000	-0.079272000
C	2.965555000	-0.403465000	-0.334718000
C	-0.513048000	-3.053978000	-0.109132000
C	1.884693000	-2.354436000	-0.172113000
C	-3.155158000	0.423004000	0.031412000
C	2.280922000	1.991831000	-0.309279000
C	-2.067024000	2.369833000	0.066417000
C	0.329691000	3.059542000	-0.096465000
C	-2.757359000	-3.395984000	0.001016000
C	3.962345000	-1.455542000	-0.385868000
C	-1.557352000	-4.057532000	-0.013293000
C	3.301037000	-2.651119000	-0.278765000
C	-4.156023000	1.474468000	0.125220000
C	2.563357000	3.415919000	-0.335341000
C	-3.488317000	2.668869000	0.148537000
C	1.367542000	4.069934000	-0.200985000
H	-3.749820000	-3.817887000	0.074788000
H	5.024920000	-1.289085000	-0.493922000
H	-1.382932000	-5.122738000	0.044478000
H	3.719859000	-3.647577000	-0.288839000
H	-5.222839000	1.305327000	0.166108000
H	3.549526000	3.845088000	-0.443320000
H	-3.904022000	3.664652000	0.211025000
H	1.189831000	5.135932000	-0.180396000
C	-3.411696000	-0.947446000	-0.012895000
C	3.222816000	0.966532000	-0.393610000
C	-1.036718000	3.310681000	0.024565000
C	0.861203000	-3.300184000	-0.117149000
H	-4.453230000	-1.248521000	0.041015000
H	4.260551000	1.263383000	-0.506993000
H	-1.333155000	4.354064000	0.068259000
H	1.166911000	-4.341492000	-0.090548000
O	-0.138684000	-0.052171000	1.659044000
H	0.901727000	-0.140304000	2.185392000
O	-0.210799000	0.056830000	-1.943847000
H	-0.696039000	-0.720759000	-2.295873000
H	2.583734000	0.746810000	2.299502000
H	1.854708000	0.008599000	3.825229000
H	2.547486000	-1.077755000	2.503141000
C	2.114539000	-0.114759000	2.772815000

2-⁴ts1_(is) (π -pathway)

Fe	-0.121676000	0.012260000	-0.125235000
N	-1.149124000	-1.713152000	-0.113532000
N	1.607817000	-1.038249000	-0.210660000
N	-1.820472000	1.038709000	0.000418000
N	0.929484000	1.727368000	-0.179701000
C	-2.524690000	-1.852837000	-0.143123000
C	2.873344000	-0.523955000	-0.434176000
C	-0.627430000	-2.992238000	0.021108000
C	1.756105000	-2.405839000	-0.068407000
C	-3.104729000	0.528320000	-0.050403000
C	2.284660000	1.861203000	-0.420715000
C	-1.947461000	2.409595000	0.152670000
C	0.427317000	3.001851000	-0.027667000
C	-2.874694000	-3.254370000	-0.061616000
C	3.840494000	-1.597662000	-0.423091000
C	-1.707050000	-3.954484000	0.054734000
C	3.154026000	-2.756682000	-0.181692000
C	-4.062726000	1.606724000	0.075141000
C	2.640564000	3.265171000	-0.419774000
C	-3.350081000	2.762908000	0.214831000
C	1.497200000	3.968099000	-0.163736000
H	-3.887449000	-3.631045000	-0.071829000
H	4.902302000	-1.463539000	-0.572787000
H	-1.568409000	-5.021957000	0.150326000
H	3.539197000	-3.763436000	-0.104868000
H	-5.134913000	1.472681000	0.064896000
H	3.640068000	3.641284000	-0.585138000
H	-3.718942000	3.771559000	0.333831000
H	1.367128000	5.037889000	-0.084480000
C	-3.438712000	-0.811303000	-0.152955000
C	3.187150000	0.820253000	-0.564156000
C	-0.908452000	3.322561000	0.165578000

C	0.717550000	-3.315867000	0.071065000
H	-4.492286000	-1.066895000	-0.176433000
H	4.226545000	1.077356000	-0.736788000
H	-1.162492000	4.370852000	0.277465000
H	0.978398000	-4.363559000	0.173157000
O	-0.062599000	-0.012439000	1.673365000
H	1.017129000	-0.036859000	2.143837000
O	-0.109856000	0.035345000	-1.942499000
H	-0.041230000	-0.869306000	-2.317433000
H	2.710623000	0.844242000	2.237894000
H	2.033072000	0.065615000	3.762771000
H	2.680960000	-0.982818000	2.394950000
C	2.247546000	-0.029248000	2.697074000

2-⁴ts1_(is) (δ-pathway)

Fe	-0.082075000	0.022765000	-0.123739000
N	-1.101423000	-1.807163000	-0.174134000
N	1.719122000	-0.980699000	-0.185639000
N	-1.906837000	1.005024000	0.004228000
N	0.920989000	1.812551000	-0.160086000
C	-2.469512000	-1.975065000	-0.079323000
C	2.965516000	-0.403706000	-0.334749000
C	-0.513297000	-3.053940000	-0.109124000
C	1.884498000	-2.354587000	-0.172088000
C	-3.155114000	0.423254000	0.031374000
C	2.281078000	1.991644000	-0.309329000
C	-2.066823000	2.369993000	0.066450000
C	0.329943000	3.059514000	-0.096433000
C	-2.757639000	-3.395766000	0.000977000
C	3.962221000	-1.455865000	-0.385880000
C	-1.557683000	-4.057410000	-0.013293000
C	3.300818000	-2.651386000	-0.278738000
C	-4.155896000	1.474796000	0.125207000
C	2.563624000	3.415708000	-0.335435000
C	-3.488093000	2.669142000	0.148570000
C	1.367868000	4.069821000	-0.201025000
H	-3.750134000	-3.817590000	0.074732000
H	5.024809000	-1.289496000	-0.493946000
H	-1.383347000	-5.122629000	0.044497000
H	3.719560000	-3.647877000	-0.288790000
H	-5.222725000	1.305740000	0.166078000
H	3.549820000	3.844797000	-0.443476000
H	-3.903717000	3.664957000	0.211086000
H	1.190242000	5.135833000	-0.180449000
C	-3.411773000	-0.947172000	-0.012957000
C	3.222886000	0.966269000	-0.393675000
C	-1.036444000	3.310761000	0.024619000
C	0.860934000	-3.300254000	-0.117114000
H	-4.453334000	-1.248157000	0.040937000
H	4.260641000	1.263034000	-0.507097000
H	-1.332799000	4.354167000	0.068327000
H	1.166561000	-4.341585000	-0.090488000
O	-0.138678000	-0.052240000	1.659062000
H	0.901728000	-0.140377000	2.185426000
O	-0.210795000	0.056870000	-1.943827000
H	-0.696117000	-0.720702000	-2.295785000
H	2.583719000	0.746748000	2.299611000
H	1.854633000	0.008512000	3.825296000
H	2.547485000	-1.077821000	2.503235000
C	2.114512000	-0.114832000	2.772892000

2-²ts1_(is)

Fe	-0.094114000	0.013192000	-0.117637000
N	0.976668000	-1.694896000	-0.199010000
N	1.591738000	1.072570000	-0.199835000
N	-1.795448000	-1.074981000	-0.031533000
N	-1.169354000	1.706964000	-0.069654000
C	0.497050000	-2.982166000	-0.017736000
C	1.710007000	2.446744000	-0.074994000
C	2.337361000	-1.807745000	-0.423383000
C	2.867457000	0.587525000	-0.442023000
C	-1.894990000	-2.444013000	0.137972000

C	-0.678575000	2.991582000	0.035250000
C	-3.085798000	-0.584014000	-0.066687000
C	-2.545590000	1.811046000	-0.122489000
C	1.588988000	-3.923862000	-0.127966000
C	3.098466000	2.827177000	-0.207265000
C	2.720179000	-3.201927000	-0.391950000
C	3.808445000	1.684014000	-0.450166000
C	-3.290400000	-2.822574000	0.206909000
C	-1.778744000	3.934585000	0.048644000
C	-4.024296000	-1.678099000	0.066920000
C	-2.928891000	3.207644000	-0.063661000
H	1.482690000	-4.994463000	-0.026095000
H	3.460228000	3.843451000	-0.143732000
H	3.728221000	-3.561357000	-0.541873000
H	4.870720000	1.573552000	-0.614861000
H	-3.641723000	-3.836356000	0.335691000
H	-1.662489000	5.006341000	0.122892000
H	-5.098754000	-1.562937000	0.066266000
H	-3.949764000	3.560840000	-0.091107000
C	-0.831345000	-3.331934000	0.168628000
C	0.661479000	3.340345000	0.069911000
C	-3.439317000	0.753894000	-0.148458000
C	3.216244000	-0.746065000	-0.574010000
H	-1.059281000	-4.384301000	0.297358000
H	0.906674000	4.393328000	0.153387000
H	-4.497005000	0.992075000	-0.174093000
H	4.261011000	-0.977629000	-0.749172000
O	-0.096901000	-0.051439000	1.658107000
H	-0.429061000	-0.888526000	-2.286523000
H	0.949212000	-0.013178000	2.149323000
H	2.546236000	1.045352000	2.425790000
H	1.990123000	-0.111706000	3.750415000
H	2.711256000	-0.767615000	2.183170000
C	2.198056000	0.047943000	2.691511000
O	-0.225758000	0.002929000	-1.931582000

2-²ts1_(ls)

Fe	0.089784000	0.011802000	-0.119765000
N	1.851561000	0.990281000	0.008417000
N	-0.891791000	1.749811000	-0.178459000
N	1.083850000	-1.752143000	-0.140484000
N	-1.656903000	-0.975306000	-0.196275000
C	3.115031000	0.434608000	-0.017490000
C	-2.246458000	1.933965000	-0.392970000
C	2.020821000	2.353450000	0.129237000
C	-0.337913000	3.011130000	-0.050568000
C	2.457058000	-1.929112000	-0.126517000
C	-2.910679000	-0.425608000	-0.401340000
C	0.523143000	-3.013451000	-0.029364000
C	-1.839630000	-2.345468000	-0.095184000
C	4.109677000	1.482935000	0.096637000
C	-2.549374000	3.348541000	-0.399424000
C	3.434728000	2.665199000	0.197615000
C	-1.375490000	4.011384000	-0.176544000
C	2.762693000	-3.340816000	-0.051709000
C	-3.905559000	-1.473410000	-0.406574000
C	1.571526000	-4.007950000	0.019986000
C	-3.247693000	-2.655104000	-0.203311000
H	5.176747000	1.312464000	0.102672000
H	-3.537674000	3.759359000	-0.548491000
H	3.834781000	3.664115000	0.296392000
H	-1.204866000	5.076474000	-0.112116000
H	3.763894000	-3.747094000	-0.035668000
H	-4.964352000	-1.307384000	-0.545097000
H	1.399217000	-5.071807000	0.099461000
H	-3.657562000	-3.653649000	-0.151077000
C	3.403717000	-0.917158000	-0.103416000
C	-3.188046000	0.926257000	-0.519176000
C	-0.833509000	-3.291984000	0.010191000
C	1.006222000	3.296026000	0.123339000
H	4.448252000	-1.208767000	-0.100994000
H	-4.220376000	1.217335000	-0.678161000
H	-1.130128000	-4.332216000	0.087985000
H	1.289065000	4.338963000	0.214351000

O	0.110672000	-0.043567000	1.655879000
H	-0.928932000	-0.079001000	2.162695000
O	0.201438000	0.054875000	-1.935258000
H	0.535247000	-0.786467000	-2.313426000
H	-2.604435000	0.854433000	2.224338000
H	-2.618245000	-0.966966000	2.458747000
H	-1.931727000	0.124735000	3.778935000
C	-2.168126000	-0.010158000	2.722582000

2⁻⁶int1_(hs)

Fe	0.075902000	0.006397000	0.187538000
N	-1.868853000	-0.504132000	-0.369221000
N	-0.412550000	2.010154000	-0.132045000
N	2.108169000	0.501045000	0.050077000
N	0.639441000	-2.003047000	-0.135864000
C	-2.372817000	-1.787443000	-0.462060000
C	-3.808167000	-1.718628000	-0.655916000
H	-4.457860000	-2.575810000	-0.763546000
C	-4.149655000	-0.390133000	-0.684410000
H	-5.131646000	0.042128000	-0.815195000
C	-2.928908000	0.370087000	-0.505131000
C	-2.837667000	1.766207000	-0.471828000
C	-1.679263000	2.525692000	-0.318079000
C	-1.596127000	3.976851000	-0.374991000
H	-2.439714000	4.638242000	-0.514060000
C	-0.275091000	4.308556000	-0.242578000
H	0.169369000	5.293775000	-0.251201000
C	0.467377000	3.064689000	-0.102413000
C	1.858486000	2.961056000	0.013284000
C	2.616052000	1.796620000	0.069454000
C	4.058235000	1.722659000	0.166134000
H	4.714595000	2.580213000	0.211902000
C	4.406648000	0.395398000	0.192383000
H	5.398690000	-0.027930000	0.263093000
C	3.185892000	-0.377809000	0.112284000
C	3.084616000	-1.765709000	0.098340000
C	1.911268000	-2.522016000	-0.017062000
C	1.840208000	-3.972364000	-0.053973000
H	2.692659000	-4.633311000	0.016078000
C	0.519675000	-4.308484000	-0.193470000
H	0.087198000	-5.296963000	-0.259627000
C	-0.235184000	-3.068666000	-0.245025000
C	-1.617603000	-2.962659000	-0.393423000
H	-2.168559000	-3.894756000	-0.475721000
H	4.014472000	-2.321213000	0.169700000
H	-3.765681000	2.313890000	-0.605123000
H	2.410472000	3.895751000	0.036050000
O	0.902002000	0.253459000	-1.925439000
O	-0.095671000	-0.065727000	2.021011000
H	-0.913915000	-0.107881000	2.557971000
C	-3.138286000	-0.120675000	2.821709000
H	-3.216654000	-0.919237000	2.093020000
H	-3.201587000	-0.337470000	3.882989000
H	-3.095391000	0.906746000	2.477565000
H	1.357871000	-0.611858000	-2.074477000

2⁻⁴int1_(hs)

Fe	0.126594000	0.020619000	-0.124179000
N	-1.879176000	-0.515223000	-0.220849000
N	-0.406102000	2.008927000	-0.174527000
N	2.120043000	0.526033000	0.043972000
N	0.648073000	-2.000777000	-0.193205000
C	-2.380041000	-1.803919000	-0.257733000
C	-3.822832000	-1.735668000	-0.388418000
H	-4.476048000	-2.595476000	-0.438665000
C	-4.164524000	-0.409267000	-0.458025000
H	-5.150634000	0.019208000	-0.569224000
C	-2.939204000	0.359541000	-0.363031000
C	-2.847725000	1.751984000	-0.392621000
C	-1.683002000	2.513401000	-0.301935000
C	-1.612100000	3.964865000	-0.301203000
H	-2.465953000	4.621645000	-0.390454000

C	-0.293337000	4.306790000	-0.166674000
H	0.137969000	5.297065000	-0.126363000
C	0.468189000	3.071536000	-0.086484000
C	1.852839000	2.977899000	0.053844000
C	2.613511000	1.809860000	0.111385000
C	4.061698000	1.745693000	0.226514000
H	4.710276000	2.607205000	0.300270000
C	4.411892000	0.422662000	0.217184000
H	5.401990000	-0.006049000	0.282077000
C	3.184035000	-0.347145000	0.097446000
C	3.094908000	-1.738028000	0.044386000
C	1.930549000	-2.499862000	-0.065397000
C	1.860201000	-3.948509000	-0.011738000
H	2.717420000	-4.600840000	0.077915000
C	0.536612000	-4.297170000	-0.075713000
H	0.106728000	-5.288580000	-0.049221000
C	-0.229578000	-3.068765000	-0.173161000
C	-1.621002000	-2.974287000	-0.215725000
H	-2.171290000	-3.909837000	-0.224252000
H	4.027691000	-2.287893000	0.119720000
H	-3.780382000	2.297410000	-0.495940000
H	2.397860000	3.914696000	0.112906000
O	0.237538000	0.041114000	-1.939983000
O	0.036330000	-0.053812000	1.671951000
H	-0.886838000	-0.166534000	2.032725000
C	-2.692006000	-0.028761000	2.869684000
H	-3.158662000	-0.798055000	2.264421000
H	-2.342859000	-0.258576000	3.871203000
H	-2.739187000	1.003254000	2.539069000
H	0.435161000	-0.852978000	-2.296539000

2⁻⁴int1_(is)

Fe	0.140180000	0.008559000	-0.126805000
N	0.808211000	1.897304000	-0.104642000
N	2.017834000	-0.673638000	0.045909000
N	-0.543505000	-1.894918000	-0.246893000
N	-1.768678000	0.676687000	-0.222208000
C	0.042493000	3.047655000	-0.099635000
C	0.907789000	4.208774000	-0.072667000
H	0.555746000	5.230411000	-0.066137000
C	2.193349000	3.749478000	-0.060657000
H	3.112532000	4.317071000	-0.037606000
C	2.127599000	2.302683000	-0.067731000
C	3.229851000	1.468444000	0.008287000
C	3.169688000	0.087348000	0.081990000
C	4.321575000	-0.778490000	0.223335000
H	5.342734000	-0.429187000	0.277056000
C	3.855232000	-2.060899000	0.274354000
H	4.415861000	-2.979243000	0.374534000
C	2.413821000	-1.993889000	0.152657000
C	1.580168000	-3.098193000	0.101822000
C	0.209100000	-3.047864000	-0.090740000
C	-0.653998000	-4.204713000	-0.165678000
H	-0.311865000	-5.226085000	-0.079104000
C	-1.928219000	-3.746658000	-0.355948000
H	-2.841101000	-4.316686000	-0.453963000
C	-1.861677000	-2.302955000	-0.389042000
C	-2.960545000	-1.465126000	-0.492032000
C	-2.911488000	-0.082915000	-0.410217000
C	-4.065749000	0.784304000	-0.474592000
H	-5.080711000	0.438968000	-0.610008000
C	-3.613205000	2.067571000	-0.336119000
H	-4.181548000	2.986639000	-0.344244000
C	-2.175262000	1.999177000	-0.200147000
C	-1.340320000	3.102236000	-0.123152000
H	-1.804311000	4.082358000	-0.114983000
H	-3.933819000	-1.926642000	-0.617697000
H	4.209695000	1.931706000	0.041180000
H	2.036740000	-4.076708000	0.201919000
O	0.249816000	0.048346000	-1.934327000
O	0.017085000	-0.046996000	1.667750000
H	-0.902796000	0.071982000	2.016528000
C	-2.796918000	0.028341000	2.867709000
H	-2.458811000	0.201122000	3.883951000

H	-2.873632000	-0.984958000	2.488215000
H	-3.183457000	0.848155000	2.272447000
H	0.062099000	-0.826112000	-2.338485000

2⁻²int1_(is)

Fe	0.132158000	0.010494000	-0.123863000
N	0.800429000	1.899495000	-0.102439000
N	2.016071000	-0.672792000	0.040244000
N	-0.546045000	-1.893903000	-0.239443000
N	-1.770167000	0.675637000	-0.220416000
C	0.035320000	3.049296000	-0.082708000
C	0.900763000	4.210454000	-0.059390000
H	0.548962000	5.232071000	-0.043420000
C	2.186328000	3.750989000	-0.066839000
H	3.105758000	4.318489000	-0.052693000
C	2.120544000	2.304043000	-0.079985000
C	3.224124000	1.470442000	-0.017598000
C	3.166792000	0.089200000	0.061731000
C	4.320491000	-0.774635000	0.203839000
H	5.341826000	-0.424388000	0.247318000
C	3.854977000	-2.056585000	0.272879000
H	4.416687000	-2.973533000	0.379712000
C	2.412497000	-1.991027000	0.159712000
C	1.577407000	-3.095288000	0.122823000
C	0.206791000	-3.045780000	-0.072909000
C	-0.655058000	-4.203401000	-0.151462000
H	-0.313116000	-5.224241000	-0.057990000
C	-1.927478000	-3.747103000	-0.357664000
H	-2.838721000	-4.318310000	-0.463720000
C	-1.861603000	-2.303456000	-0.395064000
C	-2.959587000	-1.465790000	-0.509244000
C	-2.911335000	-0.084144000	-0.420630000
C	-4.066518000	0.781640000	-0.479826000
H	-5.080320000	0.436010000	-0.622949000
C	-3.617260000	2.064179000	-0.324036000
H	-4.187642000	2.982020000	-0.323593000
C	-2.179880000	1.997647000	-0.184527000
C	-1.347900000	3.101950000	-0.097174000
H	-1.814025000	4.080892000	-0.078691000
H	-3.931723000	-1.926982000	-0.644417000
H	4.203705000	1.934975000	0.004634000
H	2.033257000	-4.073294000	0.230921000
O	0.264720000	0.042518000	-1.931806000
O	0.029006000	-0.047037000	1.667936000
H	-0.892294000	0.043466000	2.029362000
C	-2.752846000	0.018989000	2.836275000
H	-2.404813000	0.167499000	3.853152000
H	-2.866262000	-0.986567000	2.445553000
H	-3.131900000	0.856160000	2.260961000
H	0.163286000	-0.849749000	-2.327567000

2⁻²int1_(ls)

Fe	-0.129132000	0.014235000	-0.125856000
N	-2.033336000	-0.607936000	0.048011000
N	0.487995000	-1.916445000	-0.242428000
N	-0.733883000	1.920202000	-0.113296000
N	1.794721000	0.612442000	-0.215862000
C	-3.158033000	0.190794000	0.085909000
C	1.790917000	-2.371296000	-0.375941000
C	-2.474562000	-1.913398000	0.150414000
C	-0.305949000	-3.043104000	-0.096874000
C	-2.039968000	2.369642000	-0.080075000
C	2.914851000	-0.186806000	-0.385676000
C	0.067351000	3.046082000	-0.121134000
C	2.248337000	1.920939000	-0.198666000
C	-4.340141000	-0.634613000	0.227380000
C	1.807040000	-3.816980000	-0.349317000
C	-3.918146000	-1.932275000	0.273696000
C	0.515911000	-4.230302000	-0.171615000
C	-2.058884000	3.818186000	-0.088474000
C	4.098565000	0.639708000	-0.441308000
C	-0.759322000	4.235472000	-0.106936000

C	3.688791000	1.938995000	-0.318047000
H	-5.348729000	-0.250644000	0.282600000
H	2.699917000	-4.418662000	-0.442702000
H	-4.509880000	-2.831262000	0.371006000
H	0.137123000	-5.239337000	-0.092677000
H	-2.959161000	4.415585000	-0.070779000
H	5.102669000	0.259108000	-0.562863000
H	-0.374521000	5.245260000	-0.111510000
H	4.288709000	2.837817000	-0.326514000
C	-3.169364000	1.573524000	0.006203000
C	2.918564000	-1.570232000	-0.465381000
C	1.451609000	3.053057000	-0.138199000
C	-1.678679000	-3.045586000	0.092708000
H	-4.132584000	2.070822000	0.038006000
H	3.877406000	-2.063637000	-0.581254000
H	1.949442000	4.016570000	-0.136560000
H	-2.169076000	-4.008338000	0.186869000
O	-0.030732000	-0.065315000	1.665832000
H	0.894078000	0.035042000	2.035329000
O	-0.265007000	0.040301000	-1.929380000
H	-0.101064000	-0.844141000	-2.324673000
H	2.819884000	-0.983503000	2.517441000
H	3.067211000	0.853078000	2.269926000
H	2.292528000	0.216452000	3.860197000
C	2.664596000	0.035189000	2.856970000

2⁻⁶ts2_(hs)

Fe	-0.107232000	0.013271000	-0.185541000
N	-2.176519000	0.047725000	-0.071924000
N	-0.149785000	-2.069878000	-0.054037000
N	-0.064035000	2.074356000	-0.145557000
N	1.959141000	-0.054721000	-0.337494000
C	-2.954953000	1.187253000	0.027137000
C	0.943782000	-2.907818000	-0.178092000
C	-3.007006000	-1.049928000	0.070724000
C	-1.284423000	-2.856215000	0.016006000
C	-1.153428000	2.912402000	-0.060138000
C	2.742464000	-1.187773000	-0.376557000
C	1.073761000	2.851395000	-0.192305000
C	2.791068000	1.043255000	-0.355770000
C	-4.339439000	0.788073000	0.195217000
C	0.478440000	-4.281971000	-0.151945000
C	-4.371483000	-0.581676000	0.222222000
C	-0.886314000	-4.250585000	-0.032078000
C	-0.683521000	4.288074000	-0.050772000
C	4.137598000	-0.786786000	-0.446790000
C	0.682618000	4.250326000	-0.130528000
C	4.166985000	0.582565000	-0.431175000
H	-5.167777000	1.475655000	0.292616000
H	1.120740000	-5.148259000	-0.225533000
H	-5.230866000	-1.225541000	0.345778000
H	-1.570818000	-5.086072000	0.010640000
H	-1.324436000	5.156329000	0.009816000
H	4.972747000	-1.471343000	-0.494580000
H	1.372826000	5.082002000	-0.148611000
H	5.031021000	1.231073000	-0.464946000
C	-2.484906000	2.500962000	0.011025000
C	2.271164000	-2.500122000	-0.315531000
C	2.381659000	2.376436000	-0.290265000
C	-2.595506000	-2.382998000	0.090389000
H	-3.232886000	3.283742000	0.087290000
H	3.015525000	-3.287707000	-0.377258000
H	3.167416000	3.124941000	-0.316022000
H	-3.377678000	-3.130938000	0.173196000
O	0.048651000	0.043479000	1.650821000
H	0.213927000	-0.860384000	2.000761000
O	-0.212235000	-0.048849000	-2.006773000
H	-1.135611000	-0.071426000	-2.340197000
H	2.114992000	1.086503000	2.848771000
H	2.302078000	-0.325405000	4.075732000
H	2.854145000	-0.534333000	2.287726000
C	2.423064000	0.074581000	3.074159000

2⁻⁴ts2_(hs)

Fe	0.099045000	-0.020884000	-0.132200000
N	1.940814000	0.957392000	-0.089501000
N	-0.856729000	1.840358000	-0.089858000
N	1.065150000	-1.842165000	-0.054995000
N	-1.719527000	-0.946713000	-0.276448000
C	3.171900000	0.336863000	0.011584000
C	-2.211250000	2.046881000	-0.268792000
C	2.140508000	2.321550000	0.015531000
C	-0.238444000	3.077270000	-0.060738000
C	2.426046000	-2.046003000	0.009187000
C	-2.948712000	-0.332316000	-0.402844000
C	0.446903000	-3.072258000	-0.063359000
C	-1.923333000	-2.312687000	-0.260207000
C	4.195524000	1.357533000	0.141190000
C	-2.462999000	3.475703000	-0.307510000
C	3.563807000	2.573271000	0.145099000
C	-1.254078000	4.107463000	-0.176220000
C	2.681017000	-3.476801000	0.051631000
C	-3.975169000	-1.356108000	-0.475278000
C	1.466190000	-4.106531000	0.009147000
C	-3.347413000	-2.569868000	-0.382482000
H	5.253756000	1.156214000	0.230497000
H	-3.438900000	3.924033000	-0.430499000
H	4.007324000	3.554695000	0.237270000
H	-1.054421000	5.169809000	-0.173368000
H	3.663146000	-3.924951000	0.105697000
H	-5.032999000	-1.158659000	-0.576374000
H	1.264753000	-5.168405000	0.021057000
H	-3.793640000	-3.554188000	-0.398761000
C	3.393006000	-1.041358000	0.034346000
C	-3.172088000	1.044133000	-0.406091000
C	-0.929183000	-3.285208000	-0.151434000
C	1.138152000	3.293145000	0.013426000
H	4.427220000	-1.363520000	0.103841000
H	-4.200958000	1.369312000	-0.523633000
H	-1.261629000	-4.318504000	-0.150647000
H	1.465557000	4.326912000	0.061916000
O	0.075873000	-0.014961000	1.682583000
H	-0.452615000	0.726610000	2.055055000
O	0.192307000	0.041104000	-1.942410000
H	0.991267000	0.529659000	-2.240667000
H	-2.447957000	-1.060082000	2.323742000
H	-2.173447000	-0.097794000	3.912934000
H	-2.907456000	0.750892000	2.400657000
C	-2.499980000	-0.133062000	2.879268000

2⁻⁴ts2_(is)

Fe	-0.116650000	0.014711000	-0.162698000
N	1.723890000	-0.849554000	-0.347789000
N	0.744977000	1.835084000	-0.170231000
N	-0.946573000	-1.822640000	-0.008662000
N	-1.926491000	0.851337000	-0.028052000
C	2.012130000	-2.203366000	-0.301364000
C	0.094086000	3.050382000	-0.107401000
C	2.940353000	-0.190317000	-0.387424000
C	2.095963000	2.115341000	-0.259979000
C	-0.288157000	-3.042866000	-0.070917000
C	-2.207981000	2.205281000	-0.004727000
C	-2.300545000	-2.110549000	0.047526000
C	-3.142313000	0.195423000	0.042533000
C	3.444343000	-2.397398000	-0.355820000
C	1.062620000	4.126156000	-0.146700000
C	4.016182000	-1.156207000	-0.409532000
C	2.297127000	3.549713000	-0.239998000
C	-1.254379000	-4.116938000	-0.016501000
C	-3.639422000	2.402909000	0.072021000
C	-2.493133000	-3.542915000	0.054214000
C	-4.215336000	1.164750000	0.099802000
H	3.930115000	-3.362671000	-0.343775000
H	0.809513000	5.176030000	-0.110416000
H	5.065220000	-0.899659000	-0.447648000
H	3.263565000	4.030015000	-0.295818000
H	-0.999358000	-5.166778000	-0.041616000
H	-4.119298000	3.370586000	0.102500000

H	-3.458043000	-4.027275000	0.099358000
H	-5.263813000	0.909851000	0.157745000
C	1.080186000	-3.223867000	-0.190490000
C	-1.277473000	3.229459000	-0.035316000
C	-3.323415000	-1.176858000	0.075891000
C	3.116231000	1.184092000	-0.362316000
H	1.450446000	-4.243221000	-0.196210000
H	-1.650129000	4.247236000	-0.002173000
H	-4.340987000	-1.548082000	0.126119000
H	4.132797000	1.558822000	-0.410368000
O	0.142341000	0.008053000	1.668083000
H	0.502424000	-0.398841000	-2.439909000
H	-0.211021000	-0.813908000	2.075031000
O	-0.268848000	-0.003210000	-1.980967000
H	2.336495000	0.980967000	2.545693000
H	1.709812000	-0.009428000	4.010550000
H	2.515542000	-0.878509000	2.548955000
C	2.183109000	0.030117000	3.036222000

2⁻²ts2_(is)

Fe	-0.098065000	0.018191000	-0.133783000
N	0.577196000	-1.890449000	-0.097246000
N	1.780313000	0.681988000	-0.293942000
N	-2.004452000	-0.675569000	-0.069954000
N	-0.778195000	1.901709000	-0.052776000
C	-0.186528000	-3.045777000	-0.015594000
C	2.192470000	2.001685000	-0.265509000
C	1.889186000	-2.301268000	-0.269158000
C	2.923702000	-0.082104000	-0.437800000
C	-2.408234000	-1.997025000	0.038259000
C	-0.013644000	3.051471000	-0.043622000
C	-3.156293000	0.090790000	-0.011560000
C	-2.098666000	2.307417000	-0.004214000
C	0.675277000	-4.203808000	-0.092395000
C	3.631859000	2.066494000	-0.401254000
C	1.952980000	-3.745225000	-0.254585000
C	4.081725000	0.781782000	-0.514954000
C	-3.850361000	-2.059241000	0.129416000
C	-0.876570000	4.211836000	0.028513000
C	-4.311507000	-0.773116000	0.093669000
C	-2.162572000	3.753266000	0.046710000
H	0.327483000	-5.225836000	-0.044099000
H	4.202513000	2.984042000	-0.408913000
H	2.864262000	-4.315733000	-0.363610000
H	5.097166000	0.430438000	-0.629015000
H	-4.416402000	-2.975763000	0.215477000
H	-0.523687000	5.232926000	0.051062000
H	-5.331919000	-0.421519000	0.147728000
H	-3.080887000	4.321084000	0.091130000
C	-1.568671000	-3.098978000	0.066487000
C	1.366993000	3.105097000	-0.131992000
C	-3.205339000	1.475132000	0.000739000
C	2.980798000	-1.465494000	-0.437194000
H	-2.029013000	-4.078238000	0.138719000
H	1.834198000	4.083602000	-0.118857000
H	-4.183249000	1.941677000	0.046311000
H	3.953824000	-1.928453000	-0.559279000
O	-0.057203000	0.029447000	1.679084000
H	-1.035650000	-0.396576000	-2.258526000
H	0.308097000	-0.798686000	2.059010000
O	-0.188343000	-0.018253000	-1.938313000
H	2.524747000	0.923107000	2.283496000
H	2.117492000	0.006604000	3.869943000
H	2.813277000	-0.921747000	2.387172000
C	2.484692000	0.002533000	2.849682000

2⁻²ts2_(ls)

Fe	-0.117282000	0.010145000	-0.128039000
N	-0.168060000	-2.011814000	-0.042028000
N	1.885764000	-0.060388000	-0.345586000
N	-2.125498000	0.066165000	-0.010551000
N	-0.045896000	2.014941000	-0.105687000

C	-1.301598000	-2.802911000	0.050335000
C	2.755997000	1.019862000	-0.344315000
C	0.903393000	-2.879410000	-0.182734000
C	2.678054000	-1.198216000	-0.416454000
C	-2.982183000	-1.012616000	0.079691000
C	1.086907000	2.807249000	-0.132931000
C	-2.915583000	1.197090000	-0.003248000
C	-1.125990000	2.875699000	-0.056303000
C	-0.925345000	-4.198324000	0.009111000
C	4.116797000	0.548944000	-0.450002000
C	0.432805000	-4.245690000	-0.137574000
C	4.068918000	-0.817112000	-0.499678000
C	-4.352939000	-0.545151000	0.133261000
C	0.707186000	4.203219000	-0.082865000
C	-4.311899000	0.817935000	0.078419000
C	-0.657181000	4.245300000	-0.041112000
H	-1.625271000	-5.019305000	0.070996000
H	4.984011000	1.193130000	-0.474194000
H	1.071945000	-5.113301000	-0.218463000
H	4.888825000	-1.517355000	-0.572102000
H	-5.215160000	-1.192572000	0.204497000
H	1.407925000	5.025813000	-0.090134000
H	-5.133419000	1.519635000	0.097808000
H	-1.304393000	5.109798000	-0.003720000
C	-2.606684000	-2.344666000	0.120678000
C	2.390584000	2.351836000	-0.237507000
C	-2.459213000	2.503989000	-0.026214000
C	2.226132000	-2.506441000	-0.355724000
H	-3.394713000	-3.086426000	0.190276000
H	3.183009000	3.091980000	-0.248756000
H	-3.200096000	3.295452000	-0.001081000
H	2.964412000	-3.296646000	-0.436569000
O	0.015142000	0.048550000	1.679721000
H	0.213742000	-0.827410000	2.074332000
O	-0.313394000	-0.038924000	-1.926964000
H	0.547021000	0.071867000	-2.386153000
H	2.325896000	1.037376000	2.534280000
H	2.211618000	-0.323846000	3.818434000
H	3.078493000	-0.639235000	2.178262000
C	2.539729000	0.024074000	2.844534000

2-⁶P_(hs)

Fe	-0.070750000	0.008655000	-0.429774000
N	1.638911000	-1.184250000	-0.151166000
N	-1.239233000	-1.683422000	-0.021062000
N	-1.752965000	1.188251000	-0.064257000
N	1.134403000	1.687756000	-0.165369000
C	2.947574000	-0.742443000	-0.187047000
C	3.835610000	-1.891709000	-0.159984000
H	4.915202000	-1.836755000	-0.176901000
C	3.047665000	-3.011222000	-0.108365000
H	3.360693000	-4.045511000	-0.076241000
C	1.665307000	-2.564128000	-0.104474000
C	0.543156000	-3.394388000	-0.057813000
C	-0.794503000	-2.995449000	-0.032791000
C	-1.942131000	-3.881271000	-0.008145000
H	-1.886461000	-4.960892000	-0.007465000
C	-3.064649000	-3.093935000	0.007793000
H	-4.098378000	-3.409863000	0.024298000
C	-2.623807000	-1.712605000	-0.004379000
C	-3.455541000	-0.591485000	0.015622000
C	-3.056007000	0.746220000	0.010134000
C	-3.941395000	1.895983000	0.110291000
H	-5.018579000	1.839634000	0.181856000
C	-3.152269000	3.014172000	0.106598000
H	-3.460206000	4.048266000	0.173452000
C	-1.772603000	2.565326000	0.000565000
C	-0.649195000	3.392790000	-0.021463000
C	0.687823000	2.994234000	-0.089309000
C	1.834864000	3.882492000	-0.075283000
H	1.777659000	4.960640000	-0.019860000
C	2.958516000	3.098923000	-0.136748000
H	3.991991000	3.416342000	-0.139981000
C	2.517362000	1.717732000	-0.187833000

C	3.348094000	0.594809000	-0.2111759000
H	4.417416000	0.782048000	-0.229139000
H	-0.832459000	4.461462000	0.035441000
H	0.730547000	-4.463665000	-0.044067000
H	-4.523873000	-0.780554000	0.054210000
O	-0.129621000	-0.027826000	-2.270447000
O	-0.039990000	-0.031728000	1.938994000
H	-0.492434000	-0.891415000	2.056636000
C	1.220642000	0.032314000	2.671758000
H	1.702070000	0.949962000	2.335628000
H	1.033152000	0.079185000	3.751239000
H	1.863680000	-0.820046000	2.427999000
H	0.321495000	0.526060000	-2.932579000

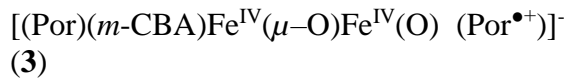
2-⁴P_(ls)

Fe	-0.054190000	0.016121000	-0.309739000
N	1.409361000	1.407935000	-0.130273000
N	1.341074000	-1.443550000	-0.173908000
N	-1.509292000	-1.387444000	-0.010251000
N	-1.445645000	1.469099000	-0.100202000
C	1.243614000	2.781387000	-0.086770000
C	2.536888000	3.432279000	-0.107436000
H	2.683077000	4.502725000	-0.077365000
C	3.480919000	2.446058000	-0.177323000
H	4.556466000	2.545471000	-0.215541000
C	2.773769000	1.182815000	-0.197123000
C	3.381993000	-0.061702000	-0.260504000
C	2.714344000	-1.277634000	-0.248878000
C	3.362986000	-2.569935000	-0.275996000
H	4.432309000	-2.716291000	-0.332498000
C	2.376405000	-3.515428000	-0.217814000
H	2.475280000	-4.591682000	-0.218671000
C	1.115068000	-2.810002000	-0.157249000
C	-0.126661000	-3.426058000	-0.087025000
C	-1.344149000	-2.764454000	-0.029543000
C	-2.636977000	-3.413120000	0.000518000
H	-2.784125000	-4.483868000	-0.001295000
C	-3.582139000	-2.424650000	0.017048000
H	-4.658252000	-2.524173000	0.033174000
C	-2.877283000	-1.161270000	0.000695000
C	-3.486587000	0.084537000	-0.009174000
C	-2.819201000	1.301087000	-0.037970000
C	-3.467554000	2.593185000	0.027324000
H	-4.537264000	2.738151000	0.080455000
C	-2.479703000	3.538664000	0.023301000
H	-2.577538000	4.613940000	0.071589000
C	-1.217855000	2.834187000	-0.048407000
C	0.027098000	3.446353000	-0.047747000
H	0.050669000	4.530340000	-0.011665000
H	-4.570738000	0.110966000	0.019643000
H	4.465121000	-0.087201000	-0.315253000
H	-0.146464000	-4.510660000	-0.091517000
O	-0.115522000	-0.020149000	-2.193448000
O	-0.053280000	-0.047085000	2.069609000
H	-0.583785000	-0.862254000	2.174815000
C	1.244549000	-0.155522000	2.732270000
H	1.119517000	-0.195596000	3.821058000
H	1.786669000	0.746707000	2.451156000
H	1.795863000	-1.031127000	2.373312000
H	-0.633080000	0.646332000	-2.688197000

2-²P_(ls)

Fe	-0.055436000	0.018677000	-0.178547000
N	1.221623000	1.571371000	-0.137383000
N	1.530086000	-1.230721000	-0.176268000
N	-1.328432000	-1.552403000	-0.029118000
N	-1.636544000	1.258640000	-0.030073000
C	0.866449000	2.910018000	-0.105697000
C	2.055063000	3.735377000	-0.148771000
H	2.048332000	4.816130000	-0.134360000
C	3.129161000	2.892402000	-0.213227000
H	4.179656000	3.142166000	-0.261765000

C	2.607576000	1.542782000	-0.208213000
C	3.381128000	0.391824000	-0.255161000
C	2.875875000	-0.900148000	-0.238492000
C	3.678887000	-2.102721000	-0.263877000
H	4.758589000	-2.116792000	-0.312446000
C	2.814676000	-3.161333000	-0.216704000
H	3.044097000	-4.217628000	-0.220994000
C	1.474634000	-2.616102000	-0.166188000
C	0.319611000	-3.383902000	-0.117451000
C	-0.976253000	-2.891809000	-0.074339000
C	-2.168210000	-3.714277000	-0.092073000
H	-2.165215000	-4.794755000	-0.122634000
C	-3.240196000	-2.866381000	-0.079681000
H	-4.292690000	-3.111799000	-0.095670000
C	-2.713734000	-1.518309000	-0.049538000
C	-3.484522000	-0.365971000	-0.041614000
C	-2.977341000	0.924456000	-0.030151000
C	-3.787917000	2.126857000	-0.010892000
H	-4.868680000	2.135768000	-0.006204000
C	-2.926989000	3.186008000	-0.003268000
H	-3.156889000	4.242081000	0.007208000
C	-1.583363000	2.638980000	-0.022987000
C	-0.428018000	3.404730000	-0.048393000
H	-0.546012000	4.483360000	-0.035316000
H	-4.563084000	-0.482343000	-0.052173000
H	4.458173000	0.510693000	-0.307205000
H	0.441133000	-4.462143000	-0.133359000
O	-0.179347000	0.016501000	-1.979095000
O	-0.033515000	-0.029970000	1.883181000
H	-0.738736000	-0.640648000	2.173064000
C	1.213865000	-0.188942000	2.635518000
H	1.031277000	0.035566000	3.691134000
H	1.899549000	0.536555000	2.202353000
H	1.615022000	-1.198578000	2.506042000
H	0.710281000	0.155046000	-2.371057000



¹⁰3_(hs, hs) Or 3-¹⁰R_(hs, hs)

Fe	-2.402265000	0.104296000	1.508908000
N	-1.359120000	1.748731000	2.244217000
N	-1.163243000	-1.146440000	2.617968000
N	-3.125961000	-1.557672000	0.486137000
N	-3.3111034000	1.338238000	0.101156000
C	-1.561900000	3.068320000	1.876857000
C	-0.710483000	3.917761000	2.695718000
H	-0.662764000	4.994467000	2.619725000
C	-0.005670000	3.096346000	3.530910000
H	0.726806000	3.370491000	4.277099000
C	-0.414287000	1.730940000	3.233158000
C	0.100317000	0.576569000	3.844143000
C	-0.235791000	-0.740272000	3.563039000
C	0.339024000	-1.919940000	4.191277000
H	1.095177000	-1.897527000	4.962614000
C	-0.244922000	-3.010948000	3.610291000
H	-0.064536000	-4.056068000	3.818899000
C	-1.185378000	-2.514537000	2.615921000
C	-1.972255000	-3.313492000	1.771697000
C	-2.856609000	-2.880610000	0.793547000
C	-3.630967000	-3.734198000	-0.094592000
H	-3.609332000	-4.814225000	-0.080485000
C	-4.343074000	-2.912666000	-0.923339000
H	-5.023667000	-3.189798000	-1.716051000
C	-4.012226000	-1.543078000	-0.555795000
C	-4.497629000	-0.390124000	-1.192590000
C	-4.175559000	0.927921000	-0.899325000
C	-4.664037000	2.102329000	-1.605465000
H	-5.351431000	2.075531000	-2.438559000
C	-4.079286000	3.193643000	-1.025240000
H	-4.201358000	4.235380000	-1.286663000
C	-3.222837000	2.702388000	0.044545000

