

Supporting Information

Mechanistic Insights on the Intramolecular ortho-amination/hydroxylation by Nonheme FeIV=NTs/FeIV=O Species: The σ vs. the π channels

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Table S1. B3LYP computed structural parameters for *ortho*-amination.

	Fe-NTs	Fe-N _{ax}	Fe-N(L)	Fe-N2	Fe-N3	Fe-N4	N _{eq} avg	N-Fe-NTs	C1-N	TsN—H _{or}	H _{or} —C1	H _{or} —C2	Fe-N-C
⁷ I _(HS,T)	1.968	2.243	2.248	2.209	2.197	2.257	2.228	172.03	2.765				92.55
⁵ I _(HS,S)	1.75	2.076	2.107	2.259	2.06	2.258	2.171	175.9	3.225				93.29
³ I _(IS,S)	1.767	2.055	2.01	2.036	1.981	2.133	2.04	176.5	3.278				93.93
¹ I _(LS,S)	1.736	2.084	2.001	2.016	2.026	2.065	2.027	172.8	3.150				96.43
⁷ I-ts1	1.959	2.26	2.227	2.181	2.213	2.287	2.227	163.14	2.012				107.33
⁵ I-ts1	1.904	2.272	2.236	2.195	2.212	2.245	2.222	166.76	2.131				105.15
³ I-ts1	1.99	2.072	1.998	2.018	2.03	2.114	2.040	173.17	1.990				108.47
¹ I- ts 1	1.891	2.063	2.001	2.04	2.053	2.065	2.039	172.64	2.122				104.52
⁵ ts1a	1.834	2.054	2.207	2.112	2.144	2.235	2.175	175.53	2.575	1.176	1.402		104.94
³ ts1a	1.852	2.043	2.005	1.993	1.987	2.145	2.032	176.40	2.565	1.179	1.393		105.04
⁷ I- ts 2	2.002	2.253	2.213	2.197	2.196	2.169	2.194	158.59	1.407				
⁵ I- ts 2	2.103	2.293	2.293	2.196	2.282	2.327	2.274	150.62	1.399				
³ I- ts 2	2.13	2.248	1.98	2.131	2.002	2.338	2.113	153.3	1.399				
¹ I- ts 2	2.109	2.038	2.005	2.018	2.022	2.036	2.020	169.3	1.405				
⁵ I- ts 2a	2.171	2.274	2.247	2.217	2.278	2.351	2.273	148.97	1.476	1.428	1.227		127.89
³ I- ts 2a	2.185	2.245	1.978	2.141	2.005	2.351	2.11875	151.76	1.475	1.442	1.22		124.86
⁵ I- ts 2b	2.206	2.260	2.272	2.162	2.244	2.297	2.244	154.97	1.416	1.530	1.736	1.381	112.0
³ I- ts 2b	2.211	2.234	1.979	2.105	2.000	2.350	2.109	152.79	1.416	1.533	1.735	1.377	112.74
⁵ I- ts 3	2.506	2.216	1.975	2.253	1.982	2.39	2.150	146.9	1.305				
³ I- ts 3	2.529	2.215	1.975	2.246	1.982	2.394	2.149	146.5	1.302				
⁵ I- ts3 _{HOH}	2.211	2.291	2.265	2.290	2.263	2.271	2.272	154.03	1.369				131.13
³ I- ts3 _{HOH}	2.274	2.255	1.980	2.182	2.008	2.194	2.091	158.6	1.368				125.74

L=CH₃CN

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Table S2. B3LYP computed Mulliken spin densities for *ortho*-amination.

	Fe	NTs	N _{ax}	C (1)	C(2)	N1	N2	N3	N4	H _{or}	Freq (cm ⁻¹)
⁷ I _(HS,T)	3.891	1.310	0.076	0.048	0.026	0.037	0.090	0.086	0.076	-0.002	
⁵ I _(HS,S)	2.692	0.955	-0.049	0.007	0.0003	0.013	0.085	0.023	0.081	-0.0003	
³ I _(IS,S)	0.716	1.137	-0.015	0.011	-0.003	0.004	-0.004	-0.008	0.011	-0.0004	
¹ I _(LS,S)	0	0	0	0	0	0	0	0	0	0	
⁷ I- <i>ts1</i>	3.914	0.979	0.072	-0.028	0.257	0.031	0.082	0.076	0.103	0.009	
⁵ I- <i>ts1</i>	3.881	0.045	0.059	-0.011	-0.130	0.025	0.073	0.078	0.057	-0.004	-221.6
³ I- <i>ts1</i>	0.648	0.754	-0.012	-0.0735	0.271	-0.005	-0.009	-0.007	0.034	0.0168	-380.9
¹ I- <i>ts 1</i>	0	0	0	0	0	0	0	0	0	0	
⁵ <i>ts1a</i>	2.739	0.468	-0.051	0.631	-0.037	0.019	0.034	0.060	0.022	-0.053	-1191.1
³ <i>ts1a</i>	0.776	0.618	-0.015	0.634	-0.038	-0.004	-0.013	-0.012	-0.003	-0.064	-1231.6
⁷ I- <i>ts 2</i>	3.993	0.320	0.106	-0.076	-0.076	0.039	0.090	0.106	0.251	0.131	-1707.0
⁵ I- <i>ts 2</i>	3.739	0.059	0.048	-0.003	0.002	0.012	0.043	0.040	0.034	0.002	-871.5
³ I- <i>ts 2</i>	1.957	0.017	0.032	-0.00	0.000	-0.009	0.027	-0.025	0.027	0.001	-852.7
¹ I- <i>ts 2</i>	0	0	0	0	0	0	0	0	0	0	
⁵ I- <i>ts 2a</i>	3.742	0.042	0.052	0.002	0.001	0.016	0.045	0.038	0.035	-0.002	-1428.4
³ I- <i>ts 2a</i>	1.961	0.015	0.037	0.003	-0.003	-0.01	0.022	-0.026	0.027	-0.001	-1401.3
⁵ I- <i>ts 2b</i>	3.739	0.033	0.052	-0.01	0.006	0.019	0.052	0.039	0.035	0.000	-1833.9
³ I- <i>ts 2b</i>	1.961	0.011	0.038	-0.005	0.002	-0.011	0.023	-0.026	0.027	0.001	-1821.2
⁵ I- <i>ts 3</i>	1.965	0.183	0.038	-0.052	0.225	-0.006	0.024	-0.028	0.032	-0.087	-1355.0

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<i>³I- ts 3</i>	1.966	-0.136	0.038	0.043	-0.175	-0.007	0.025	-0.028	0.013	0.049	-648.5
<i>⁵I- ts3_{HOH}</i>	3.743	0.038	0.051	-0.004	0.004	0.017	0.038	0.039	0.045		-1032.8
<i>³I- ts3_{HOH}</i>	1.954	0.016	0.044	-0.002	0.001	-0.008	0.015	-0.027	0.031		-1039.2

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Table S3. B3LYP computed structural parameters for *ortho*-hydroxylation.

	Fe-O	Fe-N_{ax}	Fe-N(L)	Fe-N2	Fe-N3	Fe-N4	N_{eq} avg	N-Fe-O	C—O	Fe-O-C
⁵ 2_(HS)	1.623	2.102	2.328	2.063	2.139	2.088	2.155	176.35	3.044	97.48
³ 2_(IS)	1.629	2.098	2.03	1.998	1.962	2.053	2.011	173.85	3.75	103.8
⁵ 2-ts1	1.685	2.226	2.276	2.119	2.183	2.202	2.195	168.56	2.224	117.05
³ 2-ts1	1.726	2.089	2.029	1.995	2.012	2.035	2.018	175.49	1.887	113.99
⁵ 2Int1	1.92	2.268	2.288	2.202	2.266	2.275	2.25775	158.18	1.336	126.6
³ 2Int1	1.948	2.226	1.987	2.167	1.988	2.331	2.11825	156.31	1.328	126.4
⁵ 2-ts2	1.938	2.265	2.285	2.201	2.257	2.265	2.252	158.39	1.318	128.10
³ 2-ts2	1.963	2.225	1.986	2.161	1.987	2.316	2.113	156.73	1.316	127.22
⁵ 2Int2	2.037	2.247	2.271	2.188	2.220	2.211	2.2225	159.92	1.253	133.15
³ 2Int2	2.054	2.224	1.986	2.117	1.990	2.204	2.07425	160.98	1.25	132.84
⁵ 2-ts3_{HOH}	2.002	2.262	2.310	2.215	2.232	2.209	2.242	161.16	1.321	124.96
³ 2-ts3_{HOH}	2.051	2.234	1.990	2.143	1.990	2.200	2.080	161.25	1.315	124.52

L=CH₃CN

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Table S4. B3LYP computed Mulliken spin densities for *ortho*-hydroxylation.

	Fe	O	N _{ax}	C (1)	C(2)	N1	N2	N3	N4	Freq (cm ⁻¹)
<i>⁵2_(HS)</i>	2.904	0.823	-0.031	0.0134	-0.004	0.039	0.049	0.096	0.0435	
<i>³2_(IS)</i>	0.998	1.020	-0.015	-0.006	0.013	0.009	-0.001	-0.014	-0.00	
<i>⁵2-ts1</i>	3.645	0.339	0.031	-0.084	-0.108	0.035	0.063	0.084	0.071	-484.25
<i>³2-ts1</i>	0.768	0.759	-0.013	-0.098	0.279	-0.001	-0.009	-0.007	0.021	-435.63
<i>⁵2Int1</i>	3.704	0.125	0.041	-0.003	-0.003	0.021	0.039	0.041	0.042	
<i>³2Int1</i>	1.936	0.047	0.028	-0.000	-0.007	-0.005	0.029	-0.023	0.036	
<i>⁵2-ts2</i>	3.706	0.106	0.044	-0.003	0.003	0.021	0.040	0.041	0.044	-424.49
<i>³2-ts2</i>	1.935	0.043	0.029	0.00	-0.004	-0.005	0.029	-0.023	0.037	-563.61
<i>⁵2Int2</i>	3.719	0.055	0.051	0.004	0.005	0.023	0.044	0.042	0.049	
<i>³2Int2</i>	1.939	0.039	0.038	-0.008	-0.008	-0.007	0.019	-0.028	0.036	
<i>⁵2-ts3_{HOH}</i>	3.717	0.072	0.048	-0.007	0.007	0.021	0.038	0.042	0.052	-1036.9
<i>³2-ts3_{HOH}</i>	1.932	0.035	0.041	-0.002	0.003	-0.005	0.021	-0.027	0.040	-1116.6

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Table S5. B3LYP-D3 computed structural parameters for ortho-amination.

	Fe-NTs	Fe-N _{ax}	Fe-N(L)	Fe-N2	Fe-N3	Fe-N4	N _{eq-avg}	N-Fe-NTs	C-N	TsN-H _{or}	H _{or} -C	H _{or} -C2	Fe-N-C
⁷ I _(HS,T)	1.922	2.234	2.196	2.206	2.171	2.212	2.196	171.49	2.463		1.081		95.34
⁵ I _(HS,S)	1.731	2.068	2.136	2.203	2.088	2.175	2.151	175.88	2.907		1.082		94.78
³ I _(LS,S)	1.751	2.053	1.997	2.023	1.977	2.095	2.023	176.31	2.972				96.66
¹ I _(LS,S)	-	-	-	-	-	-	-	-	-	-	-	-	-
⁵ I- <i>ts1</i>	1.876	2.267	2.201	2.159	2.182	2.205	2.187	169.02	2.141		1.083		102.95
³ I- <i>ts1</i>	1.837	2.069	1.988	1.966	2.019	2.086	2.015	174.29	2.006		1.08		107.41
⁵ <i>ts1a</i>	1.827	2.049	2.18	2.08	2.13	2.177	2.141	176.37	2.563	1.153	1.416		103.74
³ <i>ts1a</i>	1.841	2.041	1.995	1.98	1.974	2.099	2.012	177.65	2.548	1.158	1.399		104.62
⁵ I- <i>ts2</i>	2.078	2.272	2.228	2.162	2.229	2.26	2.219	154.87	1.396		1.243		120.17
³ I- <i>ts2</i>	2.095	2.24	1.963	2.105	1.989	2.26	2.079	157.15	1.395		1.237		118.34
⁵ I- <i>ts2a</i>	2.171	2.257	2.213	2.148	2.208	2.258	2.207	156.25	1.416	1.524	1.379		110.52
³ I- <i>ts2a</i>	2.138	2.239	1.96	2.121	1.994	2.285	2.09	155.18	1.471	1.433	1.222		122.81
⁵ I- <i>ts2b</i>	2.171	2.257	2.213	2.148	2.208	2.258	2.206	156.25	110.52	1.524	1.379	1.379	110.52
³ I- <i>ts2b</i>	2.175	2.233	1.960	2.083	1.987	2.283	2.078	155.48	110.85	1.531	1.375	1.375	110.85
C1-C2													
⁵ I- <i>ts3</i>	2.174	2.232	1.960	2.182	1.978	2.212	2.083	157.88	1.317			1.497	128.63
³ I- <i>ts3</i>	2.209	2.229	1.960	2.166	1.979	2.204	2.077	157.79	1.311			1.506	127.68
⁵ I- <i>ts3</i> _{HOH}	2.156	2.28	2.212	2.246	2.246	2.197	2.225	126.35	1.37				126.35
³ I- <i>ts3</i> _{HOH}	2.205	2.252	1.960	2.160	1.991	2.159	2.068	124.33	1.365				124.33