C	-2.415935000	3.499633000	0.871412000
Fe	0.301701000	-0.073122000	-0.949255000
N	0.744150000	1.946235000	-0.666864000
N	-0.987128000	0.422329000	-2.488707000
N	-0.066509000	-2.088379000	-1.251217000
N	1.681399000	-0.560493000	0.534096000
C	1.584543000	2.470021000	0.297845000
C	1.565764000	3.918821000	0.196310000
H	2.131305000	4.587266000	0.829303000
C	0.706899000	4.240193000	-0.820963000
H	0.439020000	5.222894000	-1.182953000
C	0.185238000	2.989983000	-1.350271000
C	-0.760506000	2.870536000	-2.385490000
C	-1.298722000	1.702090000	-2.909892000
C	-2.276671000	1.610908000	-3.982742000
H	-2.701561000	2.458095000	-4.501447000
C	-2.533718000	0.281597000	-4.181713000
H	-3.206168000	-0.168255000	-4.898446000
C	-1.718992000	-0.458532000	-3.229364000
C	-1.691454000	-1.858773000	-3.086992000
C	-0.932836000	-2.605939000	-2.195957000
C	-0.908411000	-4.058407000	-2.100830000
H	-1.489954000	-4.724243000	-2.721825000
C	-0.026779000	-4.381890000	-1.107863000
H	0.260706000	-5.364907000	-0.763182000
C	0.497321000	-3.131241000	-0.579201000
C	1.443039000	-3.010887000	0.452134000
C	1.992451000	-1.840184000	0.961049000
C	2.973775000	-1.749452000	2.027184000
H	3.404253000	-2.597199000	2.539908000
C	3.223499000	-0.419804000	2.234691000
H	3.904909000	0.028516000	2.943467000
C	2.397187000	0.321313000	1.298208000
C	2.338283000	1.720229000	1.193136000
H	-1.112167000	3.800917000	-2.820677000
H	-2.333151000	-2.419185000	-3.759742000
H	2.965796000	2.277305000	1.881226000
H	1.797566000	-3.938738000	0.889102000
H	-2.453678000	4.569726000	0.693693000
H	-5.187294000	-0.548681000	-2.015615000
H	0.855337000	0.731830000	4.608259000
H	-1.864044000	-4.387276000	1.886628000
O	-0.933636000	0.033296000	0.164377000
O	-3.624127000	0.168877000	2.617086000
O	1.702730000	-0.182425000	-2.267196000
C	2.841142000	-0.870804000	-2.092719000
O	2.952790000	-2.100878000	-2.271128000
C	4.008186000	-0.043612000	-1.638198000
C	3.961432000	1.357782000	-1.666655000
C	5.141126000	-0.700984000	-1.130653000
C	5.043414000	2.103871000	-1.188904000
H	3.068582000	1.837359000	-2.045946000
C	6.190106000	0.065701000	-0.645755000
H	5.163128000	-1.783138000	-1.119537000
C	6.172299000	1.459414000	-0.664045000
H	5.009637000	3.188377000	-1.213568000
H	7.014057000	2.023883000	-0.281127000
Cl	7.670639000	-0.789395000	0.063012000

⁸3_(hs, hs) or 3-⁸R_(hs, hs)

Fe	-2.410587629	0.114056289	1.500364877
N	-1.398249374	1.787964562	2.212063270
N	-1.164737366	-1.097882186	2.646777120
N	-3.102498180	-1.576945667	0.504463186
N	-3.323445853	1.306648115	0.059641023
C	-1.611885738	3.095611843	1.812834406
C	-0.768437619	3.972450527	2.612536341
H	-0.730939781	5.047509929	2.511099593
C	-0.055567180	3.177432240	3.465683988
H	0.674288927	3.475396327	4.205287347
C	-0.451982577	1.800962473	3.200128054
C	0.075526788	0.666704838	3.836914285
C	-0.242683667	-0.659950531	3.581522295
C	0.356284601	-1.819796431	4.226344919

H	1.113811104	-1.771158803	4.995177585
C	-0.206867593	-2.930000526	3.662181825
H	-0.005832216	-3.968434945	3.884872047
C	-1.159214936	-2.466019702	2.662064210
C	-1.929207362	-3.291906476	1.828487966
C	-2.814493155	-2.889057987	0.838364667
C	-3.571391948	-3.771442428	-0.038033653
H	-3.533294504	-4.850566175	-0.002733163
C	-4.291613064	-2.977023581	-0.885349183
H	-4.964588838	-3.279155686	-1.675441376
C	-3.983450588	-1.595076862	-0.542080882
C	-4.484964382	-0.462199824	-1.201828918
C	-4.179897624	0.865085245	-0.933793915
C	-4.682749935	2.019386013	-1.664232761
H	-5.368393810	1.966701110	-2.497586766
C	-4.113913957	3.129427745	-1.104962552
H	-4.250117328	4.164266855	-1.386136676
C	-3.253942549	2.670877884	-0.022617615
C	-2.464632051	3.496019814	0.793447028
Fe	0.305279729	-0.082820874	-0.938049755
N	0.678134787	1.960242364	-0.749128402
N	-1.016056556	0.298853375	-2.481246810
N	0.004692982	-2.119313950	-1.142810398
N	1.714318081	-0.455813231	0.556096924
C	1.501520796	2.554897498	0.189258688
C	1.429048770	3.996883477	0.025785338
H	1.972220625	4.712008277	0.626624499
C	0.557779846	4.242386440	-1.001898398
H	0.252915119	5.197984009	-1.404787073
C	0.080260264	2.951955312	-1.474009691
C	-0.867980353	2.754766925	-2.496192939
C	-1.368822039	1.546841123	-2.962001948
C	-2.339751597	1.372486924	-4.031745891
H	-2.790646439	2.179750908	-4.590647698
C	-2.547218448	0.027321314	-4.172068923
H	-3.199332790	-0.478363448	-4.870109934
C	-1.709892111	-0.639158549	-3.185022779
C	-1.629181394	-2.031081857	-2.983363045
C	-0.841464752	-2.708947176	-2.064524362
C	-0.756990716	-4.154557331	-1.911826694
H	-1.311339371	-4.867589648	-2.504656844
C	0.141830658	-4.401775956	-0.912658751
H	0.472106511	-5.357509269	-0.531594277
C	0.615657020	-3.110423900	-0.436578861
C	1.561425867	-2.913037289	0.584705389
C	2.069415520	-1.703527855	1.040256663
C	3.044403784	-1.530229984	2.102680036
H	3.504682652	-2.338213152	2.652462542
C	3.245194482	-0.184454164	2.250506373
H	3.907591537	0.319402533	2.939755628
C	2.394401743	0.483545124	1.280668845
C	2.282888184	1.874293660	1.114634292
H	-1.253222618	3.652074302	-2.970223976
H	-2.248579892	-2.643497893	-3.630935427
H	2.885928909	2.484405087	1.779101965
H	1.948338168	-3.808559095	1.059755585
H	-2.513270807	4.561401215	0.592155962
H	-5.169358557	-0.646331218	-2.023726166
H	0.830146381	0.847473665	4.595700468
H	-1.802557329	-4.361695849	1.959822314
O	-0.911920554	0.034318932	0.194750154
O	-3.645088781	0.183728646	2.594058599
O	1.696103075	-0.206495862	-2.261752638
C	2.837920859	-0.889565149	-2.075503673
O	2.950974646	-2.121140596	-2.240320033
C	4.002712656	-0.053533381	-1.634586797
C	3.949562066	1.347269919	-1.678074826
C	5.141392439	-0.700790225	-1.127146270
C	5.031849918	2.102773769	-1.216212173
H	3.052104451	1.818703770	-2.056719632
C	6.190535332	0.075367368	-0.657873537
H	5.168482817	-1.782646511	-1.104668726
C	6.166846236	1.468647442	-0.691991933
H	4.993958683	3.186781897	-1.253222681
H	7.008926204	2.040735865	-0.321336823

Cl	7.678750458	-0.765975532	0.050040635
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$2^3_{(hs, hs)}$ or $3^{-2}R_{(hs, hs)}$

Fe	-2.358730672	0.105317279	1.519177599
N	-2.888529460	1.873052120	0.556476339
N	-0.978178800	1.161795188	2.667333741
N	-1.551794206	-1.679899011	2.226483154
N	-3.469581050	-0.968570428	0.122076390
C	-3.773910352	1.992900417	-0.488587651
C	-3.905907663	3.396307649	-0.838540407
H	-4.538129603	3.777539386	-1.627956804
C	-3.087845659	4.100368385	0.006313655
H	-2.923123851	5.168118055	0.040831202
C	-2.446092962	3.134732372	0.881234613
C	-1.499090263	3.430639087	1.864396813
C	-0.817370047	2.527175489	2.684364003
C	0.203305422	2.871521629	3.658717905
H	0.532085724	3.877739193	3.877095989
C	0.644486104	1.697387854	4.211319492
H	1.402961390	1.558920652	4.968927547
C	-0.101546183	0.622475712	3.580208412
C	0.071950358	-0.741918425	3.823275090
C	-0.587301390	-1.804234180	3.198291221
C	-0.335486846	-3.214691742	3.438009526
H	0.378849963	-3.600573713	4.151375124
C	-1.155742993	-3.918534742	2.595447001
H	-1.241600086	-4.990611738	2.487771062
C	-1.917985534	-2.945960649	1.831551596
C	-2.841259348	-3.243258185	0.826716222
C	-3.552771974	-2.337871145	0.034145454
C	-4.457041497	-2.689009762	-1.047250169
H	-4.705638899	-3.699656417	-1.338783774
C	-4.898331825	-1.514899778	-1.599584060
H	-5.579359528	-1.381083541	-2.428239167
C	-4.268929040	-0.433419649	-0.861406378
C	-4.410314040	0.929005369	-1.134169257
Fe	0.288021117	-0.074090819	-0.959004047
N	-0.992922906	0.521685515	-2.469166926
N	-0.138054850	-2.066093700	-1.346629916
N	1.677062029	-0.661146435	0.477014999
N	0.798839588	1.920934491	-0.607583029
C	-1.279229034	1.813877303	-2.829563832
C	-2.288598054	1.799040290	-3.873951866
H	-2.698509245	2.679727887	-4.347775841
C	-2.594292421	0.485404106	-4.119353376
H	-3.300984126	0.086432040	-4.833241446
C	-1.774922989	-0.317398737	-3.227940959
C	-1.786662527	-1.711258378	-3.138681156
C	-1.032528479	-2.519800716	-2.279305739
C	-1.078884289	-3.972243265	-2.222078421
H	-1.697207092	-4.594290978	-2.853499742
C	-0.200222920	-4.363779495	-1.247731451
H	0.042435755	-5.368063498	-0.930867105
C	0.393395217	-3.155843311	-0.699472647
C	1.345281097	-3.098570415	0.315911449
C	1.938571217	-1.952692196	0.862853350
C	2.905947838	-1.936959677	1.942852605
H	3.302560947	-2.817707304	2.427186522
C	3.199051183	-0.623034825	2.203241351
H	3.885181066	-0.224906269	2.936987327
C	2.416201977	0.179458811	1.283097272
C	2.401697975	1.571797916	1.225874430
C	1.655905051	2.380867870	0.359238689
C	1.672194371	3.831146618	0.328016575
H	2.265688934	4.455543889	0.980734350
C	0.806619652	4.221624785	-0.662157804
H	0.558225878	5.226506980	-0.973630469
C	0.253001932	3.012444203	-1.245654235
C	-0.699111600	2.957155717	-2.266154176
H	-2.465465527	-2.228642293	-3.808553528
H	1.664956623	-4.047363843	0.732988819
H	-1.041899313	3.909970088	-2.656066663
H	3.039861252	2.088060552	1.934629540
H	-5.067039887	1.189814837	-1.957516668

H	-3.004046335	-4.295563092	0.618370656
H	-1.245236492	4.478253753	1.988250451
H	0.820061929	-1.008318328	4.562653047
O	-0.922108930	0.008683825	0.177271286
O	-3.561446602	0.181038935	2.639744339
O	1.670898691	-0.166739972	-2.299496973
C	2.811532170	-0.856638957	-2.144294186
O	2.923175335	-2.083386519	-2.342600486
C	3.980107759	-0.035834124	-1.682047392
C	3.939156965	1.365729537	-1.704264322
C	5.106508593	-0.700075460	-1.168896583
C	5.019734532	2.105394022	-1.213418990
H	3.050316726	1.850532390	-2.086236652
C	6.153856363	0.060227647	-0.670355579
H	5.124313916	-1.782373027	-1.162422665
C	6.141399743	1.454059513	-0.681534115
H	4.989882066	3.190137415	-1.232369732
H	6.981546732	2.013410581	-0.287649884
Cl	7.624386809	-0.804082523	0.048177985

${}^6_3\text{R}_{(\text{is, is})}$ or $3\text{-}^6\text{R}_{(\text{is, is})}$

Fe	-2.321302076	0.064357338	1.488911121
N	-3.607426273	-0.032823175	-0.067010808
N	-2.248961662	2.075646244	1.289330625
N	-0.836283816	0.154178998	2.856619591
N	-2.192743321	-1.952843154	1.498423532
C	-4.143634700	-1.164395189	-0.624988685
C	-5.068213417	-0.812586364	-1.685876619
H	-5.622661679	-1.528537459	-2.275638630
C	-5.072789477	0.548889467	-1.771523454
H	-5.627418877	1.181789695	-2.448759740
C	-4.156267214	1.037880307	-0.760295603
C	-3.867122125	2.367317705	-0.538391236
C	-2.974636346	2.847882890	0.419228325
C	-2.668300378	4.251805330	0.617891460
H	-3.114025401	5.060018356	0.055834481
C	-1.738647232	4.317026415	1.614257384
H	-1.259322878	5.188593314	2.035535683
C	-1.472099758	2.954438333	2.031590740
C	-0.562920697	2.593627235	3.003113311
C	-0.265793057	1.284715930	3.382143389
C	0.728426522	0.930420448	4.377061918
H	1.314235241	1.645135045	4.937244048
C	0.762258639	-0.431985325	4.435314146
H	1.384210963	-1.067302414	5.048650920
C	-0.214751116	-0.918854485	3.481305649
C	-0.470795496	-2.249466820	3.227917950
C	-1.396466369	-2.728146420	2.301195431
C	-1.636066757	-4.134810140	2.039596446
H	-1.131784218	-4.945064600	2.546382263
C	-2.582782853	-4.199640127	1.059950809
H	-3.012025402	-5.073064120	0.591352697
C	-2.928305269	-2.833940403	0.716768044
C	-3.832734684	-2.474069065	-0.258884139
Fe	0.311035213	-0.042870004	-0.990786861
N	-0.930201463	0.681202845	-2.397980664
N	-0.208832230	-1.924045503	-1.478485027
N	1.610473803	-0.762189899	0.380424695
N	0.873601861	1.843799149	-0.517536124
C	-1.149658148	1.996791251	-2.711695215
C	-2.151091706	2.101756913	-3.754964129
H	-2.494718244	3.033633085	-4.180700677
C	-2.541538635	0.829907076	-4.058476169
H	-3.273273595	0.501975463	-4.782100143
C	-1.776098980	-0.059956924	-3.208937781
C	-1.874281315	-1.435284473	-3.217358906
C	-1.128077575	-2.301383622	-2.418715315
C	-1.222725096	-3.748299268	-2.475182623
H	-1.873622420	-4.291940651	-3.144714830
C	-0.345793257	-4.237817016	-1.553477270
H	-0.128260752	-5.266296733	-1.306089118
C	0.289365193	-3.095362029	-0.927749076
C	1.239955266	-3.171700086	0.064225616
C	1.857658725	-2.078514919	0.672380757

C	2.843805955	-2.181407746	1.727546115
H	3.221199945	-3.113714430	2.121867003
C	3.174106271	-0.907406243	2.088275816
H	3.878084423	-0.579016702	2.838337686
C	2.398845577	-0.017226485	1.250764261
C	2.453012118	1.356887573	1.303164758
C	1.744898514	2.223062812	0.469431531
C	1.858182044	3.666352869	0.510521300
H	2.489728044	4.210021865	1.198421360
C	1.032067078	4.156808007	-0.459964610
H	0.840465125	5.185747843	-0.727525498
C	0.409235922	3.015676280	-1.098880807
C	-0.523296980	3.089395153	-2.112188896
H	-2.578531644	-1.882274352	-3.910174388
H	1.541012040	-4.159024937	0.395342662
H	-0.802139013	4.076380997	-2.464944372
H	3.117677709	1.803420348	2.033625702
H	-4.331910023	-3.272144574	-0.797547072
H	0.097885617	-2.983983045	3.787541545
H	-4.366152691	3.099016691	-1.164377721
H	-0.021078294	3.389906864	3.501789333
O	-0.901300374	0.025019904	0.149750051
O	-3.526251309	0.106393540	2.626822852
O	1.689099107	-0.109710611	-2.338759628
C	2.820182546	-0.805852118	-2.186348865
O	2.935526877	-2.029769000	-2.410184105
C	3.984346141	-0.003231719	-1.676399874
C	3.959834709	1.398860282	-1.682609357
C	5.083032719	-0.685502754	-1.128509775
C	5.027587077	2.120990823	-1.140160342
H	3.091774482	1.898152521	-2.093147252
C	6.116059561	0.057295959	-0.576593166
H	5.089002526	-1.767872496	-1.135716624
C	6.119228274	1.451112371	-0.569976947
H	5.009395059	3.206124886	-1.146513877
H	6.947990174	1.996209415	-0.134191593
Cl	7.544942222	-0.832522344	0.195792555

${}^4_3\text{R}_{(\text{is, is})}$ or $3\text{-}^4\text{R}_{(\text{is, is})}$

Fe	-2.306136507	0.065095684	1.471676231
N	-3.601195052	-0.034299965	-0.077622991
N	-2.242375935	2.077998077	1.278315901
N	-0.832688929	0.157541115	2.853033753
N	-2.188679827	-1.953567555	1.494501884
C	-4.137665988	-1.165830498	-0.632717736
C	-5.063833925	-0.815178454	-1.693545313
H	-5.619186466	-1.531727789	-2.281738700
C	-5.068771651	0.546037148	-1.780542275
H	-5.624753887	1.178076739	-2.457495657
C	-4.150648114	1.036452804	-0.770464945
C	-3.861840174	2.365685934	-0.548847185
C	-2.969202357	2.848161698	0.409148132
C	-2.665916541	4.253319163	0.608706525
H	-3.113326871	5.060936092	0.047111128
C	-1.737030569	4.320084234	1.605434644
H	-1.260326595	5.192597667	2.027750808
C	-1.467754011	2.957291906	2.022639268
C	-0.561385051	2.597257100	2.996565060
C	-0.265188799	1.287995707	3.378926897
C	0.724179102	0.934924016	4.380175216
H	1.307309766	1.650268186	4.942364537
C	0.756831064	-0.427196215	4.441244975
H	1.374854918	-1.061608901	5.059501747
C	-0.216063722	-0.915582725	3.482766099
C	-0.472738496	-2.245937599	3.230667619
C	-1.396236182	-2.726591321	2.301231737
C	-1.636759413	-4.134404081	2.042729392
H	-1.135068202	-4.943902236	2.553299293
C	-2.580835676	-4.200866633	1.060900354
H	-3.010246160	-5.075152799	0.594038203
C	-2.924166331	-2.835077489	0.713005959
C	-3.826914391	-2.475877539	-0.263978790
Fe	0.303495785	-0.043648419	-0.979264958
N	-0.928647169	0.701546482	-2.382909500

N	-0.227341873	-1.916906526	-1.484795794	C	-1.457703702	2.953264793	2.032029322
N	1.596365864	-0.783836318	0.387639791	C	-0.552778724	2.588244931	3.005852872
N	0.879172335	1.834685839	-0.488004792	C	-0.261042663	1.277480865	3.386453046
C	-1.138684710	2.021330221	-2.684764072	C	0.726437059	0.919506902	4.387452557
C	-2.135201365	2.142173852	-3.731118095	H	1.311451361	1.631820792	4.951529802
H	-2.471272750	3.080139975	-4.149443082	C	0.755134400	-0.443065284	4.445451521
C	-2.532049360	0.875733112	-4.048303371	H	1.370929974	-1.080560453	5.062790721
H	-3.262522639	0.559128988	-4.778232275	C	-0.218513472	-0.926227103	3.485399306
C	-1.775559071	-0.027074465	-3.204159781	C	-0.478145006	-2.255734401	3.229101402
C	-1.881916332	-1.401443720	-3.226655365	C	-1.401675527	-2.732022691	2.297664326
C	-1.145027725	-2.279421650	-2.432372994	C	-1.644931624	-4.138312034	2.034926367
C	-1.250782280	-3.725166343	-2.500330296	H	-1.145652498	-4.950470707	2.543638463
H	-1.902529383	-4.258375235	-3.177397399	C	-2.588149070	-4.199832551	1.051649965
C	-0.383062525	-4.228595658	-1.577489868	H	-3.018974970	-5.071870582	0.581875217
H	-0.175127666	-5.260602775	-1.336599864	C	-2.928023874	-2.832443318	0.707477030
C	0.258466244	-3.096008387	-0.940019379	C	-3.829160330	-2.468225694	-0.269747526
C	1.204308261	-3.187903022	0.054973221	Fe	0.301384461	-0.043780847	-0.980867222
C	1.830442128	-2.104411308	0.671334377	N	0.882493843	1.832099268	-0.483093802
C	2.813852988	-2.223378800	1.727524895	N	-0.929985374	0.710616972	-2.379533878
H	3.181537994	-3.161846996	2.116376932	N	-0.233610053	-1.912901871	-1.493390130
C	3.155771559	-3.159547325	2.096896706	N	1.594547325	-0.791201877	-0.382388083
H	3.861270202	-0.638096818	2.850468143	C	1.759319208	2.190540245	0.506224572
C	2.390159080	-0.051856879	1.264134205	C	1.888345592	3.632466819	0.563371048
C	2.456438276	1.321123536	1.327205127	H	2.527695443	4.160950316	1.255874087
C	1.754680033	2.199094633	0.500747014	C	1.065890204	4.142757213	-0.399366652
C	1.879498288	3.641193481	0.552892597	H	0.884941399	5.176614800	-0.655103500
H	2.516842811	4.174137408	1.243827314	C	0.429483637	3.015546007	-1.050629785
C	1.055979259	4.145776122	-0.412309219	C	-0.500789561	3.111310050	-2.063142505
H	0.872294968	5.178238279	-0.671724847	C	-1.135754762	2.031520386	-2.677417562
C	0.423346399	3.014691249	-1.059800676	C	-2.131409466	2.158753552	-3.724186926
C	-0.507053678	3.104314771	-2.073468272	H	-2.464251293	3.099133888	-4.139651154
H	-2.586073695	-1.837406916	-3.926472110	C	-2.531884622	0.894716165	-4.045616034
H	1.494573455	-4.180087816	0.380960496	H	-3.262607752	0.582592734	-4.777221272
H	-0.778633288	4.096332488	-2.417463589	C	-1.778387121	-0.013285180	-3.204023174
H	3.124154653	1.756501879	2.061513094	C	-1.887961515	-1.386848144	-3.232147744
H	-4.326186119	-3.274421460	-0.801834488	C	-1.152483833	-2.269658499	-2.441335589
H	0.093133818	-2.980010649	3.793686404	C	-1.261518244	-3.715154532	-2.514666951
H	-4.361523078	3.096967061	-1.174780928	H	-1.914992397	-4.244275868	-3.193274065
H	-0.021284586	3.393974184	3.496391064	C	-0.394252275	-4.223948910	-1.594516866
O	-0.908502677	0.020151031	0.156802798	H	-0.188293560	-5.257311986	-1.357770457
O	-3.511298680	0.110287093	2.605938692	C	0.250457120	-3.095127011	-0.953087893
O	1.682570409	-0.104947263	-2.323661540	C	1.196345377	-3.193014901	0.040849297
C	2.813269597	-0.803271966	-2.175853777	C	1.824696999	-2.113091609	0.661641237
O	2.924979750	-2.027654127	-2.398275325	C	2.806947532	-2.238355997	1.718696181
C	3.981709965	-0.001673008	-1.674398389	H	3.171645618	-3.179189436	2.104633065
C	3.956241759	1.400465483	-1.674227237	C	3.151864877	-0.972450874	2.092741579
C	5.086998855	-0.685582496	-1.141846079	H	3.857509922	-0.659906583	2.848016862
C	5.029644439	2.120909663	-1.140686191	C	2.389367277	-0.064033461	1.262155664
H	3.083639223	1.901052910	-2.073337099	C	2.459299522	1.308179511	1.329839964
C	6.126166582	0.055500241	-0.599300627	H	-0.769910537	-4.105057086	-2.403955202
H	5.093341065	-1.767919513	-1.153871447	H	-2.593389465	-1.818504556	-3.933308387
C	6.128432942	1.449308184	-0.586543651	H	3.127733685	1.739591316	2.065797446
H	5.010529372	3.206033296	-1.141825991	H	1.484135894	-4.187048587	0.363312325
H	6.961974265	1.993054370	-0.158274623	H	-4.330023749	-3.264268205	-0.809865139
Cl	7.565425721	-0.836546478	0.150960384	H	0.085551748	-2.992570719	3.790747449
				H	-4.348981487	3.108139585	-1.166752510
				H	-0.010791618	3.382414646	3.507740344
				O	-0.904954570	0.017824056	0.161013989
				O	-3.509984225	0.110414010	2.605163108
				O	1.679429425	-0.102028677	-2.327256214
				C	2.809963922	-0.800871158	-2.180501118
				O	2.921426283	-2.024923726	-2.404985108
				C	3.978533288	-0.000427057	-1.677538209
				C	3.953983035	1.401722999	-1.676387217
				C	5.082775147	-0.685438480	-1.144245607
				C	5.027226443	2.121089695	-1.141083111
				H	3.082127951	1.903162041	-2.076062151
				C	6.121719747	0.054581712	-0.599805875
				H	5.088498702	-1.767769163	-1.157086886
				C	6.124862424	1.448374890	-0.586007303
				H	5.008802031	3.206220852	-1.141447471
				H	6.958196574	1.991273789	-0.156263643
				Cl	7.559355846	-0.838967892	0.151757511

${}^2\mathbf{3}_{(is, is)}$ Or ${}^3\mathbf{-2}\mathbf{R}_{(is, is)}$

Fe	-2.302319726	0.064402035	1.472981589
N	-3.596745291	-0.027838857	-0.077752447
N	-2.233921487	2.077888717	1.285156015
N	-0.831621219	0.149606434	2.857907899
N	-2.191727840	-1.954931737	1.492044189
C	-4.136507402	-1.156767824	-0.635520212
C	-5.061387279	-0.801037393	-1.695488028
H	-5.618721267	-1.514550119	-2.285502018
C	-5.062367496	0.560521656	-1.779368665
H	-5.616487451	1.195660934	-2.454946028
C	-4.143173400	1.045891998	-0.768079991
C	-3.851171786	2.374072398	-0.542566301
C	-2.958478908	2.852120838	0.417462628
C	-2.652090245	4.255841116	0.620969139
H	-3.097174382	5.066075181	0.061298161
C	-1.723301484	4.317684685	1.618305785
H	-1.244701499	5.187955735	2.043109140

${}^3\mathbf{-10}\mathbf{ts1}_{(hs, hs)}$

Fe	-2.348568000	-0.126335000	1.184895000
N	-1.349434000	1.230830000	2.461909000
N	-1.354245000	-1.667820000	2.064219000
N	-3.103750000	-1.459132000	-0.270854000
N	-3.203932000	1.437227000	0.193781000
C	-1.492534000	2.603216000	2.442821000
C	-0.671830000	3.175214000	3.502374000
H	-0.588083000	4.231064000	3.716605000
C	-0.050632000	2.133070000	4.135013000
H	0.634159000	2.172415000	4.970682000
C	-0.483163000	0.912454000	3.465081000
C	-0.082567000	-0.396875000	3.774634000
C	-0.473967000	-1.567811000	3.135580000
C	0.005875000	-2.897184000	3.468462000
H	0.708078000	-3.112489000	4.260796000
C	-0.572211000	-3.770562000	2.589153000
H	-0.439051000	-4.841285000	2.525127000
C	-1.413811000	-2.991003000	1.698457000
C	-2.139662000	-3.524378000	0.618765000
C	-2.918213000	-2.826731000	-0.293852000
C	-3.669855000	-3.385084000	-1.410190000
H	-3.700930000	-4.433047000	-1.671584000
C	-4.293537000	-2.339442000	-2.033858000
H	-4.939409000	-2.368862000	-2.900324000
C	-3.926680000	-1.129671000	-1.306037000
C	-4.342625000	0.177600000	-1.607161000
C	-4.011826000	1.344145000	-0.928671000
C	-4.430030000	2.683967000	-1.313601000
H	-5.064351000	2.907456000	-2.159158000
C	-3.858196000	3.555249000	-0.430521000
H	-3.937798000	4.632969000	-0.406628000
C	-3.077479000	2.763343000	0.510265000
C	-2.291357000	3.298990000	1.545194000
Fe	0.466221000	0.206644000	-1.007592000
N	0.960534000	2.068487000	-0.182903000
N	-0.701465000	1.137815000	-2.424766000
N	0.028463000	-1.651546000	-1.827942000
N	1.697342000	-0.711420000	0.390344000
C	1.745459000	2.284423000	0.933882000
C	1.781554000	3.710378000	1.210557000
H	2.321748000	4.165827000	2.027962000
C	1.006169000	4.323931000	0.262761000
H	0.794885000	5.378525000	0.154205000
C	0.482566000	3.277686000	-0.602652000
C	-0.396312000	3.469148000	-1.684946000
C	-0.938657000	2.498066000	-2.517404000
C	-1.851036000	2.733131000	-3.625923000
H	-2.210845000	3.705555000	-3.929866000
C	-2.144026000	1.513932000	-4.172993000
H	-2.786817000	1.296562000	-5.014336000
C	-1.418536000	0.513399000	-3.403656000
C	-1.455597000	-0.875632000	-3.629073000
C	-0.787657000	-1.866200000	-2.921891000
C	-0.819696000	-3.294504000	-3.203550000
H	-1.381499000	-3.750153000	-4.005953000
C	-0.018597000	-3.904764000	-2.279403000
H	0.209847000	-4.956661000	-2.183588000
C	0.509859000	-2.858111000	-1.416623000
C	1.380075000	-3.049024000	-0.331378000
C	1.927077000	-2.073368000	0.493874000
C	2.826032000	-2.309252000	1.609032000
H	3.183440000	-3.282051000	1.913845000
C	3.109939000	-1.091233000	2.165142000
H	3.752048000	-0.875113000	3.006989000
C	2.387650000	-0.091839000	1.398349000
C	2.397974000	1.289598000	1.651554000
H	-0.689605000	4.494650000	-1.887591000
H	-2.072443000	-1.207644000	-4.458233000
H	2.992106000	1.614848000	2.499300000
H	1.671653000	-4.073232000	-0.122688000
H	-2.303959000	4.380307000	1.641121000
H	-4.986490000	0.293022000	-2.473573000
H	0.623362000	-0.509854000	4.591499000
H	-2.067331000	-4.598603000	0.480809000
O	-0.854316000	0.109852000	0.030852000

O	-3.797435000	-0.259138000	2.229431000
O	1.938863000	0.353070000	-2.218574000
C	3.043163000	-0.409803000	-2.144068000
O	3.131301000	-1.561018000	-2.615487000
C	4.195876000	0.228383000	-1.427172000
C	4.193094000	1.596237000	-1.117563000
C	5.268071000	-0.584290000	-1.022787000
C	5.259395000	2.154420000	-0.405472000
H	3.344185000	2.193730000	-1.423059000
C	6.300473000	-0.006464000	-0.299503000
H	5.257283000	-1.637276000	-1.273402000
C	6.326475000	1.350495000	0.018814000
H	5.259861000	3.213441000	-0.168194000
H	7.154397000	1.766372000	0.580446000
Cl	7.696867000	-1.075818000	0.276871000
H	-3.750044000	-1.058149000	2.995052000
C	-3.749928000	-2.108926000	4.011127000
H	-4.687499000	-1.897380000	4.524723000
H	-2.838441000	-1.894762000	4.566252000
H	-3.729431000	-3.012465000	3.404145000

3-⁸ts1_(hs, hs)

Fe	-2.333181000	-0.108662000	1.198883000
N	-1.343372000	1.300268000	2.424955000
N	-1.318004000	-1.610291000	2.122452000
N	-3.083984000	-1.496811000	-0.206838000
N	-3.221560000	1.412654000	0.168208000
C	-1.505514000	2.669512000	2.363931000
C	-0.691963000	3.284691000	3.405156000
H	-0.622688000	4.347660000	3.586921000
C	-0.058782000	2.270684000	4.070551000
H	0.625136000	2.344411000	4.904574000
C	-0.474908000	1.024473000	3.437596000
C	-0.055012000	-0.269905000	3.785967000
C	-0.431313000	-1.464487000	3.184121000
C	0.076611000	-2.775536000	3.548122000
H	0.789157000	-2.955935000	4.339915000
C	-0.487996000	-3.682093000	2.694572000
H	-0.333869000	-4.751242000	2.656955000
C	-1.351758000	-2.942807000	1.790206000
C	-2.077444000	-3.519185000	0.732716000
C	-2.876073000	-2.860926000	-0.191930000
C	-3.626770000	-3.463633000	-1.286063000
H	-3.642820000	-4.519136000	-1.516700000
C	-4.272913000	-2.446759000	-1.933929000
H	-4.924294000	-2.511525000	-2.794311000
C	-3.919694000	-1.210531000	-1.244468000
C	-4.354130000	0.081525000	-1.584321000
C	-4.032960000	1.273331000	-0.946640000
C	-4.463122000	2.595883000	-1.376948000
H	-5.102879000	2.784406000	-2.226930000
C	-3.892540000	3.502182000	-0.528976000
H	-3.979479000	4.579492000	-0.543212000
C	-3.101706000	2.749545000	0.435470000
C	-2.315427000	3.327042000	1.448251000
Fe	0.458194000	0.187588000	-1.021074000
N	0.903074000	2.098640000	-0.280562000
N	-0.739808000	1.024392000	-2.471143000
N	0.061794000	-1.716871000	-1.751304000
N	1.706310000	-0.634624000	0.417057000
C	1.678946000	2.383123000	0.826929000
C	1.677990000	3.821061000	1.040426000
H	2.204292000	4.325739000	1.837789000
C	0.890751000	4.372038000	0.064594000
H	0.652881000	5.414996000	-0.091187000
C	0.395968000	3.274833000	-0.754270000
C	-0.488341000	3.395150000	-1.842884000
C	-1.008360000	2.373197000	-2.626311000
C	-1.928345000	2.534600000	-3.742475000
H	-2.310495000	3.483282000	-4.091008000
C	-2.191783000	1.284978000	-4.232440000
H	-2.829798000	1.013376000	-5.061584000
C	-1.441163000	0.338703000	-3.418891000
C	-1.445358000	-1.060461000	-3.581049000

C	-0.751902000	-2.000065000	-2.832331000
C	-0.746853000	-3.440366000	-3.051016000
H	-1.297784000	-3.945189000	-3.831276000
C	0.074872000	-3.987743000	-2.106294000
H	0.333250000	-5.027738000	-1.966565000
C	0.578206000	-2.889920000	-1.292358000
C	1.459213000	-3.009935000	-0.204176000
C	1.978648000	-1.984560000	0.575451000
C	2.889427000	-2.145509000	1.694822000
H	3.278553000	-3.093294000	2.037341000
C	3.138037000	-0.897411000	2.197608000
H	3.776363000	-0.626724000	3.026475000
C	2.382572000	0.047123000	1.393122000
C	2.355607000	1.438257000	1.587647000
H	-0.807103000	4.402505000	-2.092276000
H	-2.055514000	-1.444400000	-4.392464000
H	2.939826000	1.814646000	2.420930000
H	1.780951000	-4.015395000	0.046616000
H	-2.338131000	4.410745000	1.508202000
H	-5.003511000	0.161394000	-2.450567000
H	0.655725000	-0.347761000	4.602703000
H	-1.985452000	-4.595069000	0.622862000
O	-0.862981000	0.109022000	0.023840000
O	-3.774555000	-0.220488000	2.257881000
O	1.924687000	0.311999000	-2.236844000
C	3.032191000	-0.446887000	-2.143821000
O	3.123944000	-1.604936000	-2.596497000
C	4.181502000	0.207767000	-1.437669000
C	4.172961000	1.580768000	-1.151993000
C	5.257488000	-0.593174000	-1.020213000
C	5.237716000	2.155851000	-0.451210000
H	3.321067000	2.169028000	-1.466713000
C	6.288135000	0.001634000	-0.308300000
H	5.251368000	-1.650401000	-1.252403000
C	6.308679000	1.364092000	-0.014147000
H	5.233999000	3.218887000	-0.232734000
H	7.135383000	1.793325000	0.539154000
Cl	7.689052000	-1.051638000	0.285653000
H	-3.719060000	-1.008434000	3.035412000
C	-3.7111705000	-2.048455000	4.057790000
H	-4.650248000	-1.838499000	4.570394000
H	-2.801581000	-1.828938000	4.613072000
H	-3.687485000	-2.954924000	3.455164000

3-²ts1_(hs, hs)

Fe	2.592410180	-0.135656057	0.933414950
N	2.717676944	-1.953825334	0.021530629
N	1.497219426	-1.016367988	2.518923859
N	2.294658065	1.706315746	1.750859744
N	3.425917614	0.774206091	-0.792503759
C	3.270265667	-2.207349264	-1.217544122
C	3.140202445	-3.620658652	-1.511744315
H	3.488536714	-4.093184513	-2.419251827
C	2.488284846	-4.196454686	-0.451556911
H	2.204759354	-5.231509626	-0.323272262
C	2.214269214	-3.143630275	0.505547157
C	1.517610901	-3.322507257	1.707344604
C	1.178114088	-2.344889363	2.644224089
C	0.421797058	-2.539214314	3.872634114
H	0.040388008	-3.488020110	4.223201225
C	0.298451185	-1.308026658	4.463144509
H	-0.204300384	-1.059151116	5.387209554
C	0.976236100	-0.353554106	3.598294949
C	1.062078922	1.028810416	3.789953799
C	1.656818496	1.970650746	2.943855963
C	1.647797654	3.406062984	3.167476061
H	1.210854480	3.890227760	4.029373812
C	2.273267133	3.985187596	2.096090340
H	2.446553446	5.035646706	1.909893128
C	2.673484093	2.911996291	1.202810780
C	3.299441913	3.097023995	-0.034678693
C	3.652847313	2.114608665	-0.963623648
C	4.291660574	2.330067368	-2.253328830
H	4.581950173	3.293504491	-2.648453220

C	4.440488420	1.097646718	-2.835479790
H	4.876379113	0.862409011	-3.796432035
C	3.892564538	0.122065980	-1.904893583
C	3.818915861	-1.259875736	-2.090309174
Fe	-0.575559508	0.240357763	-0.711428709
N	0.195153354	-0.478787111	-2.496949578
N	-0.094748825	2.174233405	-1.264250899
N	-1.459822867	0.944627502	1.024566652
N	-1.155301765	-1.709326516	-0.188241746
C	0.260385243	-1.796725547	-2.880545218
C	0.970385067	-1.883133037	-4.145269604
H	1.162606835	-2.801133975	-4.682662674
C	1.326925091	-0.606592907	-4.495088934
H	1.865647063	-0.280474161	-5.373553659
C	0.837091091	0.274973404	-3.449462514
C	1.003593564	1.662612918	-3.406320127
C	0.574153733	2.539478479	-2.405848127
C	0.785089997	3.977873430	-2.386842795
H	1.281194493	4.538015634	-3.166777552
C	0.238352529	4.448602009	-1.222134306
H	0.198244455	5.468656494	-0.867322972
C	-0.313005840	3.304094587	-0.516463506
C	-0.941051243	3.335594276	0.728916054
C	-1.463917746	2.253194027	1.442962957
C	-2.085276227	2.327314196	2.751582511
H	-2.230539033	3.239443637	3.312620008
C	-2.443398460	1.051374269	3.101917069
H	-2.936464653	0.719556914	4.004571089
C	-2.042436429	0.180845313	2.011807819
C	-2.207018946	-1.205281074	1.975327462
C	-1.803532565	-2.082135539	0.963017306
C	-1.990887146	-3.521616102	0.955806784
H	-2.479645286	-4.084431836	1.738590875
C	-1.442060053	-3.992124898	-0.210222306
H	-1.395946654	-5.013600939	-0.561340171
C	-0.916021302	-2.843566672	-0.927781647
C	-0.259124476	-2.877932294	-2.161638049
H	1.540908443	2.107776632	-4.237080925
H	-1.028844077	4.308449288	1.200473235
H	-0.126444126	-3.858144066	-2.608081574
H	-2.693605729	-1.653343849	2.835188891
H	4.202314588	-1.645612268	-3.029453182
H	3.515979364	4.124338675	-0.309274748
H	1.182782257	-4.333425539	1.916034532
H	0.586675744	1.424051734	4.681892387
O	0.890411293	0.036857338	0.050189913
O	4.171248820	-0.295826259	1.752695258
O	-2.267050369	0.365014655	-1.603993144
C	-3.366582472	1.008984203	-1.197731768
O	3.441015358	2.237838081	-0.987724353
C	-4.554448789	0.110457050	-0.996435092
C	-4.439852027	-1.284252989	-1.110602136
C	-5.783234483	0.689557226	-0.636878176
C	-5.549230874	-2.099199442	-0.862885884
H	-3.480363508	-1.705047827	-1.380996666
C	-6.865515148	-0.145012474	-0.400151942
H	-5.852083988	1.766286155	-0.545553369
C	-6.780298508	-1.532634767	-0.503839361
H	-5.460617816	-3.177798779	-0.945368133
H	-7.648082149	-2.151492706	-0.309532267
Cl	-8.487930206	0.606189520	0.079192047
C	5.280562611	-2.617841020	1.666013474
H	4.642391290	-1.290136885	1.678337743
H	5.308743257	-2.861093710	0.605434617
H	6.236649478	-2.387449237	2.135522327
H	4.580600575	-3.198581718	2.264707426

3-⁶ts1_(is, is)

Fe	2.519402000	-0.368659000	0.861733000
N	3.456576000	-0.236776000	-0.924708000
N	2.124899000	-2.320313000	0.530830000
N	1.459495000	-0.473202000	2.575645000
N	2.744761000	1.620308000	1.108487000
C	3.953614000	0.888051000	-1.524063000

C	4.562618000	0.553458000	-2.800177000
H	5.028631000	1.268990000	-3.462549000
C	4.419405000	-0.792572000	-2.964418000
H	4.735771000	-1.409610000	-3.792860000
C	3.715841000	-1.286509000	-1.793796000
C	3.315557000	-2.592602000	-1.608090000
C	2.557808000	-3.066883000	-0.534261000
C	2.070956000	-4.428468000	-0.422944000
H	2.280644000	-5.212943000	-1.136085000
C	1.317000000	-4.489276000	0.713687000
H	0.778774000	-5.331408000	1.123281000
C	1.350363000	-3.169654000	1.310931000
C	0.723335000	-2.816503000	2.487759000
C	0.793408000	-1.558716000	3.086960000
C	0.184386000	-1.224104000	4.357887000
H	-0.391562000	-1.911570000	4.960735000
C	0.480550000	0.085549000	4.606066000
H	0.188743000	0.695372000	5.448688000
C	1.263931000	0.560293000	3.482856000
C	1.689186000	1.862638000	3.315342000
C	2.361701000	2.358333000	2.197278000
C	2.723015000	3.751689000	2.012608000
H	2.531663000	4.534448000	2.732727000
C	3.316797000	3.847014000	0.787965000
H	3.711115000	4.723401000	0.294911000
C	3.336049000	2.511126000	0.224005000
C	3.884852000	2.178588000	-0.997004000
Fe	-0.542978000	0.368251000	-0.806095000
N	0.185777000	-0.307962000	-2.559407000
N	0.109445000	2.216840000	-1.250194000
N	-1.305657000	1.037941000	0.934173000
N	-1.244014000	-1.485402000	-0.374694000
C	0.168242000	-1.601957000	-3.011754000
C	0.858468000	-1.696124000	-4.284276000
H	0.977265000	-2.610124000	-4.848458000
C	1.298399000	-0.441554000	-4.590845000
H	1.856926000	-0.113694000	-5.455327000
C	0.880228000	0.427202000	-3.508834000
C	1.147194000	1.777640000	-3.433534000
C	0.775722000	2.611421000	-2.378787000
C	1.072039000	4.030645000	-2.315975000
H	1.583152000	4.582806000	-3.091586000
C	0.585219000	4.483229000	-1.125471000
H	0.614320000	5.483402000	-0.718912000
C	-0.016786000	3.346886000	-0.456021000
C	-0.619360000	3.393649000	0.780105000
C	-1.227282000	2.315087000	1.420979000
C	-1.890150000	2.403591000	2.706455000
H	-1.973271000	3.309981000	3.288384000
C	-2.372958000	1.160385000	2.991044000
H	-2.928253000	0.832334000	3.857341000
C	-2.006705000	0.302544000	1.882539000
C	-2.315040000	-1.036389000	1.789754000
C	-1.958470000	-1.869903000	0.729310000
C	-2.286852000	-3.278208000	0.649501000
H	-2.857001000	-3.815899000	1.393410000
C	-1.742266000	-3.745968000	-0.511937000
H	-1.767903000	-4.747999000	-0.914953000
C	-1.088859000	-2.623294000	-1.153558000
C	-0.424817000	-2.683201000	-2.361173000
H	1.694153000	2.227647000	-4.254791000
H	-0.642342000	4.350026000	1.289848000
H	-0.364556000	-3.649436000	-2.850059000
H	-2.880584000	-1.478140000	2.602446000
H	4.310934000	2.981198000	-1.589130000
H	1.450130000	2.569817000	4.102516000
H	3.577090000	-3.308828000	-2.379871000
H	0.147047000	-3.580025000	2.998519000
O	0.923750000	0.011188000	-0.063317000
O	4.085148000	-0.702708000	1.657302000
O	-2.201613000	0.734615000	-1.690001000
C	-3.289112000	1.302810000	-1.167419000
O	-3.367435000	2.500175000	-0.814633000
C	-4.461120000	0.372927000	-1.010353000
C	-4.374068000	-0.977608000	-1.382397000

C	-5.640552000	0.867029000	-0.427917000
C	-5.458073000	-1.834874000	-1.167702000
H	-3.452246000	-1.333839000	-1.822706000
C	-6.697603000	-0.007833000	-0.225709000
H	-5.690015000	1.910828000	-0.144390000
C	-6.637439000	-1.354244000	-0.581761000
H	-5.388600000	-2.880484000	-1.449950000
H	-7.484595000	-2.006613000	-0.407004000
Cl	-8.251484000	0.628844000	0.555493000
H	4.012458000	-1.279652000	2.596695000
C	3.915452000	-2.078481000	3.825581000
H	4.967855000	-2.168943000	4.094404000
H	3.306428000	-1.451957000	4.475242000
H	3.435328000	-2.986180000	3.463177000

3-⁴ts1_(is, is)

Fe	-2.282124174	-0.265365357	1.170446828
N	-3.498071969	0.114108892	-0.396916220
N	-2.286539168	1.707417006	1.619082512
N	-0.946108743	-0.620859594	2.637191307
N	-2.175091794	-2.206680151	0.647069177
C	-4.033287279	-0.810831639	-1.252199697
C	-4.885284610	-0.157951262	-2.230145490
H	-5.425553579	-0.672446036	-3.012068376
C	-4.843971134	1.178625385	-1.959987867
H	-5.341068314	1.987722957	-2.474797917
C	-3.980186490	1.348639192	-0.806852506
C	-3.705486791	2.554376528	-0.196078488
C	-2.926598964	2.715539190	0.950910746
C	-2.687656343	3.987637708	1.610011535
H	-3.086877989	4.934817913	1.276298640
C	-1.890552330	3.730477605	2.686594739
H	-1.494435721	4.423654509	3.414430584
C	-1.631426756	2.301829750	2.686401267
C	-0.813116531	1.649160587	3.584694782
C	-0.478960910	0.293494702	3.546788873
C	0.478735136	-0.331533314	4.438630781
H	0.983531423	0.177256232	5.247513412
C	0.607955120	-1.629829874	4.036663001
H	1.241133119	-2.403719644	4.444970456
C	-0.282741387	-1.810966532	2.908649510
C	-0.466527540	-2.995785471	2.226145830
C	-1.373067199	-3.183029088	1.183196418
C	-1.620513418	-4.452517842	0.529968528
H	-1.115884484	-5.375912731	0.775816451
C	-2.577978072	-4.230575807	-0.417485968
H	-3.011918418	-4.932079194	-1.115093422
C	-2.912215683	-2.821369909	-0.358220352
C	-3.777275395	-2.183164874	-1.223428351
Fe	0.469242401	0.326608083	-1.007494452
N	0.964509580	1.987315543	0.040855520
N	-0.698849732	1.445261893	-2.206024754
N	-0.016208759	-1.329380045	-2.033485618
N	1.679590951	-0.779246107	0.175994851
C	1.741821248	2.044740853	1.168169292
C	1.823057036	3.408533348	1.650523043
H	2.381708130	3.715591648	2.523141603
C	1.077717580	4.175367047	0.800916339
H	0.891633157	5.238867751	0.838487696
C	0.532444903	3.283611999	-0.202188162
C	-0.313765662	3.664780043	-1.222771563
C	-0.890255714	2.800703336	-2.154199765
C	-1.818008257	3.214930136	-3.189617932
H	-2.126788214	4.236251657	-3.360982829
C	-2.196978956	2.085966470	-3.855523247
H	-2.881231646	1.988305915	-4.685538366
C	-1.493947830	0.977343351	-3.240149115
C	-1.596184880	-0.339416537	-3.637254333
C	-0.892457833	-1.407709147	-3.082136164
C	-0.976631412	-2.774684161	-3.562156593
H	-1.596499841	-3.094592272	-4.387358734
C	-0.133072585	-3.517968187	-2.791133171
H	0.080745633	-4.575014083	-2.848187675
C	0.468474280	-2.613624711	-1.832318554

C	1.377368013	-2.982950165	-0.867036846	N	-0.668891949	1.558241643	-2.135546669
C	1.945406229	-2.120446808	0.071198585	N	-0.067875019	-1.233668148	-2.136084054
C	2.876399114	-2.529591649	1.102124013	N	1.636922442	-0.867899209	0.115776818
H	3.260262111	-3.533052210	1.216047551	C	1.785796407	1.886188570	1.268981479
C	3.146956186	-1.423110237	1.853648662	C	1.913735495	3.218214851	1.824938214
H	3.800294156	-1.331258820	2.708586674	H	2.487177405	3.457851381	2.708917568
C	2.393689137	-0.327716511	1.280158316	C	1.189956191	4.054255996	1.024388960
C	2.405643928	0.965622017	1.752135024	H	1.038968571	5.119569418	1.120944366
H	-0.568415382	4.716561525	-1.296024421	C	0.610760019	3.237625887	-0.023321045
H	-2.263501691	-0.561834772	-4.462496130	C	-0.225371157	3.702426321	-1.015986292
H	3.003487296	1.169285380	2.633090617	C	-0.824996031	2.911880174	-1.997049389
H	1.678501333	-4.023761448	-0.832273472	C	-1.739426721	3.415178496	-3.004417526
H	-4.272961910	-2.794230614	-1.970374273	H	-2.020559120	4.453243878	-3.110027785
H	0.118314315	-3.853165646	2.539807744	C	-2.145083745	2.342175504	-3.742643951
H	-4.147240223	3.446098704	-0.627366797	H	-2.828591951	2.316298245	-4.578604677
H	-0.356163697	2.246514540	4.366674380	C	-1.473465924	1.177910598	-3.199789761
O	-0.839658553	0.088699428	0.050162868	C	-1.609918606	-0.105980001	-3.681822456
O	-3.707623879	-0.496971550	2.230807067	C	-0.939207658	-1.225899355	-3.190449756
O	1.914855705	0.648982931	-2.220085274	C	-1.062782293	-2.560726967	-3.747634733
C	3.019970347	-0.106554298	-2.242065080	H	-1.686809579	-2.813952003	-4.592629943
O	3.124930750	-1.189053309	-2.855921781	C	-0.248787024	-3.371912134	-3.014754311
C	4.160695279	0.434315649	-1.427208937	H	-0.067485796	-4.430384024	-3.129352809
C	4.157980219	1.756698416	-0.960186430	C	0.374788376	-2.541678671	-2.003084062
C	5.211673914	-0.431496033	-1.083197878	C	1.261567875	-2.995662437	-1.054354405
C	5.199668179	2.215151078	-0.147793894	C	1.850630177	-2.209344611	-0.063896189
H	3.325486054	2.395515068	-1.224666679	C	2.756545611	-2.712361343	0.948759736
C	6.218617499	0.044789668	-0.257020817	H	3.098387351	-3.735521331	1.008157247
H	5.202190190	-1.447614615	-1.455962095	C	3.064878022	-1.661751031	1.762696444
C	6.242596795	1.353804459	0.221002204	H	3.712983571	-1.643985281	2.626312307
H	5.198387983	3.239015570	0.212334233	C	2.359084210	-0.506660659	1.247308834
H	7.049980251	1.690259371	0.860406027	C	2.415084011	0.756221758	1.791234777
Cl	7.582068134	-1.103835965	0.245286937	H	-0.451189446	4.763093980	-1.025546091
H	-3.701606403	-1.450419223	-2.792461014	H	-2.280095012	-0.257198886	-4.520583551
C	-3.670259303	-2.717598557	3.510588281	H	3.017260653	0.890476715	2.682382706
H	-4.536632878	-2.611856105	4.163547074	H	1.525532758	-4.046754030	-1.076856191
H	-2.697296931	-2.680816928	3.997201735	H	-4.284403024	-2.662375202	-2.118853265
H	-3.765219711	-3.444161307	2.705089749	H	0.006522177	-3.983927895	2.419835419
				H	-4.092827255	3.512364062	-0.513730708
				H	-0.308984491	2.069670388	4.421220696
				O	-0.832939029	0.045025956	0.029174592
				O	-3.728665908	-0.550220713	2.193357664
				O	1.927571411	0.679828879	-2.179384919
				C	3.034610147	-0.069632323	-2.211357147
				O	3.143908099	-1.145679952	-2.836897964
				C	4.175851990	0.465918030	-1.392844156
				C	4.160278177	1.775446012	-0.890848155
				C	5.242163430	-0.394082139	-1.082299435
				C	5.204379174	2.226757813	-0.077301226
				H	3.316715782	2.409716989	-1.129977676
				C	6.252579459	0.074930408	-0.256088185
				H	5.241894613	-1.400266370	-1.481439286
				C	6.263838023	1.371230631	0.256187031
				H	5.192302582	3.240330327	0.310603676
				H	7.074174288	1.702349319	0.894688219
				Cl	7.639623621	-1.065678671	0.197996178
				H	-3.641224459	-1.409061566	2.876184295
				C	-3.527182279	-2.551198200	3.798099615
				H	-4.514360453	-2.538152187	4.259751857
				H	-2.696120163	-2.248772180	4.433474938
				H	-3.326042293	-3.378386083	3.119473620

3⁻²ts1(is, is)

Fe	-2.297499588	-0.294221968	1.148566804
N	-3.500507259	0.164146505	-0.406888617
N	-2.246619015	1.662016673	1.654558692
N	-0.975605538	-0.730301329	2.612031003
N	-2.219709389	-2.221216560	0.552348487
C	-4.039769806	-0.717661395	-1.303555021
C	-4.881737022	-0.015234614	-2.256893505
H	-5.423983933	-0.491011629	-3.061651586
C	-4.828927461	1.307844637	-1.930216207
H	-5.316237518	2.142889046	-2.412023260
C	-3.965422593	1.420212135	-0.768955742
C	-3.666080634	2.597565414	-0.117267138
C	-2.871402014	2.704051143	1.026292744
C	-2.602123096	3.948736206	1.725180243
H	-2.984804857	4.914126464	1.426025506
C	-1.803472308	3.640297102	2.786868902
H	-1.388829881	4.300715569	3.534577463
C	-1.575111624	2.206994392	2.739693110
C	-0.779627956	1.507164550	3.621782677
C	-0.488244845	0.141788362	3.550367699
C	0.440497026	-0.537964031	4.433911599
H	0.953608741	-0.068330393	5.261052301
C	0.532839690	-1.827699582	3.995806633
H	1.137013537	-2.632692253	4.387899775
C	-0.350785717	-1.947663662	2.853373533
C	-0.553823420	-3.102617234	2.128201990
C	-1.445290945	-3.231780309	1.061831626
C	-1.693811108	-4.467559610	0.344865095
H	-1.207986493	-5.408685789	0.559595945
C	-2.624562661	-4.187918766	-0.613689449
H	-3.052951282	-4.850297919	-1.351818256
C	-2.943840612	-2.778341358	-0.494008674
C	-3.792916149	-2.091952153	-1.337845357
Fe	0.450622177	0.340054170	-0.997974951
N	1.001858138	1.916384927	0.145274759

3⁻¹²int1(hs, hs)

Fe	2.481805000	-0.270208000	1.292633000
N	2.404531000	-2.164196000	0.380145000
N	0.971092000	-0.899649000	2.608864000
N	2.131011000	1.698121000	1.873264000
N	3.537997000	0.441771000	-0.373119000
C	3.080115000	-2.543385000	-0.750377000
C	2.818300000	-3.950262000	-1.011778000
H	3.230610000	-4.510882000	-1.839087000
C	1.956721000	-4.387083000	-0.040854000
H	1.526853000	-5.371360000	0.075947000
C	1.682745000	-3.256627000	0.829761000
C	0.817501000	-3.259199000	1.919205000

C	0.478773000	-2.170662000	2.738532000
C	-0.481819000	-2.201535000	3.832835000
H	-1.020998000	-3.081231000	4.155414000
C	-0.564697000	-0.930406000	4.330965000
H	-1.189023000	-0.567428000	5.134485000
C	0.344241000	-0.103598000	3.550475000
C	0.528890000	1.266617000	3.697061000
C	1.344302000	2.103962000	2.917930000
C	1.451909000	3.547978000	3.063752000
H	0.938715000	4.131416000	3.815189000
C	2.292490000	3.990512000	2.079353000
H	2.594363000	5.005665000	1.865913000
C	2.713897000	2.824803000	1.318198000
C	3.532987000	2.838249000	0.195785000
C	3.907012000	1.739704000	-0.596246000
C	4.722563000	1.804891000	-1.801281000
H	5.152428000	2.710276000	-2.206360000
C	4.814496000	0.532182000	-2.293765000
H	5.326651000	0.195558000	-3.183631000
C	4.057941000	-0.329954000	-1.397560000
C	3.858365000	-1.695978000	-1.557192000
Fe	-0.468852000	0.372373000	-0.926451000
N	0.700870000	0.197170000	-2.620266000
N	-0.089699000	2.406528000	-0.837054000
N	-1.742665000	0.548728000	0.715414000
N	-0.935156000	-1.659893000	-1.035318000
C	0.954742000	-0.948704000	-3.317732000
C	1.858346000	-0.645794000	-4.417713000
H	2.220776000	-1.368328000	-5.135359000
C	2.136580000	0.692595000	-4.351740000
H	2.774322000	1.274830000	-5.001002000
C	1.405123000	1.227055000	-3.213946000
C	1.402140000	2.551083000	-2.788644000
C	0.701129000	3.103613000	-1.701755000
C	0.703165000	4.509657000	-1.319133000
H	1.242484000	5.288922000	-1.838816000
C	-0.097909000	4.626205000	-0.217869000
H	-0.341048000	5.518319000	0.340565000
C	-0.603287000	3.296114000	0.086178000
C	-1.470066000	2.964167000	1.116263000
C	-2.007292000	1.696342000	1.407471000
C	-2.926532000	1.399602000	2.493751000
H	-3.314786000	2.130325000	3.188805000
C	-3.188586000	0.057594000	2.444203000
H	-3.830995000	-0.521757000	3.091071000
C	-2.437095000	-0.484493000	1.325603000
C	-2.417719000	-1.811074000	0.922264000
C	-1.726161000	-2.361758000	-0.172211000
C	-1.759906000	-3.756890000	-0.578883000
H	-2.318735000	-4.532968000	-0.075058000
C	-0.965440000	-3.870659000	-1.688558000
H	-0.743392000	-4.758784000	-2.262693000
C	-0.438563000	-2.546403000	-1.975309000
C	0.426635000	-2.215772000	-3.012505000
H	2.003380000	3.243162000	-3.370021000
H	-1.789426000	3.776983000	1.760348000
H	0.730739000	-3.029917000	-3.663317000
H	-3.018364000	-2.500709000	1.506331000
H	4.324642000	-2.154362000	-2.423739000
H	3.903203000	3.808102000	-0.121006000
H	0.323976000	-4.200331000	2.140351000
H	-0.043958000	1.750074000	4.482060000
O	0.838860000	0.040767000	0.049989000
O	3.926525000	-0.618278000	2.383472000
O	-1.967010000	0.769211000	-2.101513000
C	-3.119381000	1.301178000	-1.681655000
O	-3.306477000	2.520919000	-1.485143000
C	-4.210921000	0.301326000	-1.421113000
C	-4.105557000	-1.023582000	-1.868619000
C	-5.323898000	0.702104000	-0.663599000
C	-5.106279000	-1.949833000	-1.558315000
H	-3.228296000	-1.309368000	-2.434319000
C	-6.289933000	-0.243737000	-0.354255000
H	-5.392687000	1.729399000	-0.329369000
C	-6.211582000	-1.566894000	-0.785618000

H	-5.025093000	-2.974930000	-1.905390000
H	-6.989456000	-2.275451000	-0.527260000
Cl	-7.737966000	0.261872000	0.683838000
H	4.380066000	-1.469995000	2.550980000
C	4.532727000	-3.730765000	2.546574000
H	4.435957000	-3.739268000	1.467119000
H	5.495794000	-3.908001000	3.013736000
H	3.641627000	-3.631999000	3.156592000

3-¹⁰int1_(hs, hs)

Fe	2.478732000	-0.270953000	1.293998000
N	2.398755000	-2.164418000	0.382851000
N	0.966489000	-0.896221000	2.610528000
N	2.133560000	1.698385000	1.875156000
N	3.536169000	0.438591000	-0.372697000
C	3.077437000	-2.547262000	-0.744508000
C	2.826367000	-3.958038000	-0.994855000
H	3.242432000	-4.522048000	-1.817996000
C	1.969678000	-4.394397000	-0.019102000
H	1.547989000	-5.381327000	0.105473000
C	1.687451000	-3.259500000	0.842948000
C	0.822932000	-3.259872000	1.933191000
C	0.478453000	-2.168141000	2.745949000
C	-0.482344000	-2.197176000	3.840219000
H	-1.018959000	-3.077036000	4.166644000
C	-0.568993000	-0.924156000	4.332892000
H	-1.194157000	-0.559636000	5.135070000
C	0.338390000	-0.098321000	3.549477000
C	0.523277000	1.272220000	3.693212000
C	1.341923000	2.107190000	2.914985000
C	1.446729000	3.552009000	3.055484000
H	0.929662000	4.137570000	3.802603000
C	2.289673000	3.992108000	2.072071000
H	2.589909000	5.006987000	1.855054000
C	2.715122000	2.824081000	1.316646000
C	3.533455000	2.835502000	0.193498000
C	3.906002000	1.735938000	-0.597718000
C	4.719726000	1.799238000	-1.804127000
H	5.149784000	2.703802000	-2.210836000
C	4.809756000	0.525924000	-2.295414000
H	5.319991000	0.187998000	-3.185888000
C	4.053688000	-0.334599000	-1.397157000
C	3.853674000	-1.700891000	-1.554422000
Fe	-0.471399000	0.374455000	-0.925741000
N	0.699334000	0.196103000	-2.618577000
N	-0.098337000	2.409858000	-0.843885000
N	-1.746399000	0.552959000	0.715165000
N	-0.930825000	-1.659949000	-1.026324000
C	0.956427000	-0.951522000	-3.311885000
C	1.858391000	-0.649858000	-4.413562000
H	2.222653000	-1.373908000	-5.128755000
C	2.132677000	0.689575000	-4.352565000
H	2.768357000	1.271349000	-5.004268000
C	1.400368000	1.225930000	-3.216184000
C	1.394614000	2.551239000	-2.794905000
C	0.692492000	3.105649000	-1.709680000
C	0.692746000	4.512645000	-1.330389000
H	1.231621000	5.291263000	-1.851514000
C	-0.109503000	4.631035000	-0.230139000
H	-0.354058000	5.524276000	0.325901000
C	-0.613660000	3.301131000	0.076743000
C	-1.480342000	2.970536000	1.107388000
C	-2.014553000	1.702384000	1.402791000
C	-2.933328000	1.407105000	2.489888000
H	-3.323920000	2.139306000	3.182080000
C	-3.191528000	0.064168000	2.445280000
H	-3.832438000	-0.514613000	3.094142000
C	-2.438057000	-0.479934000	1.328994000
C	-2.414395000	-1.807998000	0.930730000
C	-1.720212000	-2.360842000	-0.160958000
C	-1.748849000	-3.757816000	-0.561758000
H	-2.305399000	-4.533645000	-0.055041000
C	-0.953092000	-3.873576000	-1.670248000
H	-0.727440000	-4.763353000	-2.240390000

C	-0.430565000	-2.548680000	-1.962242000
C	0.433175000	-2.219264000	-3.001061000
H	1.994469000	3.242792000	-3.378358000
H	-1.801777000	3.784693000	1.748772000
H	0.739850000	-3.034996000	-3.648677000
H	-3.013183000	-2.497237000	1.517153000
H	4.320562000	-2.161085000	-2.419699000
H	3.902788000	3.804971000	-0.125563000
H	0.334913000	-4.202419000	2.160732000
H	-0.051693000	1.757921000	4.475279000
O	0.837112000	0.051305000	0.052166000
O	3.915286000	-0.648298000	2.373104000
O	-1.971557000	0.760814000	-2.102582000
C	-3.125529000	1.290779000	-1.685143000
O	-3.316371000	2.510547000	-1.492053000
C	-4.214477000	0.288573000	-1.422294000
C	-4.104623000	-1.037704000	-1.864683000
C	-5.329554000	0.688812000	-0.667595000
C	-5.102977000	-1.965776000	-1.552157000
H	-3.225853000	-1.322997000	-2.428309000
C	-6.293170000	-0.258742000	-0.355955000
H	-5.401810000	1.717143000	-0.337297000
C	-6.210403000	-1.583252000	-0.782287000
H	-5.018330000	-2.991914000	-1.895320000
H	-6.986513000	-2.293138000	-0.522269000
Cl	-7.744050000	0.246439000	0.678466000
H	4.367981000	-1.509166000	2.525597000
C	4.642866000	-3.601788000	2.492428000
H	4.500902000	-3.637648000	1.418564000
H	5.641770000	-3.636416000	2.914900000
H	3.777106000	-3.668062000	3.142103000

3-⁴int1_(hs, hs)

Fe	2.749215845	-0.132210247	1.059530515
N	2.782289539	-1.932783600	-0.029196218
N	1.510308281	-1.074825865	2.474174573
N	2.224981159	1.716135392	1.872671901
N	3.470356316	0.859258099	-0.645415789
C	3.354088121	-2.114643421	-1.272082680
C	3.218561790	-3.509341413	-1.652471426
H	3.580538523	-3.934196823	-2.578347480
C	2.542488858	-4.140240224	-0.638413329
H	2.249356592	-5.178877747	-0.577393044
C	2.260337237	-3.139960712	0.373360179
C	1.537758171	-3.359411956	1.553001111
C	1.180089195	-2.412436622	2.512906601
C	0.350544060	-2.660061676	3.681431399
H	-0.051690373	-3.624365454	3.958907606
C	0.184438308	-1.458050673	4.318675903
H	-0.382117018	-1.250283938	5.215455965
C	0.906738771	-0.461861669	3.545240093
C	0.926380333	0.913086040	3.809302716
C	1.512206906	1.916099880	3.035518220
C	1.407922379	3.343964796	3.284317466
H	0.903217710	3.787204909	4.131285994
C	2.048583087	3.980502785	2.252724483
H	2.164888023	5.043277077	2.093661025
C	2.550840857	2.949642934	1.361594594
C	3.207342438	3.176919112	0.145849880
C	3.620110519	2.221403899	-0.783898898
C	4.229745698	2.500951809	-2.073863345
H	4.463466651	3.489289405	-2.444267210
C	4.429393637	1.295069764	-2.694210150
H	4.855001469	1.108852973	-3.670272691
C	3.941241140	0.265699039	-1.791740591
C	3.902815532	-1.106070617	-2.067149165
Fe	-0.570399458	0.284540564	-0.740084202
N	0.277487417	-0.243746276	-2.555717723
N	-0.172676294	2.283181480	-1.113703358
N	-1.548102851	0.807669852	1.020745130
N	-1.082302758	-1.718568554	-0.401089002
C	0.412470398	-1.518845127	-3.048027103
C	1.154043228	-1.466026676	-4.296294531
H	1.401323772	-2.324861502	-4.904195432

C	1.456950847	-0.149274934	-4.527824786
H	1.999280781	0.274616594	-5.361019249
C	0.902676304	0.615629090	-3.424088740
C	0.995068709	2.003076474	-3.260056853
C	0.496513627	2.775159061	-2.205982378
C	0.616255339	4.218726142	-2.075320916
H	1.092601976	4.866370826	-2.797624535
C	0.011810118	4.565283275	-0.896277048
H	-0.102504764	5.551024732	-0.468563814
C	-0.482361444	3.337959153	-0.294451375
C	-1.154168791	3.235884587	0.925381209
C	-1.643353782	2.075594289	1.536540296
C	-2.325173891	2.016852985	2.816090762
H	-2.545239659	2.873593607	3.436827286
C	-2.628554833	0.701011987	3.050743835
H	-3.142465466	0.274928358	3.900532969
C	-2.133835479	-0.058226389	1.916658554
C	-2.230118618	-1.442282943	1.755439334
C	-1.754026108	-2.213531097	0.688362613
C	-1.886376804	-3.652177274	0.551285079
H	-2.379886384	-4.297997207	1.263746286
C	-1.280581320	-3.999693318	-0.629579117
H	-1.182482118	-4.984303575	-1.064726178
C	-0.775549725	-2.775108429	-1.225000394
C	-0.078546451	-2.676393266	-2.434675825
H	1.523359925	2.541748766	-4.039892940
H	-1.317984753	4.163955408	1.462668020
H	0.109418892	-3.609748049	-2.955561295
H	-2.729858647	-1.982913101	2.552316764
H	4.297516195	-1.414135793	-3.029921060
H	3.376899576	4.214976699	-0.120809391
H	1.180438663	-4.371084887	1.715342917
H	0.379842429	1.240690277	4.687599940
O	0.872823822	0.092483852	0.045140558
O	4.363258065	-0.369941047	1.925760106
O	-2.260473320	0.438727219	-1.681482066
C	-3.378017172	1.024932123	-1.252517108
O	-3.501436679	2.246539634	-1.013209927
C	-4.529543591	0.077971272	-1.049675171
C	-4.378938042	-1.302779443	-1.253430235
C	-5.756417579	0.592799415	-0.598277648
C	-5.448499075	-2.168447359	-1.002842397
H	-3.421186806	-1.672529086	-1.595095658
C	-6.798445900	-0.290733949	-0.358230558
H	-5.854196940	1.659766923	-0.442289585
C	-6.676290042	-1.666192675	-0.549237655
H	-5.331387069	-3.236515086	-1.156425970
H	-7.513667953	-2.324237142	-0.350260054
Cl	-8.416793808	0.375189909	0.246444777
H	4.884575016	-1.197041224	1.996238080
C	5.311108256	-3.383497607	1.726778528
H	5.126666209	-3.255365803	0.666457062
H	6.325434943	-3.469483068	2.102118537
H	4.468997591	-3.511477410	2.397885232

3-²int1_(hs, hs)

Fe	2.492362000	-0.282264000	1.297542000
N	2.435395000	-2.156122000	0.343903000
N	0.985620000	-0.956189000	2.600635000
N	2.113717000	1.672863000	1.917858000
N	3.532321000	0.479896000	-0.358724000
C	3.115334000	-2.504554000	-0.793645000
C	2.879899000	-3.911815000	-1.077331000
H	3.299154000	-4.451074000	-1.915295000
C	2.030364000	-4.381085000	-0.110596000
H	1.619719000	-5.375344000	-0.009364000
C	1.737454000	-3.270167000	0.779207000
C	0.871860000	-3.304833000	1.867995000
C	0.512020000	-2.235796000	2.705677000
C	-0.455248000	-2.300465000	3.793034000
H	-0.984021000	-3.193236000	4.096381000
C	-0.560689000	-1.039303000	4.312098000
H	-1.195702000	-0.699649000	5.117491000
C	0.342011000	-0.186112000	3.552309000

C	0.506411000	1.184043000	3.722674000
C	1.314259000	2.048111000	2.963365000
C	1.392720000	3.492076000	3.131088000
H	0.863604000	4.054609000	3.887390000
C	2.228964000	3.965247000	2.157417000
H	2.510808000	4.989215000	1.959220000
C	2.676037000	2.818447000	1.381345000
C	3.492574000	2.864323000	0.257506000
C	3.881744000	1.786929000	-0.557255000
C	4.690104000	1.888856000	-1.764861000
H	5.103727000	2.808565000	-2.154251000
C	4.797753000	0.627974000	-2.283733000
H	5.309401000	0.317276000	-3.183264000
C	4.058472000	-0.263260000	-1.401077000
C	3.877238000	-1.628672000	-1.586972000
Fe	-0.482149000	-0.387002000	-0.927354000
N	0.693917000	0.233972000	-2.618625000
N	-0.117981000	2.420612000	-0.818220000
N	-1.759167000	0.537240000	0.715104000
N	-0.929759000	-1.649420000	-1.052267000
C	0.955607000	-0.902474000	-3.326244000
C	1.854809000	-0.582294000	-4.425817000
H	2.221452000	-1.295633000	-5.150505000
C	2.121634000	0.757512000	-4.348682000
H	2.752160000	1.351292000	-4.994599000
C	1.387354000	1.276018000	-3.204444000
C	1.373895000	2.595286000	-2.768286000
C	0.666689000	3.131278000	-1.676187000
C	0.657384000	4.534345000	-1.280730000
H	1.190864000	5.322291000	-1.793348000
C	-0.144747000	4.634601000	-0.178928000
H	-0.396264000	5.519811000	0.386828000
C	-0.640541000	3.297623000	0.112808000
C	-1.504280000	2.950915000	1.139436000
C	-2.030120000	1.675248000	1.419213000
C	-2.941438000	1.359638000	2.507883000
H	-3.332565000	2.080410000	3.211703000
C	-3.190289000	0.015937000	2.447779000
H	-3.823865000	-0.575645000	3.092349000
C	-2.439368000	-0.509242000	1.319650000
C	-2.408005000	-1.831522000	0.906592000
C	-1.712337000	-2.365265000	-0.194464000
C	-1.730688000	-3.758816000	-0.610653000
H	-2.280623000	-4.544206000	-0.111464000
C	-0.934908000	-3.856416000	-1.720341000
H	-0.703276000	-4.737908000	-2.300912000
C	-0.422505000	-2.523654000	-1.998628000
C	0.439569000	-2.178119000	-3.032075000
H	1.969337000	3.297901000	-3.342793000
H	-1.828742000	3.754806000	1.791972000
H	0.752449000	-2.984065000	-3.688743000
H	-2.998023000	-2.532690000	1.487562000
H	4.347164000	-2.063023000	-2.463933000
H	3.845227000	3.845814000	-0.043311000
H	0.394132000	-4.257858000	2.072925000
H	-0.079210000	1.645991000	4.511270000
O	0.812292000	0.053449000	0.049743000
O	3.937759000	-0.654656000	2.371562000
O	-1.973475000	0.777714000	-2.099083000
C	-3.129074000	1.299223000	-1.666038000
O	-3.320825000	2.516226000	-1.462154000
C	-4.213392000	0.291572000	-1.411997000
C	-4.101288000	-1.028764000	-1.871306000
C	-5.327697000	0.680127000	-0.649923000
C	-5.097081000	-1.962708000	-1.568213000
H	-3.223079000	-1.305235000	-2.440054000
C	-6.288476000	-0.273370000	-0.347953000
H	-5.401975000	1.703856000	-0.306114000
C	-6.203544000	-1.592209000	-0.791256000
H	-5.010830000	-2.984260000	-1.924258000
H	-6.977432000	-2.307058000	-0.538277000
Cl	-7.737642000	0.215559000	0.695876000
H	4.399260000	-1.514937000	2.499813000
C	4.699533000	-3.605628000	2.425567000
H	4.554634000	-3.622198000	1.351625000

H	5.700030000	-3.637629000	2.844405000
H	3.836573000	-3.692426000	3.076527000

3-⁸int1(is, is)

Fe	-2.411900000	0.908516000	0.902603000
N	-3.583475000	-0.357819000	-0.183237000
N	-2.327952000	2.168549000	-0.681619000
N	-0.941573000	2.011774000	1.824102000
N	-2.185997000	-0.528044000	2.311913000
C	-4.045226000	-1.587681000	0.207304000
C	-4.917059000	-2.139054000	-0.812959000
H	-5.414375000	-3.096047000	-0.742848000
C	-4.961613000	-1.228939000	-1.830671000
H	-5.497453000	-1.290297000	-2.766785000
C	-4.120067000	-0.115148000	-1.437503000
C	-3.869840000	1.002188000	-2.209849000
C	-3.027066000	2.056981000	-1.858084000
C	-2.741484000	3.192100000	-2.715321000
H	-3.171137000	3.340843000	-3.695751000
C	-1.851803000	3.982522000	-2.046732000
H	-1.396896000	4.907952000	-2.368835000
C	-1.585824000	3.338836000	-0.774698000
C	-0.700906000	3.814758000	0.173617000
C	-0.390744000	3.187338000	1.380977000
C	0.581150000	3.673981000	2.339552000
H	1.148038000	4.587471000	2.229023000
C	0.627558000	2.761967000	3.356929000
H	1.246960000	2.771715000	4.241918000
C	-0.317903000	1.713998000	3.027087000
C	-0.538287000	0.574844000	3.777965000
C	-1.402023000	-0.466638000	3.437800000
C	-1.576014000	-1.670112000	4.230242000
H	-1.069979000	-1.864447000	5.165147000
C	-2.464190000	-2.461675000	3.562074000
H	-2.832081000	-3.440490000	3.832946000
C	-2.842990000	-1.749337000	2.356673000
C	-3.706416000	-2.236787000	1.395557000
Fe	0.466856000	-0.829190000	-0.761409000
N	-0.715411000	-1.378343000	-2.292804000
N	0.018766000	-2.532676000	0.215494000
N	1.706819000	-0.298246000	0.747587000
N	0.962416000	0.865705000	-1.750074000
C	-0.940870000	-0.688253000	-3.454384000
C	-1.905026000	-1.393060000	-4.276375000
H	-2.245406000	-1.056188000	-5.245061000
C	-2.270151000	-2.512615000	-3.585984000
H	-2.972129000	-3.282713000	-3.870118000
C	-1.522659000	-2.504029000	-2.344849000
C	-1.596215000	-3.480484000	-1.373038000
C	-0.857506000	-3.500928000	-0.189523000
C	-0.913875000	-4.569664000	0.790579000
H	-1.528228000	-5.453486000	0.696241000
C	-0.055127000	-4.230612000	1.793886000
H	0.180308000	-4.775961000	2.695826000
C	0.526617000	-2.952461000	1.435829000
C	1.431458000	-2.257462000	2.205452000
C	1.979194000	-1.013936000	1.883262000
C	2.902792000	-0.284832000	2.727183000
H	3.288235000	-0.648079000	3.668740000
C	3.168435000	0.896443000	2.096822000
H	3.818571000	1.698646000	2.412561000
C	2.417451000	0.891919000	0.859898000
C	2.426809000	1.905388000	-0.071196000
C	1.754175000	1.885519000	-1.294775000
C	1.831061000	2.941147000	-2.283181000
H	2.402069000	3.850585000	-2.162697000
C	1.065071000	2.548060000	-3.343566000
H	0.870385000	3.072790000	-4.267606000
C	0.512789000	1.252434000	-3.005570000
C	-0.360101000	0.533957000	-3.796090000
H	-2.270178000	-4.311343000	-1.550846000
H	1.747015000	-2.710046000	3.138671000
H	-0.636547000	0.963127000	-4.753174000
H	3.029535000	2.779065000	0.148663000

H	-4.143156000	-3.214340000	1.569323000
H	0.025273000	0.468132000	4.698526000
H	-4.350233000	1.056199000	-3.180789000
H	-0.184837000	4.742155000	-0.050503000
O	-0.800402000	-0.045084000	-0.031407000
O	-3.851673000	1.773826000	1.754679000
O	1.938517000	-1.771779000	-1.644472000
C	3.062304000	-2.081038000	-0.998449000
O	3.224524000	-3.103263000	-0.294906000
C	4.160138000	-1.059332000	-1.126217000
C	4.128108000	-0.081261000	-2.130351000
C	5.187905000	-1.051341000	-0.169258000
C	5.117086000	0.906179000	-2.180244000
H	3.310311000	-0.097576000	-2.839249000
C	6.139033000	-0.043674000	-0.227666000
H	5.199779000	-1.815135000	0.597380000
C	6.133672000	0.939892000	-1.215133000
H	5.093338000	1.661685000	-2.959122000
H	6.898815000	1.706864000	-1.230628000
Cl	7.462791000	0.013930000	1.067958000
H	-3.731008000	2.565891000	2.320908000
C	-2.865741000	4.468318000	3.233951000
H	-3.691661000	4.733406000	3.885343000
H	-2.871842000	4.778769000	2.195087000
H	-2.007151000	3.935185000	3.624865000

3⁻⁶int1_(is, is)

Fe	2.474891000	0.646315000	1.019353000
N	1.580663000	-0.204912000	2.625842000
N	1.308582000	2.319028000	1.290098000
N	3.063197000	1.373782000	-0.775393000
N	3.326479000	-1.147285000	0.557562000
C	1.800174000	-1.487890000	3.106956000
C	1.041793000	-1.686011000	4.327093000
H	1.037252000	-2.601511000	4.900539000
C	0.360181000	-0.527769000	4.565377000
H	-0.314189000	-0.296897000	5.377830000
C	0.694615000	0.388838000	3.491410000
C	0.158223000	1.670731000	3.362425000
C	0.432278000	2.557258000	2.338420000
C	-0.160207000	3.870666000	2.188686000
H	-0.879671000	4.299741000	2.870649000
C	0.351942000	4.410010000	1.041330000
H	0.138259000	5.371677000	0.596759000
C	1.258312000	3.426318000	0.481071000
C	1.951004000	3.575393000	-0.721452000
C	2.773037000	2.626839000	-1.298371000
C	3.442624000	2.787026000	-2.575015000
H	3.376118000	3.671724000	-3.191290000
C	4.121716000	1.628261000	-2.817100000
H	4.732993000	1.370585000	-3.670289000
C	3.871038000	0.747788000	-1.691192000
C	4.361723000	-0.554676000	-1.590562000
C	4.101298000	-1.431303000	-0.555240000
C	4.576301000	-2.799492000	-0.481375000
H	5.199227000	-3.272235000	-1.226751000
C	4.076769000	-3.331719000	0.673388000
H	4.213033000	-4.327900000	1.069752000
C	3.291132000	-2.292151000	1.311266000
C	2.588438000	-2.450139000	2.506424000
Fe	-0.501169000	-0.624942000	-0.877021000
N	-0.818108000	-2.031918000	0.545235000
N	0.661784000	-1.917385000	-1.892480000
N	-0.227704000	0.768839000	-2.301854000
N	-1.725658000	0.644370000	0.118732000
C	-1.544806000	-1.876533000	1.716814000
C	-1.481532000	-3.093558000	2.497215000
H	-1.965102000	-3.231306000	3.453214000
C	-0.709647000	-3.975579000	1.795260000
H	-0.432351000	-4.986730000	2.056884000
C	-0.291130000	-3.296684000	0.586021000
C	0.557059000	-3.849312000	-0.375311000
C	0.997271000	-3.209612000	-1.514690000
C	1.896470000	-3.786364000	-2.493833000

H	2.306512000	-4.783875000	-2.433185000
C	2.100092000	-2.836388000	-3.452571000
H	2.708494000	-2.895978000	-4.343555000
C	1.328044000	-1.673026000	-3.062024000
C	1.288557000	-0.476615000	-3.781374000
C	0.564006000	0.642222000	-3.433171000
C	0.514566000	1.869225000	-4.204268000
H	1.044356000	2.027770000	-5.132024000
C	-0.313108000	2.722333000	-3.536820000
H	-0.610398000	3.725402000	-3.806272000
C	-0.767738000	2.023926000	-2.350233000
C	-1.632461000	2.570880000	-1.402795000
C	-2.078040000	1.931172000	-0.265304000
C	-2.965029000	2.510070000	0.719803000
H	-3.396050000	3.497719000	0.648333000
C	-3.128273000	1.577601000	1.703804000
H	-3.727285000	1.641886000	2.600475000
C	-2.343558000	0.423027000	1.323427000
C	-2.244451000	-0.743862000	2.079274000
H	0.905871000	-4.862171000	-0.204864000
H	1.871111000	-0.429062000	-4.695018000
H	-2.783151000	-0.770331000	3.019804000
H	-1.989032000	3.579190000	-1.580940000
H	2.652578000	-3.416201000	2.995514000
H	4.983934000	-0.912548000	-2.403779000
H	-0.548058000	1.989013000	4.121688000
H	1.812043000	4.505906000	-1.261423000
O	0.815178000	-0.062499000	-0.038369000
O	3.939479000	1.318585000	1.973334000
O	-2.032977000	-1.299323000	-1.885548000
C	-3.135754000	-0.581097000	-2.093834000
O	-3.269487000	0.278646000	-2.993727000
C	-4.252197000	-0.847624000	-1.120159000
C	-4.213227000	-1.953367000	-0.258601000
C	-5.315046000	0.066982000	-1.042579000
C	-5.231796000	-2.148214000	0.679477000
H	-3.370610000	-2.629055000	-0.328545000
C	-6.298924000	-0.140132000	-0.087198000
H	-5.332469000	0.912404000	-1.718437000
C	-6.288267000	-1.231687000	0.779255000
H	-5.205007000	-3.007169000	1.342715000
H	-7.079536000	-1.362620000	1.507716000
Cl	-7.680621000	1.086246000	0.055251000
H	3.922937000	2.180856000	2.449873000
C	3.289293000	3.881219000	3.583028000
H	4.274772000	4.301258000	3.754115000
H	2.882252000	3.155726000	4.278377000
H	2.666159000	4.256006000	2.779622000

3⁻⁴int1_(is, is)

Fe	-2.285704000	-0.352316000	1.106879000
N	-3.513998000	0.164878000	-0.407424000
N	-2.268787000	1.571104000	1.721615000
N	-0.973206000	-0.854863000	2.556617000
N	-2.210463000	-2.254173000	0.432390000
C	-4.048503000	-0.677804000	-1.343470000
C	-4.902801000	0.062118000	-2.256976000
H	-5.444684000	-0.379196000	-3.081386000
C	-4.862547000	1.367671000	-1.865014000
H	-5.362088000	2.220117000	-2.301708000
C	-3.994883000	1.431501000	-0.703182000
C	-3.708276000	2.578000000	0.006778000
C	-2.913085000	2.634985000	1.152683000
C	-2.666213000	3.842814000	1.921477000
H	-3.066696000	4.816462000	1.677456000
C	-1.862903000	3.488769000	2.965040000
H	-1.461562000	4.112367000	3.750699000
C	-1.609366000	2.064446000	2.837244000
C	-0.805526000	1.329429000	3.682630000
C	-0.495737000	-0.025216000	3.538960000
C	0.444554000	-0.737973000	4.382810000
H	0.952880000	-0.305564000	5.232896000
C	0.556428000	-2.000736000	3.875483000
H	1.175101000	-2.815616000	4.221764000