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Table S6. B3LYP-D3 computed Mulliken spin densities for *ortho*-amination

	Fe	NTs	N _{ax}	C (1)	C(2)	N1	N2	N3	N4	H _{or}	Freq (cm ⁻¹)
<i>⁷I_(HS,T)</i>	3.897	1.177	0.077	0.059	0.076	0.026	0.088	0.088	0.086		
<i>⁵I_(HS,S)</i>	2.671	0.947	-0.051	0.013	0.005	0.019	0.067	0.047	0.070		
<i>³I_(LS,S)</i>	0.705	1.123	-0.014	0.015	-0.000	0.005	-0.003	-0.007	0.012		
<i>¹I_(LS,S)</i>	-	-	-	-	-	-	-	-	-	-	-
<i>⁵I-ts1</i>	3.893	0.006	0.064	-0.012	-0.138	0.023	0.081	0.083	0.063		-193.2
<i>³I-ts1</i>	0.688	0.737	-0.013	-0.071	0.256	-0.005	-0.009	-0.007	0.031		-374.8
<i>⁵ts1a</i>	2.724	0.437	-0.052	0.659	-0.04	0.019	0.033	0.068	0.022	-0.05	-903.4
<i>³ts1a</i>	0.795	0.58	-0.016	0.652	-0.04	-0.004	-0.001	-0.012	-0.003	-0.06	-960.1
<i>⁵I-ts 2</i>	3.719	0.061	0.051	-0.004	0.002	0.009	0.046	0.042	0.038	0.002	-891.6
<i>³I- ts 2</i>	1.941	0.025	0.034	-0.001	0.001	-0.007	0.029	-0.023	0.030	0.002	-877.2
<i>⁵I- ts 2a</i>	3.723	0.048	0.055	0.001	0.001	0.014	0.047	0.039	0.040	-0.002	-1457.4
<i>³I- ts 2a</i>	1.950	0.020	0.039	0.003	-0.002	0.009	0.025	-0.025	0.030	-0.001	-1422.9

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<i>⁵I- ts 2b</i>	3.723	0.034	0.054	-0.011	0.007	0.015	0.052	0.041	0.038	0.000	-1846.5
<i>³I- ts 2b</i>	1.951	0.014	0.041	-0.005	0.002	-0.01	0.025	-0.025	0.028	0.002	-1835.4
<i>⁵I- ts 3</i>	2.000	0.196	0.048	-0.063	0.198	-0.007	0.018	-0.031	0.047	-0.077	-1034.0
<i>³I- ts 3</i>	1.932	-0.125	0.045	0.038	-0.138	-0.008	0.015	-0.03	0.021	0.038	-332.5
<i>⁵I- ts3_{HOH}</i>	1.945	0.019	0.045	-0.002	0.002	-0.008	0.016	-0.027	0.034	0.000	-996.8
<i>³I- ts3_{HOH}</i>	3.722	0.041	0.055	-0.041	0.006	0.012	0.037	0.044	0.050	0.001	-1027.0

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Table S7. B3LYP-D3 computed structural parameters for *ortho*-hydroxylation.

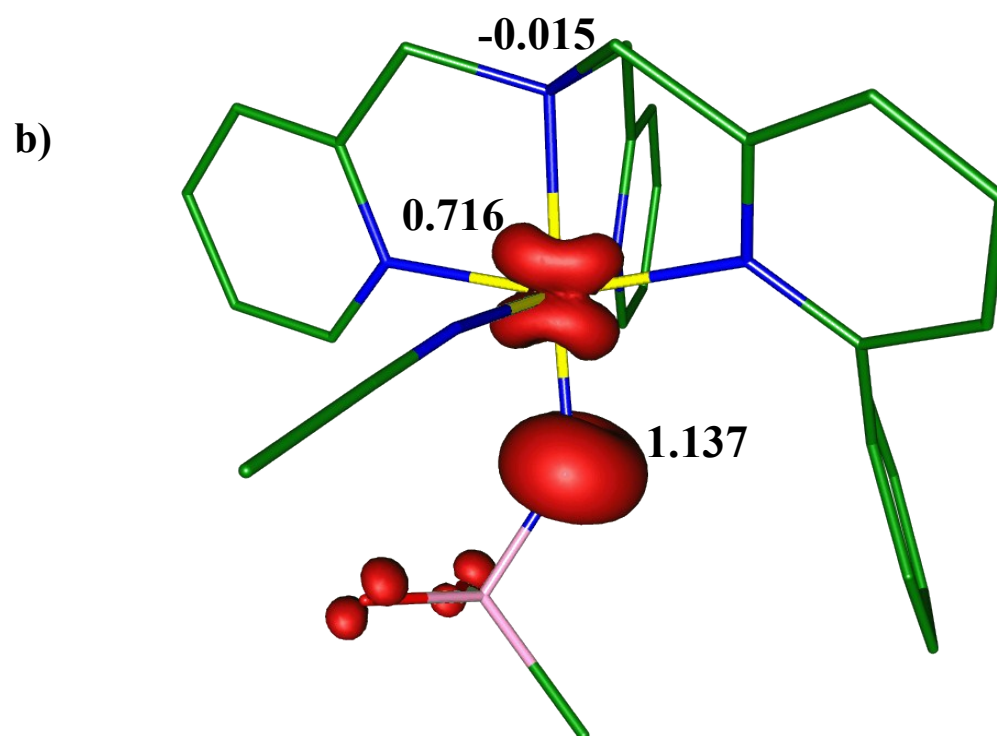
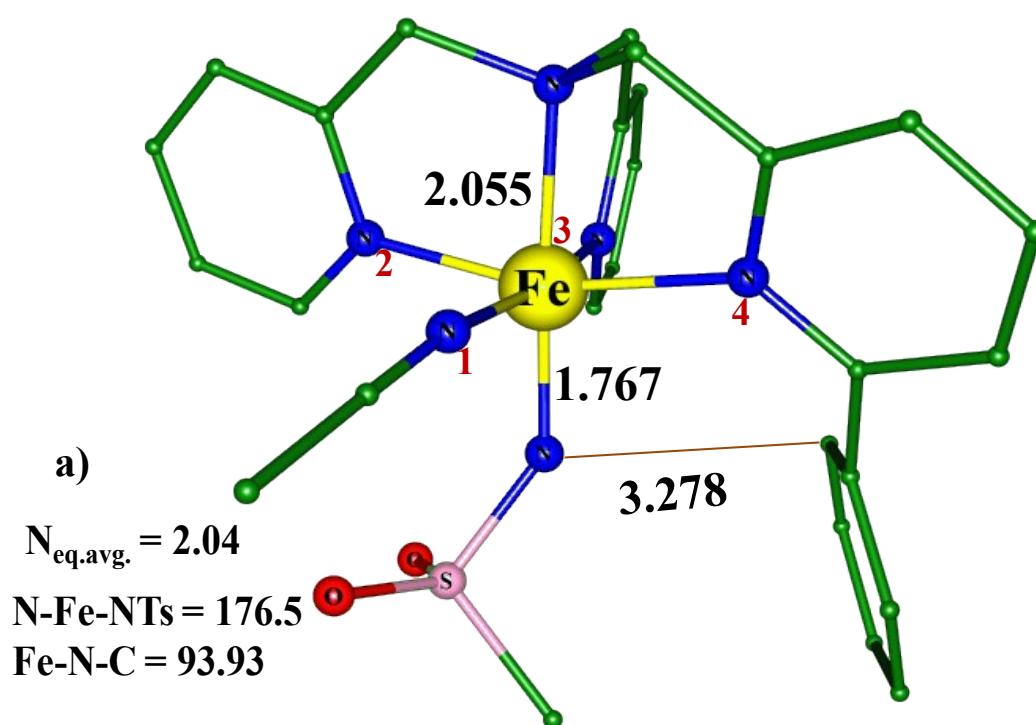
	Fe-O	Fe-N _{ax}	Fe-N(L)	Fe-N2	Fe-N3	Fe-N4	N _{eq} avg	N-Fe-O	C—O	Fe-O-C
⁵ 2 _(HS)	1.622	2.109	2.263	2.068	2.128	2.076	2.134	176.69	2.91	94.54
³ 2 _(IS)	1.784	2.064	2.358	2.03	2.212	1.954	2.138	176.06	1.43	115.09
⁵ 2- <i>ts1</i>	1.683	2.229	2.218	2.11	2.171	2.181	2.17	169.54	2.215	111.89
³ 2- <i>ts1</i>	1.724	2.088	2.008	1.988	2.005	2.029	2.007	175.98	1.89	111.7
⁵ 2Int1	1.917	2.273	2.219	2.195	2.232	2.248	2.223	158.27	1.338	122.66
³ 2Int1	1.945	2.225	1.966	2.151	1.977	2.287	2.095	157.72	1.328	123.39
⁵ 2- <i>ts2</i>	1.938	2.271	2.214	2.194	2.22	2.241	2.217	158.35	1.318	124.56
³ 2- <i>ts2</i>	1.96	2.226	1.965	2.144	1.975	2.274	2.089	157.97	1.316	124.16
⁵ 2Int2	2.028	2.252	2.208	2.181	2.194	2.194	2.194	160.03	1.254	131.65
³ 2Int2	2.047	2.231	1.965	2.096	1.981	2.166	2.052	162.07	1.249	130.75
⁵ 2- <i>ts3</i> _{HOH}	1.99	2.267	2.23	2.208	2.199	2.194	2.208	161.04	1.32	122.94
³ 2- <i>ts3</i> _{HOH}	2.033	2.235	1.967	2.216	1.978	2.174	2.083	161.84	1.314	122.67

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Table S8. B3LYP-D3 computed Mulliken spin densities for *ortho*-hydroxylation.

	Fe	O	N _{ax}	C (1)	C(2)	N1	N2	N3	N4	Freq (cm ⁻¹)
⁵ 2 _(HS)	2.899	0.813	-0.032	0.015	-0.002	0.040	0.053	0.094	0.047	
³ 2 _(IS)	2.655	0.054	-0.027	0.031	-0.322	0.026	-0.001	0.085	-0.059	
⁵ 2-ts1	3.637	1.345	0.031	-0.088	0.100	0.035	0.063	0.085	0.071	-603.5
³ 2-ts1	0.766	0.762	-0.014	-0.098	0.277	0.000	-0.008	-0.006	0.024	-483.1
⁵ 2Int1	3.693	0.127	0.043	-0.003	-0.003	0.021	0.041	0.041	0.044	
³ 2Int1	1.930	0.050	0.028	-0.001	-0.006	-0.004	0.03	-0.022	0.038	
⁵ 2-ts2	3.695	0.105	0.045	-0.004	0.003	0.022	0.041	0.042	0.045	-583.1
³ 2-ts2	1.929	0.045	0.030	-0.00	-0.004	-0.004	0.029	-0.022	0.038	-434.3
⁵ 2Int2	3.708	0.055	0.052	-0.009	0.004	0.024	0.045	0.043	0.051	
³ 2Int2	1.937	0.041	0.049	-0.008	0.004	-0.006	0.019	-0.026	0.036	
⁵ 2-ts3 _{HOH}	3.705	0.074	0.05	-0.007	0.008	0.023	0.04	0.043	0.054	-1042.8
³ 2-ts3 _{HOH}	1.926	0.038	0.042	-0.002	0.004	-0.005	0.021	-0.027	0.041	-1120.4

Supporting Information



Supporting Information

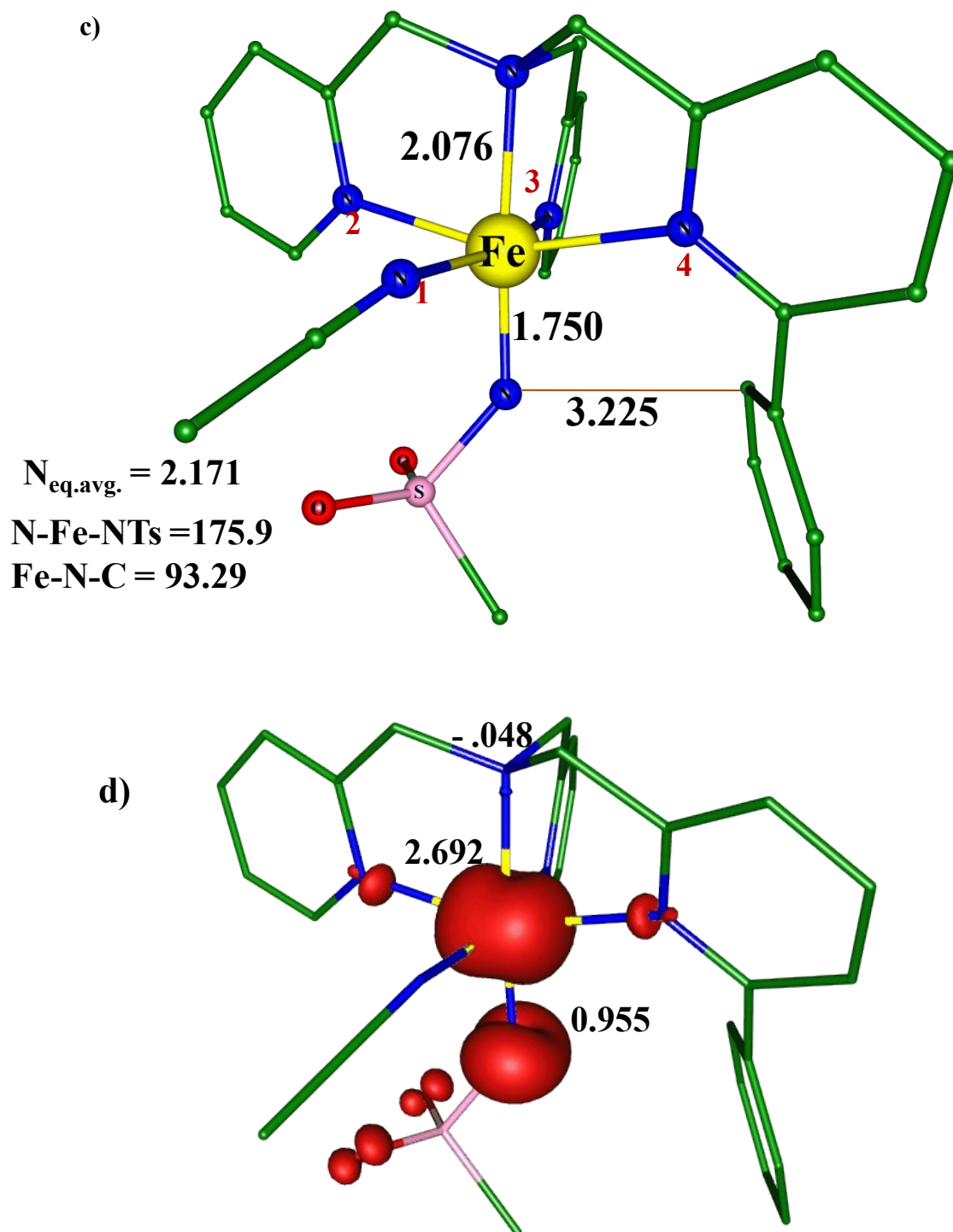
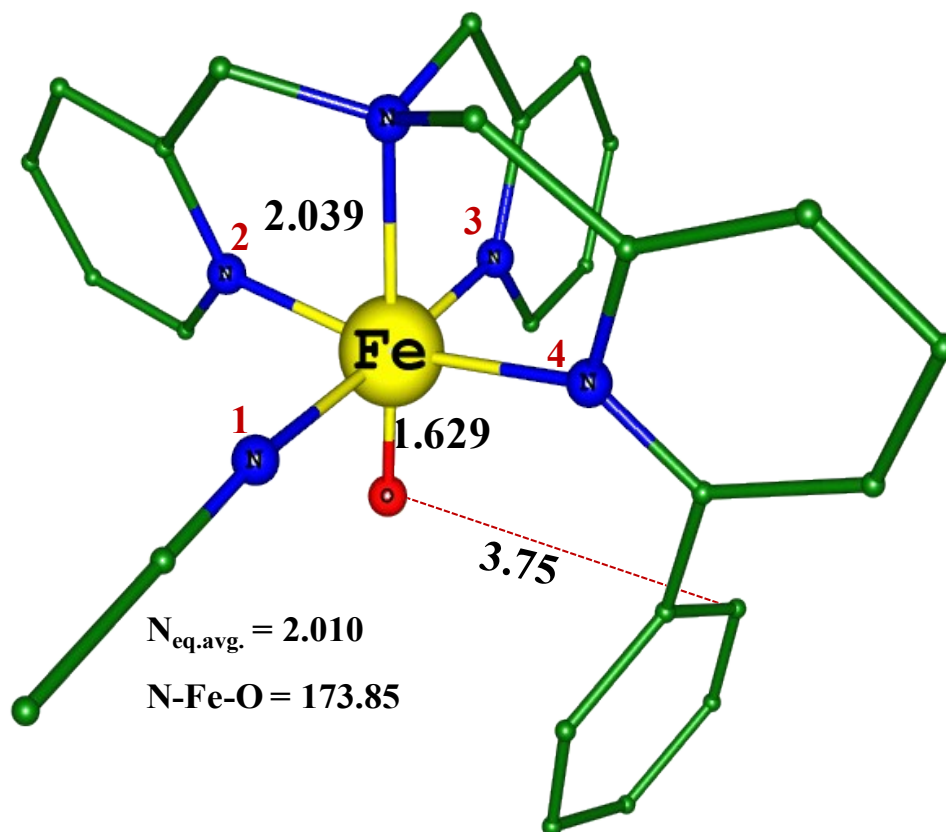


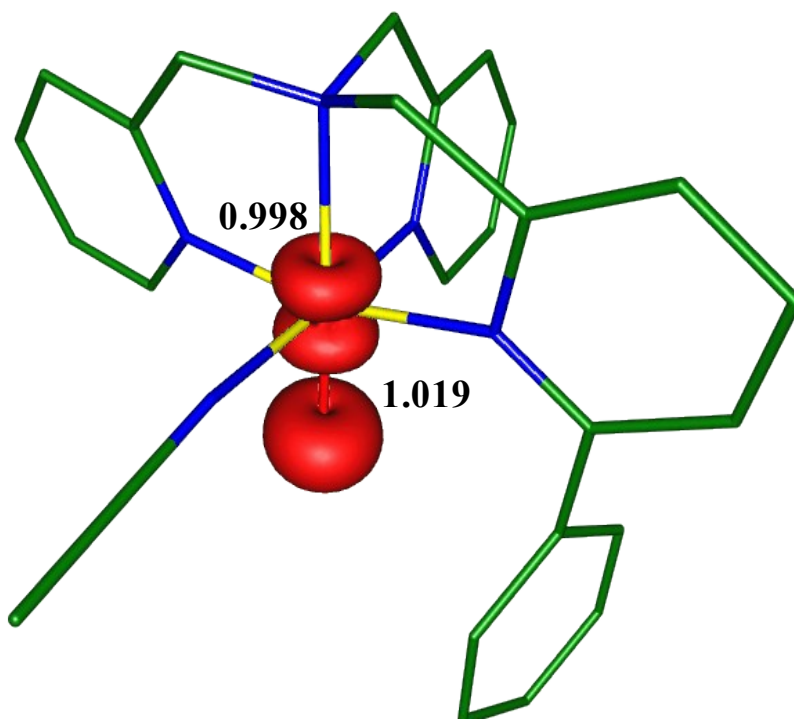
Figure S1. B3LYP optimized structures with selected structural parameters for **1** ($\text{Fe}^{\text{IV}}=\text{NTs}$) a) $^3\text{R}_{\text{Fe}^{\text{IV}}=\text{NTs}}$ and c) $^5\text{R}_{\text{Fe}^{\text{IV}}=\text{NTs}}$, spin density plots: (b) $^3\text{R}_{\text{Fe}^{\text{IV}}=\text{NTs}}$ and (d) $^5\text{R}_{\text{Fe}^{\text{IV}}=\text{NTs}}$

Supporting Information

a)



b)



Supporting Information

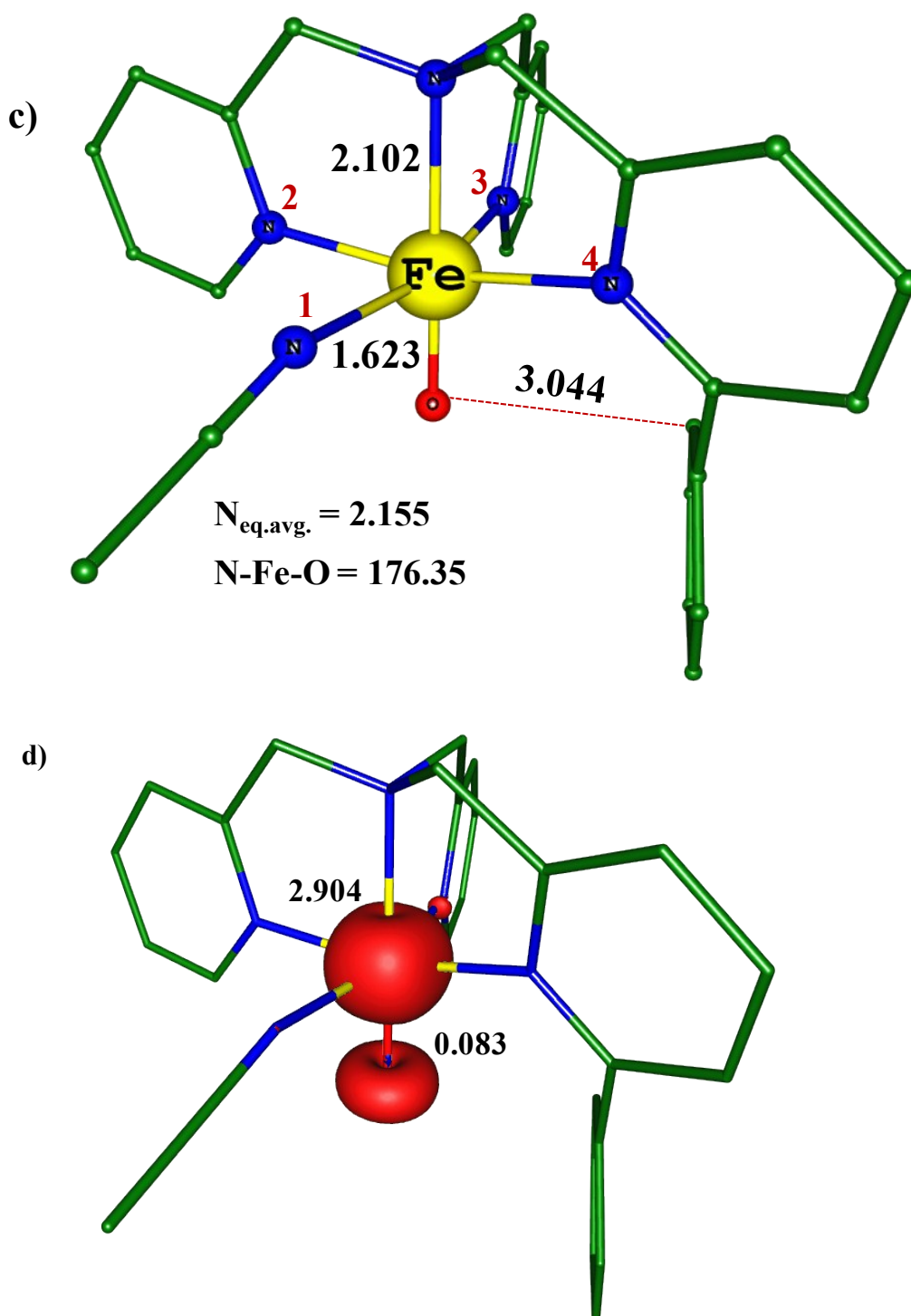


Figure S2. B3LYP optimized structures with selected structural parameters for **2** ($Fe^{IV}=O$) a) ${}^3R_{Fe^{IV}=O}$ and c) ${}^5R_{Fe^{IV}=O}$, spin density plots: (b) ${}^3R_{Fe^{IV}=O}$ and (d) ${}^5R_{Fe^{IV}=O}$

Supporting Information

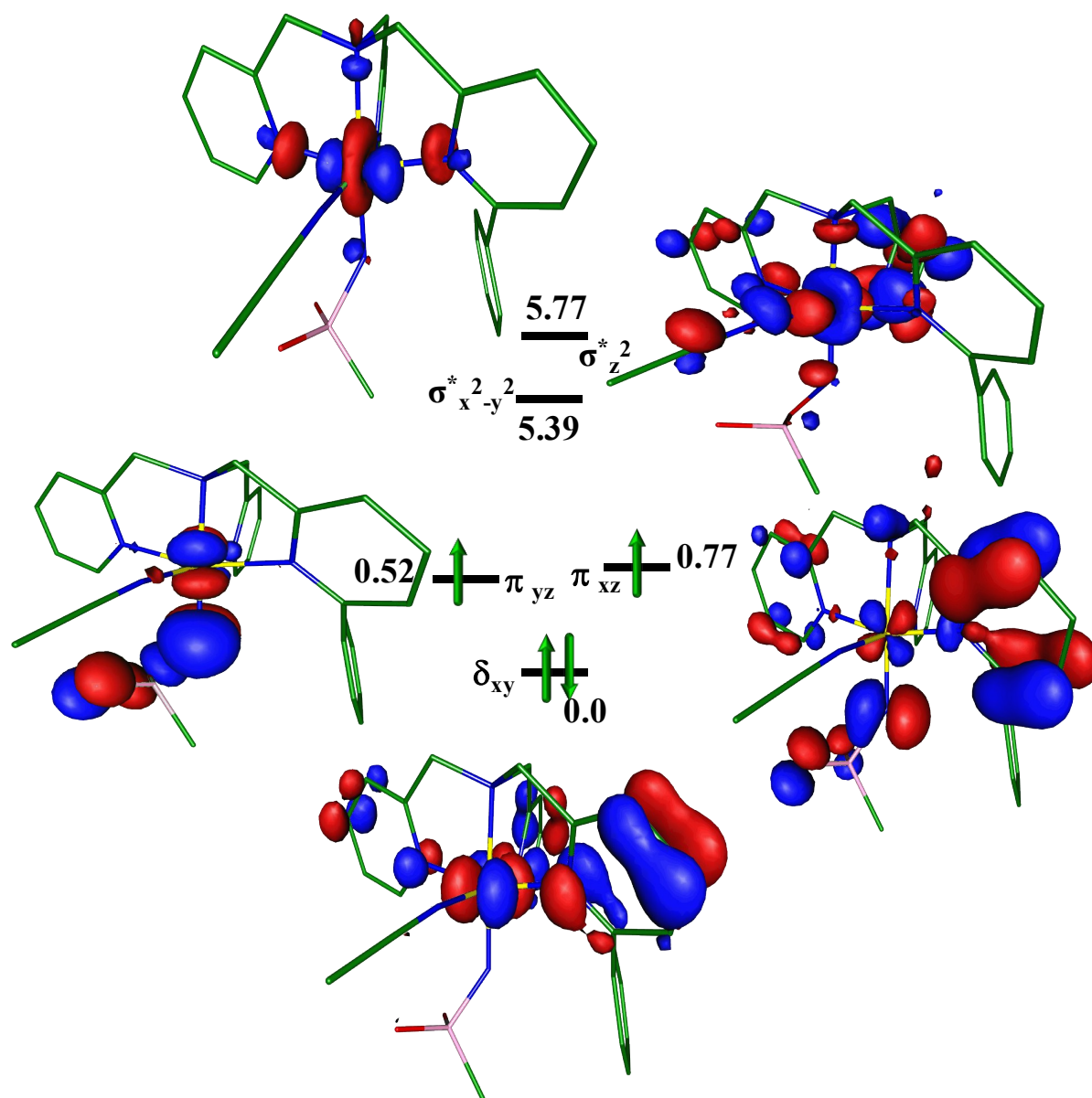


Figure S3. B3LYP computed Eigen-value plot incorporating energies computed for d-based orbitals for ground state of the $\text{Fe}^{\text{IV}}=\text{NTs}$ ($^3\mathbf{1}$) species (energies are given in eV).