C	-0.327719000	-2.073862000	2.730184000	N	-3.511317000	-0.007402000	-0.417474000
C	-0.518467000	-3.193341000	1.947435000	N	-2.350824000	1.514081000	1.689263000
C	-1.417114000	-3.279790000	0.883833000	N	-0.932507000	-0.814586000	2.576894000
C	-1.654044000	-4.478777000	0.103859000	N	-2.078675000	-2.328136000	0.469047000
H	-1.154020000	-5.423079000	0.265527000	C	-4.006630000	-0.902340000	-1.328210000
C	-2.593942000	-4.161579000	-0.834071000	C	-4.900897000	-0.228335000	-2.253372000
H	-3.017064000	-4.789911000	-1.604323000	H	-5.424318000	-0.716830000	-3.062955000
C	-2.930982000	-2.764836000	-0.639849000	C	-4.922802000	1.087394000	-1.895064000
C	-3.788884000	-2.045585000	-1.446801000	H	-5.466496000	1.902618000	-2.349647000
Fe	0.472789000	0.403180000	-0.990633000	C	-4.055128000	1.224679000	-0.739968000
N	0.966720000	1.922338000	0.249890000	C	-3.832184000	2.402053000	-0.056207000
N	-0.691136000	1.660966000	-2.047908000	C	-3.050134000	2.527104000	1.090733000
N	-0.022229000	-1.119362000	-2.200934000	C	-2.881570000	3.760316000	1.840054000
N	1.654938000	-0.850058000	0.074041000	H	-3.334628000	4.704543000	1.573383000
C	1.746482000	1.844624000	1.373720000	C	-2.074512000	3.471732000	2.900635000
C	1.847549000	3.145230000	2.004013000	H	-1.721345000	4.131443000	3.679855000
H	2.412078000	3.345749000	2.903366000	C	-1.737488000	2.062818000	2.803156000
C	1.110829000	4.011454000	1.247898000	C	-0.906812000	1.389844000	3.674816000
H	0.938336000	5.066317000	1.404354000	C	-0.518887000	0.055290000	3.555415000
C	0.551382000	3.244243000	0.153825000	C	0.449607000	-0.592254000	4.418148000
C	-0.291364000	3.747483000	-0.814721000	H	0.919572000	-0.122207000	5.270309000
C	-0.875138000	3.001135000	-1.839621000	C	0.644799000	-1.850617000	3.924182000
C	-1.799909000	3.539426000	-2.820090000	H	1.305751000	-2.623763000	4.287416000
H	-2.102662000	4.575556000	-2.871065000	C	-0.217874000	-1.989704000	2.769786000
C	-2.183160000	2.498905000	-3.614368000	C	-0.338857000	-3.133348000	2.006827000
H	-2.866543000	2.503007000	-4.450852000	C	-1.229206000	-3.295283000	0.947400000
C	-1.487140000	1.321425000	-3.131449000	C	-1.406152000	-4.526544000	0.201832000
C	-1.594617000	0.061087000	-3.679374000	H	-0.856660000	-5.438391000	0.387635000
C	-0.898631000	-1.070178000	-3.250419000	C	-2.367114000	-4.287045000	-0.737381000
C	-1.000368000	-2.374315000	-3.879528000	H	-2.761281000	-4.959121000	-1.485725000
H	-1.623670000	-2.592493000	-4.734798000	C	-2.777361000	-2.905217000	-0.580638000
C	-0.168614000	-3.210089000	-3.195073000	C	-3.679010000	-2.255365000	-1.399386000
H	0.029697000	-4.257562000	-3.368007000	Fe	0.465334000	0.460612000	-1.011045000
C	0.442728000	-2.425883000	-2.141075000	N	0.835008000	2.053656000	0.176849000
C	1.333323000	-2.916091000	-1.213684000	N	-0.782223000	1.597702000	-2.109291000
C	1.900103000	-2.174771000	-0.175564000	N	0.056175000	-1.150259000	-2.143342000
C	2.809922000	-2.713772000	0.814892000	N	1.685165000	-0.688828000	0.127381000
H	3.172849000	-3.731387000	0.822077000	C	1.611657000	2.067268000	1.306536000
C	3.091915000	-1.701854000	1.685774000	C	1.626045000	3.393275000	1.889074000
H	3.734594000	-1.717324000	2.553520000	H	2.168959000	3.662378000	2.783916000
C	2.365680000	-0.535514000	1.227117000	C	0.838985000	4.182635000	1.098920000
C	2.393940000	0.698003000	1.836907000	H	0.597667000	5.228928000	1.217305000
H	-0.537111000	4.802820000	-0.765611000	C	0.337600000	3.341488000	0.032575000
H	-2.262564000	-0.060804000	-4.524892000	C	-0.531543000	3.751402000	-0.958002000
H	2.989699000	0.795697000	2.737201000	C	-1.058052000	2.930369000	-1.956722000
H	1.617233000	-3.959349000	-1.292818000	C	-2.007545000	3.367222000	-2.962444000
H	-4.277284000	-2.581311000	-2.253910000	H	-2.379625000	4.377506000	-3.056023000
H	0.056703000	-4.080017000	2.189353000	C	-2.312757000	2.272725000	-3.718155000
H	-4.148818000	3.506088000	-0.340519000	H	-2.988555000	2.198312000	-4.557496000
H	-0.343706000	1.854876000	4.511820000	C	-1.543713000	1.165405000	-3.184174000
O	-0.867056000	0.033983000	0.028463000	C	-1.563007000	-0.121088000	-3.682922000
O	-3.723519000	-0.675485000	2.164617000	C	-0.806248000	-1.192532000	-3.204934000
O	1.925384000	0.860192000	-2.137863000	C	-0.824383000	-2.522870000	-3.784581000
C	3.033540000	0.112607000	-2.222604000	H	-1.421599000	-2.809526000	-4.638250000
O	3.143795000	-0.910546000	-2.929991000	C	0.042848000	-3.283089000	-3.056996000
C	4.170156000	0.583533000	-1.360416000	H	0.302227000	-4.323440000	-3.186259000
C	4.153197000	1.852237000	-0.762572000	C	0.591998000	-2.424761000	-2.027613000
C	5.233515000	-0.298986000	-1.109166000	C	1.498879000	-2.822752000	-1.071313000
C	5.193622000	2.239973000	0.087534000	C	2.012957000	-2.005918000	-0.061655000
H	3.311688000	2.503933000	-0.957934000	C	2.948203000	-2.444513000	0.953012000
C	6.240099000	0.105577000	-0.245156000	H	3.374251000	-3.435935000	1.006438000
H	5.234228000	-1.272693000	-1.581974000	C	3.162684000	-1.379349000	1.779496000
C	6.250187000	1.360256000	0.361846000	H	3.801168000	-1.317273000	2.648232000
H	5.181044000	3.221985000	0.549486000	C	2.368373000	-0.282580000	1.267378000
H	7.057553000	1.641732000	1.027277000	C	2.319849000	0.978403000	1.819674000
Cl	7.622707000	-1.068084000	0.130273000	H	-0.845024000	4.789905000	-0.950484000
H	-3.596761000	-1.497644000	2.702587000	H	-2.212170000	-0.316274000	-4.529594000
C	-3.367413000	-3.173780000	3.885587000	H	2.904555000	1.149609000	2.716510000
H	-4.355507000	-3.093426000	4.325559000	H	1.843628000	-3.850242000	-1.103494000
H	-2.510642000	-2.742017000	4.390411000	H	-4.144329000	-2.837165000	-2.187833000
H	-3.215076000	-3.777105000	2.997858000	H	0.285273000	-3.980059000	2.269411000
				H	-4.322866000	3.295898000	-0.425287000
				H	-0.489764000	1.953640000	4.502397000
				O	-0.912938000	0.016101000	0.060157000
				O	-3.654152000	-0.807111000	2.142203000
Fe	-2.223926000	-0.406693000	1.079554000				

3-²int1_(is, is)

O	1.906714000	0.925926000	-2.157071000
C	3.012813000	0.177712000	-2.252732000
O	3.123229000	-0.836409000	-2.972922000
C	4.149754000	0.637345000	-1.384116000
C	4.140965000	1.905147000	-0.783789000
C	5.203157000	-0.255228000	-1.127916000
C	5.180535000	2.281862000	0.072229000
H	3.306881000	2.565488000	-0.983405000
C	6.207565000	0.137446000	-0.255780000
H	5.198020000	-1.227925000	-1.602705000
C	6.226511000	1.391091000	0.352629000
H	5.176457000	3.264180000	0.533927000
H	7.032261000	1.663797000	1.023681000
Cl	7.573477000	-1.052593000	0.129077000
H	-3.465286000	-1.548190000	2.769454000
C	-3.082560000	-3.111078000	4.089955000
H	-4.074916000	-3.125128000	4.527871000
H	-2.284946000	-2.551005000	4.565736000
H	-2.857177000	-3.736543000	3.233542000

3-¹²ts₂(hs, hs)

Fe	2.244299000	-0.195303000	1.182504000
N	3.589299000	-0.003104000	-0.385096000
N	2.104798000	-2.251503000	0.808904000
N	0.952099000	-0.418102000	2.798904000
N	2.363100000	1.840797000	1.561104000
C	4.162500000	1.161796000	-0.807696000
C	5.021300000	0.881595000	-1.950796000
H	5.602600000	1.621895000	-2.482396000
C	4.934499000	-0.461405000	-2.198596000
H	5.426599000	-1.030205000	-2.974396000
C	4.023799000	-1.021804000	-1.209996000
C	3.639398000	-2.355304000	-1.113296000
C	2.759397000	-2.928703000	-0.179396000
C	2.402496000	-4.339903000	-0.106596000
H	2.779996000	-5.106803000	-0.768496000
C	1.525396000	-4.479402000	0.933904000
H	1.041396000	-5.380202000	1.283204000
C	1.336697000	-3.156602000	1.513904000
C	0.520597000	-2.840802000	2.594804000
C	0.325998000	-1.577202000	3.179804000
C	-0.607902000	-1.280601000	4.253904000
H	-1.230202000	-2.013101000	4.748604000
C	-0.551301000	0.068699000	4.478804000
H	-1.120000000	0.650999000	5.189304000
C	0.423700000	0.618798000	3.552204000
C	0.752700000	1.964198000	3.415704000
C	1.651101000	2.534797000	2.498504000
C	1.960902000	3.953197000	2.377304000
H	1.540102000	4.732098000	2.997504000
C	2.856002000	4.082197000	1.351004000
H	3.303102000	4.987196000	0.965404000
C	3.106701000	2.746297000	0.828004000
C	3.932601000	2.430496000	-0.245696000
Fe	-0.571301000	0.339799000	-1.097096000
N	0.675999000	-0.248102000	-2.638596000
N	0.089701000	2.303998000	-1.293496000
N	-1.688400000	0.888600000	0.582704000
N	-1.079002000	-1.659401000	-0.744096000
C	0.868598000	-1.528702000	-3.084796000
C	1.850598000	-1.515503000	-4.154896000
H	2.187498000	-2.389303000	-4.694596000
C	2.253299000	-0.215603000	-4.317696000
H	2.984499000	0.173197000	-5.011396000
C	1.519500000	0.585798000	-3.354596000
C	1.654200000	1.957897000	-3.158996000
C	0.990401000	2.759998000	-2.213296000
C	1.157302000	4.196698000	-2.044096000
H	1.807202000	4.818297000	-2.643596000
C	0.345702000	4.575898000	-1.009496000
H	0.208103000	5.565298000	-0.598096000
C	-0.326199000	3.377899000	-0.529796000
C	-1.219299000	3.307699000	0.532704000
C	-1.852699000	2.162900000	1.051304000

C	-2.762899000	2.139200000	2.184304000
H	-3.081699000	3.011000000	2.737804000
C	-3.122000000	0.833101000	2.387104000
H	-3.787301000	0.433701000	3.138604000
C	-2.440301000	0.039800000	1.379404000
C	-2.524902000	-1.338200000	1.224304000
C	-1.896402000	-2.129900000	0.246204000
C	-2.019103000	-3.572500000	0.117904000
H	-2.613504000	-4.200800000	0.766204000
C	-1.247903000	-3.949701000	-0.949496000
H	-1.083204000	-4.945901000	-1.333996000
C	-0.644503000	-2.742801000	-1.490096000
C	0.242097000	-2.674702000	-2.560096000
H	2.359401000	2.467797000	-3.808196000
H	-1.456298000	4.245699000	1.024604000
H	0.499497000	3.617702000	-3.032596000
H	-3.159602000	-1.864199000	1.930104000
H	4.450901000	3.261796000	-0.713796000
H	0.246901000	2.653298000	4.084904000
H	4.071097000	-3.033904000	-1.842696000
H	-0.043703000	-3.659801000	3.030004000
O	0.926699000	0.077698000	0.118504000
O	3.714999000	-0.543704000	2.299304000
O	-2.136000000	0.663100000	-2.227996000
C	-3.299000000	1.202901000	-1.849896000
O	-3.507599000	2.431301000	-1.762096000
C	-4.352401000	0.204801000	-1.460496000
C	-4.208602000	-1.159799000	-1.750996000
C	-5.470700000	0.657402000	-0.740596000
C	-5.175602000	-2.073798000	-1.320196000
H	-3.329302000	-1.485599000	-2.291496000
C	-6.403201000	-0.274697000	-0.310696000
H	-5.568800000	1.714402000	-0.528396000
C	-6.285902000	-1.636697000	-0.584596000
H	-5.062403000	-3.129698000	-1.542896000
H	-7.038302000	-2.333597000	-0.235096000
Cl	-7.858101000	0.304104000	0.677804000
H	3.447099000	-0.668504000	3.235104000
C	5.208097000	-2.644605000	2.327004000
H	4.301597000	-3.232504000	2.399704000
H	5.794798000	-2.426105000	3.212304000
H	5.485198000	-2.215605000	1.374104000

3-¹⁰ts₂(hs, hs)

Fe	2.441423338	-0.371449041	1.266962991
N	2.355852064	-2.225971863	0.289859954
N	0.973828926	-1.022274495	2.592872517
N	2.138610658	1.586685481	1.933464694
N	3.564244880	0.372161373	-0.342379253
C	3.035130127	-2.583047510	-0.844383752
C	2.776570112	-3.986124700	-1.133599222
H	3.191361963	-4.530767758	-1.970305744
C	1.919595482	-4.443876240	-0.169125765
H	1.495616199	-5.432512048	-0.068146491
C	1.644649520	-3.329892931	0.724131836
C	0.794635502	-3.359034600	1.824633344
C	0.473986850	-2.295521973	2.684586432
C	-0.475536113	-2.356393222	3.784589492
H	-1.016368421	-3.243071513	4.084351227
C	-0.549058375	-1.099843979	4.323069318
H	-1.165090264	-0.760765422	5.143345855
C	0.356912975	-0.253474632	3.563655933
C	0.545385948	1.112780288	3.748918929
C	1.359175883	1.969502866	2.990497916
C	1.478967066	3.409547944	3.175771575
H	0.972601976	3.976744049	3.944175227
C	2.321444737	3.871706043	2.202722678
H	2.630877455	4.889832249	2.015823163
C	2.732197578	2.722228329	1.409316237
C	3.554893837	2.757465570	0.289248034
C	3.927246931	1.680053198	-0.532870732
C	4.719936765	1.781743385	-1.748658139
H	5.141867815	2.699284960	-2.134314845
C	4.796586058	0.525435170	-2.287243498

H	5.285730418	0.220178743	-3.201025639	H	5.491343000	2.045145000	-2.362458000
C	4.052307899	-0.363756398	-1.409988510	C	4.902185000	-0.079259000	-2.284878000
C	3.823957242	-1.719546924	-1.623137227	H	5.397821000	-0.546860000	-3.123490000
Fe	-0.458259322	0.423748386	-0.934560614	C	4.032630000	-0.771519000	-1.344275000
N	0.704685959	0.309030802	-2.639461276	C	3.697454000	-2.121348000	-1.380426000
N	-0.084507309	2.452558730	-0.778240321	C	2.856016000	-2.821958000	-0.498039000
N	-1.723447812	0.539311406	0.720780721	C	2.539702000	-4.242501000	-0.573335000
N	-0.917462558	-1.606018686	-1.110040076	H	2.927890000	-4.923165000	-1.317960000
C	0.958836440	-0.812628116	-3.376076594	C	1.679115000	-4.517515000	0.454507000
C	1.857992186	-0.470130722	-4.467997790	H	1.225190000	-5.464245000	0.709842000
H	2.219271860	-1.166825415	-5.211368452	C	1.462127000	-3.270362000	1.174579000
C	2.133144421	0.866180229	-4.357777270	C	0.647422000	-3.092800000	2.288235000
H	2.766738221	1.471560452	-4.989854803	C	0.423364000	-1.905308000	3.008435000
C	1.404724958	1.359875101	-3.199940201	C	-0.515829000	-1.751439000	4.106994000
C	1.402742782	2.668051384	-2.727320591	H	-1.116547000	-2.549199000	4.520648000
C	0.706305368	3.180146718	-1.618483414	C	-0.496494000	-0.432008000	4.473773000
C	0.713680210	4.570355121	-1.181624110	H	-1.079911000	0.055173000	5.241671000
H	1.252998352	5.367756840	-1.673130056	C	0.460085000	0.239518000	3.610577000
C	-0.083560582	4.646741693	-0.074044441	C	0.744938000	1.602909000	3.610491000
H	-0.322113703	5.517615233	0.518918858	C	1.612388000	2.296421000	2.749915000
C	-0.591681073	3.307689532	0.181055838	C	1.861789000	3.731266000	2.765106000
C	-1.452214319	2.939203331	1.204031491	H	1.420188000	4.427557000	3.464007000
C	-1.984560080	1.661065302	1.455490916	C	2.731453000	3.997749000	1.743085000
C	-2.893088052	1.323134155	2.538695752	H	3.133340000	4.954279000	1.441443000
H	-3.277320600	2.027448013	3.262663570	C	3.026095000	2.730899000	1.088799000
C	-3.151304155	-0.017377924	2.444194565	C	3.838522000	2.556673000	-0.027901000
H	-3.786129811	-0.621284280	3.075907277	Fe	-0.554097000	0.395702000	-1.043679000
C	-2.408373890	-0.517055144	1.300336655	N	0.645349000	0.049950000	-2.629397000
C	-2.388722496	-1.828702902	0.849630915	N	-0.026729000	2.349929000	-1.056702000
C	-1.704515676	-2.338484726	-0.268568378	N	-1.719251000	0.723241000	0.595137000
C	-1.741936397	-3.717644162	-0.726142683	N	-1.016661000	-1.580461000	-0.959367000
H	-2.297859640	-4.511459625	-0.247380586	C	0.859863000	-1.152346000	-3.256746000
C	-0.953444431	-3.791120905	-1.843302548	C	1.803873000	-0.981466000	-4.341728000
H	-0.734435589	-4.657970131	-2.450092938	H	2.134883000	-1.775313000	-4.996058000
C	-0.426621921	-2.457514480	-2.084030438	C	2.169792000	0.335420000	-4.348710000
C	0.434101297	-2.090048046	-3.112983753	H	2.864206000	0.837708000	-5.006135000
H	2.001420446	3.381277814	-3.285491155	C	1.446063000	0.982247000	-3.274757000
H	-1.766501324	3.728400494	1.879221147	C	1.544050000	2.320951000	-2.946992000
H	0.735657528	-2.880559046	-3.793437013	C	0.845763000	2.957718000	-1.919566000
H	-2.983005993	-2.540232086	1.413580067	C	0.939182000	4.373189000	-1.614606000
H	4.276984562	-2.151614109	-2.510106364	H	1.556361000	5.076408000	-2.155233000
H	3.926721406	3.734088504	-0.004690827	C	0.108153000	4.606828000	-0.557263000
H	0.303338823	-4.305217311	2.028669174	H	-0.092312000	5.539247000	-0.050322000
H	-0.022267040	1.573698117	4.551130181	C	-0.496193000	3.337206000	-0.204746000
O	0.854846184	0.063654234	0.027825337	C	-1.386617000	3.148543000	0.831608000
C	3.920450015	-0.756980149	2.341675220	C	-1.952171000	1.928150000	1.206408000
O	-1.970303437	0.844389816	-2.085032356	C	-2.853493000	1.749076000	2.325923000
C	-3.117491068	1.367978001	-1.641347359	H	-3.208915000	2.548857000	2.959421000
O	-3.298895685	2.581953362	-1.407270417	C	-3.147666000	0.416365000	2.392472000
C	-4.210270403	0.364056573	-1.402119961	H	-3.790535000	-0.097216000	3.091915000
C	-4.109632654	-0.948755222	-1.885004208	C	-2.433699000	-0.228407000	1.310818000
C	-5.318147002	0.746435064	-0.627874225	C	-2.467872000	-1.578940000	1.031031000
C	-5.110211083	-1.881297363	-1.593709923	C	-1.811724000	-2.204067000	-0.030609000
H	-3.235513242	-1.220700432	-2.462244928	C	-1.900024000	-3.618845000	-0.325646000
C	-6.284131071	-0.205735435	-0.338374563	H	-2.474037000	-4.328864000	0.252340000
H	-5.382972696	1.764506929	-0.265809342	C	-1.139001000	-3.843346000	-1.438519000
C	-6.210567707	-1.517118142	-0.805075635	H	-0.952949000	-4.776270000	-1.950458000
H	-5.032596502	-2.897051019	-1.968025445	C	-0.577365000	-2.567479000	-1.831129000
H	-6.988197961	-2.230999994	-0.561026830	C	0.283756000	-2.371447000	-2.893707000
Cl	-7.725541157	0.274511921	0.720928271	H	2.210849000	2.932103000	-3.545435000
H	4.845823979	-0.840013975	2.044344706	H	-1.673633000	4.021970000	1.406420000
C	4.339041247	-3.307988421	2.729655760	H	0.548827000	-3.239890000	-3.487118000
H	4.327248569	-3.553831947	1.674708550	H	-3.075710000	-2.205449000	1.673897000
H	5.278234712	-3.192051301	3.259246551	H	4.315696000	3.450412000	-0.418535000
H	3.403917922	-3.180028896	3.255970314	H	0.222492000	2.202357000	4.349709000

3-⁴ts₂(hs, hs)

Fe	2.268827000	-0.263366000	1.143108000	O	0.927851000	0.063800000	0.161502000
N	3.578598000	0.139867000	-0.411350000	O	3.770578000	-0.678641000	2.205769000
N	2.197075000	-2.273641000	0.564092000	O	-2.137396000	0.804047000	-2.232949000
N	1.015552000	-0.695507000	2.752745000	C	-3.276563000	1.315713000	-1.785551000
N	2.336113000	1.726971000	1.739432000	O	-3.492035000	2.536519000	-1.594455000
C	4.102555000	1.362065000	-0.721081000	C	-4.327422000	0.294892000	-1.427835000
C	4.947254000	1.233151000	-1.900849000	C	-4.206242000	-1.044264000	-1.825940000
				C	-5.409258000	0.692831000	-0.625314000

C	-5.157421000	-1.986856000	-1.422248000
H	-3.352577000	-1.327184000	-2.428688000
C	-6.324540000	-0.268115000	-0.222425000
H	-5.491617000	1.731780000	-0.332563000
C	-6.229495000	-1.605617000	-0.602888000
H	-5.062204000	-3.023020000	-1.731294000
H	-6.968744000	-2.325314000	-0.271972000
Cl	-7.727774000	0.236894000	0.880229000
H	3.494673000	-0.894800000	3.122704000
C	5.066010000	-2.953017000	2.576883000
H	4.187124000	-3.379745000	2.111005000
H	5.199988000	-3.009964000	3.652453000
H	5.795446000	-2.437352000	1.966985000

3-²ts₂(_{hs, hs})

Fe	2.463500000	-0.441071000	1.224850000
N	2.407292000	-2.277171000	0.198162000
N	0.973016000	-1.149039000	2.520154000
N	2.150443000	1.479297000	1.964399000
N	3.566939000	0.360356000	-0.363213000
C	3.050010000	-2.577068000	-0.973615000
C	2.747589000	-3.950639000	-1.346647000
H	3.128570000	-4.449314000	-2.226888000
C	1.893275000	-4.446593000	-0.398555000
H	1.436451000	-5.424955000	-0.358726000
C	1.661448000	-3.384740000	0.568035000
C	0.790273000	-3.447961000	1.651329000
C	0.463486000	-2.418936000	2.550929000
C	-0.492157000	-2.523909000	3.643453000
H	-1.040879000	-3.419234000	3.899814000
C	-0.556030000	-1.294048000	4.241115000
H	-1.172141000	-0.988485000	5.074418000
C	0.360486000	-0.421022000	3.523064000
C	0.563461000	0.933808000	3.768527000
C	1.385402000	1.816984000	3.047906000
C	1.530569000	3.241713000	3.308912000
H	1.038481000	3.775602000	4.109729000
C	2.375965000	3.741424000	2.356249000
H	2.702388000	4.762710000	2.223163000
C	2.763348000	2.630411000	1.500572000
C	3.585142000	2.710616000	0.381442000
C	3.944692000	1.670299000	-0.492200000
C	4.742567000	1.819923000	-1.701297000
H	5.174267000	2.750053000	-2.043498000
C	4.809642000	0.589380000	-2.295402000
H	5.300848000	0.320245000	-3.219371000
C	4.056821000	-0.333030000	-1.458689000
C	3.828458000	-1.678342000	-1.725213000
Fe	-0.453322000	0.417302000	-0.960999000
N	0.708061000	0.338305000	-2.669094000
N	-0.005736000	2.421294000	-0.713243000
N	-1.712987000	0.504003000	0.699016000
N	-0.984187000	-1.584976000	-1.227712000
C	0.924927000	-0.758151000	-3.453046000
C	1.832551000	-0.397618000	-4.533036000
H	2.169874000	-1.073241000	-5.306536000
C	2.147427000	0.923938000	-4.368815000
H	2.796256000	1.536673000	-4.977961000
C	1.436605000	1.390952000	-3.188463000
C	1.472436000	2.678144000	-2.665257000
C	0.792760000	3.162343000	-1.533597000
C	0.828419000	4.536658000	-1.049887000
H	1.380874000	5.339618000	-1.517144000
C	0.038474000	4.590242000	0.063853000
H	-0.182392000	5.444853000	0.686539000
C	-0.495723000	3.253366000	0.275218000
C	-1.367767000	2.871940000	1.283024000
C	-1.937724000	1.601153000	1.481511000
C	-2.852049000	1.243849000	2.554307000
H	-3.213003000	1.928099000	3.308862000
C	-3.146579000	-0.083915000	2.407030000
H	-3.796383000	-0.695355000	3.015926000
C	-2.422829000	-0.557216000	1.238996000
C	-2.441119000	-1.849695000	0.738053000

C	-1.777640000	-2.331198000	-0.405227000
C	-1.842342000	-3.693815000	-0.909332000
H	-2.409794000	-4.493390000	-0.454105000
C	-1.061612000	-3.743320000	-2.033219000
H	-0.862830000	-4.592539000	-2.671353000
C	-0.511400000	-2.411566000	-2.231878000
C	0.360946000	-2.029388000	-3.244540000
H	2.087205000	3.397315000	-3.197335000
H	-1.659771000	3.642758000	1.988503000
H	0.643009000	-2.800661000	-3.954683000
H	-3.047180000	-2.568316000	1.279945000
H	4.265941000	-2.070434000	-2.638107000
H	3.970413000	3.695583000	0.137038000
H	0.278714000	-4.393639000	1.801114000
H	0.003685000	1.364180000	4.593028000
O	0.824302000	-0.054371000	-0.016477000
O	3.924085000	-0.844912000	2.323199000
O	-1.928968000	0.953970000	-2.091797000
C	-3.056634000	1.496108000	-1.609002000
O	-3.196658000	2.708113000	-1.344762000
C	-4.172414000	0.518503000	-1.379288000
C	-4.127535000	-0.774440000	-1.920184000
C	-5.245345000	0.902069000	-0.557797000
C	-5.149710000	-1.686608000	-1.640070000
H	-3.277541000	-1.049013000	-2.530921000
C	-6.232457000	-0.031471000	-0.279667000
H	-5.267590000	1.904736000	-0.150669000
C	-6.214609000	-1.322841000	-0.804214000
H	-5.115314000	-2.687171000	-2.058936000
H	-7.007424000	-2.022272000	-0.567383000
Cl	-7.624801000	0.445762000	0.843905000
H	4.694448000	-1.393507000	2.083009000
C	3.548687000	-2.946322000	3.816023000
H	3.353773000	-3.521684000	2.919398000
H	4.517797000	-2.993521000	4.300513000
H	2.771112000	-2.312276000	4.217028000

3-⁸ts₂(_{is, is})

Fe	2.362100000	-0.178690000	1.298698000
N	3.551199000	0.304913000	-0.366302000
N	2.327307000	-2.107491000	0.687898000
N	0.875402000	-0.649595000	2.755998000
N	2.134894000	1.754709000	1.721298000
C	3.984395000	1.551015000	-0.705802000
C	4.832295000	1.473118000	-1.887702000
H	5.312492000	2.316419000	-2.364302000
C	4.881599000	0.155018000	-2.251702000
H	5.403901000	-0.289080000	-3.087002000
C	4.067902000	-0.578085000	-1.292402000
C	3.821606000	-1.941386000	-1.284702000
C	3.019509000	-2.642388000	-0.370402000
C	2.782313000	-4.072489000	-0.434002000
H	3.213815000	-4.732188000	-1.173502000
C	1.928914000	-4.384892000	0.587098000
H	1.515018000	-5.349093000	0.844598000
C	1.631010000	-3.150093000	1.289298000
C	0.746510000	-3.054096000	2.355398000
C	0.371806000	-1.886397000	3.034198000
C	-0.617994000	-1.787600000	4.098698000
H	-1.166992000	-2.620502000	4.515598000
C	-0.709799000	-0.463401000	4.431998000
H	-1.351600000	-0.002903000	5.169398000
C	0.227399000	0.251402000	3.577598000
C	0.455394000	1.618003000	3.550098000
C	1.336092000	2.303406000	2.697898000
C	1.498887000	3.744507000	2.699598000
H	0.982785000	4.416305000	3.370698000
C	2.385386000	4.053310000	1.705998000
H	2.736183000	5.027911000	1.399098000
C	2.780790000	2.807011000	1.079798000
C	3.626191000	2.718014000	-0.016902000
Fe	-0.495801000	0.264800000	-0.987702000
N	0.693100000	-0.072896000	-2.572802000
N	-0.100408000	2.235501000	-1.090002000

N	-1.754302000	0.605096000	0.559198000	C	2.869370000	-4.020463000	-0.481823000
N	-0.937195000	-1.708501000	-0.898002000	H	3.306531000	-4.660907000	-1.234503000
C	0.948204000	-1.276295000	-3.176302000	C	2.040007000	-4.361225000	0.549655000
C	1.882503000	-1.098392000	-4.270602000	H	1.650968000	-5.335564000	0.807440000
H	2.237206000	-1.896191000	-4.907402000	C	1.731361000	-3.139693000	1.264759000
C	2.198799000	0.228509000	-4.309602000	C	0.877722000	-3.055098000	2.350286000
H	2.867897000	0.744311000	-4.982502000	C	0.520467000	-1.880483000	3.009246000
C	1.452897000	0.871106000	-3.246602000	C	-0.443394000	-1.803064000	4.089192000
C	1.489492000	2.220107000	-2.962902000	H	-0.955113000	-2.654326000	4.515451000
C	0.750090000	2.854004000	-1.965002000	C	-0.569449000	-0.482897000	4.417837000
C	0.771886000	4.283704000	-1.717202000	H	-1.208045000	-0.032436000	5.163565000
H	1.360883000	4.992306000	-2.281702000	C	0.322094000	0.256658000	3.547858000
C	-0.080415000	4.517701000	-0.679402000	C	0.465138000	1.631568000	3.543710000
H	-0.335718000	5.457401000	-0.212202000	C	1.295261000	2.355349000	2.690257000
C	-0.627311000	3.234500000	-0.285702000	C	1.418328000	3.801434000	2.702277000
C	-1.528210000	3.046197000	0.737498000	H	0.888025000	4.454031000	3.381052000
C	-2.055306000	1.815295000	1.128598000	C	2.298850000	4.134514000	1.714719000
C	-2.986406000	1.636192000	2.223098000	H	2.633804000	5.116101000	1.412844000
H	-3.391708000	2.441790000	2.818098000	C	2.720569000	2.896642000	1.087757000
C	-3.226701000	0.296691000	2.325098000	C	3.579705000	2.812504000	0.011142000
H	-3.869499000	-0.222911000	3.019798000	Fe	-0.530400000	0.253407000	-1.007807000
C	-2.451399000	-0.351306000	1.288898000	N	0.664861000	-0.042323000	-2.599627000
C	-2.426995000	-1.708006000	1.057998000	N	-0.181623000	2.233326000	-1.092065000
C	-1.724092000	-2.337604000	0.030498000	N	-1.785399000	0.549169000	0.550297000
C	-1.757988000	-3.763004000	-0.225002000	N	-0.926455000	-1.731427000	-0.937125000
H	-2.317185000	-4.475906000	0.363998000	C	0.945640000	-1.234573000	-3.215935000
C	-0.971087000	-3.989102000	-1.318102000	C	1.885626000	-1.027352000	-4.299235000
H	-0.744984000	-4.926301000	-1.805502000	H	2.259402000	-1.810397000	-4.943405000
C	-0.450091000	-2.703200000	-1.734702000	C	2.179336000	0.305991000	-4.318590000
C	0.415208000	-2.506097000	-2.790502000	H	2.843677000	0.841785000	-4.980617000
H	2.131790000	2.842309000	-3.576202000	C	1.412131000	0.921295000	-3.255092000
H	-1.862713000	3.923795000	1.279098000	C	1.418779000	2.269395000	-2.955544000
H	0.716711000	-3.378496000	-3.360302000	C	0.658147000	2.878954000	-1.959959000
H	-3.021892000	-2.336608000	1.710598000	C	0.642877000	4.306809000	-1.702794000
H	4.029788000	3.653615000	-0.391002000	H	1.216784000	5.033844000	-2.259206000
H	-0.111908000	2.230301000	4.243798000	C	-0.220984000	4.512838000	-0.668268000
H	4.283808000	-2.532884000	-2.068602000	H	-0.501408000	5.442866000	-0.196283000
H	0.276313000	-3.979197000	2.674298000	C	-0.735623000	3.213921000	-0.284551000
O	0.776700000	0.037204000	0.059898000	C	-1.629626000	2.994585000	0.739899000
O	3.807001000	-0.444386000	2.484198000	C	-2.116793000	1.747153000	1.129958000
O	-1.959902000	0.532295000	-2.237002000	C	-3.027942000	1.534262000	2.234684000
C	-3.105804000	1.121791000	-1.890802000	H	-3.450459000	2.323770000	2.839099000
O	-3.286908000	2.358591000	-1.848602000	C	-3.227266000	0.187307000	2.331412000
C	-4.204601000	0.172588000	-1.497102000	H	-3.847708000	-0.354656000	3.029582000
C	-4.121996000	-1.196812000	-1.787402000	C	-2.447241000	-0.430883000	1.281286000
C	-5.297202000	0.672484000	-0.769602000	C	-2.390457000	-1.785055000	1.037097000
C	-5.125093000	-2.068115000	-1.350902000	C	-1.686895000	-2.388900000	-0.005496000
H	-3.259795000	-1.557809000	-2.333302000	C	-1.688312000	-3.811606000	-0.273933000
C	-6.263999000	-0.219219000	-0.329402000	H	-2.222072000	-4.544326000	0.314246000
H	-5.349306000	1.732784000	-0.558402000	C	-0.908592000	-4.007501000	-1.378794000
C	-6.208795000	-1.584519000	-0.604302000	H	-0.665143000	-4.934377000	-1.877633000
H	-5.062290000	-3.127615000	-1.578102000	C	-0.424449000	-2.705532000	-1.787583000
H	-6.987093000	-2.248622000	-0.247902000	C	0.434446000	-2.477581000	-2.844380000
Cl	-7.681102000	0.421776000	0.677598000	H	2.052514000	2.910897000	-3.558037000
H	3.590302000	-0.558786000	3.432898000	H	-1.987337000	3.859755000	1.286631000
C	5.326307000	-2.295781000	2.085598000	H	0.752731000	-3.337713000	-3.423770000
H	4.520610000	-3.010883000	2.191198000	H	-2.961417000	-2.433938000	1.691569000
H	5.966407000	-2.057879000	2.926398000	H	3.985994000	3.740442000	-0.376512000
H	5.484006000	-1.810580000	1.132998000	H	-0.125922000	2.195926000	4.256794000
				H	4.343484000	-2.403534000	-2.092788000
				H	0.423343000	-3.976690000	2.698095000
				O	0.752581000	0.042707000	0.026395000
				O	3.857299000	-0.332865000	2.488104000
				O	-2.011729000	0.500038000	-2.254518000
				C	-3.156392000	1.079679000	-1.893627000
				O	-3.351115000	2.315358000	-1.858853000
				C	-4.237377000	0.123283000	-1.467085000
				C	-4.149857000	-1.247178000	-1.751471000
				C	-5.315130000	0.617356000	-0.714122000
				C	-5.132642000	-2.125039000	-1.283068000
				H	-3.298843000	-1.603326000	-2.317750000
				C	-6.260669000	-0.280684000	-0.241837000
				H	-5.372007000	1.678541000	-0.508528000
				C	-6.200097000	-1.647005000	-0.509820000
				H	-5.066326000	-3.185260000	-1.505954000

3-⁶ts₂(is, is)

Fe	2.380804000	-0.137034000	1.299377000
N	3.525460000	0.373265000	-0.300224000
N	2.390829000	-2.073704000	0.671144000
N	0.990431000	-0.623236000	2.708001000
N	2.099282000	1.823069000	1.712079000
C	3.944460000	1.633763000	-0.642075000
C	4.794476000	1.574507000	-1.814752000
H	5.257160000	2.433152000	-2.280182000
C	4.866311000	0.261974000	-2.187509000
H	5.394840000	-0.173566000	-3.022946000
C	4.066224000	-0.490126000	-1.241693000
C	3.861950000	-1.855720000	-1.290182000
C	3.075981000	-2.588861000	-0.401940000

H	-6.962015000	-2.316130000	-0.128194000
Cl	-7.655204000	0.353372000	0.800827000
H	3.812149000	-0.929850000	3.261202000
C	5.367987000	-2.600337000	1.939769000
H	4.534676000	-3.290596000	1.882960000
H	6.055680000	-2.640652000	2.778067000
H	5.477703000	-1.834067000	1.186617000

3-⁴ts2_(is, is)

Fe	2.326443000	-0.228393000	1.157284000
N	3.533985000	0.088831000	-0.570227000
N	2.170625000	-2.190889000	0.669094000
N	0.956917000	-0.539455000	2.786979000
N	2.344106000	1.730353000	1.563096000
C	4.055945000	1.278460000	-0.965062000
C	4.861142000	1.083857000	-2.168200000
H	5.395313000	1.862645000	-2.694711000
C	4.794972000	-0.248522000	-2.475244000
H	5.259238000	-0.765284000	-3.303200000
C	3.952318000	-0.874012000	-1.460822000
C	3.599490000	-2.212879000	-1.363403000
C	2.786741000	-2.817267000	-0.381639000
C	2.457977000	-4.233038000	-0.356775000
H	2.815048000	-4.952904000	-1.073426000
C	1.628731000	-4.435839000	0.712186000
H	1.171020000	-5.358697000	1.038289000
C	1.441080000	-3.148818000	1.360426000
C	0.632100000	-2.936572000	2.473061000
C	0.385765000	-1.722174000	3.139709000
C	-0.528952000	-1.508387000	4.256734000
H	-1.114487000	-2.278465000	4.739681000
C	-0.503106000	-0.168321000	4.539399000
H	-1.064879000	0.363897000	5.293757000
C	0.432357000	0.441710000	3.602137000
C	0.763528000	1.785321000	3.486012000
C	1.642595000	2.374091000	2.553357000
C	1.910575000	3.798138000	2.477877000
H	1.485934000	4.537899000	3.141658000
C	2.761543000	3.995741000	1.424237000
H	3.163915000	4.928281000	1.055850000
C	3.029309000	2.696612000	0.836173000
C	3.809339000	2.492110000	-0.299413000
Fe	-0.488522000	0.324194000	-0.919819000
N	-1.082563000	-1.593671000	-0.651131000
N	0.566734000	-0.228859000	-2.538764000
N	0.064870000	2.237381000	-1.199729000
N	-1.616830000	0.880651000	0.658664000
C	-1.884149000	-2.079099000	0.350958000
C	-2.061276000	-3.509484000	0.197628000
H	-2.659167000	-4.123251000	0.856056000
C	-1.350829000	-3.881870000	-0.906416000
H	-1.235882000	-4.866450000	-1.335969000
C	-0.732597000	-2.682459000	-1.435834000
C	0.079408000	-2.641026000	-2.549680000
C	0.686254000	-1.494130000	-3.055286000
C	1.562919000	-1.477840000	-4.211180000
H	1.812100000	-2.349336000	-4.799614000
C	1.980281000	-0.189931000	-4.375142000
H	2.646032000	0.215333000	-5.122870000
C	1.356748000	0.593625000	-3.327255000
C	1.524375000	1.951307000	-3.156917000
C	0.910026000	2.713690000	-2.167266000
C	1.072801000	4.149077000	-2.022698000
H	1.683783000	4.761488000	-2.670284000
C	0.313755000	4.528307000	-0.955981000
H	0.173502000	5.516118000	-0.542271000
C	-0.317875000	3.330092000	-0.438713000
C	-1.162693000	3.297422000	0.647898000
C	-1.768210000	2.151622000	1.154606000
C	-2.646718000	2.133868000	2.306910000
H	-2.937304000	3.012389000	2.864666000
C	-3.009797000	0.835228000	2.511476000
H	-3.656480000	0.425698000	3.273285000
C	-2.360627000	0.046969000	1.484527000

C	-2.480816000	-1.318585000	1.352385000
H	0.271785000	-3.575235000	-3.065428000
H	2.178004000	2.467149000	-3.851097000
H	-3.102329000	-1.838568000	2.071929000
H	-1.379116000	4.236285000	1.144362000
H	4.262008000	3.381533000	-0.727747000
H	0.283884000	2.471268000	4.177652000
H	3.988409000	-2.879100000	-2.127770000
H	0.116477000	-3.811883000	2.857133000
O	0.823823000	0.067867000	0.073186000
O	3.807625000	-0.571783000	2.220842000
O	-1.989280000	0.596844000	-2.082671000
C	-3.138782000	1.175015000	-1.713908000
O	-3.309002000	2.407361000	-1.604781000
C	-4.248424000	0.210974000	-1.401467000
C	-4.136996000	-1.153348000	-1.707399000
C	-5.389282000	0.692554000	-0.737663000
C	-5.159125000	-2.037765000	-1.348495000
H	-3.240885000	-1.500262000	-2.204738000
C	-6.378429000	-0.211131000	-0.379841000
H	-5.460984000	1.748833000	-0.511505000
C	-6.294282000	-1.571908000	-0.670719000
H	-5.071401000	-3.093491000	-1.583622000
H	-7.090041000	-2.246192000	-0.377501000
Cl	-7.868971000	0.405576000	0.530805000
H	3.672439000	-0.363088000	3.169625000
C	5.237304000	-2.582261000	2.468616000
H	6.028002000	-2.029720000	1.978494000
H	4.461419000	-3.049901000	1.878341000
H	5.202461000	-2.633786000	3.551361000

3-²ts2_(is, is)

Fe	2.399950000	-0.619095000	1.027586000
N	3.540381000	0.292905000	-0.356628000
N	2.310073000	-2.287449000	-0.151026000
N	1.035831000	-1.439833000	2.281812000
N	2.281537000	1.143044000	2.081857000
C	4.007662000	1.583975000	-0.320646000
C	4.844320000	1.839076000	-1.479099000
H	5.336447000	2.779884000	-1.680760000
C	4.863799000	0.692595000	-2.218479000
H	5.371005000	0.501422000	-3.152884000
C	4.041237000	-0.276983000	-1.521200000
C	3.781459000	-1.555186000	-1.973475000
C	2.965152000	-2.491827000	-1.335298000
C	2.671415000	-3.819272000	-1.843271000
H	3.069203000	-4.227076000	-2.761679000
C	1.820225000	-4.406203000	-0.950261000
H	1.373128000	-5.388778000	-0.991710000
C	1.589593000	-3.442258000	0.109197000
C	0.761404000	-3.637104000	1.197352000
C	0.500640000	-2.700917000	2.200642000
C	-0.401476000	-2.928025000	3.311583000
H	-0.944265000	-3.847009000	3.480601000
C	-0.418714000	-1.780069000	4.052348000
H	-0.985575000	-1.563611000	4.946151000
C	0.475436000	-0.842441000	3.402609000
C	0.699888000	0.454579000	3.829825000
C	1.529629000	1.384973000	3.204686000
C	1.698786000	2.763622000	3.626067000
H	1.216506000	3.205985000	4.486242000
C	2.545408000	3.352841000	2.729981000
H	2.892779000	4.375418000	2.704583000
C	2.902598000	2.338501000	1.756628000
C	3.711221000	2.537932000	0.653381000
Fe	-0.486040000	0.590006000	-0.902384000
N	-1.001753000	-1.319975000	-1.329151000
N	0.645737000	0.657715000	-2.560684000
N	-0.019175000	2.504989000	-0.488361000
N	-1.680204000	0.533053000	0.732446000
C	-1.783745000	-2.153822000	-0.573910000
C	-1.896443000	-3.448925000	-1.212508000
H	-2.469031000	-4.276133000	-0.818135000
C	-1.160629000	-3.390202000	-2.361527000