Supporting Information

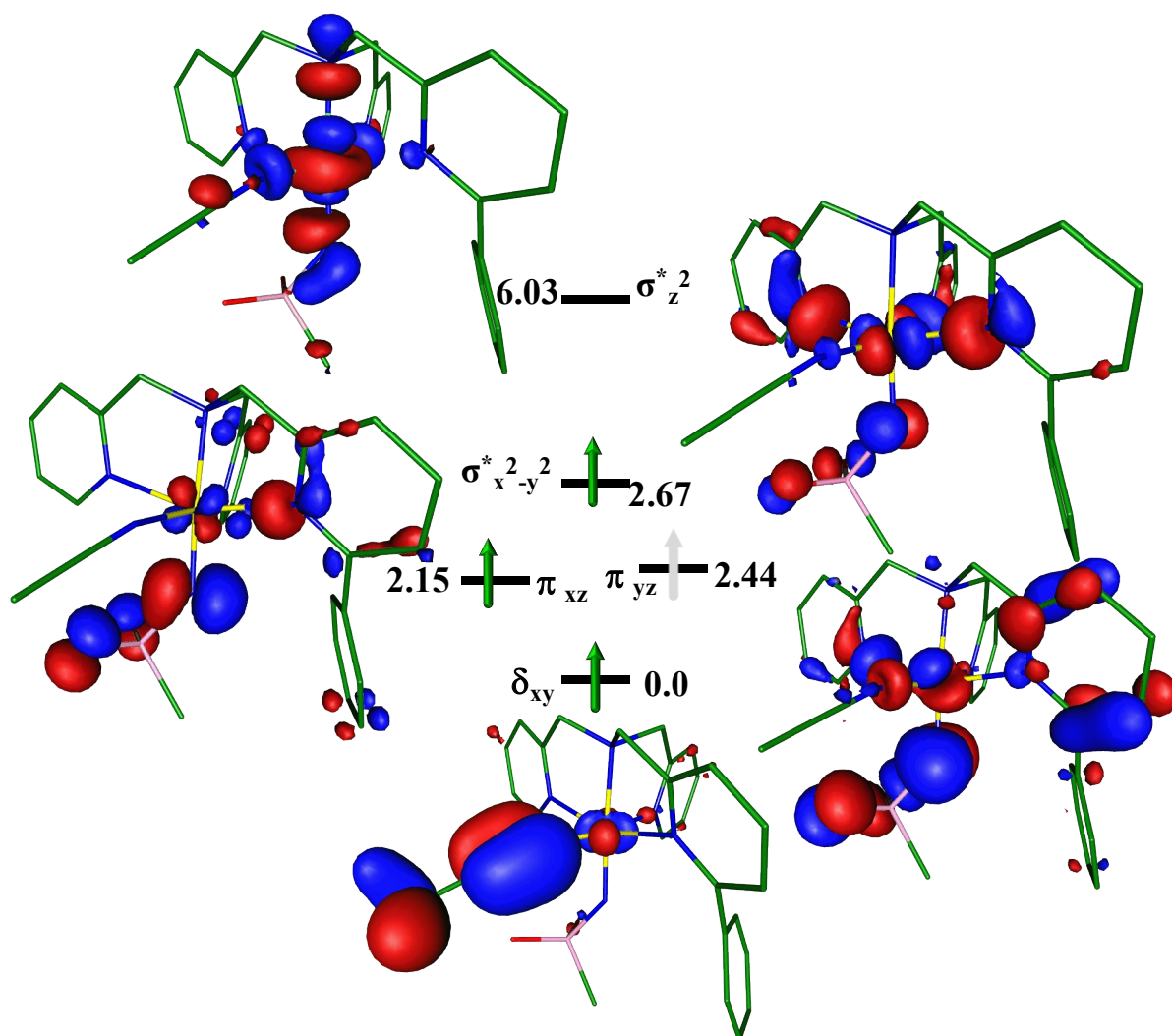


Figure S4. B3LYP computed Eigen-value plot incorporating energies computed for d-based orbitals for quintet state of the $\text{Fe}^{\text{IV}}=\text{NTs}$ ($^5\mathbf{1}$) species (energies are given in eV).

Supporting Information

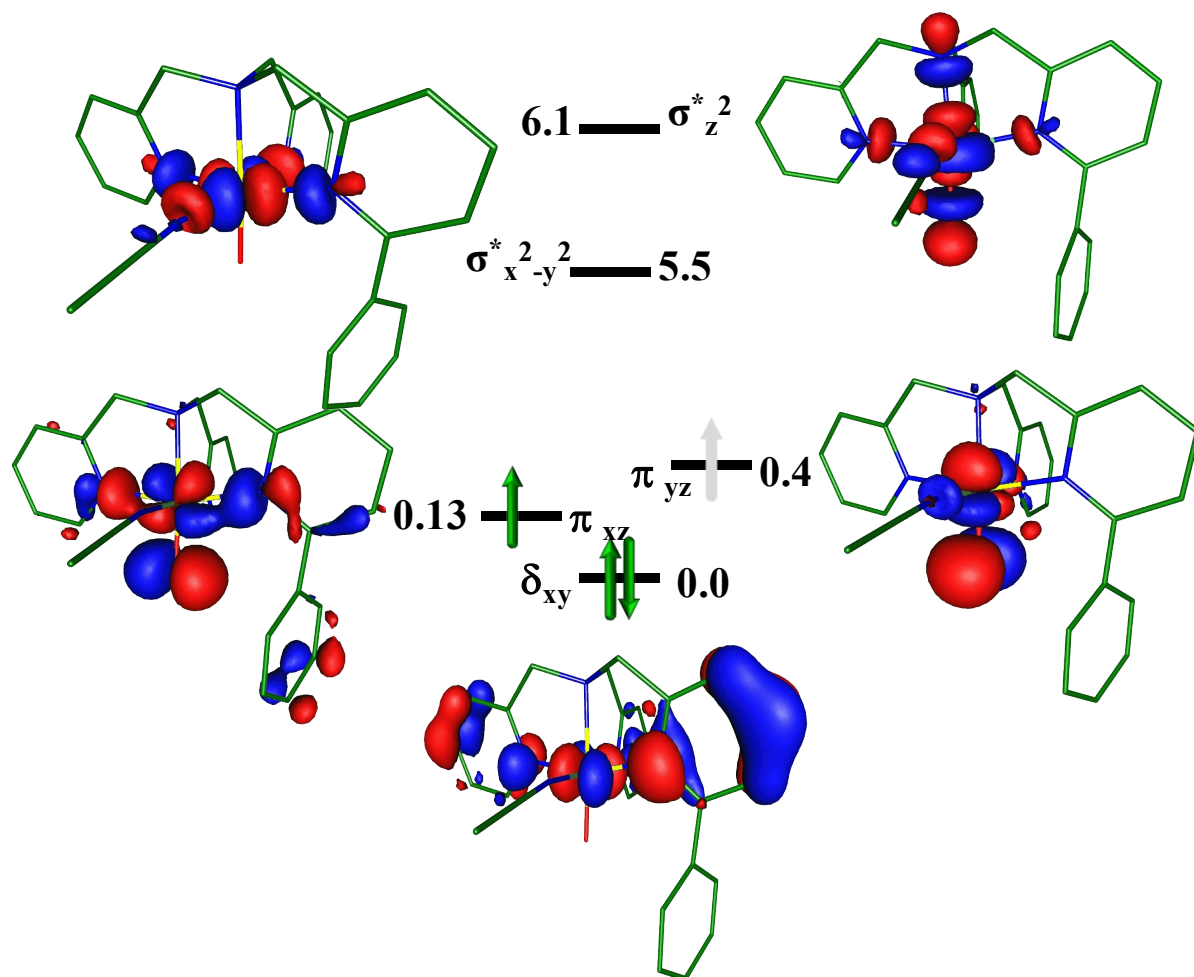


Figure S5. B3LYP computed Eigen-value plot incorporating energies computed for d-based orbitals for ground state of the $\text{Fe}^{\text{IV}}=\text{O}$ ($^3\text{2}$) species (energies are given in eV).

Supporting Information

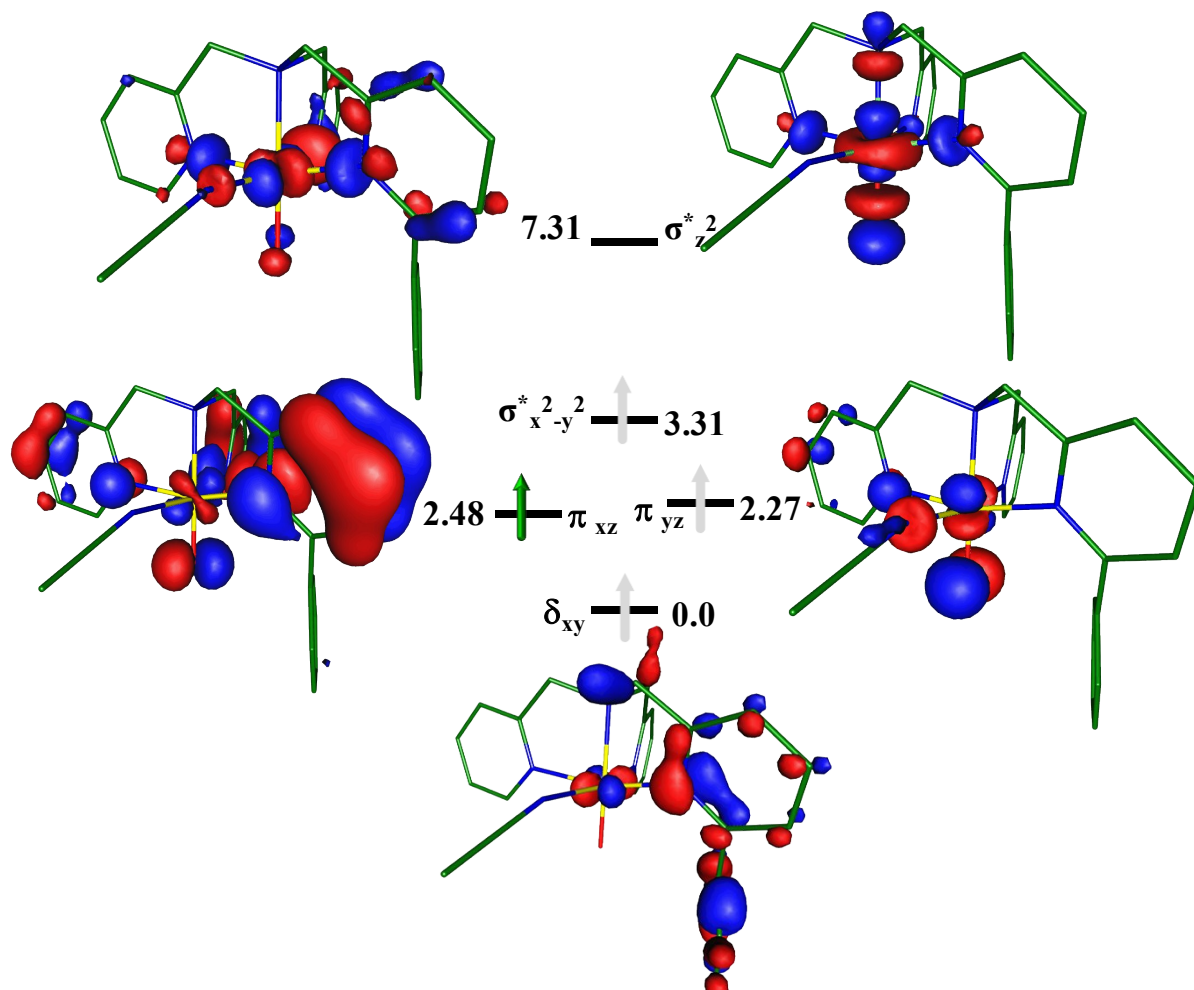
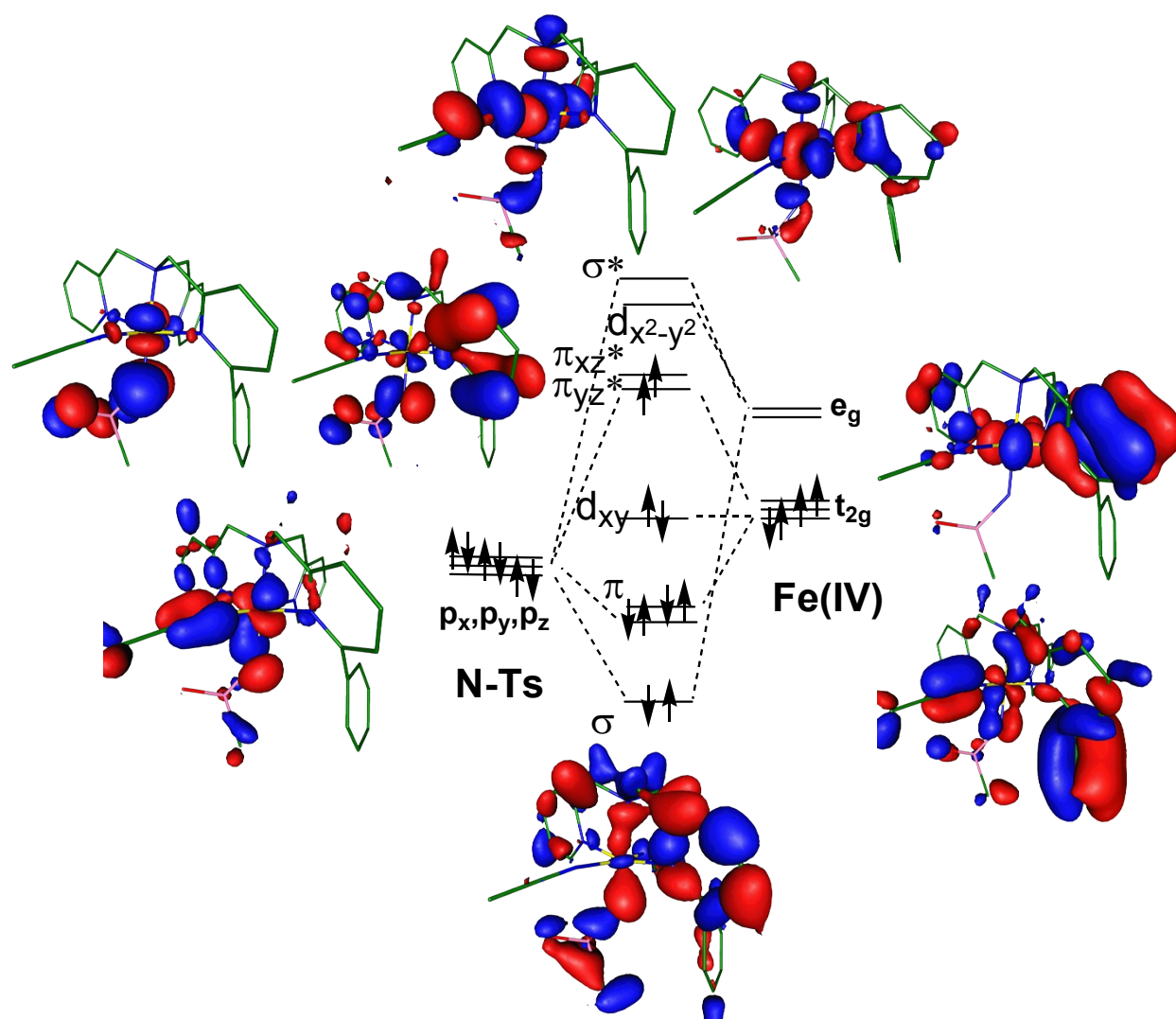