H	-0.997821000	-4.162077000	-3.099618000	C	1.518163000	2.458960000	2.618789000
C	-0.591820000	-2.059590000	-2.429628000	C	1.649964000	3.903220000	2.533681000
C	0.254301000	-1.611971000	-3.422690000	H	1.155058000	4.604495000	3.190516000
C	0.835627000	-0.345155000	-3.475019000	C	2.490152000	4.171522000	1.487613000
C	1.756380000	0.088650000	-4.507832000	H	2.815616000	5.135065000	1.121781000
H	2.063475000	-0.518779000	-5.347190000	C	2.883179000	2.895853000	0.913985000
C	2.128615000	1.364180000	-4.196734000	C	3.706586000	2.726179000	-0.198111000
H	2.804848000	2.019144000	-4.726356000	C	4.057169000	1.522433000	-0.808966000
C	1.430590000	1.722059000	-2.978303000	C	4.844562000	1.387933000	-2.019937000
C	1.526926000	2.943393000	-2.345535000	H	5.280798000	2.214397000	-2.562986000
C	0.833840000	3.309688000	-1.192115000	C	4.895251000	0.053741000	-2.326289000
C	0.918625000	4.617439000	-0.567600000	H	5.381704000	-0.420362000	-3.167082000
H	1.521404000	5.433686000	-0.939119000	C	4.141233000	-0.650175000	-1.306433000
C	0.101147000	4.588147000	0.522966000	C	3.904615000	-2.024153000	-1.268710000
H	-0.104865000	5.373302000	1.235473000	Fe	-0.693541000	0.180858000	-1.157234000
C	-0.485194000	3.263323000	0.575097000	N	0.375189000	-0.981005000	-2.483766000
C	-1.356598000	2.829204000	1.547773000	N	0.284513000	1.869627000	-1.852330000
C	-1.907453000	1.549630000	1.622813000	N	-1.493088000	1.301991000	0.408170000
C	-2.783911000	1.098473000	2.684299000	N	-1.343488000	-1.555181000	-0.192955000
H	-3.128233000	1.720593000	3.497688000	C	0.339414000	-2.360340000	-2.579654000
C	-3.065076000	-0.213961000	2.436767000	C	1.210812000	-2.777046000	-3.660207000
H	-3.688523000	-0.889734000	3.003243000	H	1.365127000	-3.803239000	-3.963603000
C	-2.371257000	-0.571037000	1.217175000	C	1.779039000	-1.644989000	-4.185339000
C	-2.412882000	-1.812331000	0.623650000	H	2.484193000	-1.569671000	-5.001403000
H	0.500887000	-2.304679000	-4.219876000	C	1.260217000	-0.515731000	-3.439654000
H	2.181775000	3.685632000	-2.788459000	C	1.619059000	0.817723000	-3.635525000
H	-3.001805000	-2.580081000	1.112069000	C	1.175749000	1.918353000	-2.901851000
H	-1.636259000	3.535651000	2.321015000	C	1.580511000	3.297237000	-3.110023000
H	4.138054000	3.526238000	0.520528000	H	2.268457000	3.626819000	-3.876053000
H	0.165090000	0.782720000	4.714702000	C	0.925891000	4.056723000	-2.176588000
H	4.236662000	-1.851601000	-2.912132000	H	0.975917000	5.126792000	-2.031743000
H	0.253456000	-4.592440000	1.272373000	C	0.114730000	3.154442000	-1.379310000
O	0.791503000	0.066635000	0.012579000	C	-0.679180000	3.522067000	-0.294942000
O	3.901218000	-1.248758000	2.028801000	C	-1.412392000	2.672864000	0.534442000
O	-1.981158000	1.227059000	-1.974983000	C	-2.174516000	3.081460000	1.698351000
C	-3.106689000	1.692305000	-1.430063000	H	-2.294972000	4.104757000	2.024926000
O	-3.267841000	2.861802000	-1.016621000	C	-2.691040000	1.945485000	2.265750000
C	-4.205525000	0.673597000	-1.296158000	H	-3.316028000	1.862573000	3.143840000
C	-4.149418000	-0.550000000	-1.978931000	C	-2.253868000	0.824593000	1.456010000
C	-5.268538000	0.940687000	-0.417696000	C	-2.538425000	-0.518401000	1.702202000
C	-5.149378000	-1.508331000	-1.785002000	C	-2.111784000	-1.614033000	0.953173000
H	-3.307942000	-0.736514000	-2.633542000	C	-2.416237000	-3.001375000	1.242123000
C	-6.231877000	-0.038582000	-0.226935000	H	-3.013136000	-3.336563000	2.078838000
H	-5.300598000	1.892117000	0.097487000	C	-1.819712000	-3.760489000	0.268274000
C	-6.202841000	-1.262565000	-0.893194000	H	-1.830352000	-4.836251000	0.159899000
H	-5.106168000	-2.454530000	-2.314870000	C	-1.138137000	-2.847667000	-0.629895000
H	-6.978149000	-1.999780000	-0.721705000	C	-0.375254000	-3.213937000	-1.739955000
Cl	-7.608445000	0.280889000	0.971782000	H	2.335185000	1.016480000	-4.425719000
H	4.066563000	-0.895998000	2.926229000	H	-0.708474000	4.578797000	-0.051981000
C	3.245306000	-3.239245000	3.881145000	H	-0.294609000	-4.276310000	-1.945111000
H	2.365484000	-2.760546000	4.294473000	H	-3.146162000	-0.733510000	2.574443000
H	4.139195000	-3.354268000	4.485560000	H	4.324772000	-2.610208000	-2.079135000
H	3.247833000	-3.549232000	2.846753000	H	4.081134000	3.631158000	-0.664625000

$3^{-10}\text{P}_{(\text{hs}, \text{hs})}$

Fe	2.267513000	-0.112231000	1.084762000	H	0.499231000	-3.882677000	2.896543000
N	2.509436000	-2.154982000	0.763092000	H	0.158010000	2.370325000	4.235757000
N	1.198872000	-0.551300000	2.830535000	O	0.938013000	0.016704000	0.093057000
N	2.286341000	1.879388000	1.630727000	O	3.943825000	-0.318221000	2.460581000
N	3.668510000	0.265871000	-0.385786000	O	-2.286525000	0.408735000	-2.187317000
C	3.140222000	-2.718001000	-0.331125000	C	-3.438960000	1.025965000	-1.873058000
C	2.861822000	-4.141790000	-0.354369000	O	-3.617725000	2.252795000	-1.990897000
H	3.233447000	-4.827327000	-1.102791000	C	-4.502142000	0.121177000	-1.325806000
C	2.048214000	-4.414118000	0.712920000	C	-4.352613000	-1.273501000	-1.333833000
H	1.626420000	-5.365246000	1.005594000	C	-5.648695000	0.704607000	-0.760214000
C	1.815420000	-3.161490000	1.407289000	C	-5.341389000	-2.086386000	-0.770740000
C	0.995955000	-2.993279000	2.523659000	H	-3.454319000	-1.699016000	-1.760550000
C	0.688602000	-1.794937000	3.166970000	C	-6.607416000	-0.127331000	-0.202339000
C	-0.256252000	-1.637643000	4.254676000	H	-5.750072000	1.782539000	-0.764932000
H	-0.798272000	-2.449492000	4.718829000	C	-6.483355000	-1.515981000	-0.192574000
C	-0.333223000	-0.299117000	4.537226000	H	-5.219347000	-3.164238000	-0.767336000
H	-0.950451000	0.191719000	5.276394000	H	-7.254842000	-2.132200000	0.253441000
C	0.564311000	0.386358000	3.628938000	Cl	-8.110785000	0.629455000	0.569675000
C	0.731518000	1.767762000	3.539527000	H	3.513642000	-0.649061000	3.275305000
				C	5.134634000	-1.091309000	2.094616000
				H	5.512178000	-0.621668000	1.188120000
				H	5.875727000	-1.024268000	2.897664000

H 4.865399000 -2.131274000 1.887154000

3-²P_(hs, hs)

Fe 2.181257000 -0.117228000 1.142850000
N 2.589591000 -2.141480000 0.758109000
N 1.061070000 -0.710107000 2.822388000
N 2.078792000 1.853376000 1.800473000
N 3.660481000 0.413786000 -0.218303000
C 3.317872000 -2.609181000 -0.313822000
C 3.125055000 -4.047641000 -0.422961000
H 3.585534000 -4.676538000 -1.172484000
C 2.264680000 -4.417713000 0.576476000
H 1.882575000 -5.404811000 0.795389000
C 1.917846000 -3.212729000 1.313656000
C 1.020643000 -3.140540000 2.381637000
C 0.605289000 -1.990467000 3.063896000
C -0.415655000 -1.939032000 4.097747000
H -0.938513000 -2.799761000 4.491316000
C -0.580723000 -0.622704000 4.440418000
H -1.268785000 -0.203599000 5.160774000
C 0.337096000 0.154535000 3.624975000
C 0.440618000 1.546832000 3.616199000
C 1.244278000 2.332466000 2.781515000
C 1.312096000 3.788122000 2.789251000
H 0.759880000 4.427915000 3.463575000
C 2.186935000 4.156199000 1.803510000
H 2.481581000 5.154272000 1.511862000
C 2.666638000 2.932832000 1.175809000
C 3.551568000 2.860216000 0.099041000
C 4.001134000 1.705749000 -0.553171000
C 4.867168000 1.674771000 -1.722069000
H 5.292788000 2.547913000 -2.197071000
C 5.015038000 0.361547000 -2.083058000
H 5.579137000 -0.042114000 -2.911987000
C 4.244313000 -0.433149000 -1.140412000
C 4.090737000 -1.820695000 -1.174315000
Fe -0.566006000 0.169831000 -1.133243000
N 0.689739000 -0.147845000 -2.759615000
N -0.211821000 2.228916000 -1.228754000
N -1.882067000 0.487913000 0.482078000
N -0.960353000 -1.888080000 -1.025726000
C 1.050751000 -1.364230000 -3.274631000
C 2.059422000 -1.162100000 -4.301982000
H 2.521341000 -1.949208000 -4.881206000
C 2.297913000 0.186804000 -4.370524000
H 2.994674000 0.707522000 -5.011464000
C 1.436937000 0.822975000 -3.387340000
C 1.392608000 2.191055000 -3.089527000
C 0.628580000 2.849269000 -2.109335000
C 0.617348000 4.282771000 -1.846692000
H 1.187031000 5.018193000 -2.396928000
C -0.241707000 4.490658000 -0.801633000
H -0.507113000 5.427227000 -0.333257000
C -0.764114000 3.188535000 -0.413348000
C -1.665093000 2.934905000 0.621538000
C -2.182178000 1.694057000 1.047298000
C -3.084245000 1.484171000 2.168507000
H -3.498187000 2.268095000 2.786429000
C -3.296838000 0.133746000 2.265065000
H -3.916844000 -0.393094000 2.975550000
C -2.530526000 -0.494728000 1.202340000
C -2.442827000 -1.861577000 0.942278000
C -1.712216000 -2.515050000 -0.071388000
C -1.613029000 -3.952865000 -0.256374000
H -2.111808000 -4.692345000 0.354242000
C -0.773486000 -4.164107000 -1.321044000
H -0.453464000 -5.107727000 -1.739230000
C -0.354208000 -2.857105000 -1.797830000
C 0.556491000 -2.604576000 -2.829492000
H 2.040631000 2.824999000 -3.687911000
H -2.010439000 3.803405000 1.174132000
H 0.957631000 -3.480313000 -3.331847000
H -3.003422000 -2.508074000 1.610632000
H 4.602910000 -2.342509000 -1.976925000

H 3.912869000 3.806083000 -0.292840000
H 0.560965000 -4.075042000 2.688461000
H -0.193282000 2.080444000 4.317724000
O 0.807485000 -0.034977000 0.031796000
O 3.888707000 -0.334007000 2.699240000
O -2.165396000 0.482922000 -2.379926000
C -3.276097000 1.087668000 -1.993368000
O -3.452397000 2.331154000 -1.962884000
C -4.353096000 0.161370000 -1.482218000
C -4.291223000 -1.220172000 -1.714773000
C -5.388164000 0.694431000 -0.697459000
C -5.254783000 -2.070343000 -1.162751000
H -3.468947000 -1.604506000 -2.304999000
C -6.315895000 -0.175605000 -0.143550000
H -5.424415000 1.763485000 -0.532007000
C -6.279446000 -1.551857000 -0.357306000
H -5.208318000 -3.139415000 -1.346060000
H -7.026607000 -2.197718000 0.088276000
Cl -7.652991000 0.512920000 0.942029000
H 3.403690000 -0.812675000 3.401389000
C 5.118832000 -1.022415000 2.308641000
H 5.832841000 -1.028174000 3.140181000
H 4.902615000 -2.041544000 1.971875000
H 5.516534000 -0.444410000 1.475249000

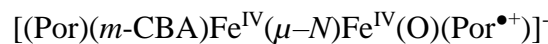
3-⁶P_(is, is)

Fe 2.340273620 -0.123844373 1.070656567
N 3.530240776 0.702889963 -0.326016456
N 2.749581120 -1.958897609 0.322004988
N 1.341876873 -0.986772829 2.607836877
N 2.045634316 1.680890653 1.900221255
C 3.770032467 2.056069035 -0.508543174
C 4.548130661 2.257397837 -1.708268257
H 4.868365152 3.223274658 -2.071591159
C 4.755549521 1.025363895 -2.264990107
H 5.281944473 0.777858192 -3.175683764
C 4.109766711 0.057945822 -1.409006288
C 4.063856134 -1.304069905 -1.657626788
C 3.423952615 -2.236137374 -0.856806923
C 3.364642958 -3.652424612 -1.132735800
H 3.811031945 -4.124411760 -1.996118677
C 2.645117848 -4.229197422 -0.122278109
H 2.381993626 -5.269012264 0.008787466
C 2.253911512 -3.170287553 0.778788781
C 1.477342592 -3.351350047 1.912607374
C 1.043513198 -2.336330255 2.750088881
C 0.1623557040 -2.524940964 3.878535483
H -0.214506931 -3.483924442 4.202619924
C -0.095167606 -1.286482964 4.399812851
H -0.726249556 -1.027822532 5.237961546
C 0.627556919 -0.327714939 3.599000411
C 0.581207946 1.044961636 3.779672769
C 1.240166301 1.971568170 2.988654495
C 1.182530014 3.402387975 3.186641474
H 0.615445629 3.886550026 3.968528012
C 1.955334759 3.973553407 2.215025435
H 2.150251780 5.021407928 2.037716052
C 2.488219895 2.897803085 1.409867381
C 3.298128378 3.076283332 0.300818928
Fe -0.603747229 0.173440662 -0.972395644
N 0.362920482 -0.591991943 -2.556903916
N -0.040145532 2.028228745 -1.507474325
N -1.632047550 0.936552151 0.589454618
N -1.179381531 -1.690664742 -0.424241963
C 0.450329100 -1.925136349 -2.910383634
C 1.285307333 -2.063721568 -4.084060846
H 1.504545112 -3.005490830 -4.567185678
C 1.708287958 -0.809726457 -4.425190176
H 2.343171791 -0.511433724 -5.247601673
C 1.130423608 0.107897274 -3.467346398
C 1.332258066 1.477819973 -3.474253669
C 0.781059005 2.363095781 -2.563951885
C 0.982958313 3.797212185 -2.589270323
H 1.580853567 4.314833965 -3.325928102

C	0.272490045	4.318379558	-1.546212688	C	0.651228637	1.102674606	3.766905146
H	0.166368299	5.352184106	-1.249754416	C	1.298282796	2.018824403	2.953096980
C	-0.363927573	3.207604757	-0.869780190	C	1.257244227	3.452573764	3.140881549
C	-1.155630569	3.329275963	0.257429979	H	0.714301379	3.947936069	3.932897020
C	-1.736158760	2.271136935	0.934000400	C	2.011583744	4.009137778	2.146901463
C	-2.520429490	2.402864366	2.140862889	H	2.212435255	5.053804280	1.957494188
H	-2.763081506	3.346548583	2.608123977	C	2.516786507	2.921600625	1.337986150
C	-2.873211869	1.141252903	2.530562922	C	3.304224638	3.082681481	0.209617921
H	-3.467502860	0.838254551	3.380854150	Fe	-0.597729722	0.153389017	-0.931940313
C	-2.310746440	0.225722084	1.563288142	N	-1.169743896	-1.703967173	-0.354355306
C	-2.437047222	-1.150858999	1.622452831	N	0.335791673	-0.632313366	-2.528306807
C	-1.909357532	-2.034739498	0.697120497	N	-0.056476205	2.002235887	-1.509110399
C	-2.079883599	-3.469689801	0.746690646	N	-1.606944138	0.936951606	0.631655879
H	-2.623504487	-3.991405286	1.521616265	C	-1.892384765	-2.032583191	0.776144044
C	-1.449070477	-3.986311346	-0.351179050	C	-2.064647983	-3.466463413	0.844549188
H	-1.365166752	-5.019414718	-0.658209141	H	-2.602827082	-3.977698442	1.630129542
C	-0.881600063	-2.870734341	-1.077391819	C	-1.441685618	-3.997679381	-0.250702837
C	-0.134524754	-2.985002891	-2.238353415	H	-1.360743412	-5.034640042	-0.545085439
H	1.967805942	1.887450668	-4.251147107	C	-0.878559336	-2.892328429	-0.995429645
H	-1.326592509	4.326501688	0.645932610	C	-0.145565604	-3.021967780	-2.163547443
H	0.027494383	-3.980911257	-2.635340674	C	0.422854507	-1.970360244	-2.861908437
H	-2.999636643	-1.567134393	2.449976223	C	1.231420647	-2.122812950	-4.052228998
H	3.548690726	4.093140004	0.021754363	H	1.446053484	-3.071145513	-4.524337101
H	-0.036980693	1.423723787	4.585156034	C	1.636694933	-0.872060124	-4.424404967
H	4.540178291	-1.664327590	-2.561927231	H	2.250101848	-0.583106470	-5.266141435
H	1.144800221	-4.358689223	2.135009094	C	1.075726233	0.057598189	-3.468197299
O	0.785940808	0.025674388	-0.008920648	C	1.267507361	1.428464331	-3.502603467
O	4.147124534	-0.417434698	2.401784818	C	0.734517347	2.324499079	-2.592355807
O	-2.166872708	0.329593346	-2.053112924	C	0.929875929	3.758676148	-2.643246709
C	-3.295632371	0.977210903	-1.734945733	H	1.506070884	4.267556031	-3.402848359
O	-3.445889764	2.213140934	-1.816424874	C	0.247492738	4.292007148	-1.587906955
C	-4.405473519	0.090914370	-1.245733934	H	0.146705889	5.329334391	-1.302294208
C	-4.305446699	-1.306724634	-1.308844031	C	-0.366678506	3.189231231	-0.878980821
C	-5.541248976	0.691008886	-0.676129771	C	-1.131086397	3.324804574	0.265113199
C	-5.333964745	-2.106015409	-0.799776634	C	-1.700543290	2.275410063	0.963755291
H	-3.413395280	-1.742727697	-1.738214582	C	-2.467825673	2.422340063	2.179632828
C	-6.538408518	-0.128149044	-0.169357471	H	-2.699110030	3.371774410	2.640886943
H	-5.603520333	1.771144589	-0.638312754	C	-2.822563500	1.166668884	2.585543534
C	-6.465635216	-1.519500005	-0.216925947	H	-3.406709533	0.874703724	3.446617880
H	-5.253338532	-3.187302708	-0.844110749	C	-2.277086359	0.238628055	1.620574130
H	-7.267220583	-2.125137006	0.188722306	C	-2.408827178	-1.136451704	1.695951894
Cl	-8.028351937	0.650722289	0.611495353	H	0.013689551	-4.023151402	-2.547941818
H	3.806626460	-0.981281525	3.124374484	H	1.880959145	1.829436104	-4.301344655
C	5.372165256	-0.958734537	1.805878371	H	-2.963382820	-1.541384395	2.534384630
H	6.174082523	-0.983682111	2.551279418	H	-1.292118061	4.326443103	0.646128337
H	5.625092825	-0.269611266	1.001247790	H	3.555907682	4.095062690	-0.084589981
H	5.189694109	-1.954862685	1.389735102	H	0.053161701	1.493090690	4.582047864

3-²P_(is, is)

Fe	2.324311126	-0.102727114	1.018977731	C	5.201639788	-1.915160516	1.328692067
N	3.517222899	0.702231979	-0.394791470				
N	2.754617697	-1.954604425	0.311432557				
N	1.380027467	-0.947280865	2.607004936				
N	2.074630985	1.714471077	1.848878065				
C	3.758188040	2.051320897	-0.596796063				
C	4.522813970	2.234125860	-1.809182527				
H	4.842374432	3.193899436	-2.189032656				
C	4.721764676	0.994033406	-2.350374465				
H	5.239275588	0.732340698	-3.262233370				
C	4.084207862	0.039661969	-1.472462302				
C	4.040437511	-1.327497328	-1.695198531				
C	3.418299372	-2.249367123	-0.868170147				
C	3.370676738	-3.672806456	-1.112174380				
H	3.813238307	-4.159514828	-1.969396295				
C	2.668661907	-4.234189569	-0.081272126				
H	2.419005013	-5.273711692	0.076255767				
C	2.276361751	-3.158992243	0.801279788				
C	1.514752809	-3.321824766	1.948559750				
C	1.088317260	-2.294293912	2.775515859				
C	0.230662319	-2.466235003	3.924518795				
H	-0.138691506	-3.420504872	4.271869202				
C	-0.018217035	-1.220326774	4.432309399				
H	-0.631012008	-0.949695173	5.280238389				
C	0.688018368	-0.272847785	3.602515074				



(4)

$^{10}4_{(hs, hs)}$ OR $4^{-10}R_{(hs, hs)}$

Fe	0.481464000	-0.036211000	-1.074647000
N	-1.101181000	0.024137000	0.212667000
N	1.193770000	1.609182000	-0.006854000
N	-0.523235000	1.241195000	-2.358394000
N	-0.477205000	-1.662526000	-1.925451000
N	1.358954000	-1.302572000	0.349759000
C	1.006226000	2.932621000	-0.347550000
C	1.722327000	3.761992000	0.603021000
H	1.746495000	4.843011000	0.579811000
C	2.319980000	2.920901000	1.507983000
H	2.930005000	3.183294000	2.361327000
C	1.983802000	1.564453000	1.124078000
C	2.413019000	0.406169000	1.775376000
H	3.023258000	0.549565000	2.660604000
C	2.126173000	-0.914024000	1.424593000
C	2.559443000	-2.102178000	2.140777000
H	3.179524000	-2.094130000	3.026413000
C	2.026250000	-3.183414000	1.490340000
H	2.125632000	-4.230034000	1.742419000
C	1.258261000	-2.674322000	0.366523000
C	0.501911000	-3.441797000	-0.521611000
H	0.517798000	-4.515092000	-0.364364000
C	-0.299854000	-2.981347000	-1.567252000
C	-1.096444000	-3.811853000	-2.452390000
H	-1.148233000	-4.890626000	-2.400173000
C	-1.742359000	-2.974808000	-3.324964000
H	-2.423685000	-3.238495000	-4.122249000
C	-1.348410000	-1.617661000	-2.990703000
C	-1.774302000	-0.456975000	-3.641525000
H	-2.490165000	-0.589389000	-4.446201000
C	-1.405405000	0.857401000	-3.347105000
C	-1.914550000	2.048279000	-4.003280000
H	-2.626031000	2.044515000	-4.817815000
C	-1.343988000	3.130194000	-3.383867000
H	-1.501326000	4.179290000	-3.594468000
C	-0.477679000	2.619566000	-2.336568000
C	0.242299000	3.393005000	-1.423917000
H	0.165521000	4.469797000	-1.535583000
Fe	-2.589084000	0.077793000	1.425071000
N	-2.531752000	2.126429000	1.015911000
N	-1.153098000	0.355169000	2.915393000
N	-2.323732000	-1.987479000	1.580374000
N	-3.708771000	-0.217801000	-0.314884000
C	-1.837739000	3.072489000	1.734715000
C	-2.100727000	4.381866000	1.157129000
H	-1.680732000	5.309844000	1.521104000
C	-2.938309000	4.192406000	0.090038000
H	-3.336622000	4.935387000	-0.587709000
C	-3.202772000	2.764329000	-0.001097000
C	-3.982606000	2.141051000	-0.977909000
H	-4.430284000	2.789668000	-1.724544000
C	-4.210396000	0.771168000	-1.128209000
C	-4.984616000	0.151008000	-2.192857000
H	-5.492124000	0.693084000	-2.979439000
C	-4.920590000	-1.204088000	-2.003454000
H	-5.364129000	-1.985281000	-2.605949000
C	-4.104576000	-1.434504000	-0.821201000
C	-3.750438000	-2.682846000	-0.306202000
H	-4.129029000	-3.549645000	-0.838930000
C	-2.924109000	-2.939680000	0.790098000
C	-2.531888000	-4.257217000	1.266614000
H	-2.854670000	-5.191414000	0.827147000
C	-1.691852000	-4.068112000	2.331993000
H	-1.193982000	-4.817686000	2.932225000
C	-1.557381000	-2.632129000	2.523450000
C	-0.758799000	-2.010391000	3.485679000
H	-0.198692000	-2.666053000	4.145114000
C	-0.566058000	-0.638874000	3.663204000
C	0.316218000	-0.025567000	4.644051000
H	0.910079000	-0.572475000	5.364018000
C	0.249171000	1.329808000	4.456705000
H	0.777295000	2.106074000	4.993987000
C	-0.674846000	1.566148000	3.357989000

C	-0.996400000	2.813644000	2.818292000
H	-0.509877000	3.673703000	3.267811000
O	-3.920368000	0.149048000	2.471204000
O	2.108357000	-0.201518000	-2.193392000
C	3.241711000	-0.865355000	-2.016914000
O	3.425329000	-2.069531000	-2.309507000
C	4.358453000	-0.057829000	-1.398504000
C	5.546954000	-0.715734000	-1.038009000
C	4.218236000	1.316555000	-1.158660000
C	6.553740000	0.023340000	-0.437267000
H	5.636392000	-1.776986000	-1.232935000
C	5.253777000	2.033796000	-0.550387000
H	3.287074000	1.795138000	-1.430008000
C	6.441127000	1.388217000	-0.178825000
H	5.131069000	3.092911000	-0.348351000
H	7.250952000	1.927152000	0.298521000
Cl	8.131876000	-0.836388000	0.056270000

 $^{84}4_{(hs, hs)}$ OR $4^{-8}R_{(hs, hs)}$

Fe	0.363274000	-0.090953000	-1.051756000
N	-0.959943000	0.018263000	0.200809000
N	0.953578000	1.766357000	-0.557826000
N	-0.868609000	0.673625000	-2.432758000
N	-0.239954000	-1.941694000	-1.513507000
N	1.610371000	-0.845937000	0.329484000
C	0.637350000	2.937307000	-1.220019000
C	1.255732000	4.057898000	-0.545346000
H	1.160623000	5.086922000	-0.862990000
C	1.916001000	3.556144000	0.541945000
H	2.488352000	4.086292000	1.290118000
C	1.733002000	2.122607000	0.525206000
C	2.347284000	1.242200000	1.399768000
H	2.938314000	1.662788000	2.203777000
C	2.317926000	-0.135763000	1.281291000
C	3.090438000	-1.048431000	2.094139000
H	3.741330000	-0.741159000	2.900057000
C	2.849698000	-2.307591000	1.622448000
H	3.252429000	-3.247937000	1.971048000
C	1.904905000	-2.180823000	0.535141000
C	1.317169000	-3.243867000	-0.128125000
H	1.640263000	-4.243019000	0.140036000
C	0.299177000	-3.126546000	-1.058004000
C	-0.421847000	-4.242151000	-1.634328000
H	-0.192704000	-5.279764000	-1.437089000
C	-1.407025000	-3.718033000	-2.420485000
H	-2.150548000	-4.235623000	-3.010181000
C	-1.279350000	-2.276459000	-2.355086000
C	-2.042117000	-1.384531000	-3.090129000
H	-2.841284000	-1.790768000	-3.698328000
C	-1.826339000	-0.017358000	-3.145404000
C	-2.527107000	0.892555000	-4.026847000
H	-3.329327000	0.599390000	-4.689424000
C	-1.969323000	2.127512000	-3.853008000
H	-2.227081000	3.060068000	-4.335469000
C	-0.942310000	1.990061000	-2.841386000
C	-0.217233000	3.042184000	-2.306069000
H	-0.392178000	4.031801000	-2.713710000
Fe	-2.428951000	0.129645000	1.566097000
N	-2.676292000	2.051631000	0.797918000
N	-0.927790000	0.849694000	2.822308000
N	-1.843234000	-1.819520000	2.019509000
N	-3.638483000	-0.614046000	0.039617000
C	-2.055968000	3.190849000	1.257190000
C	-2.514957000	4.323878000	0.468937000
H	-2.182256000	5.343401000	0.608406000
C	-3.400301000	3.840129000	-0.456952000
H	-3.934108000	4.386875000	-1.222318000
C	-3.497646000	2.403861000	-0.248514000
C	-4.284751000	1.526559000	-0.995730000
H	-4.879441000	1.966705000	-1.789939000
C	-4.356999000	0.139533000	-0.859463000
C	-5.160417000	-0.751570000	-1.680584000
H	-5.821415000	-0.427708000	-2.473176000
C	-4.895005000	-2.030550000	-1.267786000

H	-5.297173000	-2.956206000	-1.657041000
C	-3.923699000	-1.940306000	-0.189784000
C	-3.330220000	-3.021553000	0.462882000
H	-3.628216000	-4.011146000	0.130978000
C	-2.355905000	-2.967632000	1.460534000
C	-1.698153000	-4.116356000	2.063313000
H	-1.900801000	-5.146192000	1.802918000
C	-0.794222000	-3.633928000	2.971413000
H	-0.114086000	-4.192230000	3.600057000
C	-0.886112000	-2.182502000	2.939265000
C	-0.118808000	-1.303780000	3.705187000
H	0.595756000	-1.753752000	4.387036000
C	-0.141779000	0.090729000	3.657976000
C	0.698746000	0.978765000	4.444654000
H	1.418358000	0.650046000	5.182170000
C	0.411332000	2.259411000	4.052658000
H	0.850472000	3.182068000	4.407543000
C	-0.606970000	2.172951000	3.018424000
C	-1.124469000	3.248108000	2.294910000
H	-0.730092000	4.229946000	2.537309000
O	-3.644668000	0.225937000	2.699750000
O	1.789174000	-0.231627000	-2.487587000
C	2.927095000	-0.865062000	-2.300653000
C	4.026629000	-0.044833000	-1.653270000
C	5.125809000	-0.707648000	-1.080750000
C	3.948123000	1.353237000	-1.595322000
C	6.095418000	0.051605000	-0.445766000
H	5.175368000	-1.786890000	-1.144771000
C	4.953102000	2.092074000	-0.962386000
H	3.078001000	1.832158000	-2.024512000
C	6.043616000	1.441843000	-0.367857000
H	4.878250000	3.173813000	-0.908555000
H	6.823833000	1.995857000	0.140702000
Cl	7.541777000	-0.817732000	0.356010000
O	3.167012000	-2.063965000	-2.600654000

${}^2_4(\text{hs, hs})$ or $4\text{-}^2\mathbf{R}(\text{hs, hs})$

Fe	-2.477327000	0.224134000	1.390967000
N	-0.964018000	0.041122000	0.135753000
N	-1.341185000	1.718826000	2.283451000
N	-1.484559000	-1.204045000	2.543447000
N	-3.299065000	-1.303287000	0.247521000
N	-3.210082000	1.627718000	0.030348000
C	-0.469468000	1.545049000	3.335364000
C	0.040088000	2.844801000	3.736690000
H	0.751661000	3.004450000	4.535318000
C	-0.535910000	3.778037000	2.915525000
H	-0.387299000	4.849290000	2.912591000
C	-1.406244000	3.064573000	1.997282000
C	-2.167068000	3.644841000	0.981435000
H	-2.082619000	4.720989000	0.868959000
C	-2.989874000	2.984876000	0.068169000
C	-3.717715000	3.607799000	-1.026223000
H	-3.718287000	4.668178000	-1.239369000
C	-4.352556000	2.605877000	-1.710782000
H	-4.973454000	2.686979000	-2.592640000
C	-4.023717000	1.355444000	-1.044185000
C	-4.440404000	0.085086000	-1.444431000
H	-5.067719000	0.037758000	-2.328688000
C	-4.110093000	-1.134751000	-0.853210000
C	-4.555882000	-2.441570000	-1.305174000
H	-5.198562000	-2.608376000	-2.158765000
C	-3.999540000	-3.372751000	-0.468883000
H	-4.097937000	-4.448989000	-0.506129000
C	-3.202230000	-2.652049000	0.508614000
C	-2.447653000	-3.230713000	1.529651000
H	-2.453102000	-4.314612000	1.580142000
C	-1.651077000	-2.566628000	2.462921000
C	-0.830817000	-3.199808000	3.484102000
H	-0.761559000	-4.267503000	3.641487000
C	-0.176505000	-2.200864000	4.153219000
H	0.532687000	-2.291708000	4.964571000
C	-0.586358000	-0.941281000	3.551466000
C	-0.123877000	0.323449000	3.915283000

H	0.602544000	0.359975000	4.720639000
Fe	0.343664000	-0.178257000	-0.906193000
N	1.677547000	-0.119080000	0.689033000
N	0.523542000	1.899823000	-1.082918000
N	-0.911353000	-0.218094000	-2.548848000
N	0.214262000	-2.235871000	-0.737182000
C	2.222268000	1.007850000	1.260514000
C	3.068250000	0.605114000	2.371012000
H	3.633951000	1.287560000	2.990364000
C	3.005134000	-0.760012000	2.455111000
H	3.505117000	-1.410577000	3.159385000
C	2.115032000	-1.215639000	1.400863000
C	1.749266000	-2.540303000	1.162520000
H	2.187550000	-3.285669000	1.817889000
C	0.881007000	-3.012670000	0.178202000
C	0.545916000	-4.406256000	-0.062401000
H	0.934373000	-5.238382000	0.508579000
C	-0.311738000	-4.437170000	-1.128813000
H	-0.763515000	-5.300078000	-1.598949000
C	-0.512650000	-3.062334000	-1.558782000
C	-1.301504000	-2.649201000	-2.633258000
H	-1.835264000	-3.428510000	-3.167814000
C	-1.489493000	-1.342689000	-3.087935000
C	-2.338718000	-0.941698000	-4.198756000
H	-2.916198000	-1.623749000	-4.808158000
C	-2.258687000	0.422124000	-4.297641000
H	-2.756343000	1.071976000	-5.004820000
C	-1.356255000	0.876723000	-3.250727000
C	-1.005011000	2.204402000	-2.997146000
H	-1.468981000	2.954996000	-3.629381000
C	-0.151659000	2.677552000	-1.998454000
C	0.152829000	4.073767000	-1.734305000
H	-0.239436000	4.906054000	-2.303075000
C	0.990489000	4.109552000	-0.649456000
H	1.415095000	4.976557000	-0.161531000
C	1.213079000	2.735900000	-0.232978000
C	2.001840000	2.320086000	0.840662000
H	2.487124000	3.100177000	1.417737000
O	-3.762374000	0.365309000	2.434553000
O	1.858634000	-0.441079000	-2.136468000
C	2.998766000	-1.063796000	-1.888288000
C	4.136587000	-0.161120000	-1.468413000
C	4.003717000	1.233478000	-1.507067000
C	5.334159000	-0.740594000	-1.016580000
C	5.060071000	2.052036000	-1.094435000
H	3.060850000	1.647013000	-1.840310000
C	6.358545000	0.098310000	-0.607569000
H	5.417293000	-1.819837000	-0.998253000
C	6.257702000	1.487778000	-0.633258000
H	4.950828000	3.132138000	-1.116616000
H	7.083090000	2.106782000	-0.301944000
O	3.194760000	-2.298769000	-1.990889000
Cl	7.949253000	-0.655459000	0.011537000

${}^6_4(\text{is, is})$ or $4\text{-}^6\mathbf{R}(\text{is, is})$

Fe	0.473965000	-0.123208000	-1.058635000
N	-0.988772000	0.017102000	0.108594000
N	1.591026000	-1.021554000	0.380399000
N	1.051747000	1.670107000	-0.361248000
N	-0.670606000	0.787520000	-2.451950000
N	-0.278982000	-1.899730000	-1.567316000
C	2.366023000	-0.402658000	1.342426000
C	3.024363000	-1.397564000	2.164835000
H	3.697767000	-1.166945000	2.978415000
C	2.626313000	-2.619516000	1.704209000
H	2.900180000	-3.600862000	2.065642000
C	1.715857000	-2.378813000	0.603173000
C	1.018787000	-3.365910000	-0.070583000
H	1.197880000	-4.395360000	0.218618000
C	0.079644000	-3.135381000	-1.062041000
C	-0.682278000	-4.172066000	-1.719242000
H	-0.586555000	-5.226942000	-1.503373000
C	-1.502334000	-3.554788000	-2.622759000
H	-2.216970000	-3.999372000	-3.301375000

C	-1.240709000	-2.135903000	-2.532330000	N	-0.982445000	0.017996000	0.133671000
C	-1.844308000	-1.179606000	-3.334344000	N	-3.603288000	-0.310312000	-0.400028000
H	-2.595283000	-1.521920000	-4.037777000	N	-2.561789000	2.093882000	0.789844000
C	-1.567855000	0.177326000	-3.301400000	N	-1.233405000	0.538200000	2.766648000
C	-2.212085000	1.172333000	-4.138233000	N	-2.274748000	-1.865702000	1.576810000
H	-2.956754000	0.948213000	-4.889608000	C	-4.147032000	0.606130000	-1.276060000
C	-1.704348000	2.386225000	-3.773480000	C	-4.904860000	-0.086727000	-2.298720000
H	-1.948883000	3.366133000	-4.159925000	H	-5.425513000	0.405038000	-3.108827000
C	-0.755086000	2.140243000	-2.703849000	C	-4.806388000	-1.423232000	-2.032850000
C	-0.095504000	3.128931000	-1.992324000	H	-5.229052000	-2.254684000	-2.579760000
H	-0.271313000	4.159444000	-2.281704000	C	-3.987850000	-1.558650000	-0.845201000
C	0.722744000	2.906453000	-0.894461000	C	-3.637103000	-2.766167000	-0.262034000
C	1.356319000	3.952172000	-0.126248000	H	-3.994854000	-3.673679000	-0.735709000
H	1.255354000	5.008112000	-0.336098000	C	-2.839190000	-2.902886000	0.862965000
C	2.058772000	3.343331000	0.879108000	C	-2.458746000	-4.168938000	1.456319000
H	2.656649000	3.797425000	1.656925000	H	-2.765350000	-5.135162000	1.080186000
C	1.870910000	1.921295000	0.726618000	C	-1.658349000	-3.883013000	2.525789000
C	2.484602000	0.964046000	1.518482000	H	-1.172132000	-4.566178000	3.208362000
H	3.110020000	1.314447000	2.331257000	C	-1.543150000	-2.439901000	2.595308000
Fe	-2.484088000	0.147550000	1.434426000	C	-0.793987000	-1.757947000	3.541477000
N	-2.703869000	2.044862000	0.767862000	H	-0.252954000	-2.352675000	4.269235000
N	-1.090007000	0.787100000	2.753507000	C	-0.653048000	-0.381146000	3.615937000
N	-2.036588000	-1.768035000	1.902453000	C	0.153178000	0.308129000	4.603479000
N	-3.673366000	-0.509536000	-0.064388000	H	0.719434000	-0.186945000	5.380196000
C	-2.126607000	3.179622000	1.300567000	C	0.056018000	1.644333000	4.336897000
C	-2.552032000	4.345132000	0.552459000	H	0.525898000	2.472234000	4.849603000
H	-2.234018000	5.356109000	0.766865000	C	-0.810474000	1.783557000	3.183936000
C	-3.377651000	3.900971000	-0.441297000	C	-1.143814000	2.989856000	2.588244000
H	-3.879991000	4.471928000	-1.209906000	H	-0.716466000	3.892154000	3.011576000
C	-3.470318000	2.461852000	-0.301931000	C	-1.956738000	3.127919000	1.473982000
C	-4.221195000	1.641207000	-1.128081000	C	-2.284542000	4.390153000	0.842267000
H	-4.762419000	2.111585000	-1.941772000	H	-1.928868000	5.352847000	1.182715000
C	-4.317884000	0.264155000	-1.008317000	C	-3.084956000	4.104184000	-0.227299000
C	-5.106926000	-0.581323000	-1.880826000	H	-3.520962000	4.783727000	-0.946479000
H	-5.702818000	-0.217289000	-2.706445000	C	-3.253179000	2.664849000	-0.258339000
C	-4.928104000	-1.868005000	-1.457304000	C	-3.989294000	1.981972000	-1.213908000
H	-5.344668000	-2.778707000	-1.865160000	H	-4.460562000	2.571846000	-1.992538000
C	-4.021237000	-1.818657000	-0.328617000	Fe	0.351494000	-0.076881000	-0.820740000
C	-3.538759000	-2.933017000	0.339150000	N	-0.516840000	1.067383000	-2.239911000
H	-3.881709000	-3.905327000	0.002289000	N	-0.355544000	-1.731981000	-1.716356000
C	-2.601297000	-2.904454000	1.358837000	N	1.311597000	-1.221700000	0.540127000
C	-2.032332000	-4.082337000	1.981988000	N	1.138793000	1.579680000	0.029235000
H	-2.302395000	-5.097507000	1.726159000	C	-1.313840000	0.629295000	-3.275944000
C	-1.111613000	-3.646179000	2.891596000	C	-1.790685000	1.762286000	-4.043404000
H	-0.471434000	-4.228829000	3.539244000	H	-2.434975000	1.684726000	-4.908354000
C	-1.118747000	-2.198076000	2.839326000	C	-1.273511000	2.883579000	-3.460093000
C	-0.319056000	-1.382091000	3.623198000	H	-1.406030000	3.918102000	-3.745453000
H	0.369980000	-1.865276000	4.306996000	C	-0.478907000	2.443278000	-2.330868000
C	-0.317313000	0.002892000	3.585812000	C	0.208872000	3.290976000	-1.478495000
C	0.517512000	0.844498000	4.418693000	H	0.140698000	4.356382000	-1.669190000
H	1.220016000	0.471151000	5.150858000	C	0.960395000	2.884732000	-0.387415000
C	0.243520000	2.138714000	4.078530000	C	1.682038000	3.778962000	0.491426000
H	0.676800000	3.047937000	4.471879000	H	1.704309000	4.854392000	0.380693000
C	-0.753238000	2.097378000	3.027974000	C	2.287342000	3.004194000	1.441907000
C	-1.239940000	3.212171000	2.364998000	H	2.913364000	3.311781000	2.267848000
H	-0.857924000	4.180853000	2.668481000	C	1.943020000	1.630876000	1.151128000
O	-3.741729000	0.255819000	2.533253000	C	2.384786000	0.539820000	1.880840000
O	1.917999000	-0.265262000	-2.339290000	H	3.007540000	0.736485000	2.746023000
C	3.058899000	-0.906188000	-2.125370000	C	2.091515000	-0.781548000	-1.591272000
C	4.159188000	-0.056979000	-1.534341000	C	2.571562000	-1.915108000	2.354693000
C	5.295324000	-0.693231000	-1.005827000	H	3.210103000	-1.837446000	3.223559000
C	4.048243000	1.339262000	-1.478571000	C	2.070311000	-3.036379000	1.758941000
C	6.276239000	0.090948000	-0.420499000	H	2.211562000	-4.071376000	2.036925000
H	5.363669000	-1.772110000	-1.061243000	C	1.282052000	-2.597486000	0.626460000
C	5.061912000	2.102699000	-0.890160000	C	0.602772000	-3.443703000	-0.231441000
H	3.150849000	1.798695000	-1.871504000	H	0.665037000	-4.508358000	-0.037778000
C	6.193373000	1.480154000	-0.345426000	C	-0.149006000	-3.035787000	-1.318770000
H	4.962669000	3.182022000	-0.832907000	C	-0.845961000	-3.935166000	-2.213985000
H	6.982525000	2.054719000	0.125047000	H	-0.837493000	-5.012126000	-2.120625000
O	3.270613000	-2.116215000	-2.374157000	C	-1.473153000	-3.162195000	-3.148595000
Cl	7.778477000	-0.738947000	0.310649000	H	-2.089238000	-3.471953000	-3.981316000
				C	-1.163407000	-1.782783000	-2.833192000
				C	-1.618527000	-0.692708000	-3.555677000
				H	-2.269100000	-0.889504000	-4.400576000
				O	-3.857009000	0.217497000	2.233853000
²⁴ (is, is) Or 4- ² R(is, is)							
Fe	-2.469505000	0.117256000	1.221392000				

O	1.959516000	-0.163543000	-1.988078000
C	3.057199000	-0.865573000	-1.804249000
C	4.252447000	-0.055063000	-1.341195000
C	5.448480000	-0.724472000	-1.030236000
C	4.170034000	1.336626000	-1.185990000
C	6.520440000	0.021043000	-0.565330000
H	5.490127000	-1.799137000	-1.155481000
C	5.270845000	2.059465000	-0.713936000
H	3.232346000	1.822489000	-1.420192000
C	6.467960000	1.402956000	-0.394406000
H	5.196527000	3.134368000	-0.580471000
H	7.328912000	1.946218000	-0.023018000
Cl	8.113513000	-0.855032000	-0.138305000
O	3.186307000	-2.104633000	-1.974650000

4⁻¹⁰ts1_(hs, hs)

Fe	-2.516685000	0.243577000	1.004625000
N	-1.047249000	0.014513000	0.061450000
N	-1.312847000	0.723980000	2.635861000
N	-2.370495000	-1.777231000	1.499405000
N	-3.667235000	-0.241503000	-0.657254000
N	-2.505806000	2.245264000	0.420669000
C	-0.739441000	-0.176425000	3.504364000
C	0.072622000	0.554513000	4.464726000
H	0.638529000	0.097128000	5.265100000
C	-0.011496000	1.882313000	4.138761000
H	0.475275000	2.720468000	4.619126000
C	-0.872705000	1.984308000	2.969554000
C	-1.156667000	3.158278000	2.267567000
H	-0.716704000	4.071018000	2.657893000
C	-1.898415000	3.280384000	1.089168000
C	-2.146459000	4.515033000	0.359714000
H	-1.783097000	5.489786000	0.656730000
C	-2.901486000	4.191231000	-0.737255000
H	-3.274551000	4.850494000	-1.509581000
C	-3.128792000	2.754274000	-0.694254000
C	-3.862153000	2.015047000	-1.626084000
H	-4.271620000	2.570112000	-2.464638000
C	-4.109047000	0.640164000	-1.613047000
C	-4.848166000	-0.101987000	-2.626444000
H	-5.310043000	0.340337000	-3.499051000
C	-4.820136000	-1.421082000	-2.260546000
H	-5.254413000	-2.267381000	-2.775873000
C	-4.062371000	-1.506078000	-1.018386000
C	-3.745557000	-2.683256000	-0.335794000
H	-4.118134000	-3.606457000	-0.769332000
C	-2.960780000	-2.812394000	0.813412000
C	-2.605251000	-4.063003000	1.467069000
H	-2.928209000	-5.042085000	1.139465000
C	-1.798910000	-3.750455000	2.530486000
H	-1.336281000	-4.424512000	3.238780000
C	-1.650372000	-2.303035000	2.545745000
C	-0.901740000	-1.563296000	3.465718000
H	-0.365985000	-2.131965000	4.219288000
Fe	0.640749000	-0.221599000	-1.042443000
N	1.416590000	-1.315794000	0.557726000
N	1.328283000	1.537919000	-0.143152000
N	-0.273779000	0.901472000	-2.514564000
N	-0.252983000	-1.941801000	-1.781477000
C	2.138592000	-0.810251000	1.616274000
C	2.538979000	-1.911198000	2.473960000
H	3.121870000	-1.805405000	3.378560000
C	2.040147000	-3.060506000	1.917576000
H	2.136680000	-4.074403000	2.280480000
C	1.326175000	-2.680337000	0.712450000
C	0.625952000	-3.547995000	-0.129507000
H	0.633309000	-4.597046000	0.147063000
C	-0.110279000	-3.211135000	-1.264856000
C	-0.878609000	-4.133372000	-2.083318000
H	-0.948888000	-5.197952000	-1.907481000
C	-1.478103000	-3.397449000	-3.071374000
H	-2.132633000	-3.744298000	-3.859209000
C	-1.080815000	-2.012664000	-2.876972000
C	-1.473443000	-0.928010000	-3.664936000