Figure S6. B3LYP computed Eigen-value plot incorporating energies computed for d-based orbitals for quintet state of the $\text{Fe}^{\text{IV}}=\text{O}$ (52) species (energies are given in eV).

Supporting Information



Supporting Information

Figure S7. A qualitative MO diagram for $^3\mathbf{1}$ species. The molecular orbital represented here are computed at B3LYP level of theory.

Supporting Information

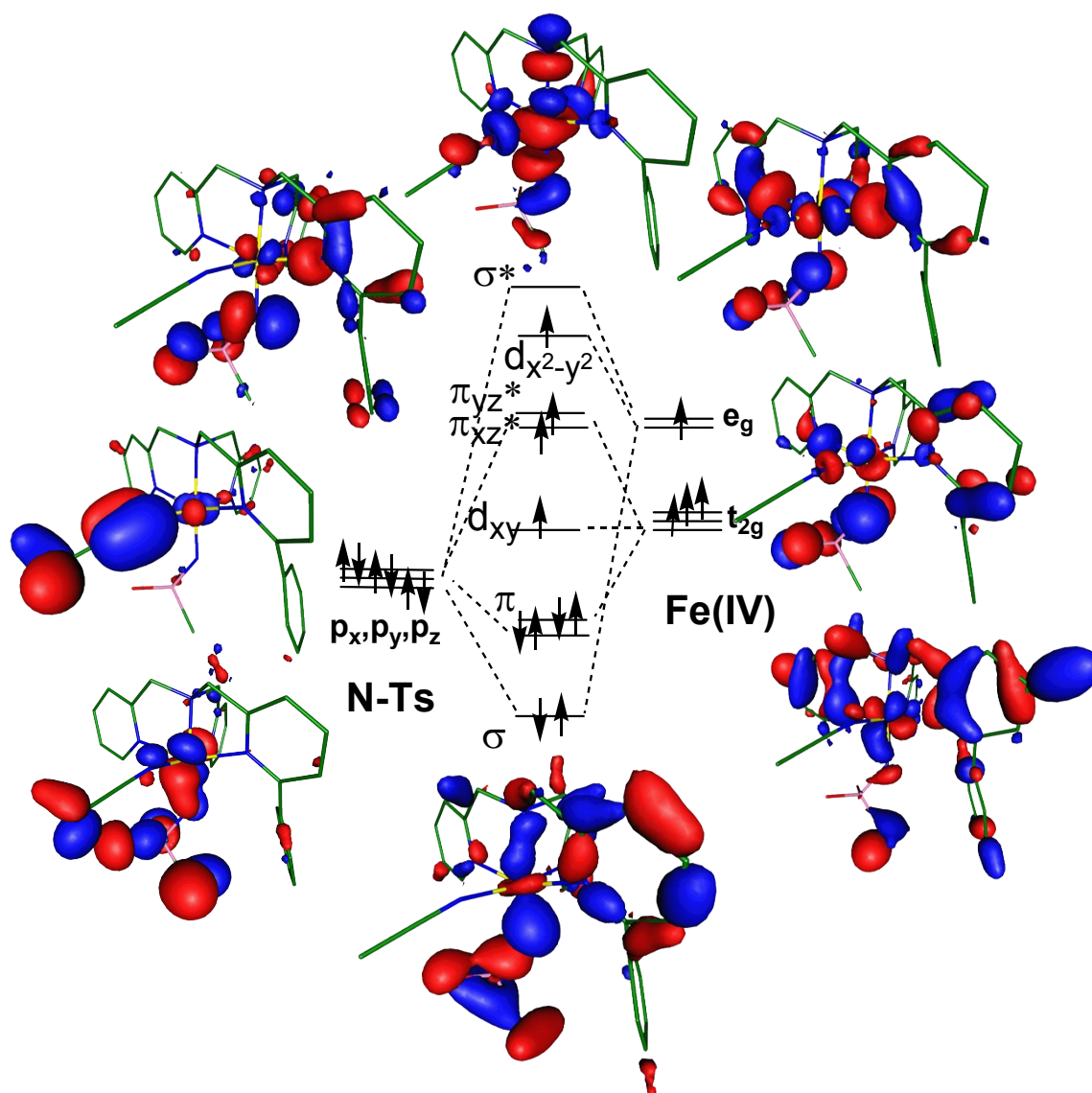
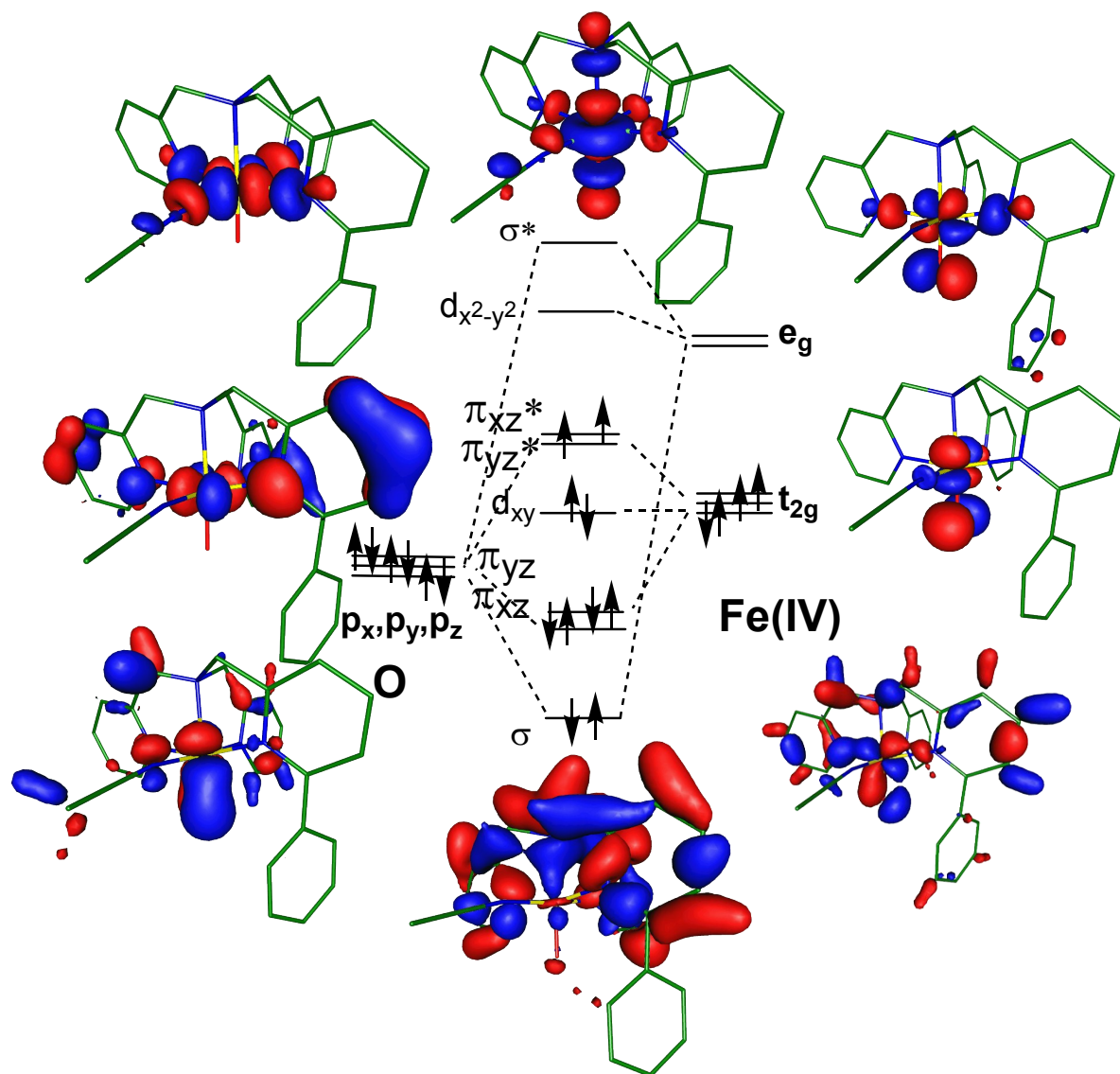