H	-2.157487000	-1.143759000	-4.479071000
C	-1.110988000	0.409751000	-3.496245000
C	-1.576171000	1.519413000	-4.307211000
H	-2.248703000	1.424777000	-5.148777000
C	-1.024774000	2.663198000	-3.789902000
H	-1.162816000	3.681708000	-4.126150000
C	-0.216952000	2.274836000	-2.648981000
C	0.461758000	3.148062000	-1.797174000
H	0.394963000	4.204796000	-2.034967000
C	1.165584000	2.813596000	-0.636428000
C	1.826791000	3.746354000	0.258367000
H	1.853573000	4.818612000	0.119340000
C	2.366938000	3.011749000	1.283323000
H	2.924870000	3.367673000	2.138459000
C	2.047664000	1.619534000	1.030639000
C	2.423561000	0.539910000	1.831395000
H	2.988301000	0.777426000	2.726772000
O	-4.103186000	0.455216000	1.947479000
O	2.336247000	-0.501814000	-2.020158000
C	3.469362000	-1.109769000	-1.701990000
C	4.554594000	-0.195779000	-1.183447000
C	4.384162000	1.195739000	-1.152231000
C	5.744985000	-0.768031000	-0.702788000
C	5.390035000	2.016097000	-0.630561000
H	3.453803000	1.609853000	-1.516139000
C	6.722708000	0.072456000	-0.194400000
H	5.858619000	-1.844196000	-0.737374000
C	6.578846000	1.457619000	-0.140911000
H	5.243323000	3.090501000	-0.588978000
H	7.366144000	2.077891000	0.270912000
O	3.677200000	-2.341947000	-1.792436000
Cl	8.302739000	-0.672483000	0.455384000
H	-3.998920000	0.448674000	3.067845000
H	-4.826067000	0.498536000	4.851561000
C	-3.810042000	0.370345000	4.473134000
H	-3.385558000	-0.625555000	4.594902000
H	-3.120788000	1.186449000	4.686212000

4⁻²ts1_(hs, hs)

Fe	2.455937000	-0.226154000	0.868877000
N	0.949380000	0.027216000	0.017304000
N	1.385107000	-1.089956000	2.416778000
N	2.261566000	1.648207000	1.767981000
N	3.520178000	0.632521000	-0.683091000
N	2.619348000	-2.104049000	-0.035887000
C	0.877175000	-0.418540000	3.507733000
C	0.148572000	-1.365879000	4.335150000
H	-0.358847000	-1.111780000	5.255811000
C	0.209136000	-2.583240000	3.709859000
H	-0.235073000	-3.518350000	4.022426000
C	0.983387000	-2.405709000	2.493508000
C	1.285168000	-3.406693000	1.568210000
H	0.871938000	-4.389713000	1.769043000
C	2.043998000	-3.272196000	0.403329000
C	2.355463000	-4.330629000	-0.545402000
H	2.026376000	-5.356845000	-0.452879000
C	3.106708000	-3.769158000	-1.544024000
H	3.508720000	-4.247547000	-2.426863000
C	3.262685000	-2.357962000	-1.224190000
C	3.921157000	-1.409451000	-2.009068000
H	4.364968000	-1.772529000	-2.930943000
C	4.037607000	-0.038910000	-1.764860000
C	4.707458000	0.921133000	-2.629664000
H	5.203043000	0.670544000	-3.557912000
C	4.572992000	2.153313000	-2.047625000
H	4.936123000	3.106455000	-2.407462000
C	3.820540000	1.967427000	-0.816108000
C	3.463019000	2.976728000	0.080761000
H	3.764578000	3.985343000	-0.183672000
C	2.752806000	2.831621000	1.273639000
C	2.413426000	3.900493000	2.202387000
H	2.669184000	4.942104000	2.062249000
C	1.724894000	3.330383000	3.239845000
H	1.307418000	3.815276000	4.111893000

C	1.631734000	1.904301000	2.959616000	C	1.213823000	-3.407288000	1.497572000
C	1.000481000	0.949471000	3.760009000	H	0.790297000	-4.388682000	1.677964000
H	0.519850000	1.316170000	4.661528000	C	1.978862000	-3.237447000	0.354275000
Fe	-0.509913000	0.271627000	-0.772471000	C	2.299510000	-4.288554000	-0.589583000
N	-1.392675000	1.058988000	0.921290000	H	1.954802000	-5.309878000	-0.504788000
N	-1.227760000	-1.625052000	-0.232904000	C	3.082836000	-3.728071000	-1.558852000
N	0.269183000	-0.520916000	-2.512015000	H	3.510274000	-4.194349000	-2.435760000
N	0.117704000	2.168654000	-1.341944000	C	3.237294000	-2.327172000	-1.221926000
C	-2.084136000	0.358312000	1.885702000	C	3.917776000	-1.403733000	-1.999757000
C	-2.497605000	1.284714000	2.926323000	H	4.381678000	-1.767363000	-2.910380000
H	-3.064315000	1.006486000	3.804336000	C	4.009513000	-0.045795000	-1.738132000
C	-2.040889000	2.524644000	2.569632000	C	4.679836000	0.910953000	-2.597208000
H	-2.161257000	3.460012000	3.098536000	H	5.188568000	0.653497000	-3.516023000
C	-1.343940000	2.380931000	1.303102000	C	4.521099000	2.140454000	-2.024155000
C	-0.737415000	3.417237000	0.593971000	H	4.874221000	3.100816000	-2.373624000
H	-0.789316000	4.402860000	1.044485000	C	3.760538000	1.943340000	-0.805860000
C	-0.069601000	3.324234000	-0.625754000	C	3.410595000	2.952954000	0.076820000
C	0.554397000	4.423529000	-1.345941000	H	3.696924000	3.966246000	-0.181794000
H	0.555746000	5.452943000	-1.014525000	C	2.731579000	2.763724000	1.269562000
C	1.112933000	3.898453000	-2.480315000	C	2.423243000	3.815496000	2.218790000
H	1.662334000	4.414220000	-3.256122000	H	2.672108000	4.857953000	2.075798000
C	0.837255000	2.469142000	-2.472234000	C	1.783590000	3.226198000	3.271605000
C	1.238347000	1.549632000	-3.442353000	H	1.394685000	3.685183000	4.170025000
H	1.828038000	1.940409000	-4.265478000	C	1.687857000	1.810934000	2.969218000
C	0.980293000	0.177256000	-3.460141000	C	1.080209000	0.872282000	3.788167000
C	1.417284000	-0.751968000	-4.490420000	H	0.643481000	1.228386000	4.714905000
H	1.997485000	-0.474575000	-5.360072000	Fe	-0.491947000	0.299868000	-0.756176000
C	0.960814000	-1.993453000	-4.137190000	N	-1.339032000	1.027691000	0.925034000
H	1.097315000	-2.930690000	-4.659422000	N	-1.198467000	-1.541904000	-0.303780000
C	0.239527000	-1.846005000	-2.882709000	N	0.272318000	-0.421679000	-2.478928000
C	-0.379273000	-2.878623000	-2.177020000	N	0.103748000	2.153785000	-1.260653000
H	-0.309603000	-3.869961000	-2.613762000	C	-2.024787000	0.310986000	1.886036000
C	-1.063135000	-2.779516000	-0.963320000	C	-2.434563000	1.195057000	2.957755000
C	-1.728892000	-3.868465000	-0.268490000	H	-2.992604000	0.878493000	3.827864000
H	-1.760437000	-4.892515000	-0.616027000	C	-1.992213000	2.445076000	2.633135000
C	-2.282142000	-3.343367000	0.871610000	H	-2.111699000	3.368929000	3.181442000
H	-2.855426000	-3.854420000	1.633190000	C	-1.310932000	2.335998000	1.360409000
C	-1.962040000	-1.927499000	0.889873000	C	-0.736867000	3.398554000	0.685601000
C	-2.350483000	-1.010539000	1.867118000	H	-0.797021000	4.376634000	1.148903000
H	-2.916725000	-1.403864000	2.704994000	C	-0.094177000	3.308934000	-0.535919000
O	4.054705000	-0.446526000	1.727176000	C	0.493655000	4.432264000	-1.236085000
O	-2.191301000	0.531922000	-1.737487000	H	0.467088000	5.452340000	-0.879066000
C	-3.282954000	1.168536000	-1.348812000	C	1.053466000	3.940692000	-2.380028000
C	-4.462009000	0.260846000	-1.071115000	H	1.584643000	4.472391000	-3.157301000
C	-4.351025000	-1.132103000	-1.195127000	C	0.809285000	2.512297000	-2.389613000
C	-5.672316000	0.833130000	-0.643218000	C	1.236198000	1.650596000	-3.386147000
C	-5.439198000	-1.954372000	-0.884132000	H	1.816224000	2.074031000	-4.198595000
H	-3.403514000	-1.544585000	-1.513796000	C	0.986171000	0.288324000	-3.420762000
C	-6.732318000	-0.009612000	-0.347833000	C	1.426364000	-0.601073000	-4.476886000
H	-5.735218000	1.909891000	-0.548685000	H	2.007659000	-0.288586000	-5.333380000
C	-6.651514000	-1.396688000	-0.453706000	C	0.967866000	-1.848779000	-4.163528000
H	-5.342661000	-3.032672000	-0.964209000	H	1.096498000	-2.774190000	-4.707781000
H	-7.503251000	-2.019155000	-0.206064000	C	0.247614000	-1.731608000	-2.911385000
O	-3.406858000	2.408279000	-1.208195000	C	-0.375758000	-2.784954000	-2.263754000
Cl	-8.344705000	0.734476000	0.225084000	H	-0.316312000	-3.763488000	-2.727624000
H	5.150166000	-2.405592000	3.664018000	C	-1.056432000	-2.688647000	-1.060320000
C	4.107172000	-2.405902000	3.342472000	C	-1.726980000	-3.791315000	-0.406312000
H	4.067234000	-1.309270000	2.456576000	H	-1.764733000	-4.799209000	-0.796545000
H	3.377318000	-2.137848000	4.105564000	C	-2.266730000	-3.301112000	0.750876000
H	3.811370000	-3.231812000	2.697242000	H	-2.842857000	-3.822115000	1.502911000

4-²ts1(is, is)

Fe	2.418377000	-0.247033000	0.847226000	H	-2.842857000	-3.822115000	1.502911000
N	0.937650000	0.030114000	0.021027000	C	-1.930525000	-1.896546000	0.811920000
N	1.391045000	-1.108500000	2.356063000	C	-2.305655000	-1.043442000	1.836602000
N	2.270813000	1.556358000	1.747280000	H	-2.864622000	-1.468924000	2.662279000
N	3.460737000	0.606712000	-0.655492000	O	4.035244000	-0.483679000	1.702773000
N	2.568165000	-2.055969000	-0.046416000	O	-2.194188000	0.606835000	-1.727376000
C	0.934223000	-0.474532000	3.494093000	C	-3.282377000	1.211384000	-1.302878000
C	0.219868000	-1.421356000	4.325492000	C	-4.456904000	0.282895000	-1.057439000
H	-0.239077000	-1.174448000	5.272821000	C	-4.340101000	-1.101007000	-1.255374000
C	0.226425000	-2.618044000	3.665298000	C	-5.664899000	0.823094000	-0.583898000
H	-0.220141000	-3.556705000	3.962496000	C	-5.418636000	-1.946366000	-0.973965000
C	0.958079000	-2.417391000	2.432650000	H	-3.393920000	-1.487968000	-1.608743000
				C	-6.715353000	-0.041524000	-0.318982000
				H	-5.731696000	1.893213000	-0.432916000
				C	-6.628619000	-1.420563000	-0.498525000
				H	-5.317288000	-3.018472000	-1.112469000

H	-7.473342000	-2.060718000	-0.272821000
O	-3.421180000	2.443034000	-1.091515000
Cl	-8.326001000	0.660332000	0.314775000
H	5.150329000	-2.563076000	3.509861000
C	4.114170000	-2.559775000	3.166504000
H	4.073890000	-1.395563000	2.357156000
H	3.365723000	-2.359756000	3.932458000
H	3.848980000	-3.348140000	2.463649000

4-¹²int1(hs, hs)

Fe	-2.731862000	0.120253000	1.389513000
N	-0.954144000	0.009193000	0.132003000
N	-1.226306000	0.381089000	2.848297000
N	-2.414481000	-1.950955000	1.505317000
N	-3.794245000	-0.167247000	-0.366641000
N	-2.560218000	2.158898000	0.921673000
C	-0.601815000	-0.622119000	3.557284000
C	0.334593000	-0.021782000	4.491565000
H	0.967707000	-0.577796000	5.169329000
C	0.278000000	1.335030000	4.306140000
H	0.856332000	2.101798000	4.803152000
C	-0.692508000	1.584573000	3.254406000
C	-0.989231000	2.832592000	2.701043000
H	-0.460718000	3.682974000	3.119759000
C	-1.832991000	3.096690000	1.621035000
C	-2.056701000	4.403328000	1.024131000
H	-1.600842000	5.321765000	1.368005000
C	-2.905350000	4.223830000	-0.035848000
H	-3.278963000	4.966989000	-0.726936000
C	-3.212725000	2.804757000	-0.103575000
C	-4.009850000	2.189874000	-1.070666000
H	-4.436787000	2.837201000	-1.829881000
C	-4.266197000	0.824092000	-1.202093000
C	-5.034578000	0.210123000	-2.269021000
H	-5.518145000	0.754136000	-3.068956000
C	-4.995777000	-1.145603000	-2.069443000
H	-5.440599000	-1.923092000	-2.675488000
C	-4.201377000	-1.382317000	-0.878462000
C	-3.859954000	-2.635797000	-0.368593000
H	-4.243055000	-3.497078000	-0.906300000
C	-3.021966000	-2.900580000	0.716095000
C	-2.612197000	-4.219832000	1.168098000
H	-2.933135000	-5.150244000	0.720077000
C	-1.746989000	-4.037683000	2.214117000
H	-1.223900000	-4.790191000	2.788213000
C	-1.617793000	-2.604288000	2.419775000
C	-0.796743000	-1.992532000	3.368624000
H	-0.204641000	-2.654043000	3.992813000
Fe	0.554650000	-0.087315000	-0.992395000
N	1.466105000	-1.324381000	0.395756000
N	1.281241000	1.578034000	0.052259000
N	-0.450137000	1.180898000	-2.283652000
N	-0.420644000	-1.721147000	-1.819580000
C	2.255861000	-0.929478000	1.453607000
C	2.695694000	-2.111665000	2.179017000
H	3.337827000	-2.094390000	3.049117000
C	2.142118000	-3.196345000	1.555046000
H	2.242694000	-4.241415000	1.814696000
C	1.356427000	-2.696113000	0.437273000
C	0.582285000	-3.479312000	-0.419153000
H	0.605205000	-4.550384000	-0.245812000
C	-0.239657000	-3.035117000	-1.456021000
C	-1.047709000	-3.873410000	-2.324402000
H	-1.096582000	-4.952322000	-2.266960000
C	-1.703484000	-3.041431000	-3.195288000
H	-2.391439000	-3.310366000	-3.985489000
C	-1.302234000	-1.682132000	-2.874541000
C	-1.726190000	-0.524115000	-3.530980000
H	-2.450603000	-0.658319000	-4.328196000
C	-1.342604000	0.790099000	-3.255572000
C	-1.852135000	1.976545000	-3.929686000
H	-2.569245000	1.962191000	-4.739431000
C	-1.269110000	3.061513000	-3.333812000
H	-1.418121000	4.109272000	-3.557798000

C	-0.396649000	2.556188000	-2.282687000
C	0.329369000	3.341286000	-1.385828000
H	0.259513000	4.416610000	-1.518202000
C	1.098106000	2.895833000	-0.306487000
C	1.840504000	3.737007000	0.613908000
H	1.875998000	4.817468000	0.569655000
C	2.459722000	2.905244000	1.514345000
H	3.102512000	3.176259000	2.341011000
C	2.106705000	1.545986000	1.155358000
C	2.555156000	0.388914000	1.795674000
H	3.195812000	0.531098000	2.660003000
O	-4.131694000	0.244844000	2.625364000
O	2.085725000	-0.194359000	-2.191145000
C	3.209412000	-0.867860000	-1.996623000
C	4.338966000	-0.052986000	-1.408123000
C	4.218097000	1.331752000	-1.224298000
C	5.516600000	-0.712725000	-1.016426000
C	5.261355000	2.058063000	-0.640422000
H	3.293545000	1.810127000	-1.517956000
C	6.530279000	0.035590000	-0.439732000
H	5.590795000	-1.781998000	-1.169190000
C	6.437339000	1.411131000	-0.236205000
H	5.152802000	3.125912000	-0.480401000
H	7.252541000	1.956730000	0.224236000
O	3.389424000	-2.079311000	-2.264343000
Cl	8.095539000	-0.826772000	0.098675000
H	-3.993439000	0.380918000	3.582027000

4-⁴int1(hs, hs)

Fe	-2.450345000	0.319449000	1.497132000
N	-0.913235000	-0.011014000	0.163397000
N	-1.007667000	1.362161000	2.616191000
N	-1.760664000	-1.488951000	2.345180000
N	-3.617103000	-0.786184000	0.144412000
N	-2.876052000	2.054748000	0.435102000
C	-0.169519000	0.819817000	3.561296000
C	0.615521000	1.892925000	4.155385000
H	1.360937000	1.757248000	4.927654000
C	0.240542000	3.058041000	3.538141000
H	0.621297000	4.055983000	3.709763000
C	-0.778316000	2.715261000	2.556284000
C	-1.384206000	3.599096000	1.656876000
H	-1.056682000	4.633217000	1.704880000
C	-2.324890000	3.294921000	0.667012000
C	-2.863489000	4.230265000	-0.308190000
H	-2.601629000	5.278174000	-0.366308000
C	-3.721151000	3.527587000	-1.114745000
H	-4.292476000	3.891777000	-1.957862000
C	-3.721902000	2.150291000	-0.646876000
C	-4.437360000	1.093116000	-1.219518000
H	-5.066260000	1.344371000	-2.068242000
C	-4.393562000	-0.257575000	-0.858174000
C	-5.106406000	-1.343498000	-1.515660000
H	-5.791306000	-1.220209000	-2.344048000
C	-4.724016000	-2.508144000	-0.902030000
H	-5.035965000	-3.517785000	-1.133729000
C	-3.774059000	-2.152003000	0.142630000
C	-3.090828000	-3.050520000	0.969691000
H	-3.283259000	-4.104620000	0.793769000
C	-2.140895000	-2.753183000	1.954296000
C	-1.357047000	-3.724683000	2.702317000
H	-1.438569000	-4.797599000	2.592586000
C	-0.503560000	-3.020910000	3.512477000
H	0.244990000	-3.409899000	4.189206000
C	-0.750920000	-1.606773000	3.274118000
C	-0.050481000	-0.543032000	3.855588000
H	0.708360000	-0.811772000	4.584395000
Fe	0.399598000	-0.244794000	-1.038823000
N	1.655728000	-0.811433000	0.420873000
N	0.947334000	1.667457000	-0.759005000
N	-0.843346000	0.328890000	-2.498485000
N	-0.158474000	-2.150216000	-1.291442000
C	2.340558000	0.017240000	1.289788000
C	3.132701000	-0.779672000	2.199207000

H	3.775202000	-0.369131000	2.964911000
C	2.928068000	-2.089065000	1.867280000
H	3.356002000	-2.974245000	2.315872000
C	1.986011000	-2.107735000	0.770702000
C	1.430955000	-3.252134000	0.225041000
H	1.780767000	-4.207129000	0.599676000
C	0.411837000	-3.263977000	-0.710917000
C	-0.282030000	-4.453645000	-1.157047000
H	-0.024510000	-5.457609000	-0.850467000
C	-1.283775000	-4.043862000	-1.989579000
H	-2.015148000	-4.641871000	-2.514868000
C	-1.191921000	-2.601448000	-2.084553000
C	-1.976614000	-1.814342000	-2.911115000
H	-2.768443000	-2.303628000	-3.465326000
C	-1.789948000	-0.458405000	-3.122164000
C	-2.513576000	0.331884000	-4.095512000
H	-3.312215000	-0.050710000	-4.715440000
C	-1.982318000	1.589970000	-4.065087000
H	-2.263696000	2.457326000	-4.645749000
C	-0.948098000	1.589202000	-3.051323000
C	-0.246845000	2.711060000	-2.639873000
H	-0.445748000	3.644477000	-3.154877000
C	0.608128000	2.748620000	-1.549727000
C	1.195417000	3.952396000	-1.002016000
H	1.080137000	4.936641000	-1.434260000
C	1.855831000	3.592401000	0.139823000
H	2.407577000	4.216615000	0.828377000
C	1.706348000	2.162055000	0.283940000
C	2.334072000	1.400463000	1.254553000
H	2.908572000	1.924084000	2.008278000
O	-3.819505000	0.503979000	2.786334000
O	1.853507000	-0.515414000	-2.455064000
C	3.004235000	-1.092430000	-2.194088000
C	4.072907000	-0.177228000	-1.624339000
C	3.960132000	1.216220000	-1.723510000
C	5.175076000	-0.743472000	-0.961203000
C	4.933557000	2.046827000	-1.158648000
H	3.086974000	1.621611000	-2.217536000
C	6.111804000	0.106756000	-0.395931000
H	5.251382000	-1.821535000	-0.903795000
C	6.026028000	1.495188000	-0.474618000
H	4.831634000	3.125581000	-1.226825000
H	6.781684000	2.122057000	-0.016026000
O	3.283279000	-2.309871000	-2.360238000
Cl	7.559788000	-0.630450000	0.527876000
H	-3.892452000	-0.155742000	3.504255000

4⁸int1_(is, is)

Fe	-2.660807000	0.174761000	1.385168000
N	-0.905593000	0.014460000	0.079533000
N	-1.239651000	0.773948000	2.765689000
N	-2.231787000	-1.753459000	1.817433000
N	-3.781046000	-0.443472000	-0.198749000
N	-2.754302000	2.073370000	0.698904000
C	-0.487531000	-0.044074000	3.582807000
C	0.388849000	0.762248000	4.407741000
H	1.088000000	0.363304000	5.129570000
C	0.169151000	2.068753000	4.064757000
H	0.653833000	2.956288000	4.447517000
C	-0.836461000	2.067899000	3.021938000
C	-1.271031000	3.190886000	2.331466000
H	-0.850721000	4.147993000	2.621071000
C	-2.136843000	3.182677000	1.247176000
C	-2.490626000	4.362229000	0.484409000
H	-2.131803000	5.358473000	0.703107000
C	-3.309658000	3.953212000	-0.530297000
H	-3.762754000	4.544987000	-1.313514000
C	-3.470453000	2.520467000	-0.394225000
C	-4.221512000	1.732899000	-1.254551000
H	-4.713144000	2.231068000	-2.082992000
C	-4.362312000	0.356391000	-1.161251000
C	-5.118919000	-0.462434000	-2.085134000
H	-5.667336000	-0.079012000	-2.934546000
C	-4.979048000	-1.760326000	-1.675154000

H	-5.387994000	-2.656261000	-2.121634000
C	-4.130365000	-1.743561000	-0.502104000
C	-3.687010000	-2.872455000	0.170701000
H	-4.022499000	-3.836733000	-0.195388000
C	-2.788494000	-2.871186000	1.227545000
C	-2.247006000	-4.067055000	1.839547000
H	-2.514732000	-5.073840000	1.550677000
C	-1.348571000	-3.660786000	2.785414000
H	-0.729933000	-4.265784000	3.433442000
C	-1.338962000	-2.212085000	2.768839000
C	-0.535444000	-1.431372000	3.587647000
H	0.135087000	-1.950951000	4.263570000
Fe	0.575302000	-0.147615000	-1.043559000
N	1.633746000	-1.080836000	0.418888000
N	1.168386000	1.629323000	-0.310341000
N	-0.522874000	0.799136000	-2.452310000
N	-0.215042000	-1.902882000	-1.578868000
C	2.399676000	-0.486913000	1.403713000
C	3.003098000	-1.502634000	2.244015000
H	3.660828000	-1.293917000	3.076284000
C	2.580439000	-2.711150000	1.770115000
H	2.814926000	-3.701001000	2.136358000
C	1.710919000	-2.440932000	0.642010000
C	1.003800000	-3.406507000	-0.053028000
H	1.147706000	-4.441403000	0.237325000
C	0.096606000	-3.148776000	-1.067836000
C	-0.680168000	-4.162836000	-1.743824000
H	-0.619342000	-5.220451000	-1.528340000
C	-1.462236000	-3.521040000	-2.664055000
H	-2.174241000	-3.944388000	-3.358908000
C	-1.162218000	-2.110009000	-2.564394000
C	-1.724835000	-1.133652000	-3.372894000
H	-2.470409000	-1.452690000	-4.093106000
C	-1.418673000	0.216591000	-3.322809000
C	-2.033650000	1.234381000	-4.155417000
H	-2.771163000	1.033339000	-4.920287000
C	-1.512155000	2.434164000	-3.765161000
H	-1.735192000	3.423542000	-4.140463000
C	-0.583465000	2.156996000	-2.684203000
C	0.075068000	3.125450000	-1.944360000
H	-0.079989000	4.162438000	-2.222950000
C	0.867926000	2.876900000	-0.832673000
C	1.500981000	3.903412000	-0.038084000
H	1.421672000	4.963505000	-0.236650000
C	2.176629000	3.270724000	0.971499000
H	2.769714000	3.705694000	1.763944000
C	1.970601000	1.853717000	0.795833000
C	2.548012000	0.875845000	1.590607000
H	3.165383000	1.205943000	2.418337000
O	-4.100184000	0.337073000	2.627978000
O	2.067936000	-0.319384000	-2.299822000
C	3.202102000	-0.949822000	-2.048953000
C	4.289023000	-0.084045000	-1.451085000
C	4.164152000	1.311525000	-1.409021000
C	5.425716000	-0.703645000	-0.904265000
C	5.162748000	2.090650000	-0.815290000
H	3.266843000	1.757263000	-1.817558000
C	6.392072000	0.095931000	-0.315491000
H	5.505038000	-1.782274000	-0.950904000
C	6.294682000	1.484730000	-0.252665000
H	5.051800000	3.169404000	-0.768511000
H	7.072961000	2.071271000	0.221198000
O	3.427446000	-2.166355000	-2.261127000
Cl	7.896815000	-0.712251000	0.438651000
H	-3.877330000	0.580603000	3.549645000

4⁴int1_(is, is)

Fe	-2.323804000	0.112292000	1.346010000
N	-0.930998000	0.000302000	0.150946000
N	-1.022688000	0.785472000	2.738909000
N	-1.928754000	-1.784543000	1.941185000
N	-3.543547000	-0.577609000	-0.105854000
N	-2.667993000	2.000227000	0.720375000
C	-0.240621000	0.033458000	3.594140000

C	0.551300000	0.909584000	4.431061000
H	1.251365000	0.567865000	5.180897000
C	0.239686000	2.191869000	4.073367000
H	0.633909000	3.117871000	4.469056000
C	-0.737571000	2.110020000	3.007956000
C	-1.260941000	3.205639000	2.338369000
H	-0.918423000	4.186920000	2.649343000
C	-2.143082000	3.149092000	1.270228000
C	-2.623730000	4.307888000	0.540360000
H	-2.352986000	5.329188000	0.770501000
C	-3.431819000	3.841871000	-0.456835000
H	-3.964778000	4.401386000	-1.213279000
C	-3.456362000	2.396171000	-0.337944000
C	-4.173218000	1.549198000	-1.168264000
H	-4.739453000	1.999224000	-1.976280000
C	-4.220268000	0.169305000	-1.046624000
C	-5.006576000	-0.705035000	-1.893297000
H	-5.623270000	-0.365938000	-2.714185000
C	-4.799166000	-1.980728000	-1.449905000
H	-5.209832000	-2.904870000	-1.832984000
C	-3.877856000	-1.895860000	-0.333850000
C	-3.391825000	-2.989676000	0.367188000
H	-3.722017000	-3.972049000	0.046496000
C	-2.473698000	-2.935865000	1.404971000
C	-1.902116000	-4.097836000	2.055114000
H	-2.159053000	-5.119811000	1.812755000
C	-0.994306000	-3.639418000	2.968096000
H	-0.356917000	-4.207902000	3.631196000
C	-1.010175000	-2.193155000	2.890489000
C	-0.221278000	-1.351787000	3.659930000
H	0.468940000	-1.810814000	4.358868000
Fe	0.361625000	-0.090078000	-0.975850000
N	1.588526000	-0.844694000	0.450512000
N	0.916934000	1.782390000	-0.456471000
N	-0.807720000	0.670566000	-2.432222000
N	-0.191590000	-1.952910000	-1.473266000
C	2.341949000	-0.124967000	1.357058000
C	3.073567000	-1.031419000	2.217371000
H	3.747848000	-0.716083000	3.001185000
C	2.744085000	-2.299574000	1.831873000
H	3.090023000	-3.240439000	2.236651000
C	1.803792000	-2.177737000	0.737509000
C	1.183617000	-3.243289000	0.108428000
H	1.435932000	-4.241900000	0.446898000
C	0.251403000	-3.131004000	-0.909033000
C	-0.410465000	-4.252948000	-1.539716000
H	-0.234913000	-5.287204000	-1.278993000
C	-1.252980000	-3.740213000	-2.484612000
H	-1.912679000	-4.266616000	-3.160428000
C	-1.108833000	-2.299752000	-2.443696000
C	-1.784006000	-1.421274000	-3.275614000
H	-2.487313000	-1.846346000	-3.983005000
C	-1.631430000	-0.044010000	-3.274676000
C	-2.322072000	0.861220000	-4.172165000
H	-3.027835000	0.548605000	-4.929392000
C	-1.905728000	2.124169000	-3.860889000
H	-2.200751000	3.063609000	-4.307956000
C	-0.963681000	1.999586000	-2.765867000
C	-0.345737000	3.067573000	-2.135905000
H	-0.581180000	4.064865000	-2.491493000
C	0.515022000	2.961850000	-1.054286000
C	1.113627000	4.084234000	-0.366016000
H	0.955702000	5.119068000	-0.636684000
C	1.863992000	3.572778000	0.657444000
H	2.453134000	4.101596000	1.393845000
C	1.738387000	2.134304000	0.597748000
C	2.398334000	1.255125000	1.441446000
H	3.019288000	1.682935000	2.219931000
O	-3.740123000	0.249778000	2.510236000
O	1.819199000	-0.185525000	-2.287437000
C	2.950154000	-0.848536000	-2.120132000
C	4.087051000	-0.024303000	-1.557464000
C	4.004160000	1.373292000	-1.486770000
C	5.227179000	-0.685307000	-1.069695000
C	5.050768000	2.113250000	-0.926713000

H	3.102121000	1.851052000	-1.846140000
C	6.240803000	0.076000000	-0.510314000
H	5.272899000	-1.764737000	-1.136101000
C	6.187598000	1.465788000	-0.423157000
H	4.975541000	3.194335000	-0.861102000
H	7.002595000	2.021892000	0.024950000
O	3.138605000	-2.060806000	-2.384432000
Cl	7.750594000	-0.787847000	0.167063000
H	-3.549565000	-0.309296000	3.295248000

4-²int1(is, is)

Fe	-2.549253000	0.206627000	1.325901000
N	-0.961235000	0.030984000	0.122521000
N	-1.784568000	2.006167000	1.845166000
N	-1.390292000	-0.677566000	2.727655000
N	-3.090429000	-1.615774000	0.637178000
N	-3.472915000	1.066057000	-0.255283000
C	-0.932542000	2.268914000	2.899527000
C	-0.671304000	3.690776000	2.977071000
H	-0.028810000	4.152592000	3.713938000
C	-1.361510000	4.279337000	1.955147000
H	-1.403597000	5.324263000	1.680498000
C	-2.051907000	3.221856000	1.247317000
C	-2.838141000	3.414129000	0.123002000
H	-2.930360000	4.426063000	-0.255758000
C	-3.488759000	2.409356000	-0.573927000
C	-4.284331000	2.622298000	-1.765500000
H	-4.445765000	3.587444000	-2.225224000
C	-4.743351000	1.398520000	-2.162294000
H	-5.358341000	1.150427000	-3.016182000
C	-4.229247000	0.427967000	-1.218028000
C	-4.450558000	-0.937110000	-1.298872000
H	-5.056651000	-1.297831000	-2.122558000
C	-3.915907000	-1.881118000	-0.437686000
C	-4.113215000	-3.310000000	-0.563754000
H	-4.714697000	-3.776237000	-1.331700000
C	-3.391258000	-3.901922000	0.433557000
H	-3.277556000	-4.954280000	0.653716000
C	-2.750075000	-2.839246000	1.179226000
C	-1.903025000	-3.038530000	2.257081000
H	-1.697732000	-4.062161000	2.549657000
C	-1.268981000	-2.031947000	2.966327000
C	-0.359539000	-2.256716000	4.071409000
H	-0.088259000	-3.233276000	4.447417000
C	0.068077000	-1.029783000	4.491513000
H	0.764113000	-0.790020000	5.283181000
C	-0.574942000	-0.045334000	3.645174000
C	-0.370306000	1.321288000	3.739386000
H	0.311657000	1.673063000	4.505691000
Fe	0.432704000	-0.163896000	-0.920975000
N	1.630713000	0.485675000	0.571807000
N	0.185250000	1.738940000	-1.564107000
N	-0.779507000	-0.798618000	-2.398824000
N	0.686372000	-2.050443000	-0.270338000
C	1.897663000	1.802477000	0.892554000
C	2.779615000	1.857747000	2.038753000
H	3.145537000	2.773464000	2.481997000
C	3.046025000	0.567799000	2.401615000
H	3.670398000	0.206940000	3.206876000
C	2.312163000	-0.285999000	1.492663000
C	2.267916000	-1.668767000	1.571359000
H	2.855025000	-2.145803000	2.348214000
C	1.497331000	-2.482821000	0.757696000
C	1.407225000	-3.922953000	0.882772000
H	1.953101000	-4.506843000	1.610622000
C	0.532517000	-4.350255000	-0.073768000
H	0.212139000	-5.358701000	-0.295797000
C	0.091222000	-3.175737000	-0.798802000
C	-0.784540000	-3.202436000	-1.871467000
H	-1.188608000	-4.166649000	-2.159362000
C	-1.177666000	-2.100667000	-2.615513000
C	-2.063905000	-2.157621000	-3.760646000
H	-2.515198000	-3.065101000	-4.137454000
C	-2.189543000	-0.881118000	-4.231560000

H	-2.767734000	-0.524295000	-5.072790000
C	-1.386802000	-0.033894000	-3.372645000
C	-1.273802000	1.341305000	-3.504269000
H	-1.825147000	1.815116000	-4.309402000
C	-0.552573000	2.162427000	-2.651721000
C	-0.514395000	3.607485000	-2.738127000
H	-1.012032000	4.186256000	-3.504136000
C	0.230998000	4.050720000	-1.681294000
H	0.472774000	5.067564000	-1.403726000
C	0.663133000	2.879083000	-0.947417000
C	1.442003000	2.913076000	0.200056000
H	1.723601000	3.887969000	0.582326000
O	-3.874968000	0.349875000	2.331514000
O	1.978508000	-0.390789000	-2.119899000
C	3.109482000	-1.019506000	-1.868580000
C	4.235403000	-0.133943000	-1.376225000
C	4.090513000	1.259178000	-1.324451000
C	5.434173000	-0.730542000	-0.950189000
C	5.131914000	2.057643000	-0.840493000
H	3.150991000	1.687815000	-1.647206000
C	6.445072000	0.088678000	-0.473415000
H	5.526423000	-1.808001000	-1.003446000
C	6.330217000	1.475336000	-0.403835000
H	5.011565000	3.135648000	-0.789733000
H	7.144386000	2.078185000	-0.019348000
Cl	8.038078000	-0.690684000	0.112477000
O	3.317055000	-2.250025000	-2.015773000

4-⁴ts₂(hs, hs)

Fe	2.304386000	-0.131791000	1.029041000
N	0.867550000	0.006657000	0.094844000
N	2.444888000	-2.160149000	0.623251000
N	1.203546000	-0.529954000	2.743155000
N	2.293752000	1.897454000	1.500888000
N	3.477058000	0.287990000	-0.658041000
C	1.866078000	-3.163370000	1.360366000
C	2.168990000	-4.439398000	0.727815000
H	1.835964000	-5.401715000	1.092761000
C	2.926208000	-4.170607000	-0.381458000
H	3.330717000	-4.870404000	-1.100267000
C	3.096111000	-2.725735000	-0.446140000
C	3.795238000	-2.028888000	-1.434990000
H	4.239840000	-2.629055000	-2.222934000
C	3.973348000	-0.646940000	-1.533679000
C	4.722923000	0.042011000	-2.574229000
H	5.221669000	-0.447397000	-3.399976000
C	4.660162000	1.382545000	-2.298137000
H	5.095822000	2.200949000	-2.855328000
C	3.871964000	1.532348000	-1.082935000
C	3.564564000	2.737788000	-0.445736000
H	3.913580000	3.643970000	-0.930856000
C	2.829410000	2.908867000	0.729622000
C	2.478356000	4.184645000	1.330748000
H	2.765266000	5.149226000	0.934273000
C	1.718816000	3.917761000	2.439552000
H	1.266223000	4.622226000	3.124106000
C	1.593037000	2.473522000	2.539895000
C	0.864679000	1.783464000	3.512246000
H	0.359559000	2.390762000	4.256604000
C	0.685020000	0.401388000	3.609434000
C	-0.088055000	-0.291666000	4.630263000
H	-0.614726000	0.195223000	5.439869000
C	-0.017917000	-1.630132000	4.349982000
H	-0.477479000	-2.449929000	4.885361000
C	0.797255000	-1.777828000	3.152367000
C	1.104516000	-2.983760000	2.518543000
H	0.690416000	-3.881674000	2.966803000
Fe	-0.511436000	0.152134000	-0.797938000
N	-1.312174000	-1.475929000	0.108324000
N	0.251712000	-1.028762000	-2.243226000
N	0.199473000	1.776422000	-1.747531000
N	-1.380911000	1.331475000	0.585885000
C	-1.168612000	-2.790782000	-0.287314000
C	-1.871579000	-3.658247000	0.634057000

H	-1.911959000	-4.735249000	0.546071000
C	-2.434771000	-2.856031000	1.586701000
H	-3.036671000	-3.137579000	2.439354000
C	-2.078756000	-1.493735000	1.256043000
C	-2.469302000	-0.380795000	1.981257000
H	-3.070274000	-0.546150000	2.868203000
C	-2.142952000	0.926840000	1.664787000
C	-2.560622000	2.082645000	2.429737000
H	-3.174108000	2.034174000	3.318525000
C	-2.041401000	3.181114000	1.807083000
H	-2.140687000	4.222909000	2.077617000
C	-1.305930000	2.706999000	0.654812000
C	-0.635635000	3.525960000	-0.236039000
H	-0.657615000	4.593100000	-0.047169000
C	0.055594000	3.088481000	-1.351539000
C	0.741717000	3.959730000	-2.283621000
H	0.775276000	5.036811000	-2.196722000
C	1.299054000	3.160497000	-3.239797000
H	1.888717000	3.443620000	-4.100646000
C	0.956621000	1.794103000	-2.899648000
C	1.339522000	0.684092000	-3.633210000
H	1.955458000	0.851016000	-4.509913000
C	1.007276000	-0.624459000	-3.323933000
C	1.416793000	-1.779718000	-4.095451000
H	2.019529000	-1.730506000	-4.991757000
C	0.907443000	-2.879967000	-3.466561000
H	1.005493000	-3.921771000	-3.738699000
C	0.182402000	-2.405694000	-2.305669000
C	-0.473819000	-3.227307000	-1.403951000
H	-0.428332000	-4.296711000	-1.578072000
O	3.921091000	-0.319725000	2.011385000
O	-2.171432000	0.263227000	-1.888176000
C	-3.278721000	0.924505000	-1.626982000
C	-4.450044000	0.052774000	-1.217119000
C	-4.326130000	-1.342552000	-1.143925000
C	-5.664578000	0.667106000	-0.866502000
C	-5.403719000	-2.123779000	-0.713243000
H	-3.375285000	-1.785731000	-1.407816000
C	-6.713159000	-0.135785000	-0.446212000
H	-5.737622000	1.745704000	-0.926291000
C	-6.619326000	-1.523001000	-0.355679000
H	-5.297349000	-3.201848000	-0.641733000
H	-7.462786000	-2.112322000	-0.015782000
O	-3.434593000	2.170743000	-1.685662000
Cl	-8.330618000	0.666947000	0.031197000
H	4.198497000	0.573457000	2.313525000
C	6.202244000	-0.814607000	1.148944000
H	6.062030000	0.001594000	0.451549000
H	6.710486000	-0.652607000	2.093375000
H	5.737486000	-1.767908000	0.940392000

4-⁸ts₂(is, is)

Fe	2.479150000	-0.467156000	1.032567000
N	0.945233000	0.050577000	-0.059009000
N	1.221139000	-1.673950000	2.137884000
N	1.960138000	1.171025000	2.236407000
N	3.663244000	0.763151000	-0.123065000
N	2.729368000	-2.013594000	-0.365051000
C	0.507714000	-1.293650000	3.250927000
C	-0.228420000	-2.445848000	3.752856000
H	-0.875241000	-2.431630000	4.619677000
C	0.041611000	-3.493580000	2.914920000
H	-0.341965000	-4.503858000	2.961251000
C	0.944534000	-2.998279000	1.885134000
C	1.397490000	-3.732750000	0.786742000
H	1.052707000	-4.760191000	0.720821000
C	2.203567000	-3.278820000	-0.260304000
C	2.624289000	-4.056331000	-1.415962000
H	2.351224000	-5.086979000	-1.599166000
C	3.399095000	-3.235494000	-2.194957000
H	3.881279000	-3.467716000	-3.135044000
C	3.466253000	-1.947464000	-1.522128000
C	4.170690000	-0.821693000	-1.958282000
H	4.683716000	-0.909607000	-2.911181000