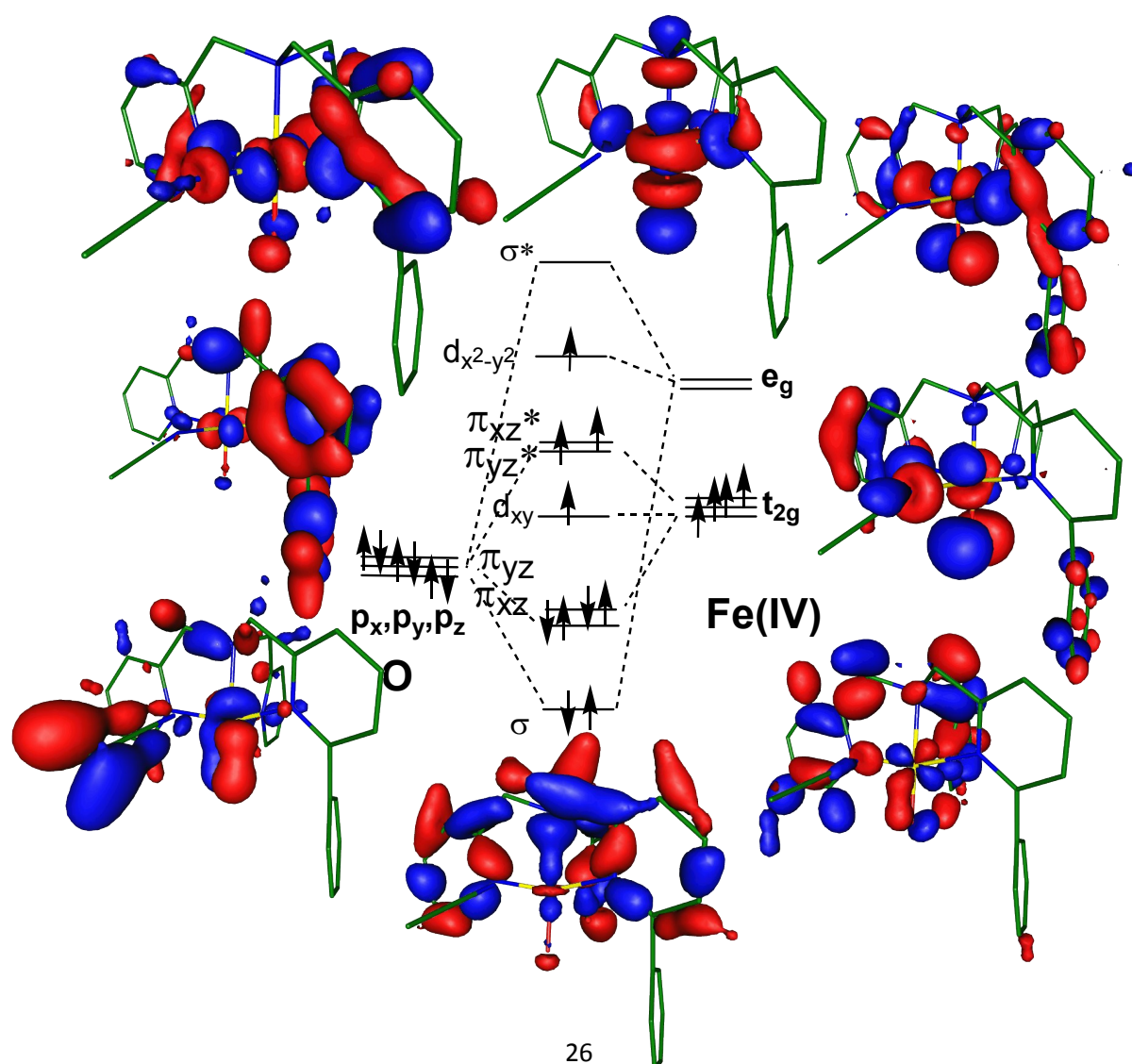
Figure S8. A qualitative MO diagram for (a) 51 species. The molecular orbital represented here are computed at B3LYP level of theory.

Supporting Information



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Figure S9. A qualitative MO diagram for $^3\mathbf{2}$ species. The molecular orbital represented here are computed at B3LYP level of theory.



Supporting Information

Figure S10. A qualitative MO diagram for $^5\mathbf{2}$ species. The molecular orbital represented here are computed at B3LYP level of theory.

Supporting Information

NBO Analysis

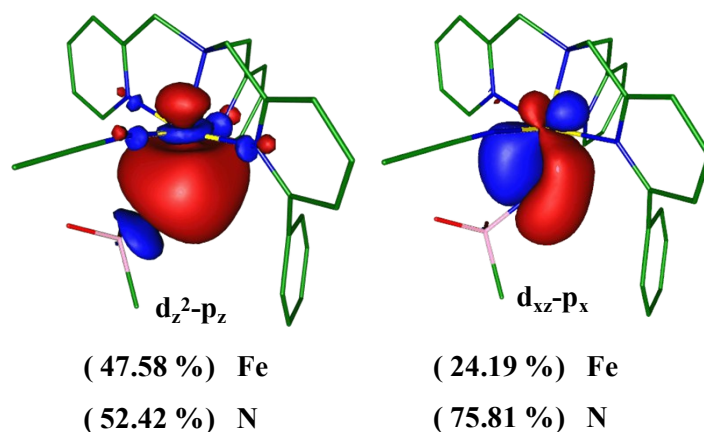


Figure S11. NBO-plot for the species ³1 showing σ -bonding and π -bonding interaction between Fe^{IV} and N atom of the -NTs group.

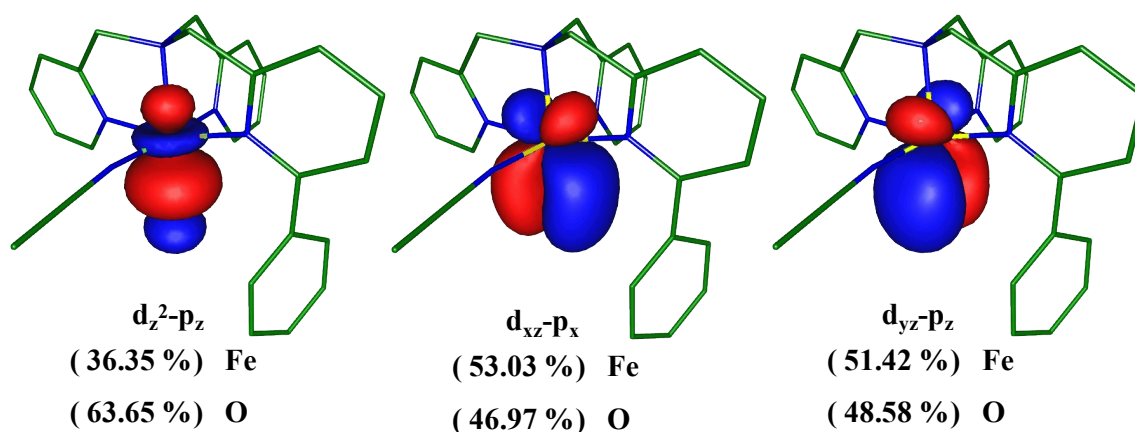


Figure S12. Difference in bonding between Fe^{IV}=O and Fe^{IV}=NTs species: For both 1 and 2 near equal distribution of spin densities on both Fe and N/O atoms are noted for the triplet state ($p_{\text{Fe}} = 0.716$; $p_{\text{NTs}} = 1.137$; $p_{\text{Fe}} = 0.998$; $p_{\text{O}} = 1.020$). NBO second-order perturbation analysis reveals significant difference present in the σ bonding interactions between these two species. The σ bonding interaction is found to be composed of Fe(d_{z^2})-N/O(p_z) orbitals and the stabilization energies for 2 is 422.7 kJ/mol which is much larger compared to species 1 (350.6 kJ/mol). Besides the Fe-N bond in species 1, is found to be more covalent in nature

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compared to the Fe-O bond in species 2. (47.58 % Fe (dz2) and 52.42% of N(pz) for 1 and 36.35 % Fe(dz2) and 63.65 % of O(pz) for 2).

Table S9. EDA Analysis

Species	EDA {(6-PhTPA)Fe ^{IV} + NTs/O}		
	ΔE_{int} (kJ/mol)	ΔE_{steric} (kJ/mol)	ΔE_{orb} (kJ/mol)
([(6-PhTPA)Fe ^{IV} =NTs] ²⁺) (31)	-3443.8	-2053.9	-1389.9
([(6-PhTPA)Fe ^{IV} =O] ²⁺) (32)	-4448.6	-2338.2	-2110.4

Probable mechanism for electron transfer via π - pathway

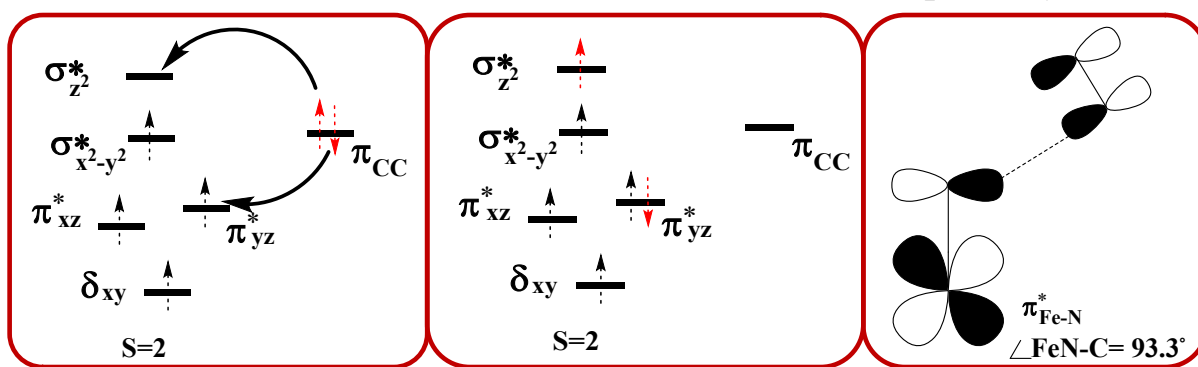


Figure S13. Orbital Occupancy Diagrams for the C-C activation by Fe^{IV}=NTs species.

Supporting Information

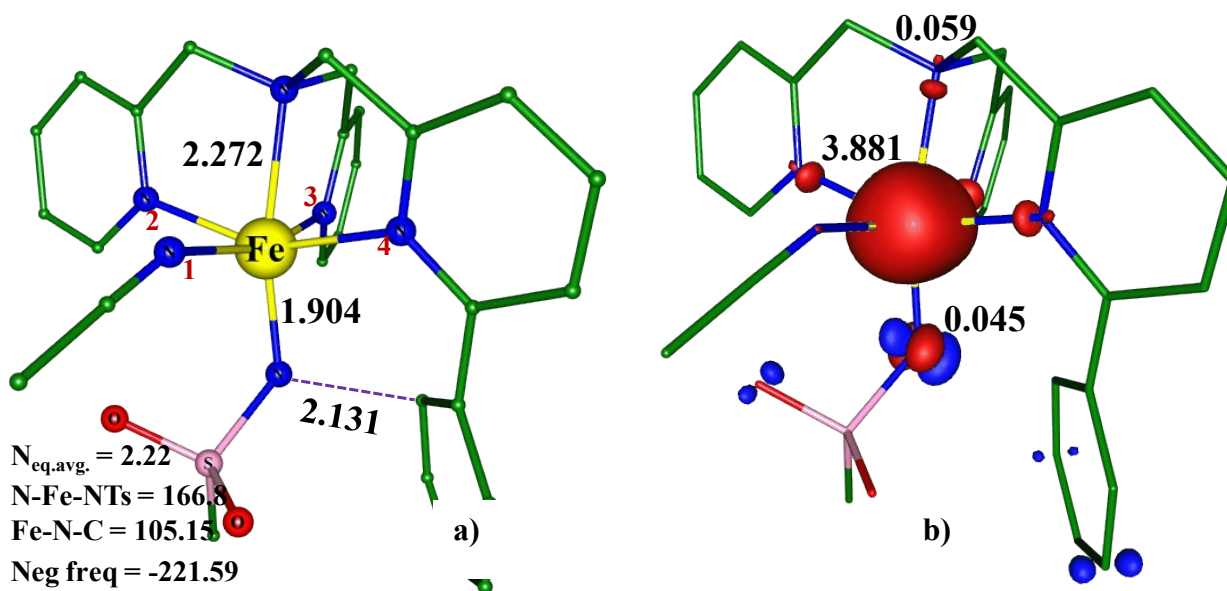


Figure S14a) B3LYP optimized structure of $^5I\text{-tsI}$ with selected structural parameters and (b) Spin density plot of $^5I\text{-tsI}$

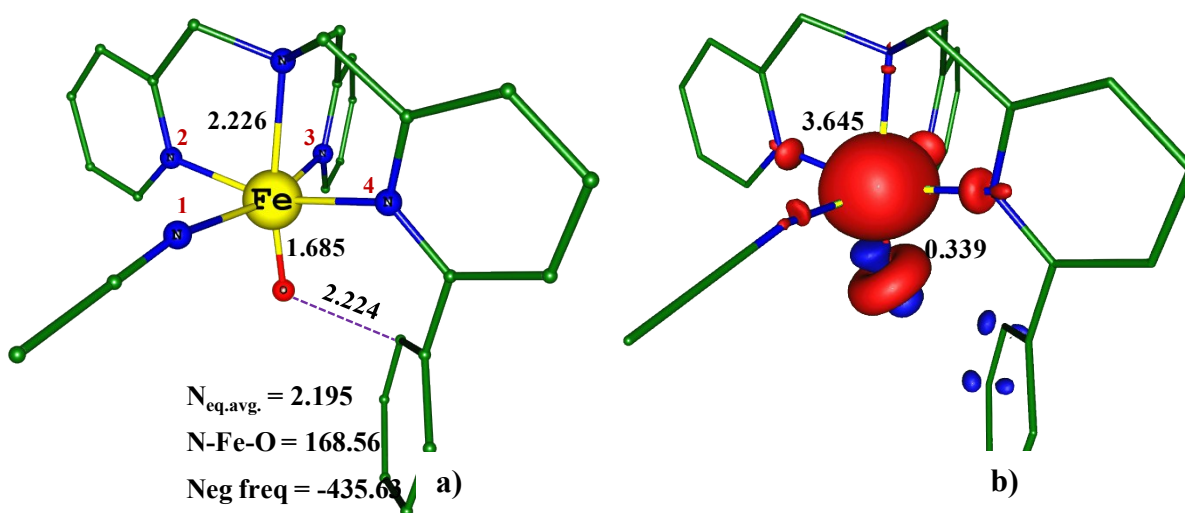


Figure S15. a) B3LYP optimized structure of $^52\text{-tsI}$ with selected structural parameters and b) Spin density plot of $^52\text{-tsI}$

Supporting Information

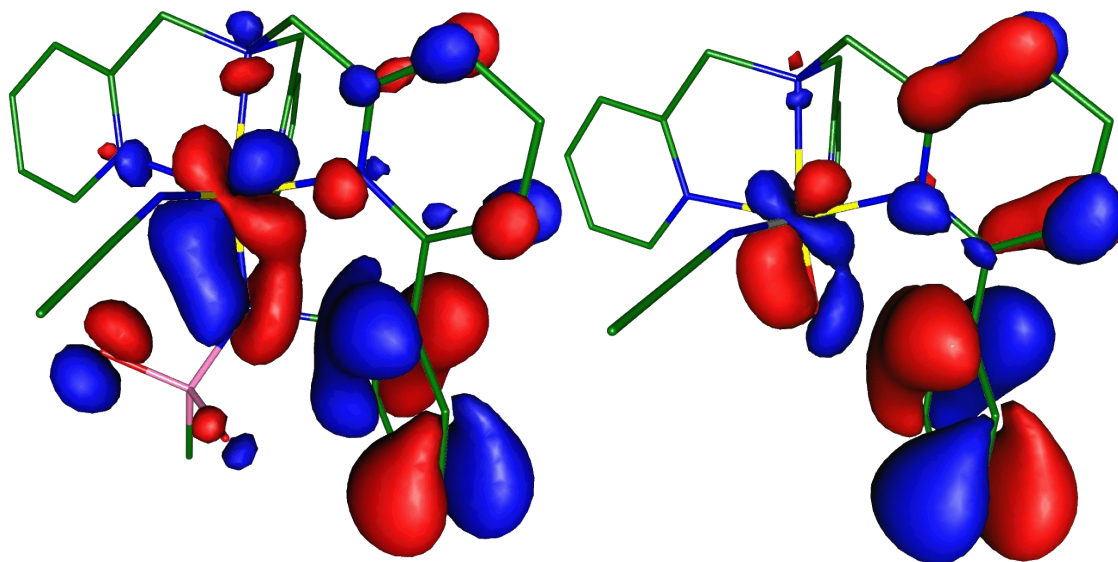


Figure S16. a) B3LYP Computed molecular orbital plot of HOMO of the transition state a) $^5I\text{-}tsI$ and b) $^52\text{-}tsI$.

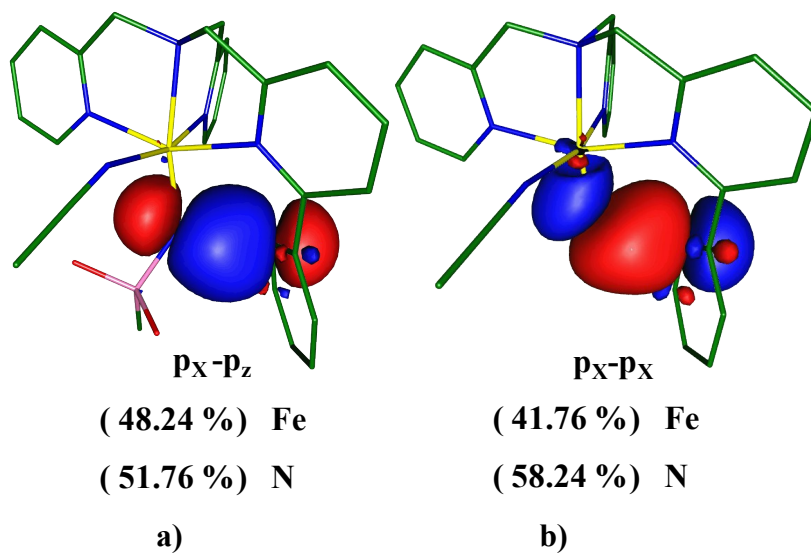


Figure S17. NBO-plot of the first transition state showing σ -bonding interaction **a)** between N atom of -NTs group with *ortho*-carbon atom in $^5I\text{-}tsI$ and **b)** O atom of -oxo group with *ortho*-carbon in $^52\text{-}tsI$.

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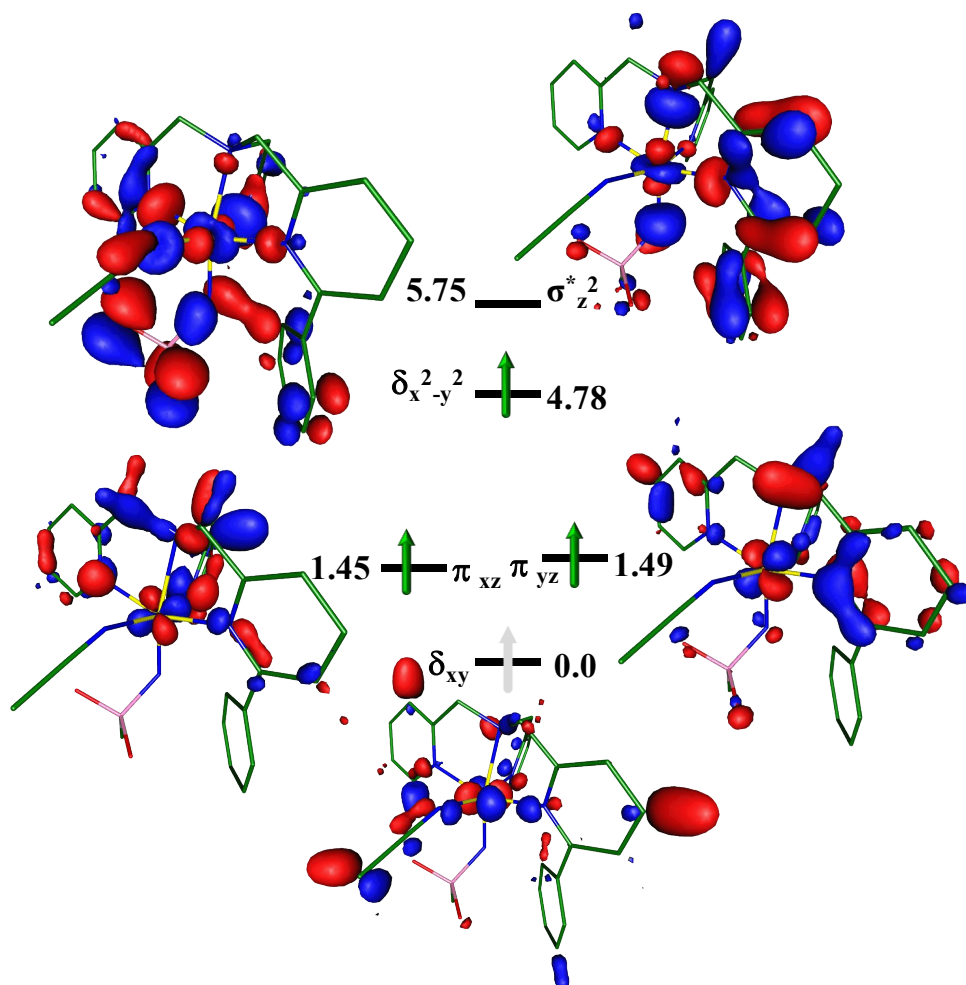


Figure S18. B3LYP computed Eigen-value plot incorporating energies computed for d-based orbitals for quintet state of the $^5I\text{-tsI}$ species (energies are given in eV).

Supporting Information

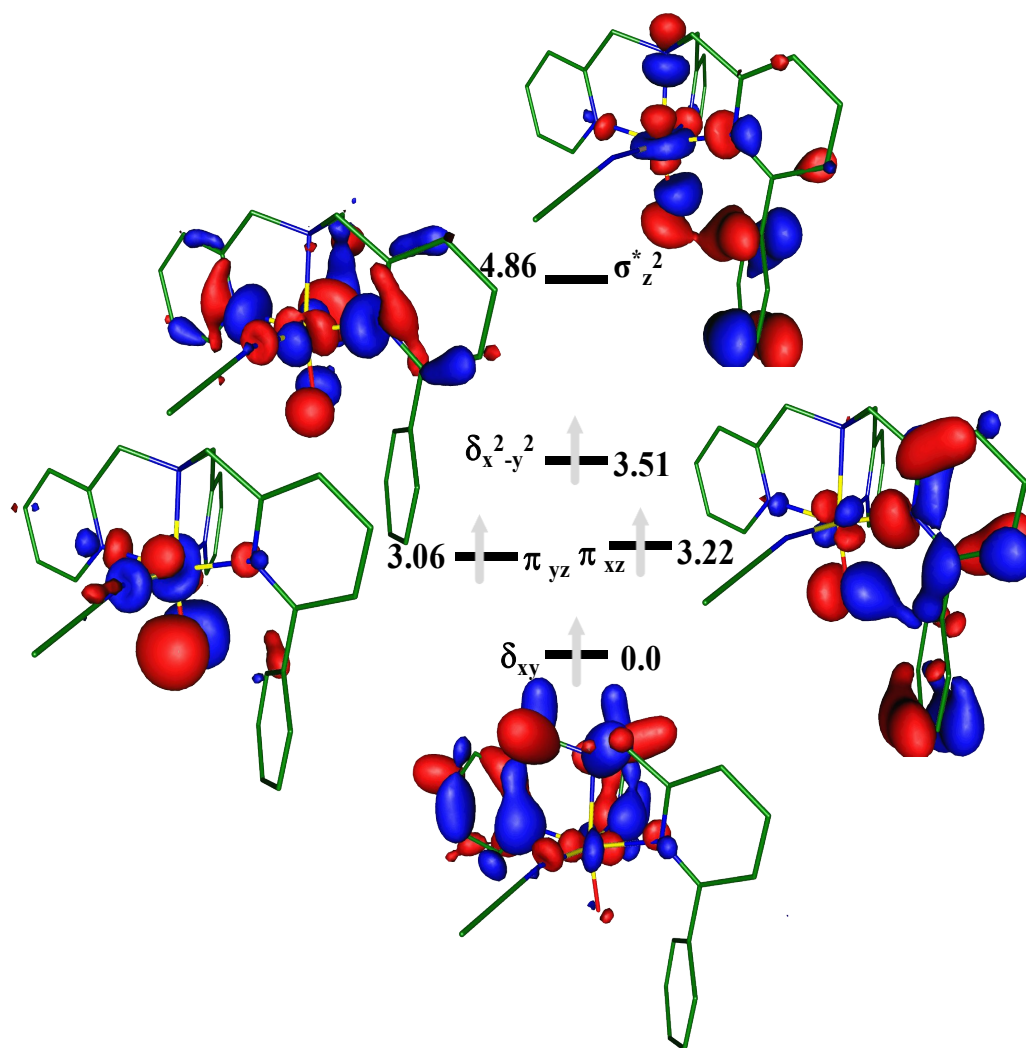


Figure S19. B3LYP computed Eigen-value plot incorporating energies computed for d-based orbitals for quintet state of the $^52\text{-ts1}$ species (energies are given in eV).

Supporting Information

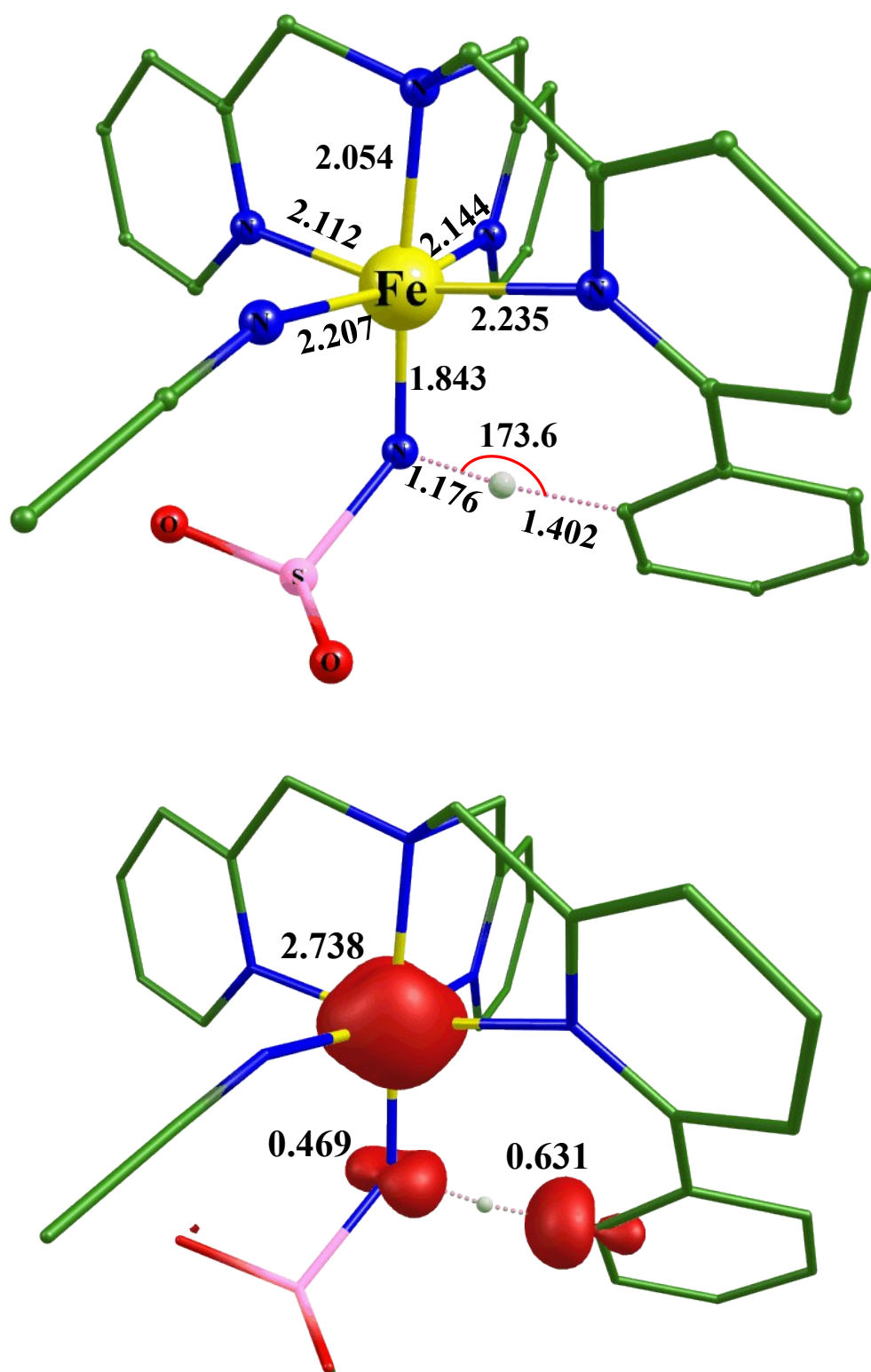


Figure S20a) B3LYP optimized structure of $^5I\text{-ts1a}$ with selected structural parameters and (b) Spin density plot of $^5I\text{-ts1a}$