C	4.250222000	0.422249000	-1.326945000	Fe	2.428982000	-0.364580000	0.997579000
C	4.901214000	1.599131000	-1.879112000	N	0.871274000	0.038041000	0.012624000
H	5.441213000	1.617748000	-2.816284000	N	1.808883000	-2.329314000	1.055934000
C	4.661992000	2.637706000	-1.019112000	N	1.316673000	0.038436000	2.739806000
H	4.967166000	3.670860000	-1.116594000	N	2.988434000	1.608038000	0.902770000
C	3.859076000	2.116128000	0.074851000	N	3.393085000	-0.721863000	-0.845096000
C	3.309743000	2.884743000	1.104449000	C	1.034505000	-2.902418000	2.038485000
H	3.559141000	3.941431000	1.100347000	C	0.854900000	-4.312528000	1.727355000
C	2.424582000	2.456478000	2.097019000	H	0.285539000	-5.007354000	2.329968000
C	1.839241000	3.282392000	3.142024000	C	1.516756000	-4.555563000	0.552975000
H	2.022850000	4.340888000	3.268380000	H	1.595560000	-5.488330000	0.010824000
C	1.030985000	2.468552000	3.892849000	C	2.113025000	-3.298270000	0.126581000
H	0.426505000	2.734600000	4.749443000	C	2.850565000	-3.110489000	-1.046764000
C	1.112822000	1.134377000	3.317742000	H	2.962190000	-3.981319000	-1.685715000
C	0.454215000	-0.004756000	3.787410000	C	3.433077000	-1.925386000	-1.503867000
H	-0.191441000	0.131105000	4.649506000	C	4.170168000	-1.751707000	-2.748683000
Fe	-0.629648000	0.505438000	-0.980186000	H	4.351563000	-2.534134000	-3.473400000
N	-1.645968000	0.793651000	0.753152000	C	4.554758000	-0.437321000	-2.809602000
N	-1.123324000	-1.442044000	-0.926353000	H	5.111925000	0.059067000	-3.592890000
N	0.418967000	0.190873000	-2.676889000	C	4.058352000	0.208718000	-1.601908000
N	0.027173000	2.388848000	-0.890892000	C	4.212336000	1.553808000	-1.253879000
C	-2.324151000	-0.158451000	1.489651000	H	4.743786000	2.181371000	-1.962756000
C	-2.936960000	0.455904000	2.649848000	C	3.715918000	2.195895000	-0.115246000
H	-3.532339000	-0.076673000	3.378180000	C	3.844954000	3.614950000	0.167464000
C	-2.613275000	1.781732000	2.614457000	H	4.366454000	4.320292000	-0.465356000
H	-2.883123000	2.562838000	3.311312000	C	3.171586000	3.862391000	1.334717000
C	-1.792133000	1.984028000	1.438626000	H	3.034851000	4.809315000	1.839310000
C	-1.192796000	3.182895000	1.096158000	C	2.616979000	2.599636000	1.790972000
H	-1.382683000	4.040135000	1.731967000	C	1.804697000	2.436471000	2.917267000
C	-0.333484000	3.359180000	0.024856000	H	1.598419000	3.333570000	3.492660000
C	0.340509000	4.598775000	-0.285222000	C	1.198165000	1.257130000	3.358506000
H	0.224602000	5.512463000	0.280731000	C	0.351665000	1.105686000	4.534319000
C	1.114314000	4.368251000	-1.388883000	H	0.078291000	1.907337000	5.207113000
H	1.762176000	5.054921000	-1.915862000	C	-0.017358000	-0.212660000	4.596207000
C	0.908512000	2.988682000	-1.770473000	H	-0.650818000	-0.694125000	5.329082000
C	1.485101000	2.393078000	-2.882050000	C	0.596440000	-0.883962000	3.457882000
H	2.177426000	2.991609000	-3.463754000	C	0.477148000	-2.238188000	3.135799000
C	1.245952000	1.096038000	-3.306010000	H	-0.138560000	-2.839894000	3.797471000
C	1.850215000	0.483411000	-4.474248000	Fe	-0.576252000	0.453466000	-0.864106000
H	2.538913000	0.985951000	-5.139427000	N	-1.656376000	-0.707430000	0.389858000
C	1.387950000	-0.800096000	-4.533498000	N	-0.263616000	-1.134143000	-2.079981000
H	1.623609000	-1.571893000	-5.253204000	N	0.514049000	1.596313000	-2.111162000
C	0.508342000	-0.982953000	-3.394334000	N	-0.898634000	2.021142000	0.352674000
C	-0.089351000	-2.182432000	-3.043759000	C	-1.833274000	-2.074255000	0.290788000
H	0.077626000	-3.035958000	-3.691875000	C	-2.650377000	-2.541994000	1.389412000
C	-0.829194000	-2.393627000	-1.889631000	H	-2.939111000	-3.573285000	1.536862000
C	-1.395895000	-3.665709000	-1.506439000	C	-2.967904000	-1.449894000	2.146082000
H	-1.304961000	-4.572738000	-2.088095000	H	-3.567067000	-1.400554000	3.044368000
C	-2.018844000	-3.481387000	-0.301370000	C	-2.330349000	-0.308287000	1.527867000
H	-2.548973000	-4.203845000	0.303335000	C	-2.359324000	0.981302000	2.033425000
C	-1.851660000	-2.092960000	0.054131000	H	-2.928424000	1.152361000	2.940116000
C	-2.407050000	-1.503645000	1.178503000	C	-1.677727000	2.057612000	1.490251000
H	-2.959034000	-2.143847000	1.856687000	C	-1.663983000	3.391648000	2.052518000
O	3.911826000	-0.997158000	2.088002000	H	-2.201045000	3.681740000	2.944631000
O	-2.180484000	0.996321000	-2.023984000	C	-0.867788000	4.153575000	1.247525000
C	-3.309918000	1.483783000	-1.529343000	H	-0.618221000	5.201474000	1.339171000
C	-4.361062000	0.443898000	-1.219827000	C	-0.399298000	3.294479000	0.179371000
C	-4.221895000	-0.881720000	-1.654657000	C	0.410616000	3.714147000	-0.862304000
C	-5.479990000	0.818678000	-0.456585000	H	0.741212000	4.746618000	-0.850291000
C	-5.189904000	-1.835874000	-1.324257000	C	0.822292000	2.927389000	-1.926718000
H	-3.339473000	-1.146640000	-2.222020000	C	1.633166000	3.399068000	-3.030735000
C	-6.415772000	-0.152540000	-0.138919000	H	2.008929000	4.408683000	-3.122641000
H	-5.572016000	1.847863000	-0.133809000	C	1.804614000	2.342393000	-3.879775000
C	-6.303757000	-1.478849000	-0.551936000	H	2.351739000	2.305078000	-4.811707000
H	-5.068877000	-2.864407000	-1.649199000	C	1.104830000	1.215466000	-3.297969000
H	-7.057496000	-2.207332000	-0.277225000	C	1.060867000	-0.055133000	-3.849423000
O	-3.549811000	2.695642000	-1.318889000	H	1.592469000	-0.216183000	-4.780958000
Cl	-7.894716000	0.322814000	0.893909000	C	0.433988000	-1.147509000	-3.271831000
H	4.567555000	-1.724756000	4.605452000	C	0.465718000	-2.492510000	-3.806250000
C	4.216554000	-2.526729000	3.966713000	H	0.951038000	-2.769464000	-4.731902000
H	3.156850000	-2.644813000	3.787158000	C	-0.195657000	-3.291484000	-2.915943000
H	4.926268000	-3.125960000	3.408455000	H	-0.366975000	-4.358151000	-2.962186000
H	4.748251000	-0.561656000	1.807631000	C	-0.645733000	-2.438912000	-1.835292000
				C	-1.357062000	-2.881117000	-0.729835000
				H	-1.562976000	-3.943456000	-0.661779000

O	3.947750000	-0.830976000	1.967019000
O	-2.181612000	0.934160000	-1.879532000
C	-3.324268000	1.401529000	-1.412056000
C	-4.384875000	0.352420000	-1.156427000
C	-4.181665000	-0.985567000	-1.520742000
C	-5.580343000	0.734018000	-0.524183000
C	-5.161283000	-1.945611000	-1.247160000
H	-3.244546000	-2.983882000	-1.991921000
C	-6.529121000	-0.242189000	-0.264985000
H	-5.718376000	1.773680000	-0.255256000
C	-6.355034000	-1.580984000	-0.608760000
H	-4.995203000	-2.983882000	-1.518033000
H	-7.121203000	-2.313062000	-0.382393000
O	-3.585934000	2.608983000	-1.187404000
Cl	-8.114926000	0.245267000	0.591568000
H	4.520822000	-0.049322000	2.134379000
H	5.836676000	-2.734469000	2.097749000
C	4.959829000	-2.892606000	2.714474000
H	4.954226000	-2.562096000	3.746278000
H	4.054621000	-3.282422000	2.270128000

4-¹⁰P_(hs, hs)

Fe	2.463267000	-0.334325000	0.953862000
N	0.838483000	0.048425000	-0.057797000
N	1.336849000	-0.838329000	2.640765000
N	2.597404000	1.628556000	1.694418000
N	3.702518000	0.155296000	-0.629297000
N	2.519414000	-2.330742000	0.373988000
C	0.821959000	0.035731000	3.574939000
C	-0.068184000	-0.695733000	4.460678000
H	-0.621764000	-0.255265000	5.278754000
C	-0.086941000	-1.998412000	4.032524000
H	-0.657602000	-2.824113000	4.435524000
C	0.789374000	-2.084018000	2.876713000
C	1.017650000	-3.232983000	2.112023000
H	0.483067000	-4.125815000	2.421831000
C	1.794925000	-3.350496000	0.955484000
C	1.938357000	-4.550783000	0.144392000
H	1.469531000	-5.500830000	0.362001000
C	2.730972000	-4.223293000	-0.924049000
H	3.033766000	-4.856034000	-1.747601000
C	3.084038000	-2.818039000	-0.784561000
C	3.819046000	-2.061384000	-1.702113000
H	4.174728000	-2.585162000	-2.584281000
C	4.098262000	-0.691912000	-1.640151000
C	4.817926000	0.078222000	-2.641797000
H	5.235099000	-0.331203000	-3.551925000
C	4.832712000	1.381828000	-2.217639000
H	5.266396000	2.239805000	-2.713414000
C	4.121993000	1.428379000	-0.949555000
C	3.876395000	2.580793000	-0.194547000
H	4.239614000	3.513669000	-0.615181000
C	3.160362000	2.684414000	1.001220000
C	2.829644000	3.923857000	1.686253000
H	3.133339000	4.908214000	1.357149000
C	2.047339000	3.597203000	2.763074000
H	1.591615000	4.264757000	3.481937000
C	1.885285000	2.152014000	2.755820000
C	1.087391000	1.409021000	3.631376000
H	0.568114000	1.967756000	4.403919000
Fe	-0.714437000	0.395240000	-1.012583000
N	-1.547177000	1.261903000	0.695471000
N	-1.375903000	-1.474697000	-0.358076000
N	0.203203000	-0.519031000	-2.648571000
N	0.179125000	2.197514000	-1.498233000
C	-2.247140000	0.609051000	1.683537000
C	-2.618509000	1.572112000	2.711945000
H	-3.185762000	1.334075000	3.601620000
C	-2.111077000	2.784164000	2.329296000
H	-2.183687000	3.732350000	2.844949000
C	-1.423032000	2.581656000	1.061089000
C	-0.702246000	3.551930000	0.363768000
H	-0.695820000	4.549213000	0.793116000
C	0.042798000	3.377584000	-0.805742000

C	0.816547000	4.404789000	-1.482331000
H	0.887485000	5.434735000	-1.159502000
C	1.409777000	3.815517000	-2.569747000
H	2.057991000	4.272539000	-3.305600000
C	1.005044000	2.419325000	-2.575637000
C	1.397997000	1.457297000	-3.511668000
H	2.083383000	1.791586000	-4.284908000
C	1.046094000	0.105862000	-3.538241000
C	1.560073000	-0.886573000	-4.474328000
H	2.245043000	-0.671792000	-5.283684000
C	1.033860000	-2.096185000	-4.108793000
H	1.204060000	-3.064063000	-4.561555000
C	0.192220000	-1.862101000	-2.941259000
C	-0.461610000	-2.847114000	-2.197381000
H	-0.368855000	-3.867292000	-2.558224000
C	-1.173632000	-2.674596000	-1.005561000
C	-1.815146000	-3.729222000	-0.241035000
H	-1.815928000	-4.775700000	-0.515971000
C	-2.387618000	-3.142132000	0.860103000
H	-2.951549000	-3.616311000	1.652179000
C	-2.104716000	-1.721414000	0.785659000
C	-2.512255000	-0.760791000	1.714956000
H	-3.077400000	-1.124689000	2.567311000
O	4.291847000	-0.626537000	2.293703000
O	-2.357501000	0.781142000	-2.055162000
C	-3.488759000	1.311070000	-1.632790000
C	-4.536853000	0.306735000	-1.197853000
C	-4.350961000	-1.069313000	-1.391628000
C	-5.702315000	0.774112000	-0.566194000
C	-5.314248000	-1.980628000	-0.945985000
H	-3.436004000	-1.400605000	-1.863580000
C	-6.635431000	-0.154973000	-0.134791000
H	-5.828019000	1.840947000	-0.430719000
C	-6.475912000	-1.528842000	-0.304107000
H	-5.152939000	-3.045772000	-1.077800000
H	-7.229100000	-2.220444000	0.054733000
O	-3.750705000	2.537943000	-1.570379000
Cl	-8.183112000	0.448282000	0.722338000
H	5.199673000	-1.872576000	3.736503000
C	4.233029000	-1.745322000	3.233162000
H	3.427626000	-1.602995000	3.960965000
H	4.005209000	-2.617095000	2.619594000
H	4.248551000	0.242469000	2.743751000

4-²P_(hs, hs)

Fe	2.318666000	-0.277668000	0.763142000
N	0.787929000	0.060920000	-0.064926000
N	1.491003000	-0.958460000	2.578600000
N	2.592101000	1.607739000	1.696412000
N	3.628141000	0.328163000	-0.743136000
N	2.599466000	-2.260778000	0.191176000
C	1.002480000	-0.159504000	3.590094000
C	0.224391000	-0.979332000	4.505292000
H	-0.282125000	-0.607809000	5.385667000
C	0.247891000	-2.260326000	4.019939000
H	-0.236905000	-3.137352000	4.426961000
C	1.037862000	-2.242951000	2.799264000
C	1.281103000	-3.341897000	1.971743000
H	0.834554000	-4.283055000	2.277387000
C	1.997421000	-3.355736000	0.770659000
C	2.208231000	-4.514596000	-0.082365000
H	1.838486000	-5.509237000	0.126968000
C	2.926075000	-4.089993000	-1.169921000
H	3.255845000	-4.671398000	-2.020316000
C	3.164678000	-2.665810000	-0.998360000
C	3.829485000	-1.834685000	-1.904806000
H	4.197300000	-2.307150000	-2.810526000
C	4.048287000	-0.459495000	-1.789618000
C	4.739119000	0.377415000	-2.760418000
H	5.168252000	0.020532000	-3.686858000
C	4.717285000	1.658134000	-2.276247000
H	5.126964000	2.550900000	-2.729059000
C	4.013781000	1.621901000	-1.001656000
C	3.753822000	2.722798000	-0.180001000

H	4.076412000	3.689943000	-0.553170000	C	0.763598000	-0.768099000	3.498037000
C	3.084791000	2.725830000	1.046687000	C	-0.061294000	-1.734407000	4.198362000
C	2.745954000	3.905578000	1.821921000	H	-0.629307000	-1.519297000	5.093511000
H	3.003147000	4.918467000	1.543563000	C	0.014621000	-2.905017000	3.496938000
C	2.028154000	3.485449000	2.912010000	H	-0.478572000	-3.846398000	3.698440000
H	1.589342000	4.089375000	3.694597000	C	0.886595000	-2.662529000	2.363844000
C	1.915752000	2.040863000	2.822627000	C	1.194547000	-3.602600000	1.391626000
C	1.202820000	1.219660000	3.700501000	H	0.741066000	-4.584195000	1.488477000
H	0.711079000	1.713728000	4.532552000	C	1.991766000	-3.377832000	0.277827000
Fe	-0.632553000	0.346100000	-0.859661000	C	2.252276000	-4.357587000	-0.759590000
N	-1.481536000	1.173839000	0.847123000	H	1.864554000	-5.367527000	-0.758601000
N	-1.356175000	-1.533116000	-0.281771000	C	3.033702000	-3.744087000	-1.698340000
N	0.143995000	-0.492380000	-2.592186000	H	3.417720000	-4.147132000	-2.625745000
N	0.042008000	2.216273000	-1.446893000	C	3.257797000	-2.386587000	-1.239581000
C	-2.132802000	0.488633000	1.846744000	C	3.970147000	-1.425448000	-1.942044000
C	-2.488420000	1.427347000	2.900156000	H	4.398348000	-1.721895000	-2.894651000
H	-3.019440000	1.163362000	3.804715000	C	4.141922000	-0.106093000	-1.550790000
C	-2.031056000	2.659038000	2.514286000	C	4.850877000	0.895959000	-2.327137000
H	-2.116195000	3.599323000	3.042063000	H	5.333623000	0.705955000	-3.276411000
C	-1.389971000	2.494406000	1.218957000	C	4.762054000	2.069309000	-1.634681000
C	-0.758473000	3.503935000	0.491443000	H	5.154721000	3.042083000	-1.898277000
H	-0.769150000	4.494863000	0.934943000	C	3.999464000	1.791036000	-0.430337000
C	-0.093900000	3.378394000	-0.729099000	C	3.665170000	2.742188000	0.522904000
C	0.601125000	4.446210000	-1.434723000	H	3.991718000	3.761790000	0.343255000
H	0.651623000	5.473452000	-1.099567000	C	2.908348000	2.508736000	1.661766000
C	1.151336000	3.894683000	-2.560794000	C	2.502735000	3.528880000	2.607204000
H	1.740407000	4.383018000	-3.325611000	H	2.771760000	4.573947000	2.532196000
C	0.799510000	2.480780000	-2.561427000	C	1.725320000	2.914661000	3.549948000
C	1.188671000	1.540983000	-3.518771000	H	1.225973000	3.353721000	4.403026000
H	1.810658000	1.907437000	-4.330024000	C	1.649339000	1.513687000	3.188216000
C	0.897578000	0.174450000	-3.529753000	C	0.909293000	0.560148000	3.873407000
C	1.368690000	-0.785443000	-4.517578000	H	0.363167000	0.891991000	4.750936000
H	1.983138000	-0.536215000	-5.372368000	Fe	-0.687539000	0.506497000	-1.012951000
C	0.898286000	-2.016014000	-4.142427000	N	-1.443111000	1.240021000	0.718604000
H	1.053507000	-2.968829000	-4.630879000	N	-1.409994000	-1.331340000	-0.533357000
C	0.133914000	-1.828564000	-2.917516000	N	0.177022000	-0.267610000	-2.661117000
C	-0.475134000	-2.843378000	-2.175183000	N	0.195205000	2.287601000	-1.384223000
H	-0.381496000	-3.851164000	-2.569046000	C	-2.160260000	0.544395000	1.672430000
C	-1.153492000	-2.712557000	-0.960318000	C	-2.519492000	1.433290000	2.755979000
C	-1.746406000	-3.798753000	-0.194582000	H	-3.088464000	1.135121000	3.625450000
H	-1.737817000	-4.838663000	-0.493171000	C	-2.005107000	2.662743000	2.451356000
C	-2.284070000	-3.247336000	0.939619000	H	-2.064151000	3.579558000	3.020714000
H	-2.804023000	-3.748514000	1.745059000	C	-1.326689000	2.535294000	1.180317000
C	-2.026647000	-1.817362000	0.884882000	C	-0.627879000	3.557283000	0.557974000
C	-2.390365000	-0.883645000	1.857168000	H	-0.613844000	4.522731000	1.051260000
H	-2.913576000	-1.269693000	2.726475000	C	0.088237000	3.432756000	-0.620975000
O	4.434737000	-0.542469000	2.006382000	C	0.876524000	4.490829000	-1.217320000
O	-2.356010000	0.657272000	-1.823521000	H	0.960604000	5.489885000	-0.812715000
C	-3.452745000	1.229747000	-1.377783000	C	1.465847000	3.969285000	-2.335021000
C	-4.578296000	0.264871000	-1.051714000	H	2.134214000	4.451805000	-3.034460000
C	-4.425510000	-1.116863000	-1.238574000	C	1.036000000	2.590153000	-2.434908000
C	-5.777708000	0.771425000	-0.522208000	C	1.422987000	1.714129000	-3.437178000
C	-5.458618000	-1.993679000	-0.890671000	H	2.111325000	2.085697000	-4.188246000
H	-3.484431000	-1.475640000	-1.632728000	C	1.026473000	0.389365000	-3.533337000
C	-6.781967000	-0.124215000	-0.190557000	C	1.476813000	-0.526885000	-4.557108000
H	-5.872996000	1.841014000	-0.383281000	H	2.152141000	-0.260655000	-5.358486000
C	-6.658911000	-1.501979000	-0.357481000	C	0.905628000	-1.740839000	-4.289441000
H	-5.328342000	-3.063684000	-1.020880000	H	1.020206000	-2.673645000	-4.823978000
H	-7.468398000	-2.166508000	-0.079043000	C	0.104825000	-1.578868000	-3.096373000
O	-3.637789000	2.461676000	-1.207056000	C	-0.580113000	-2.607713000	-2.467941000
Cl	-8.381410000	0.532572000	0.521318000	H	-0.531190000	-3.590766000	-2.923679000
H	5.451142000	-1.646275000	3.494356000	C	-1.267412000	-2.492049000	-1.268851000
C	4.500436000	-1.656444000	2.943479000	C	-1.920249000	-3.586374000	-0.584262000
H	3.654542000	-1.642250000	3.638417000	H	-1.950404000	-4.603674000	-0.949797000
H	4.436244000	-2.556735000	2.330308000	C	-2.441843000	-3.079035000	0.574392000
H	4.194593000	0.302737000	2.444833000	H	-2.993619000	-3.592536000	1.349094000
				C	-2.116774000	-1.671235000	0.604863000
				C	-2.475545000	-0.804460000	1.624341000
				H	-3.032674000	-1.217232000	2.457588000
				O	4.231223000	-0.881025000	2.158616000
				O	-2.421831000	1.051206000	-1.984377000
				C	-3.534580000	1.510702000	-1.455847000
				C	-4.568702000	0.450717000	-1.125994000
				C	-4.395246000	-0.882368000	-1.524387000
				C	-5.702872000	0.816485000	-0.380978000
Fe	2.458314000	-0.439675000	0.963063000				
N	1.028753000	-0.005029000	0.064311000				
N	1.346834000	-1.356910000	2.389221000				
N	2.394347000	1.278453000	2.042082000				
N	3.639584000	0.457644000	-0.393947000				
N	2.628491000	-2.186523000	-0.023945000				

4-⁶P (is, is)

C	-5.339217000	-1.852827000	-1.172446000
H	-3.503458000	-1.136661000	-2.081395000
C	-6.617303000	-0.169409000	-0.045804000
H	-5.819665000	1.852136000	-0.087471000
C	-6.469163000	-1.503579000	-0.419137000
H	-5.188821000	-2.887030000	-1.465402000
H	-7.206705000	-2.243074000	-0.130107000
O	-3.787717000	2.714293000	-1.188635000
Cl	-8.121488000	0.297162000	0.960292000
H	5.255154000	-2.334668000	3.294352000
C	4.303590000	-2.211834000	2.761654000
H	3.452588000	-2.382019000	3.428529000
H	4.242046000	-2.904461000	1.923157000
H	4.121252000	-0.178216000	2.831847000



⁶4a_(hs) or 4a-⁶R_(hs)

Fe	0.000009000	-0.000016000	0.228963000
N	2.110513000	-0.003388000	0.012807000
N	0.003463000	2.073567000	-0.007614000
N	-0.003516000	-2.073560000	-0.007891000
N	-2.110518000	0.003465000	0.012952000
C	2.907798000	-1.109683000	-0.030368000
C	-1.105595000	2.872950000	-0.046046000
C	2.911458000	1.100217000	-0.030480000
C	1.115066000	2.869340000	-0.046176000
C	1.105560000	-2.872897000	-0.046212000
C	-2.907836000	1.109747000	-0.030323000
C	-1.115099000	-2.869327000	-0.046307000
C	-2.911430000	-1.100148000	-0.030433000
C	4.281723000	-0.700684000	-0.088598000
C	-0.674605000	4.264611000	-0.112878000
C	4.284056000	0.686639000	-0.088686000
C	0.688633000	4.262398000	-0.112925000
C	0.674585000	-4.264598000	-0.112855000
C	-4.281741000	0.700713000	-0.088762000
C	-0.688642000	-4.262413000	-0.112838000
C	-4.284039000	-0.686609000	-0.088743000
H	5.134509000	-1.373070000	-0.130729000
H	-1.345628000	5.118071000	-0.161042000
H	5.139087000	1.356169000	-0.130747000
H	1.362436000	5.113664000	-0.161190000
H	1.345631000	-5.118045000	-0.160934000
H	-5.134535000	1.373081000	-0.131014000
H	-1.362440000	-5.113691000	-0.160969000
H	-5.139042000	-1.356168000	-0.130921000
C	2.429248000	-2.446818000	-0.037672000
C	-2.429294000	2.446874000	-0.037579000
C	-2.437395000	-2.438934000	-0.037620000
C	2.437381000	2.438974000	-0.037606000
H	3.188719000	-3.227535000	-0.075843000
H	-3.188756000	3.227596000	-0.075871000
H	-3.199507000	-3.217052000	-0.076013000
H	3.199448000	3.217133000	-0.076087000
O	-0.000008000	-0.000317000	1.915797000
N	0.000190000	0.000015000	-1.757313000

⁴4a_(hs) or 4a-⁴R_(hs)

Fe	0.000704000	-0.000053000	-0.019021000
N	2.110751000	0.019030000	0.048060000
N	-0.019387000	2.092891000	-0.038781000
N	0.018572000	-2.092902000	-0.038262000
N	-2.110644000	-0.018894000	0.047901000
C	2.918503000	-1.080716000	0.014415000
C	-1.138674000	2.876469000	-0.031760000
C	2.898640000	1.133183000	0.014383000
C	1.085951000	2.896268000	-0.031921000
C	1.138050000	-2.876329000	-0.031536000
C	-2.918628000	1.080710000	0.014279000
C	-1.086591000	-2.896420000	-0.031732000

C	-2.898679000	-1.133016000	0.014419000
C	4.288406000	-0.655536000	-0.021429000
C	-0.720886000	4.275012000	-0.040260000
C	4.275902000	0.732834000	-0.021393000
C	0.643219000	4.287127000	-0.040357000
C	0.720406000	-4.274909000	-0.040334000
C	-4.288547000	0.655543000	-0.021292000
C	-0.643707000	-4.287200000	-0.040475000
C	-4.275983000	-0.732773000	-0.021277000
H	5.150077000	-1.317583000	-0.047266000
H	-1.398784000	5.124617000	-0.039699000
H	5.125513000	1.410306000	-0.047258000
H	1.305881000	5.148659000	-0.039867000
H	1.398388000	-5.124449000	-0.040031000
H	-5.150200000	1.317619000	-0.047095000
H	-1.306243000	-5.148830000	-0.040269000
H	-5.125520000	-1.410342000	-0.047067000
C	2.454773000	-2.426197000	-0.003454000
C	-2.455317000	2.426296000	-0.003608000
C	-2.411067000	-2.469920000	-0.003655000
C	2.410545000	2.469962000	-0.003697000
H	3.227260000	-3.195229000	-0.012459000
H	-3.227956000	3.195174000	-0.012431000
H	-3.169678000	-3.252659000	-0.012577000
H	3.168915000	3.252938000	-0.012453000
O	0.000713000	0.000210000	1.847058000
N	0.000774000	-0.000530000	-1.718823000

⁴4a_(is) or 4a-⁴R_(is)

Fe	-0.000023000	0.000021000	0.032132000
N	1.417590000	1.465908000	-0.014633000
N	-1.483146000	1.418023000	0.001787000
N	1.483105000	-1.418051000	0.001092000
N	-1.417645000	-1.465863000	-0.013882000
C	2.780997000	1.289645000	-0.031801000
C	-2.838881000	1.194656000	-0.019903000
C	1.184087000	2.811318000	-0.008473000
C	-1.307035000	2.772009000	0.000047000
C	2.838828000	-1.194654000	-0.020391000
C	-2.781059000	-1.289631000	-0.031540000
C	1.307014000	-2.772028000	-0.000074000
C	-1.184113000	-2.811278000	-0.008150000
C	3.437026000	2.582436000	-0.039622000
C	-3.541235000	2.438348000	-0.029481000
C	2.452907000	3.524570000	-0.024102000
C	-2.579761000	3.433137000	-0.016799000
C	3.541210000	-2.438343000	-0.029377000
C	-3.437054000	-2.582434000	-0.039830000
C	2.579754000	-3.433144000	-0.016636000
C	-2.452918000	-3.524548000	-0.024268000
H	4.514094000	2.725153000	-0.053964000
H	-4.622936000	2.539804000	-0.044169000
H	2.548427000	4.606775000	-0.023970000
H	-2.717704000	4.510711000	-0.020954000
H	4.622910000	-2.539792000	-0.044210000
H	-4.514116000	-2.725172000	-0.054465000
H	2.717720000	-4.510716000	-0.020552000
H	-2.548411000	-4.606755000	-0.024406000
C	3.441208000	0.076636000	-0.033961000
C	-3.441277000	-0.076630000	-0.033639000
C	0.057070000	-3.429470000	0.007037000
C	-0.057107000	3.429482000	0.006931000
H	4.530310000	0.103691000	-0.048497000
H	-4.530373000	-0.103675000	-0.048600000
H	0.072599000	-4.518244000	0.006151000
H	-0.072676000	4.518256000	0.006103000
O	0.000949000	-0.000009000	1.799774000
N	-0.000589000	-0.000157000	-1.759776000

²4a_(is) or 4a-²R_(is)

Fe	-0.000663000	0.000053000	0.064736000
N	-0.001092000	2.036242000	-0.017196000

N	-2.055348000	-0.001389000	-0.009242000
N	2.055332000	0.001460000	-0.008851000
N	0.001645000	-2.036261000	-0.017482000
C	1.101539000	2.849847000	-0.021258000
C	-2.870884000	-1.100992000	-0.015982000
C	-1.105053000	2.848163000	-0.020316000
C	-2.872514000	1.096933000	-0.015161000
C	2.871041000	1.100943000	-0.015865000
C	-1.101043000	-2.849827000	-0.021296000
C	2.872617000	-1.096811000	-0.014897000
C	1.105532000	-2.848182000	-0.020475000
C	0.677339000	4.241329000	-0.030076000
C	-4.241442000	-0.695940000	-0.022662000
C	-0.683107000	4.240273000	-0.029403000
C	-4.242499000	0.689877000	-0.022134000
C	4.241622000	0.695934000	-0.022732000
C	-0.676891000	-4.241331000	-0.030001000
C	4.242637000	-0.689846000	-0.022096000
C	0.683551000	-4.240290000	-0.029435000
H	1.356308000	5.089506000	-0.037020000
H	-5.089315000	-1.375329000	-0.028527000
H	-1.363499000	5.087315000	-0.035719000
H	-5.091442000	1.367899000	-0.027525000
H	5.089481000	1.375340000	-0.028788000
H	-1.355855000	-5.089514000	-0.036860000
H	5.091538000	-1.367922000	-0.027641000
H	1.363940000	-5.087335000	-0.035747000
C	2.420523000	2.439190000	-0.018871000
C	-2.420086000	-2.439181000	-0.018889000
C	2.423900000	-2.435682000	-0.017410000
C	-2.423503000	2.435740000	-0.017473000
H	3.184529000	3.215440000	-0.024741000
H	-3.183997000	-3.215528000	-0.024552000
H	3.189086000	-3.210776000	-0.022462000
H	-3.188563000	3.210961000	-0.022517000
O	-0.000775000	-0.000264000	1.757777000
N	-0.000311000	-0.000081000	-1.780753000

²4a_(ts) or 4a-²R_(ts)

Fe	-0.000218000	-0.001565000	0.027737000
N	-2.037592000	0.065808000	-0.028449000
N	-0.065461000	-2.050761000	0.008579000
N	0.065397000	2.050556000	0.008382000
N	2.037823000	-0.064129000	-0.028554000
C	-2.814650000	1.194068000	-0.026681000
C	1.006960000	-2.903185000	-0.002715000
C	-2.884519000	-1.011107000	-0.027312000
C	-1.189589000	-2.833282000	-0.003438000
C	-1.006728000	2.903459000	-0.002676000
C	2.814633000	-1.192706000	-0.026510000
C	1.189463000	2.833409000	-0.003531000
C	2.884885000	1.012418000	-0.027569000
C	-4.218787000	0.815681000	-0.034737000
C	0.557446000	-4.260302000	-0.012603000
C	-4.261947000	-0.544637000	-0.035154000
C	-0.827219000	-4.216302000	-0.013138000
C	-0.557271000	4.260598000	-0.012354000
C	4.218872000	-0.814592000	-0.034584000
C	0.827263000	4.216495000	-0.012979000
C	4.262257000	0.545729000	-0.035208000
H	-5.044987000	1.521298000	-0.037464000
H	1.209132000	-5.129580000	-0.020867000
H	-5.130952000	-1.196822000	-0.038253000
H	-1.532476000	-5.042685000	-0.021907000
H	-1.209048000	5.129811000	-0.020405000
H	5.044988000	-1.520312000	-0.037039000
H	1.532727000	5.042710000	-0.021637000
H	5.131347000	1.197798000	-0.038212000
C	-2.359397000	2.498567000	-0.012384000
C	2.359443000	-2.497362000	-0.012251000
C	2.513661000	2.343380000	-0.013800000
C	-2.513555000	-2.342238000	-0.013522000
H	-3.109190000	3.288610000	-0.016486000
H	3.109590000	-3.287086000	-0.016362000

H	3.312130000	3.084160000	-0.018584000
H	-3.312435000	-3.082592000	-0.018243000
O	-0.000130000	-0.001319000	1.823189000
N	-0.000375000	-0.001846000	-1.791721000

4a-⁶ts₁(_{hs})

Fe	0.097615000	-0.000002000	-0.020399000
N	0.105864000	2.069317000	-0.171355000
N	-1.998198000	-0.000035000	-0.254222000
N	2.214093000	0.000040000	0.053855000
N	0.105938000	-2.069316000	-0.171374000
C	1.217312000	2.867357000	-0.119517000
C	-2.794398000	-1.104195000	-0.339061000
C	-0.997745000	2.871216000	-0.268352000
C	-2.794445000	1.104093000	-0.339013000
C	3.011907000	1.102773000	0.056335000
C	-0.997636000	-2.871258000	-0.268396000
C	3.011946000	-1.102664000	0.056365000
C	1.217415000	-2.867313000	-0.119478000
C	0.795935000	4.260734000	-0.203962000
C	-4.166715000	-0.691880000	-0.457644000
C	-0.564719000	4.263688000	-0.294192000
C	-4.166744000	0.691727000	-0.457611000
C	4.392088000	0.691283000	0.089368000
C	-0.564557000	-4.263713000	-0.294201000
C	4.392114000	-0.691123000	0.089387000
C	0.796094000	-4.260706000	-0.203915000
H	1.470013000	5.113123000	-0.192264000
H	-5.018435000	-1.362110000	-0.536893000
H	-1.230992000	5.118586000	-0.373116000
H	-5.018493000	1.361923000	-0.536828000
H	5.247222000	1.361972000	0.103082000
H	-1.230794000	-5.118639000	-0.373135000
H	5.247272000	-1.361780000	0.103119000
H	1.470205000	-5.113069000	-0.192172000
C	2.535711000	2.436832000	-0.000541000
C	-2.320632000	-2.440289000	-0.323908000
C	2.535796000	-2.436738000	-0.000481000
C	-2.320726000	2.440203000	-0.323830000
H	3.295959000	3.217908000	0.018059000
H	-3.079761000	-3.218942000	-0.397096000
H	3.296071000	-3.217788000	0.018148000
H	-3.079884000	3.218831000	-0.396989000
O	0.067482000	-0.000027000	1.844053000
H	-0.948477000	-0.000055000	2.254128000
H	-2.743333000	-0.912181000	2.409260000
H	-2.156507000	-0.000054000	3.899810000
H	-2.743232000	0.912254000	2.409336000
C	-2.308833000	-0.000004000	2.816544000
N	0.242347000	0.000016000	-1.885747000

4a-⁴ts₁(_{hs})

Fe	0.110822000	0.002783000	-0.153623000
N	0.823816000	1.964227000	-0.124278000
N	-1.874835000	0.742132000	-0.236419000
N	2.074798000	-0.738221000	0.004268000
N	-0.627716000	-1.952964000	-0.193589000
C	2.146538000	2.316268000	-0.066711000
C	-3.005629000	-0.016260000	-0.366091000
C	0.064577000	3.095694000	-0.133091000
C	-2.237554000	2.055177000	-0.237816000
C	3.209039000	0.023619000	0.026861000
C	-1.945014000	-2.309180000	-0.312224000
C	2.434950000	-2.049712000	0.026420000
C	0.132349000	-3.084074000	-0.129002000
C	2.234202000	3.770048000	-0.055417000
C	-4.146349000	0.847532000	-0.431921000
C	0.957305000	4.250985000	-0.092777000
C	-3.667938000	2.147748000	-0.348064000
C	4.352632000	-0.841363000	0.077297000
C	-2.029399000	-3.763671000	-0.323166000
C	3.869541000	-2.141482000	0.077815000

C	-0.755839000	-4.240514000	-0.209331000
H	3.161978000	4.334724000	-0.013833000
H	-5.178101000	0.518005000	-0.522272000
H	0.630558000	5.287501000	-0.091375000
H	-4.236597000	3.073603000	-0.371306000
H	5.387796000	-0.511539000	0.111958000
H	-2.952936000	-4.330814000	-0.405016000
H	4.438455000	-3.067075000	0.108215000
H	-0.427944000	-5.276271000	-0.180358000
C	3.227145000	1.442571000	-0.001959000
C	-3.024515000	-1.435991000	-0.395100000
C	1.521028000	-3.140284000	-0.016077000
C	-1.328586000	3.148776000	-0.168655000
H	4.213961000	1.904707000	0.035715000
H	-4.008634000	-1.896101000	-0.485803000
H	1.962696000	-4.136073000	0.015292000
H	-1.775227000	4.142754000	-0.175069000
O	0.121067000	0.000573000	1.768360000
H	-0.926611000	0.002995000	2.211052000
H	-2.591331000	-0.992847000	2.306112000
H	-2.064999000	-0.088767000	3.815304000
H	-2.695287000	0.823749000	2.348869000
C	-2.195246000	-0.068506000	2.727660000
N	0.222925000	-0.002285000	-1.843136000

4a-⁴ts1_(is)

Fe	-0.097628000	0.003565000	-0.072724000
N	0.245936000	-1.974155000	-0.210491000
N	1.906477000	0.358080000	-0.245903000
N	-2.119030000	-0.353103000	0.032084000
N	-0.457060000	1.982075000	-0.161870000
C	-0.694567000	-2.972260000	-0.144125000
C	2.522343000	1.579868000	-0.264429000
C	1.467276000	-2.594341000	-0.327399000
C	2.903877000	-0.575751000	-0.348552000
C	-2.730843000	-1.572118000	0.074419000
C	0.479048000	2.983010000	-0.211029000
C	-3.117318000	0.581044000	0.065071000
C	-1.686246000	2.597750000	-0.115879000
C	-0.045829000	-4.268911000	-0.246479000
C	3.944246000	1.421566000	-0.353639000
C	1.289065000	-4.034935000	-0.360894000
C	4.182503000	0.062897000	-0.409832000
C	-4.155809000	-1.415445000	0.157234000
C	-0.180559000	4.278278000	-0.224247000
C	-4.398357000	-0.057808000	0.149864000
C	-1.518405000	4.038463000	-0.168965000
H	-0.571347000	-5.219450000	-0.227074000
H	4.659179000	2.238820000	-0.381157000
H	2.100346000	-4.751152000	-0.455725000
H	5.133038000	-0.457650000	-0.483619000
H	-4.869010000	-2.233459000	0.205956000
H	0.339741000	5.230771000	-0.269452000
H	-5.350720000	0.463146000	0.194313000
H	-2.337730000	4.751734000	-0.155083000
C	-2.057887000	-2.805702000	0.008879000
C	1.851232000	2.815416000	-0.230364000
C	-2.910322000	1.968895000	-0.002166000
C	2.695378000	-1.965415000	-0.381889000
H	-2.668593000	-3.706766000	0.046546000
H	2.464842000	3.714587000	-0.260840000
H	-3.794839000	2.604065000	0.028658000
H	3.578034000	-2.597754000	-0.467021000
O	-0.084974000	-0.008465000	1.800256000
H	0.928272000	-0.029733000	2.222625000
H	2.762906000	0.811581000	2.340736000
H	2.127605000	0.001309000	3.868533000
H	2.663786000	-1.008320000	2.426056000
C	2.276017000	-0.055454000	2.785876000
N	-0.238673000	0.002674000	-1.964306000

4a-²ts1_(is)

Fe	0.108624000	0.019812000	-0.173920000
N	-0.984006000	1.839449000	-0.267310000
N	-1.663168000	-1.046746000	-0.367451000
N	1.889798000	1.082894000	-0.024436000
N	1.213356000	-1.798827000	-0.164129000
C	-0.446342000	3.085369000	-0.161213000
C	-1.773188000	-2.406761000	-0.313387000
C	-2.331958000	1.953119000	-0.323080000
C	-2.911871000	-0.510900000	-0.389377000
C	1.995744000	2.443611000	0.023312000
C	0.671764000	-3.045973000	-0.169780000
C	3.138207000	0.547681000	0.062863000
C	2.558168000	-1.912183000	-0.036333000
C	-1.513330000	4.061992000	-0.164475000
C	-3.183634000	-2.763655000	-0.320595000
C	-2.692909000	3.356072000	-0.264009000
C	-3.888915000	-1.593420000	-0.367094000
C	3.400610000	2.800775000	0.162968000
C	1.732168000	-4.023531000	-0.051659000
C	4.108026000	1.631752000	0.187464000
C	2.912164000	-3.317611000	0.029914000
H	-1.382822000	5.138730000	-0.090970000
H	-3.571006000	-3.778340000	-0.281575000
H	-3.706511000	3.747953000	-0.285993000
H	-4.967264000	-1.460107000	-0.369334000
H	3.782361000	3.816046000	0.234827000
H	1.595627000	-5.101823000	-0.027229000
H	5.182629000	1.500147000	0.283689000
H	3.920308000	-3.710033000	0.135892000
C	0.935021000	3.353940000	-0.046449000
C	-0.712422000	-3.316923000	-0.246007000
C	3.451982000	-0.818410000	0.041017000
C	-3.224739000	0.856345000	-0.394198000
H	1.210286000	4.407386000	0.018859000
H	-0.993408000	-4.370368000	-0.218408000
H	4.509256000	-1.068139000	0.133276000
H	-4.286450000	1.102593000	-0.405652000
O	0.008466000	0.004266000	1.642292000
H	-0.982101000	-0.160117000	2.102592000
H	-2.734078000	-1.268689000	2.317504000
H	-2.027926000	-0.615140000	3.875182000
H	-2.890609000	0.500977000	2.713817000
C	-2.297622000	-0.409745000	2.832402000
N	0.242334000	0.057577000	-1.934762000

4a-²ts1_(is)

Fe	0.105409000	0.005055000	-0.176481000
N	1.984163000	0.746575000	-0.028002000
N	-0.639053000	1.884079000	-0.198556000
N	0.849181000	-1.882406000	-0.118075000
N	-1.771661000	-0.739669000	-0.286171000
C	3.146576000	0.031886000	0.015700000
C	-1.950119000	2.246043000	-0.318362000
C	2.341221000	2.062954000	0.034165000
C	0.071980000	3.046839000	-0.106772000
C	2.164248000	-2.242401000	-0.059948000
C	-2.930956000	-0.027145000	-0.401551000
C	0.133435000	-3.044979000	-0.118271000
C	-2.134434000	-2.057235000	-0.255815000
C	4.285524000	0.924210000	0.108058000
C	-2.080533000	3.689560000	-0.299894000
C	3.782049000	2.192595000	0.122547000
C	-0.817978000	4.189363000	-0.164673000
C	2.292623000	-3.686135000	-0.029458000
C	-4.070626000	-0.918797000	-0.444914000
C	1.023730000	-4.187613000	-0.061043000
C	-3.574221000	-2.186688000	-0.347828000
H	5.321508000	0.601582000	0.160052000
H	-3.021632000	4.226728000	-0.374915000
H	4.315688000	3.136644000	0.185809000
H	-0.497872000	5.225912000	-0.109055000
H	3.235910000	-4.222661000	0.019786000
H	-5.104750000	-0.596547000	-0.523926000
H	0.700041000	-5.224502000	-0.049305000

H	-4.112151000	-3.130209000	-0.340682000
C	3.238711000	-1.357213000	-0.013823000
C	-3.019765000	1.361857000	-0.433590000
C	-1.255019000	-3.132568000	-0.168168000
C	1.456199000	3.137179000	0.009741000
H	4.237473000	-1.789820000	0.032374000
H	-4.015838000	1.794318000	-0.517645000
H	-1.691075000	-4.130759000	-0.155570000
H	1.885511000	4.136630000	0.070118000
O	0.088830000	-0.029482000	1.803416000
H	-0.891647000	-0.253754000	2.218448000
H	-2.553141000	0.963736000	2.408446000
H	-2.857941000	-0.828894000	2.366441000
H	-2.151354000	-0.056361000	3.871929000
C	-2.255415000	-0.016231000	2.781191000
N	0.244032000	0.005638000	-1.967035000

$[(\text{NH})\text{Fe}^{\text{IV}}(\text{O})(\text{Por}^{\bullet+})]^+$ (**4b**)

${}^6\mathbf{4b}_{(\text{hs})}$ Or $\mathbf{4b-}{}^6\mathbf{R}_{(\text{hs})}$

Fe	0.000010000	0.007358000	-0.162646000
N	1.470843000	-1.470596000	0.007144000
N	-1.480111000	-1.461310000	0.006467000
N	1.481645000	1.473405000	-0.019632000
N	-1.472334000	1.482737000	-0.020387000
C	2.814148000	-1.258798000	0.018244000
C	-2.822039000	-1.240960000	0.017836000
C	1.249056000	-2.813414000	0.017119000
C	-1.266864000	-2.805512000	0.016898000
C	2.822067000	1.254674000	0.013596000
C	-2.814110000	1.272502000	0.013260000
C	1.266267000	2.814026000	0.014599000
C	-1.248450000	2.821951000	0.014414000
C	3.495783000	-2.541942000	0.036425000
C	-3.511792000	-2.519749000	0.036438000
C	2.526990000	-3.504329000	0.035716000
C	-2.549155000	-3.488295000	0.035862000
C	3.511946000	2.534271000	0.058708000
C	-3.495861000	2.556424000	0.059074000
C	2.547925000	3.500135000	0.059587000
C	-2.525720000	3.516141000	0.059990000
H	4.572231000	-2.673552000	0.049450000
H	-4.589061000	-2.644473000	0.049629000
H	2.650887000	-4.581703000	0.048295000
H	-2.679934000	-4.564847000	0.048777000
H	4.588712000	2.659664000	0.091972000
H	-4.571793000	2.688656000	0.092741000
H	2.675769000	4.576593000	0.093662000
H	-2.646677000	4.593383000	0.094559000
C	3.437961000	-0.003561000	0.020478000
C	-3.437927000	0.018154000	0.020075000
C	0.010845000	3.436291000	0.021049000
C	-0.010842000	-3.427878000	0.022268000
H	4.525631000	-0.007523000	0.041653000
H	-4.525594000	0.021022000	0.041522000
H	0.014251000	4.523770000	0.052005000
H	-0.014231000	-4.515668000	0.035208000
O	0.000539000	-0.023067000	-1.842553000
N	-0.000526000	0.004561000	1.828339000
H	-0.002757000	-1.004448000	2.066412000

${}^4\mathbf{4b}_{(\text{hs})}$ Or $\mathbf{4b-}{}^4\mathbf{R}_{(\text{hs})}$

Fe	0.008284000	0.002775000	-0.016987000
N	-1.734071000	1.155664000	0.002141000
N	1.162479000	1.742312000	-0.023847000
N	-1.144734000	-1.739993000	-0.002101000
N	1.749938000	-1.152669000	-0.022113000
C	-3.006729000	0.674973000	-0.010654000
C	2.519410000	1.795351000	-0.011975000
C	-1.786431000	2.513940000	0.008559000
C	0.682328000	3.013477000	0.003500000

C	-2.504271000	-1.794154000	-0.013037000
C	3.020031000	-0.671926000	-0.010539000
C	-0.663442000	-3.011280000	0.005985000
C	1.804375000	-2.510200000	0.005253000
C	-3.933862000	1.794367000	-0.008331000
C	2.939023000	3.188146000	0.016086000
C	-3.178656000	2.932564000	0.003507000
C	1.801469000	3.942672000	0.025349000
C	-2.921239000	-3.186575000	-0.009892000
C	3.950197000	-1.790247000	0.018192000
C	-1.781889000	-3.939876000	0.001896000
C	3.197486000	-2.928965000	0.027815000
H	-5.014975000	1.707294000	-0.017057000
H	3.969000000	3.527965000	0.029112000
H	-3.519039000	3.962397000	0.006168000
H	1.713249000	5.023479000	0.047819000
H	-3.950624000	-3.528309000	-0.017570000
H	5.031077000	-1.700662000	0.031260000
H	-1.693038000	-5.020843000	0.005497000
H	3.538405000	-3.958383000	0.050670000
C	-3.360283000	-0.682682000	-0.016017000
C	3.375321000	0.684638000	-0.013543000
C	0.694148000	-3.365866000	0.013064000
C	-0.673797000	3.368923000	0.013169000
H	-4.426422000	-0.899664000	-0.021478000
H	4.441550000	0.900949000	-0.001195000
H	0.910060000	-4.432161000	0.026556000
H	-0.889825000	4.435210000	0.025898000
O	-0.038229000	-0.005288000	-1.825660000
N	-0.039605000	-0.008039000	1.828143000
H	-1.016138000	-0.191728000	2.115361000

${}^4\mathbf{4b}_{(\text{is})}$ Or $\mathbf{4b-}{}^4\mathbf{R}_{(\text{is})}$

Fe	0.000012214	0.009273884	-0.093065704
N	1.436324174	1.436151038	-0.012648012
N	1.436876323	-1.422429747	-0.001064631
N	-1.435478052	1.437020392	-0.013174063
N	-1.437797774	-1.421545841	-0.001516574
C	1.237355746	2.784125102	0.004987278
C	1.236897087	-2.773031689	0.000380240
C	2.786079496	1.242045087	0.004791170
C	2.786968413	-1.229290841	0.004857948
C	-1.235649821	2.784857229	0.004660408
C	-1.238659861	-2.772274733	0.000265038
C	-2.785334663	1.243767750	0.004520751
C	-2.787755400	-1.227558188	0.004717681
C	2.509602757	3.476953384	0.027689193
C	2.508473423	-3.465138946	0.009205755
C	3.474386932	2.516592960	0.027715970
C	3.473601056	-2.503966902	0.011533364
C	-2.507445835	3.478506651	0.027595688
C	-2.510692126	-3.463574544	0.009355141
C	-3.472846259	2.518770482	0.027600763
C	-3.475198108	-2.501785655	0.011833192
H	2.622948687	4.555102021	0.045598223
H	2.622444338	-4.543360541	0.013163712
H	4.552053659	2.634390256	0.044960719
H	4.551274260	-2.622758506	0.018303817
H	-2.620022786	4.556731654	0.045632558
H	-2.625415632	-4.541717536	0.013506609
H	-4.550434768	2.637271245	0.044969762
H	-4.552948709	-2.619844454	0.018883983
C	0.001039047	3.420331000	0.007254422
C	-0.001080369	-3.407138595	0.002164185
C	-3.424260485	0.009457710	0.007447534
C	3.424231719	0.007332357	0.007603568
H	0.001362517	4.507285359	0.023096406
H	-0.001425653	-4.494257020	0.007018000
H	-4.511248536	0.010430517	0.018894979
H	4.511224443	0.007582330	0.018811022
O	0.000653648	-0.036646690	-1.780666488
N	-0.000558037	-0.008544035	1.882151117
H	0.000798498	-1.013243164	2.138889820

²4b_(is) or 4b-²R_(is)

Fe	0.006721000	0.000247000	-0.074917000
N	-1.430543000	-1.433700000	0.001038000
N	-1.431186000	1.433223000	0.001309000
N	1.440991000	-1.433438000	-0.009086000
N	1.439926000	1.434687000	-0.008616000
C	-1.231351000	-2.783053000	-0.000693000
C	-1.232972000	2.782753000	-0.000701000
C	-2.781550000	-1.238124000	0.003342000
C	-2.782140000	1.236772000	0.003335000
C	1.243544000	-2.781598000	-0.000879000
C	1.241820000	2.782802000	-0.000545000
C	2.788621000	-1.235679000	0.008146000
C	2.787736000	1.237667000	0.008478000
C	-2.503865000	-3.473855000	0.001860000
C	-2.505925000	3.472697000	0.001544000
C	-3.468962000	-2.512344000	0.005234000
C	-3.470366000	2.510531000	0.004883000
C	2.517485000	-3.472452000	0.016261000
C	2.515358000	3.474307000	0.016514000
C	3.479764000	-2.509480000	0.021969000
C	3.478145000	2.511828000	0.022291000
H	-2.619111000	-4.551973000	0.001991000
H	-2.621892000	4.550738000	0.001504000
H	-4.546709000	-2.630949000	0.007759000
H	-4.548194000	2.628370000	0.007224000
H	2.633789000	-4.550425000	0.025465000
H	2.631078000	4.552341000	0.025643000
H	4.557714000	-2.625239000	0.037121000
H	4.556033000	2.628168000	0.037441000
C	0.006891000	-3.417692000	-0.000872000
C	0.004825000	3.418222000	-0.000733000
C	3.424320000	0.001217000	0.013843000
C	-3.417821000	-0.000828000	0.007848000
H	0.007152000	-4.504823000	0.003547000
H	0.004412000	4.505352000	0.003491000
H	4.511334000	0.001630000	0.028322000
H	-4.504916000	-0.001071000	0.012334000
O	-0.009889000	-0.001833000	-1.757949000
N	0.019150000	-0.002931000	1.860200000
H	-0.986031000	-0.000930000	2.118944000

²4b_(is) or 4b-²R_(is)

Fe	-0.006454000	-0.001009000	-0.056322000
N	1.450297000	1.414827000	0.000554000
N	1.420222000	-1.445330000	0.002760000
N	-1.430887000	1.446212000	-0.008657000
N	-1.462140000	-1.414646000	-0.013036000
C	1.262263000	2.765736000	-0.007508000
C	1.202752000	-2.791711000	-0.005470000
C	2.799244000	1.207522000	0.006161000
C	2.773045000	-1.266874000	0.008246000
C	-1.215274000	2.791335000	-0.005935000
C	-1.275093000	-2.763988000	-0.009009000
C	-2.780937000	1.266531000	0.011115000
C	-2.807848000	-1.206301000	0.008135000
C	2.541046000	3.445589000	-0.005219000
C	2.466584000	-3.498865000	-0.002481000
C	3.497897000	2.475859000	0.004295000
C	3.444173000	-2.549940000	0.007025000
C	-2.480026000	3.499325000	0.011813000
C	-2.554735000	-3.445026000	0.009089000
C	-3.455303000	2.549345000	0.022849000
C	-3.509507000	-2.474562000	0.020205000
H	2.665805000	4.522660000	-0.009726000
H	2.568268000	-4.578359000	-0.006912000
H	4.576606000	2.585477000	0.008329000
H	4.520256000	-2.682838000	0.011088000
H	-2.582170000	4.578788000	0.017107000
H	-2.679776000	-4.522068000	0.015198000
H	-4.531561000	2.679877000	0.039212000
H	-4.588288000	-2.582143000	0.037455000

C	0.029875000	3.412101000	-0.010648000
C	-0.043437000	-3.411155000	-0.011166000
C	-3.431441000	0.037010000	0.017599000
C	3.423212000	-0.036391000	0.014949000
H	0.041532000	4.499245000	-0.010629000
H	-0.055165000	-4.498306000	-0.010602000
H	-4.518382000	0.048875000	0.033996000
H	4.510230000	-0.047858000	0.021143000
O	0.029919000	0.001339000	-1.762849000
N	-0.019942000	-0.007744000	1.845922000
H	0.979310000	0.025705000	2.124435000

4b-⁶ts1_(hs)

Fe	-0.101284000	-0.000995000	-0.104219000
N	-1.349918000	-1.683198000	-0.080088000
N	1.567611000	-1.235089000	-0.225830000
N	-1.770401000	1.242761000	-0.039872000
N	1.147761000	1.678241000	-0.198281000
C	-2.705573000	-1.662576000	-0.023200000
C	2.859235000	-0.827934000	-0.358485000
C	-0.938812000	-2.975166000	-0.087708000
C	1.547087000	-2.595173000	-0.216743000
C	-3.063953000	0.829766000	0.018862000
C	2.502249000	1.661439000	-0.320875000
C	-1.750205000	2.601586000	0.000787000
C	0.737450000	2.974796000	-0.139281000
C	-3.200220000	-3.031668000	0.004277000
C	3.721758000	-1.995973000	-0.418154000
C	-2.104968000	-3.845269000	-0.033880000
C	2.909776000	-3.089922000	-0.326504000
C	-3.929418000	1.996451000	0.096878000
C	2.993012000	3.029075000	-0.333733000
C	-3.116512000	3.092983000	0.086793000
C	1.900475000	3.841844000	-0.219457000
H	-4.245959000	-3.316163000	0.048929000
H	4.801434000	-1.967833000	-0.516820000
H	-2.074517000	-4.929501000	-0.026880000
H	3.191535000	-4.137226000	-0.339860000
H	-5.012009000	1.964599000	0.154478000
H	4.035701000	3.315834000	-0.417136000
H	-3.399806000	4.138868000	0.134662000
H	1.871924000	4.925779000	-0.192577000
C	-3.495075000	-0.505010000	0.017264000
C	3.290597000	0.504347000	-0.405029000
C	-0.596509000	3.398092000	-0.043897000
C	0.397856000	-3.395410000	-0.141723000
H	-4.571018000	-0.659077000	0.067894000
H	4.363106000	0.658994000	-0.501627000
H	-0.755795000	4.473834000	-0.008957000
H	0.563808000	-4.470749000	-0.144127000
O	-0.105957000	0.018152000	1.733263000
H	0.917961000	-0.071048000	2.176225000
H	2.737558000	0.698644000	2.352583000
H	1.997849000	-0.093189000	3.837206000
H	2.585217000	-1.121746000	2.431118000
C	2.204481000	-0.156850000	2.766436000
N	-0.211695000	0.044145000	-1.959962000
H	-0.185853000	1.046078000	-2.219061000

4b-⁴ts1_(hs)

Fe	-0.108360000	0.006893000	-0.075172000
N	-0.990512000	-1.889524000	-0.162919000
N	1.778310000	-0.870146000	-0.261901000
N	-1.982147000	0.899937000	-0.004057000
N	0.804556000	1.902595000	-0.157414000
C	-2.323101000	-2.132107000	-0.055200000
C	2.969544000	-0.214023000	-0.347248000
C	-0.333403000	-3.077949000	-0.156834000
C	2.030196000	-2.210323000	-0.262980000
C	-3.168053000	0.242359000	0.038659000
C	2.132455000	2.158721000	-0.277079000
C	-2.227690000	2.233915000	0.010516000

C	0.141145000	3.087708000	-0.130225000
C	-2.537181000	-3.569793000	-0.000165000
C	4.045251000	-1.186911000	-0.396888000
C	-1.304714000	-4.156197000	-0.061329000
C	3.464399000	-2.422982000	-0.342137000
C	-4.249001000	1.216901000	0.095688000
C	2.340464000	3.598301000	-0.313033000
C	-3.666225000	2.450941000	0.078420000
C	1.105184000	4.173886000	-0.222914000
H	-3.504707000	-4.053058000	0.083576000
H	5.100762000	-0.945117000	-0.459091000
H	-1.064181000	-5.213645000	-0.037661000
H	3.949808000	-3.392847000	-0.358885000
H	-5.305703000	0.975212000	0.135764000
H	3.304027000	4.088948000	-0.400009000
H	-4.150037000	3.421363000	0.107406000
H	0.857144000	5.229924000	-0.220304000
C	-3.324673000	-1.151953000	0.019986000
C	3.133364000	1.179255000	-0.361151000
C	-1.251184000	3.239663000	-0.042179000
C	1.060845000	-3.224304000	-0.212228000
H	-4.347261000	-1.518706000	0.083813000
H	4.156699000	1.539980000	-0.442404000
H	-1.618985000	4.263826000	-0.028542000
H	1.437607000	-4.245085000	-0.209525000
O	-0.141902000	-0.019807000	1.753691000
H	0.890286000	-0.083092000	2.211714000
H	2.639833000	0.789101000	2.392482000
H	1.993120000	-0.126741000	3.847203000
H	2.618728000	-1.037443000	2.378732000
C	2.174083000	-0.121685000	2.769419000
N	-0.272049000	0.009726000	-1.968955000
H	0.358102000	-0.762038000	-2.259202000

4b-⁴ts1_(is)

Fe	-0.100874000	0.013091000	-0.121217000
N	-1.293896000	-1.630096000	-0.085924000
N	1.546840000	-1.150492000	-0.244601000
N	-1.755168000	1.184017000	-0.026602000
N	1.084976000	1.652298000	-0.183328000
C	-2.654939000	-1.662737000	-0.035202000
C	2.842701000	-0.744737000	-0.383072000
C	-0.870767000	-2.926458000	-0.050941000
C	1.571012000	-2.515639000	-0.184672000
C	-3.055512000	0.775987000	0.002903000
C	2.440373000	1.690385000	-0.340621000
C	-1.773924000	2.544818000	0.021630000
C	0.666102000	2.948439000	-0.116922000
C	-3.120254000	-3.033878000	0.021637000
C	3.725243000	-1.890528000	-0.404777000
C	-2.008716000	-3.820927000	0.016764000
C	2.934194000	-2.992932000	-0.274013000
C	-3.939389000	1.923079000	0.071849000
C	2.904236000	3.062087000	-0.360186000
C	-3.140624000	3.025039000	0.088022000
C	1.799517000	3.845275000	-0.215615000
H	-4.162284000	-3.330050000	0.067940000
H	4.803852000	-1.835985000	-0.499999000
H	-1.941524000	-4.902484000	0.055239000
H	3.224278000	-4.037283000	-0.244938000
H	-5.021660000	1.866684000	0.106399000
H	3.940573000	3.361321000	-0.470035000
H	-3.425049000	4.070306000	0.135882000
H	1.733078000	4.927109000	-0.184962000
C	-3.485132000	-0.545963000	-0.011160000
C	3.267430000	0.578560000	-0.446865000
C	-0.654820000	3.370662000	-0.005953000
C	0.456224000	-3.343343000	-0.087464000
H	-4.557264000	-0.722558000	0.025538000
H	4.334123000	0.756218000	-0.557083000
H	-0.829132000	4.443045000	0.035752000
H	0.638998000	-4.414662000	-0.054258000
O	-0.101124000	-0.069059000	1.721388000
H	0.929140000	-0.074444000	2.151802000

H	2.694600000	0.808323000	2.326801000
H	2.019756000	-0.044179000	3.807891000
H	2.668922000	-1.018586000	2.392507000
C	2.222433000	-0.084859000	2.735220000
N	-0.191679000	-0.032323000	-1.983931000
H	-0.108520000	-1.018498000	-2.286628000

4b-²ts1_(is)

Fe	-0.100063000	0.007461000	-0.128834000
N	1.089978000	-1.634358000	-0.192936000
N	1.551374000	1.171662000	-0.227429000
N	-1.754449000	-1.160495000	-0.039459000
N	-1.284294000	1.651928000	-0.074951000
C	0.671071000	-2.930814000	-0.104499000
C	1.577323000	2.534156000	-0.182048000
C	2.445223000	-1.672321000	-0.342491000
C	2.845928000	0.764415000	-0.382663000
C	-1.771825000	-2.523352000	0.029152000
C	-0.861554000	2.946580000	-0.052902000
C	-3.052910000	-0.751163000	-0.002378000
C	-2.646515000	1.686340000	-0.040645000
C	1.805339000	-3.826634000	-0.187655000
C	2.940572000	3.011969000	-0.289730000
C	2.909871000	-3.043277000	-0.341517000
C	3.729793000	1.909733000	-0.423060000
C	-3.137763000	-3.000413000	0.107816000
C	-1.999585000	3.843774000	-0.003893000
C	-3.935727000	-1.897009000	0.083849000
C	-3.111703000	3.058817000	-0.001844000
H	1.741421000	-4.907890000	-0.137593000
H	3.230083000	4.056798000	-0.274352000
H	3.947047000	-3.343201000	-0.440978000
H	4.806967000	1.853949000	-0.532995000
H	-3.423410000	-4.044437000	0.172315000
H	-1.931057000	4.925647000	0.021673000
H	-5.017642000	-1.839872000	0.126906000
H	-4.153947000	3.356284000	0.029314000
C	-0.652252000	-3.348736000	0.007557000
C	0.464474000	3.364581000	-0.084901000
C	-3.479423000	0.573863000	-0.018093000
C	3.270643000	-0.556790000	-0.452076000
H	-0.827534000	-4.420347000	0.064117000
H	0.647376000	4.436069000	-0.061107000
H	-4.551215000	0.752843000	0.015712000
H	4.337024000	-0.733683000	-0.567031000
O	-0.116566000	-0.059389000	1.725770000
H	0.923126000	-0.034737000	2.170412000
H	2.543896000	1.065666000	2.398602000
H	2.019492000	0.006688000	3.801346000
H	2.748489000	-0.745377000	2.294443000
C	2.190820000	0.086990000	2.724766000
N	-0.229087000	-0.087541000	-1.970376000
H	-0.331408000	-1.075910000	-2.257688000

4b-²ts1_(ls)

Fe	0.096081000	0.003069000	-0.120919000
N	-1.135119000	1.610760000	-0.194116000
N	-1.524302000	-1.205298000	-0.226753000
N	1.721608000	1.215166000	-0.041631000
N	1.332288000	-1.605124000	-0.087707000
C	-0.751421000	2.916864000	-0.123229000
C	-1.511404000	-2.567341000	-0.176596000
C	-2.489232000	1.611005000	-0.353093000
C	-2.827328000	-0.834463000	-0.379714000
C	1.700592000	2.577859000	0.020395000
C	0.940949000	-2.911422000	-0.051697000
C	3.033438000	0.843806000	0.003646000
C	2.695296000	-1.604560000	-0.035032000
C	-1.908458000	3.783068000	-0.221720000
C	-2.861567000	-3.083987000	-0.277032000
C	-2.990731000	2.969464000	-0.370703000
C	-3.680697000	-2.003999000	-0.411227000

C	3.051706000	3.094140000	0.105037000
C	2.100550000	-3.776651000	0.018083000
C	3.882122000	2.014596000	0.089735000
C	3.193355000	-2.963288000	0.022778000
H	-1.872460000	4.866249000	-0.187225000
H	-3.122341000	-4.136193000	-0.256247000
H	-4.034798000	3.240192000	-0.480901000
H	-4.759258000	-1.978014000	-0.518105000
H	3.306672000	4.146220000	0.166049000
H	2.059917000	-4.859479000	0.057679000
H	4.964997000	1.989478000	0.138405000
H	4.242045000	-3.234388000	0.070786000
C	0.559013000	3.372439000	-0.009065000
C	-0.374116000	-3.364391000	-0.082301000
C	3.497808000	-0.467931000	-0.010747000
C	-3.285943000	0.475762000	-0.455594000
H	0.704931000	4.448750000	0.039608000
H	-0.526263000	-4.440589000	-0.050883000
H	4.573773000	-0.617147000	0.031683000
H	-4.356191000	0.624901000	-0.573017000
O	0.105398000	-0.010874000	1.725933000
H	-0.934133000	-0.035626000	2.170484000
N	0.175041000	0.009154000	-1.993136000
H	1.189684000	-0.052145000	-2.209019000
H	-2.628056000	-1.019457000	2.410909000
H	-2.028608000	0.004002000	3.809965000
H	-2.708803000	0.800850000	2.304340000
C	-2.207099000	-0.066472000	2.733963000

$[(\text{NH}_2)\text{Fe}^{\text{IV}}(\text{O})(\text{Por}^{\bullet+})]$ (**4c**)

${}^6\mathbf{4c}_{(\text{hs})}$ or $\mathbf{4c-}{}^6\mathbf{R}_{(\text{hs})}$

Fe	-0.031601000	0.004677000	-0.205274000
N	-0.289742000	-2.048238000	0.012317000
N	-2.066437000	0.280605000	0.077524000
N	2.032108000	-0.276190000	0.006798000
N	0.267626000	2.051616000	0.012778000
C	0.690483000	-2.996795000	-0.012047000
C	-2.713716000	1.480001000	0.063432000
C	-1.493571000	-2.695704000	0.017389000
C	-3.010489000	-0.702325000	0.063898000
C	2.685180000	-1.485258000	-0.001332000
C	-0.719891000	2.996619000	0.016847000
C	2.984115000	0.714928000	0.000033000
C	1.465286000	2.704195000	-0.010727000
C	0.085336000	-4.312861000	-0.016909000
C	-4.144871000	1.251587000	0.063995000
C	-1.265984000	-4.126086000	0.000855000
C	-4.328667000	-0.100155000	0.064329000
C	4.110193000	-1.247879000	-0.009817000
C	-0.119075000	4.314473000	0.000522000
C	4.294117000	0.105991000	-0.008930000
C	1.233142000	4.134049000	-0.016103000
H	0.634309000	-5.246573000	-0.031291000
H	-4.896446000	2.031625000	0.062161000
H	-2.047034000	-4.876632000	0.005646000
H	-5.261096000	-0.651447000	0.062799000
H	4.864721000	-2.024990000	-0.024677000
H	-0.671840000	5.246051000	0.004690000
H	5.228489000	0.653904000	-0.023051000
H	2.011069000	4.887712000	-0.029953000
C	2.065630000	-2.734754000	-0.014984000
C	-2.091335000	2.732736000	0.045039000
C	2.720663000	2.084376000	-0.012747000
C	-2.745018000	-2.075640000	0.046052000
H	2.723335000	-3.599321000	-0.029276000
H	-2.748851000	3.597744000	0.042172000
H	3.585142000	2.742221000	-0.026174000
H	-3.609213000	-2.734218000	0.043654000
O	-0.132167000	0.018929000	-1.825363000
N	0.374483000	-0.052655000	1.851083000
H	0.695126000	-0.940982000	2.243656000

H	0.935794000	0.706915000	2.243432000
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${}^4\mathbf{4c}_{(\text{hs})}$ or $\mathbf{4c-}{}^4\mathbf{R}_{(\text{hs})}$

Fe	-0.030278000	0.000026000	-0.197031000
N	-0.018650000	-2.068119000	0.023484000
N	-2.087260000	0.003462000	0.053528000
N	2.046519000	-0.003370000	0.029884000
N	-0.011808000	2.068172000	0.023272000
C	1.079125000	-2.877949000	-0.009463000
C	-2.889964000	1.104954000	0.052845000
C	-1.125091000	-2.870568000	0.013461000
C	-2.893614000	-1.095361000	0.052757000
C	2.855196000	-1.113292000	0.008204000
C	-1.115578000	2.874291000	0.013451000
C	2.858873000	1.103863000	0.008077000
C	1.088642000	2.874369000	-0.009630000
C	0.654774000	-4.262698000	-0.029922000
C	-4.278174000	0.689134000	0.067267000
C	-0.709392000	-4.257644000	-0.015780000
C	-4.280448000	-0.674925000	0.067198000
C	4.237009000	-0.689820000	-0.010890000
C	-0.695276000	4.259996000	-0.015677000
C	4.239284000	0.675794000	-0.010978000
C	0.668898000	4.260507000	-0.029920000
H	1.323140000	-5.114834000	-0.052109000
H	-5.126610000	1.362493000	0.075872000
H	-1.383750000	-5.105316000	-0.023091000
H	-5.131136000	-1.345434000	0.075751000
H	5.087469000	-1.360415000	-0.031559000
H	-1.366789000	5.109922000	-0.022851000
H	5.091987000	1.343529000	-0.031736000
H	1.340115000	5.110402000	-0.052062000
C	2.406888000	-2.434314000	-0.009686000
C	-2.439775000	2.429625000	0.036567000
C	2.414922000	2.426362000	-0.009894000
C	-2.447798000	-2.421529000	0.036463000
H	3.173679000	-3.203662000	-0.032521000
H	-3.206510000	3.199567000	0.032678000
H	3.184280000	3.193144000	-0.032766000
H	-3.217105000	-3.188900000	0.032445000
O	-0.050029000	-0.000094000	-1.823342000
N	0.353276000	-0.000513000	1.879871000
H	0.835161000	-0.829881000	2.237343000
H	0.837998000	0.827266000	2.237193000

${}^4\mathbf{4c}_{(\text{is})}$ or $\mathbf{4c-}{}^4\mathbf{R}_{(\text{is})}$

Fe	0.000080000	0.026831000	-0.144882000
N	2.015799000	0.012068000	-0.006113000
N	-0.004788000	-1.995504000	-0.010078000
N	0.004908000	2.029452000	0.038815000
N	-2.015660000	0.021778000	-0.006205000
C	2.841543000	1.105057000	0.002511000
C	-1.107142000	-2.820040000	-0.016210000
C	2.836700000	-1.082803000	-0.029131000
C	1.093491000	-2.825470000	-0.016032000
C	1.099988000	2.848525000	0.040050000
C	-2.841957000	-1.069032000	-0.029375000
C	-1.086106000	2.853912000	0.040084000
C	-2.836011000	1.118836000	0.002582000
C	4.223581000	0.688611000	-0.010660000
C	-0.691574000	-4.199474000	-0.015833000
C	4.220912000	-0.672423000	-0.030383000
C	0.671067000	-4.202876000	-0.015700000
C	0.690719000	4.233393000	0.055632000
C	-4.224162000	-0.651770000	-0.030566000
C	-0.669965000	4.236787000	0.055671000
C	-4.220042000	0.709258000	-0.010623000
H	5.068594000	1.365938000	-0.003798000
H	-1.370682000	-5.043097000	-0.022917000
H	5.062859000	-1.353504000	-0.043853000
H	1.345883000	-5.049928000	-0.022653000
H	1.372911000	5.074442000	0.064155000

H	-5.069544000	-1.328586000	-0.044116000
H	-1.347887000	5.081271000	0.064245000
H	-5.061621000	1.390855000	-0.003624000
C	2.422899000	2.427082000	0.028481000
C	-2.425832000	-2.395139000	-0.032824000
C	-2.411057000	2.438802000	0.028632000
C	2.414233000	-2.406869000	-0.032502000
H	3.191130000	3.194335000	0.033360000
H	-3.196192000	-3.160085000	-0.046481000
H	-3.175491000	3.209835000	0.033551000
H	3.180816000	-3.175604000	-0.046057000
O	0.000394000	0.097278000	-1.773024000
N	-0.001344000	-0.358151000	1.913309000
H	-0.831481000	-0.824760000	2.289097000
H	0.825357000	-0.830650000	2.289309000

²4c_(is) or 4c-²R_(is)

Fe	-0.034547000	0.000062000	-0.126864000
N	1.999191000	-0.001798000	-0.001967000
N	-0.023932000	-2.015645000	0.003900000
N	-0.020202000	2.015689000	0.003910000
N	-2.033281000	0.001904000	0.022559000
C	2.825195000	1.097084000	-0.019749000
C	-1.118460000	-2.838643000	0.003919000
C	2.823204000	-1.102193000	-0.019305000
C	1.070655000	-2.838042000	-0.018206000
C	1.075848000	2.836137000	-0.018765000
C	-2.856499000	-1.090946000	0.023205000
C	-1.113256000	2.840657000	0.004446000
C	-2.854545000	1.096212000	0.023785000
C	4.204230000	0.677563000	-0.034858000
C	-0.704738000	-4.221439000	-0.008524000
C	4.203009000	-0.685171000	-0.034507000
C	0.656441000	-4.221287000	-0.022062000
C	0.664105000	4.220130000	-0.022493000
C	-4.239638000	-0.676563000	0.034501000
C	-0.697062000	4.222695000	-0.008227000
C	-4.238436000	0.684300000	0.034909000
H	5.050261000	1.353583000	-0.050432000
H	-1.383631000	-5.065227000	-0.007247000
H	5.047850000	-1.362684000	-0.049753000
H	1.335665000	-5.064758000	-0.035077000
H	1.344793000	5.062412000	-0.035870000
H	-5.083289000	-1.355578000	0.041147000
H	-1.374495000	5.067657000	-0.006620000
H	-5.080904000	1.364773000	0.041945000
C	2.400999000	2.416799000	-0.027788000
C	-2.439601000	-2.415385000	0.017227000
C	-2.435171000	2.419884000	0.018192000
C	2.396569000	-2.421134000	-0.026940000
H	3.166603000	3.186480000	-0.045193000
H	-3.209586000	-3.180892000	0.017228000
H	-3.203752000	3.186800000	0.018630000
H	3.160801000	-3.192186000	-0.043960000
O	-0.007479000	-0.000263000	-1.752489000
N	0.344928000	-0.000424000	1.898813000
H	0.790894000	-0.831992000	2.295219000
H	0.792816000	0.830076000	2.295292000

²4c_(ls) or 4c-²R_(ls)

Fe	-0.037931000	0.000067000	-0.116046000
N	2.001891000	-0.002847000	-0.001836000
N	-0.026363000	-2.016092000	0.004129000
N	-0.020555000	2.016160000	0.003958000
N	-2.033216000	0.002949000	0.012613000
C	2.826802000	1.095106000	-0.020597000
C	-1.120536000	-2.838839000	0.003852000
C	2.823633000	-1.103177000	-0.020279000
C	1.069027000	-2.837981000	-0.015341000
C	1.077173000	2.834918000	-0.015744000
C	-2.857189000	-1.089976000	0.015566000
C	-1.112364000	2.842039000	0.004129000

C	-2.854069000	1.098218000	0.015909000
C	4.206375000	0.675239000	-0.037605000
C	-0.706662000	-4.221591000	-0.005248000
C	4.204392000	-0.687337000	-0.037304000
C	0.654537000	-4.221243000	-0.017028000
C	0.666694000	4.219344000	-0.017161000
C	-4.239761000	-0.674327000	0.027300000
C	-0.694491000	4.223626000	-0.005035000
C	-4.237798000	0.686562000	0.027625000
H	5.052634000	1.350960000	-0.053972000
H	-1.385473000	-5.065436000	-0.003667000
H	5.048672000	-1.365541000	-0.053394000
H	1.333824000	-5.064689000	-0.027928000
H	1.348438000	5.060807000	-0.028161000
H	-5.083893000	-1.352730000	0.034661000
H	-1.370854000	5.069431000	-0.003198000
H	-5.079960000	1.367409000	0.035272000
C	2.402026000	2.415068000	-0.025795000
C	-2.441615000	-2.414603000	0.012952000
C	-2.434679000	2.421629000	0.013522000
C	2.395083000	-2.421906000	-0.025224000
H	3.167537000	3.184867000	-0.042121000
H	-3.212318000	-3.179356000	0.013595000
H	-3.203110000	3.188663000	0.014479000
H	3.158352000	-3.193933000	-0.041337000
O	0.025297000	-0.000223000	-1.742295000
N	0.322643000	-0.000458000	1.879595000
H	0.767851000	-0.832484000	2.275652000
H	0.771856000	0.829482000	2.275491000

4c-⁶ts1_(hs)

Fe	0.066119000	0.009473000	0.125161000
N	1.133400000	1.793826000	-0.089332000
N	-1.699020000	1.032568000	-0.217583000
N	1.871643000	-1.024290000	-0.009714000
N	-0.956900000	-1.787387000	-0.184496000
C	2.490086000	1.942887000	-0.052744000
C	-2.938944000	0.486500000	-0.400180000
C	0.579527000	3.042658000	-0.128072000
C	-1.836526000	2.392678000	-0.255606000
C	3.126532000	-0.475250000	0.026975000
C	-2.304700000	-1.933062000	-0.353074000
C	2.009248000	-2.388743000	0.024851000
C	-0.405480000	-3.037043000	-0.145178000
C	2.817758000	3.354030000	-0.072961000
C	-3.913787000	1.546296000	-0.527950000
C	1.635558000	4.033981000	-0.115541000
C	-3.232368000	2.726626000	-0.432643000
C	4.103569000	-1.537808000	0.093809000
C	-2.628583000	-3.343379000	-0.411431000
C	3.414308000	-2.717801000	0.095054000
C	-1.453889000	-4.026449000	-0.280293000
H	3.823133000	3.756900000	-0.053898000
H	-4.975823000	1.395634000	-0.679262000
H	1.478715000	5.105522000	-0.140749000
H	-3.624923000	3.734329000	-0.494544000
H	5.175578000	-1.388917000	0.139206000
H	-3.626532000	-3.744861000	-0.539716000
H	3.811215000	-3.724699000	0.139478000
H	-1.297674000	-5.098380000	-0.281224000
C	3.412158000	0.892711000	0.001105000
C	-3.221047000	-0.882241000	-0.453394000
C	0.961771000	-3.312093000	-0.031417000
C	-0.788869000	3.317687000	-0.188987000
H	4.462428000	1.168470000	0.031111000
H	-4.262659000	-1.157358000	-0.593307000
H	1.243720000	-4.360995000	-0.008922000
H	-1.069814000	4.366607000	-0.224372000
O	0.118908000	-0.040774000	1.990284000
H	-1.034593000	0.053256000	2.422439000
H	-2.760005000	-0.692417000	2.290592000
H	-2.212999000	0.046775000	3.874991000
H	-2.594052000	1.116847000	2.436046000
C	-2.258878000	0.139552000	2.787100000

N	0.432175000	-0.151434000	-2.075751000
H	1.349201000	0.279009000	-2.251216000
H	0.570967000	-1.149232000	-2.281512000

4c-⁴ts1_(hs)

Fe	-0.079854000	0.051424000	-0.032777000
N	-1.050403000	-1.823563000	-0.150047000
N	1.718152000	-0.889050000	-0.249169000
N	-1.900839000	0.979307000	-0.008144000
N	0.870335000	1.909095000	-0.246069000
C	-2.400478000	-2.027958000	-0.059224000
C	2.942772000	-0.276504000	-0.320766000
C	-0.438029000	-3.046020000	-0.181975000
C	1.934038000	-2.241298000	-0.249025000
C	-3.118812000	0.369557000	0.088946000
C	2.211219000	2.121003000	-0.325604000
C	-2.105924000	2.329800000	0.055966000
C	0.263102000	3.123122000	-0.170940000
C	-2.659659000	-3.452054000	-0.048392000
C	3.978562000	-1.284579000	-0.353320000
C	-1.448639000	-4.080588000	-0.123435000
C	3.356461000	-2.498400000	-0.308182000
C	-4.150571000	1.379333000	0.218715000
C	2.477108000	3.547571000	-0.325701000
C	-3.524465000	2.589958000	0.199174000
C	1.266594000	4.170074000	-0.229222000
H	-3.642294000	-3.902168000	0.025626000
H	5.040031000	-1.076376000	-0.410424000
H	-1.247389000	-5.145083000	-0.122448000
H	3.805159000	-3.484252000	-0.321935000
H	-5.209660000	1.171389000	0.310445000
H	3.460509000	3.998216000	-0.385018000
H	-3.966649000	3.576269000	0.270096000
H	1.060198000	5.233006000	-0.193935000
C	-3.350654000	-1.011721000	0.051092000
C	3.169873000	1.102616000	-0.364617000
C	-1.116572000	3.313663000	-0.030672000
C	0.944276000	-3.232556000	-0.222029000
H	-4.387882000	-1.325580000	0.130104000
H	4.209298000	1.414264000	-0.423299000
H	-1.460052000	4.343095000	0.026365000
H	1.295812000	-4.260582000	-0.232688000
O	-0.058037000	0.080548000	1.725114000
H	0.926049000	-0.257471000	2.160346000
N	-0.397058000	-0.288216000	-1.993133000
H	2.779548000	0.250346000	2.539899000
H	1.838459000	-0.623305000	3.858400000
H	2.426950000	-1.543090000	2.374127000
C	2.137414000	-0.587662000	2.810114000
H	-1.374310000	-0.323580000	-2.292854000
H	0.099714000	-1.083662000	-2.401002000

4c-⁴ts1_(is)

Fe	-0.127310000	0.000478000	-0.090898000
N	-0.621423000	-1.945691000	-0.147905000
N	1.844926000	-0.501998000	-0.211414000
N	-2.064117000	0.501579000	0.023488000
N	0.385945000	1.950242000	-0.209158000
C	-1.885943000	-2.467945000	-0.098269000
C	2.910837000	0.352410000	-0.318894000
C	0.237508000	-3.014667000	-0.137306000
C	2.365713000	-1.768499000	-0.193950000
C	-3.133077000	-0.349827000	0.054152000
C	1.650724000	2.471965000	-0.304958000
C	-2.578808000	1.766734000	0.094078000
C	-0.464419000	3.017693000	-0.109759000
C	-1.827619000	-3.909541000	-0.086887000
C	4.143822000	-0.395541000	-0.349001000
C	-0.509024000	-4.249120000	-0.106160000
C	3.805948000	-1.712919000	-0.266237000
C	-4.365441000	0.398924000	0.162993000
C	1.593434000	3.913630000	-0.291525000

C	-4.020744000	1.713816000	0.192167000
C	0.280079000	4.252291000	-0.166083000
H	-2.694741000	-4.557556000	-0.053901000
H	5.129072000	0.048147000	-0.422410000
H	-0.062161000	-5.235612000	-0.094957000
H	4.454556000	-2.580311000	-0.262360000
H	-5.351716000	-0.046213000	0.207637000
H	2.458309000	4.562208000	-0.357937000
H	-4.662495000	2.583330000	0.263350000
H	-0.163500000	5.238739000	-0.110490000
C	-3.061164000	-1.732890000	-0.018503000
C	2.827457000	1.737154000	-0.370306000
C	-1.843824000	2.941057000	0.035967000
C	1.623740000	-2.941176000	-0.148719000
H	-3.994733000	-2.285957000	0.016082000
H	3.757976000	2.291224000	-0.447192000
H	-2.390349000	3.876882000	0.101186000
H	2.171817000	-3.878361000	-0.137814000
O	-0.066705000	0.021630000	1.658640000
H	0.990433000	-0.019738000	2.126942000
H	2.610936000	0.970775000	2.499200000
H	1.896596000	-0.064501000	3.839461000
H	2.746533000	-0.853978000	2.412056000
C	2.195496000	0.006146000	2.792240000
N	-0.037642000	-0.033948000	-1.999836000
H	0.239022000	-0.925510000	-2.415529000
H	0.486148000	0.721496000	-2.445566000

4c-²ts1_(is)

Fe	0.073760000	0.018715000	-0.081239000
N	-1.680696000	0.966602000	-0.221515000
N	-0.887479000	-1.747751000	-0.213948000
N	1.057930000	1.773944000	-0.121237000
N	1.867294000	-0.953921000	0.007698000
C	-1.877316000	2.320815000	-0.157200000
C	-0.320656000	-2.990326000	-0.089525000
C	-2.921900000	0.410008000	-0.386858000
C	-2.232171000	-1.953430000	-0.374187000
C	0.489072000	3.017726000	-0.076046000
C	2.047733000	-2.306662000	0.105256000
C	2.413243000	1.970098000	-0.072154000
C	3.114555000	-0.392480000	0.041452000
C	-3.285637000	2.626622000	-0.252876000
C	-1.338708000	-4.009604000	-0.179019000
C	-3.933691000	1.439118000	-0.406980000
C	-2.525279000	-3.366002000	-0.363901000
C	1.513549000	4.033513000	-0.023769000
C	3.457137000	-2.612016000	0.209794000
C	2.709630000	3.382695000	-0.029458000
C	4.119924000	-1.423771000	0.163538000
H	-3.700070000	3.626836000	-0.222694000
H	-1.148741000	-5.073653000	-0.109187000
H	-4.994731000	1.254794000	-0.522252000
H	-3.516232000	-3.789044000	-0.474034000
H	1.321208000	5.098665000	0.014721000
H	3.863920000	-3.611552000	0.302726000
H	3.708779000	3.799033000	0.008246000
H	5.186142000	-1.240056000	0.214012000
C	-0.875057000	3.278339000	-0.076384000
C	1.034548000	-3.255150000	0.072601000
C	3.376460000	0.969499000	-0.016398000
C	-3.185987000	-0.949199000	-0.482422000
H	-1.183077000	4.318850000	-0.035582000
H	1.327229000	-4.297539000	0.156421000
H	4.415860000	1.281287000	0.022445000
H	-4.221286000	-1.251684000	-0.607187000
O	0.087265000	-0.023165000	1.666383000
H	-0.943314000	-0.002784000	2.105682000
H	-2.684898000	-0.875046000	2.278704000
H	-1.971281000	-0.076593000	3.780704000
H	-2.643877000	0.957084000	2.408973000
C	-2.218677000	0.004147000	2.721801000
N	0.435980000	-0.156249000	-1.988024000
H	1.255545000	0.333614000	-2.354542000

H 0.397121000 -1.095506000 -2.390412000

4c-²ts1_(ls)

Fe -0.070358000 0.003964000 -0.104417000
N -2.055351000 -0.445453000 0.024635000
N 0.366302000 -1.955416000 -0.204116000
N -0.529729000 1.966435000 -0.162489000
N 1.881337000 0.447408000 -0.198001000
C -3.094932000 0.439559000 0.074077000
C 1.611546000 -2.516112000 -0.304479000
C -2.603448000 -1.694053000 0.104679000
C -0.520131000 -2.997622000 -0.102795000
C -1.782517000 2.519917000 -0.092893000
C 2.923485000 -0.434511000 -0.314713000
C 0.353837000 3.010931000 -0.166133000
C 2.437978000 1.700141000 -0.208284000
C -4.347201000 -0.272610000 0.197872000
C 1.510096000 -3.954395000 -0.291426000
C -4.041610000 -1.598283000 0.219913000
C 0.187155000 -4.253067000 -0.163396000
C -1.685805000 3.959298000 -0.088018000
C 4.176445000 0.278900000 -0.365386000
C -0.358957000 4.264289000 -0.128806000
C 3.875573000 1.604572000 -0.294133000
H -5.319085000 0.201320000 0.259528000
H 2.354465000 -4.628968000 -0.361636000
H -4.708434000 -2.447832000 0.301260000
H -0.286371000 -5.225453000 -0.106707000
H -2.535220000 4.629658000 -0.042523000
H 5.147321000 -0.193331000 -0.450890000
H 0.113681000 5.238708000 -0.127605000
H 4.545928000 2.455017000 -0.312774000
C -2.977658000 1.820569000 0.005144000
C 2.808361000 -1.815133000 -0.369556000
C 1.737476000 2.896123000 -0.182223000
C -1.895882000 -2.886533000 0.045716000
H -3.892349000 2.403241000 0.054794000
H 3.723800000 -2.392398000 -0.453993000
H 2.315303000 3.815163000 -0.188167000
H -2.463958000 -3.809108000 0.114772000
O -0.141295000 -0.013300000 1.645513000
H 0.910755000 0.026409000 2.152047000
H 2.529690000 -0.946696000 2.441534000
H 2.610178000 0.882688000 2.471157000
H 1.793443000 -0.021562000 3.849557000
C 2.087747000 -0.016316000 2.798621000
N -0.336860000 -0.029466000 -1.972726000
H -0.653421000 -0.923346000 -2.351223000
H -0.915296000 0.721276000 -2.352200000

Methane (CH₄)

C 0.000000000 0.000000000 0.000000000
H 0.632031000 0.632031000 0.632031000
H -0.632031000 -0.632031000 0.632031000
H -0.632031000 0.632031000 -0.632031000
H 0.632031000 -0.632031000 -0.632031000

Methanol (CH₃OH)

C -0.683512000 -0.020828000 0.000000000
H -1.050488000 -0.544843000 0.895391000
H -1.083543000 0.995255000 -0.000001000
H -1.050488000 -0.544844000 -0.895390000
O 0.762888000 0.122484000 0.000000000
H 1.182485000 -0.760477000 0.000000000

Methyl radical (CH₃·)

H 0.000000000 1.084648000 0.000000000
H 0.939333000 -0.542324000 0.000000000
H -0.939333000 -0.542324000 0.000000000
C 0.000000000 0.000000000 0.000000000