Supporting Information

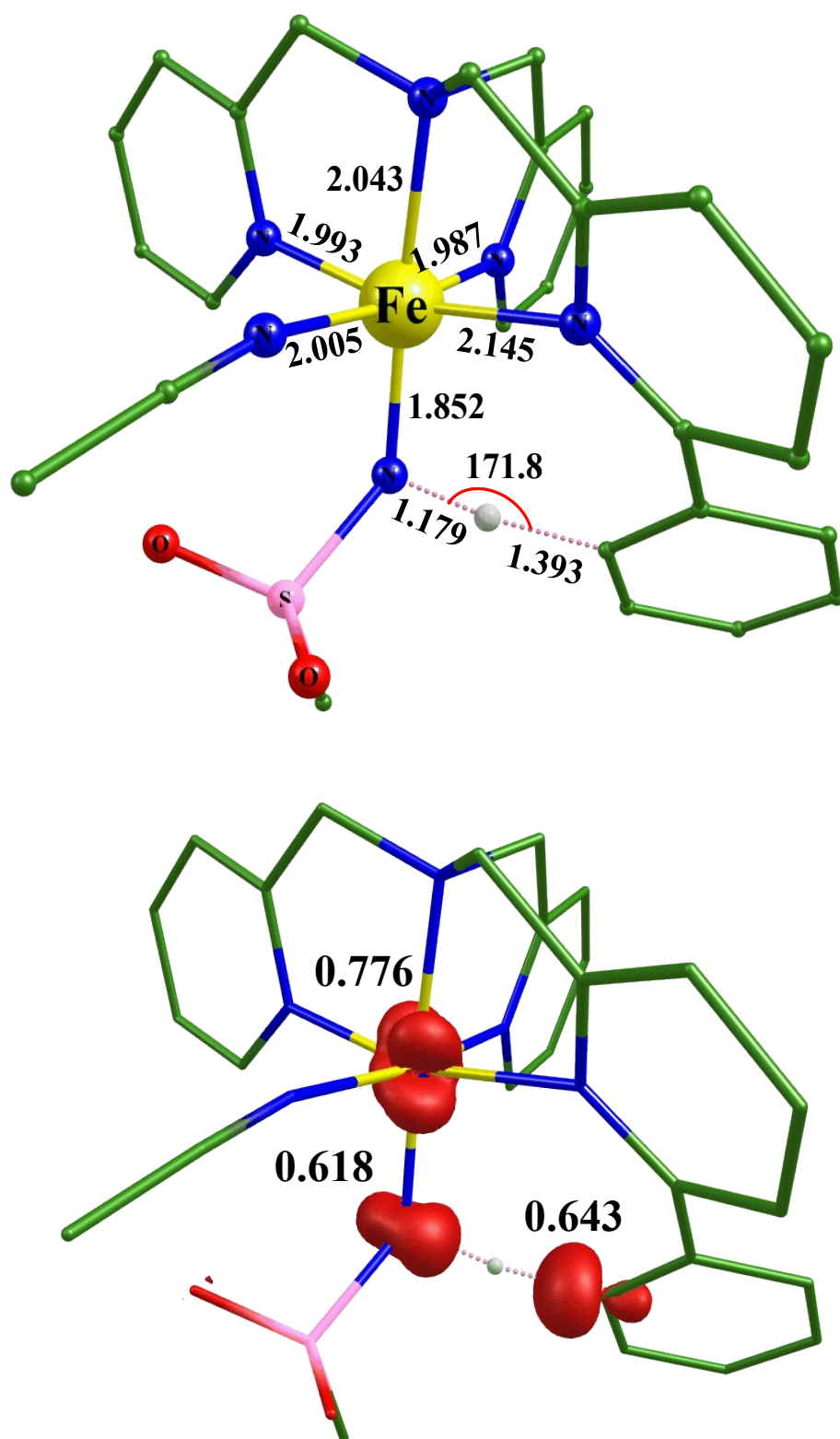


Figure S21a) B3LYP optimized structure of $^3I\text{-ts1a}$ with selected structural parameters and (b) Spin density plot of $^3I\text{-ts1a}$.

Supporting Information

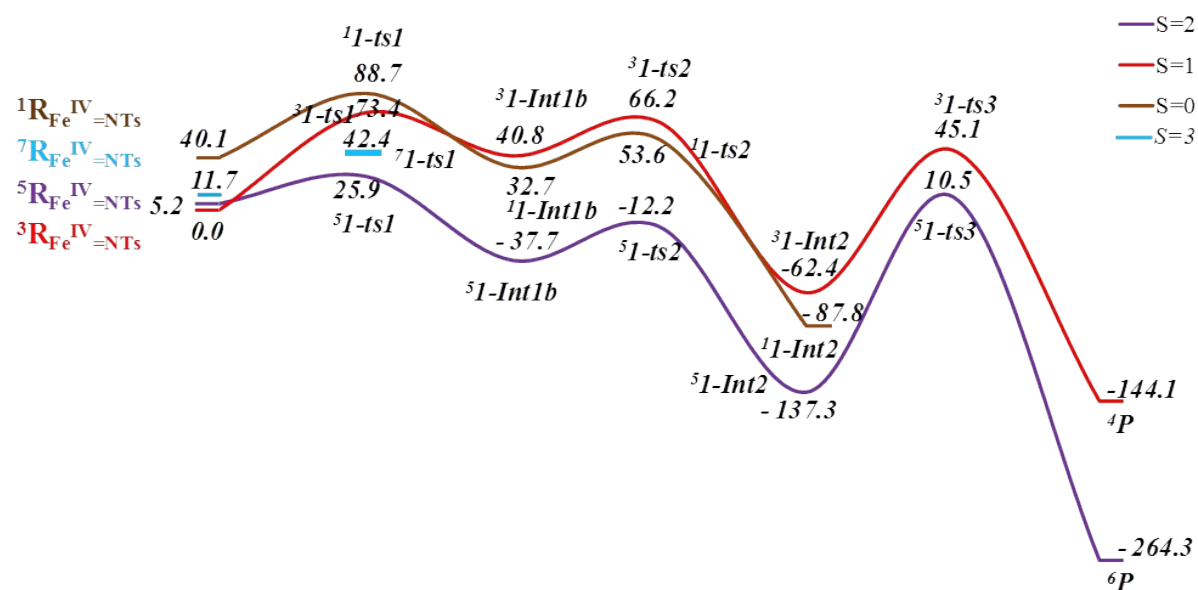


Figure S22. B3LYP computed free energy profile (ΔG in kJ/mol) of intramolecular *ortho*-amination by $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{NTs}]^{2+}$ via *ts3*.

Supporting Information

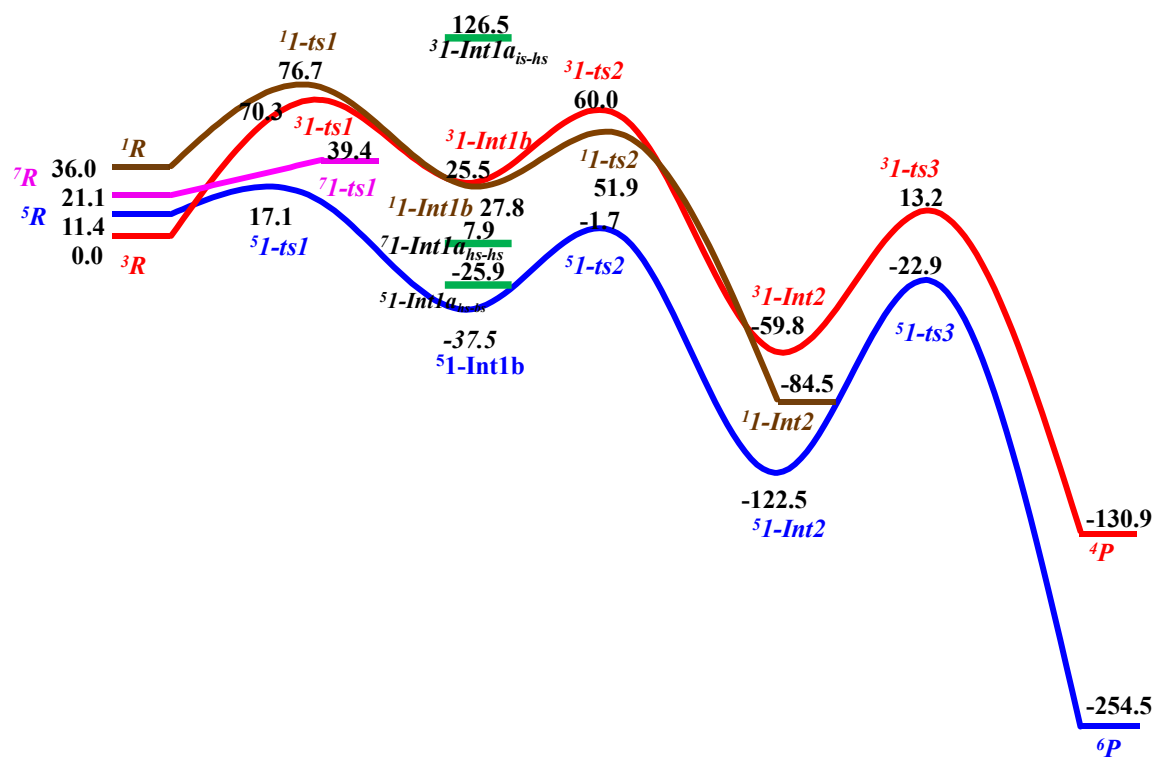


Figure S23. B3LYP-D3 computed free energy profile (ΔG in kJ/mol) of intramolecular *ortho*-amination by $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{NTs}]^{2+}$ via *ts3*.

Supporting Information

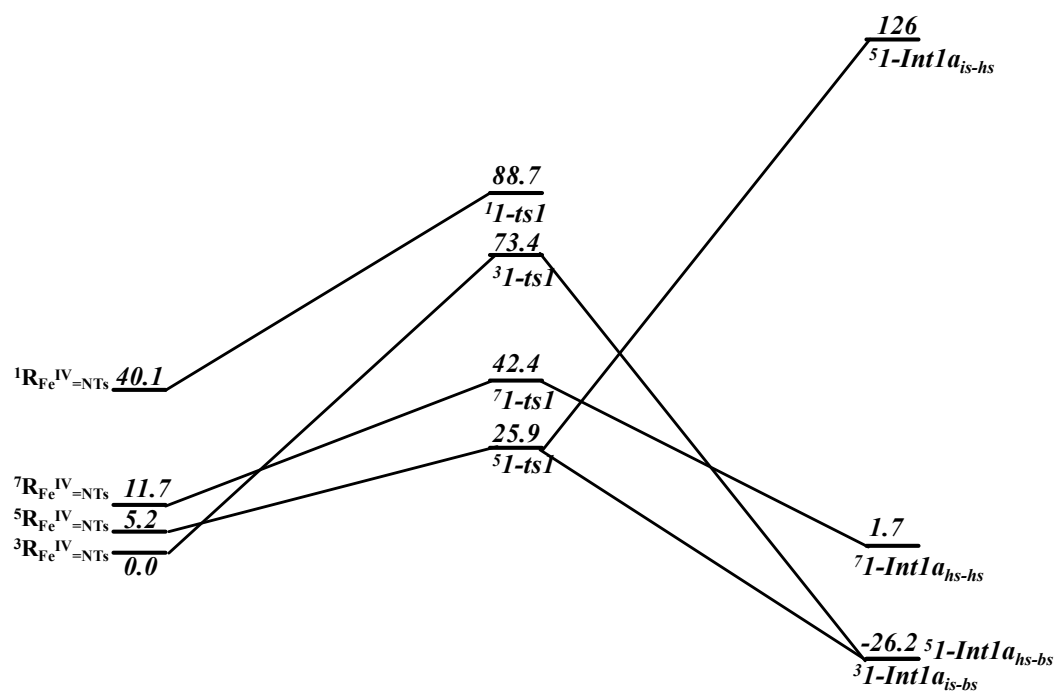


Figure S24. B3LYP Computed free energy profile (ΔG in kJ/mol) for the formation Int1a of intramolecular *ortho*-amination by $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{NTs}]^{2+}$.

Supporting Information

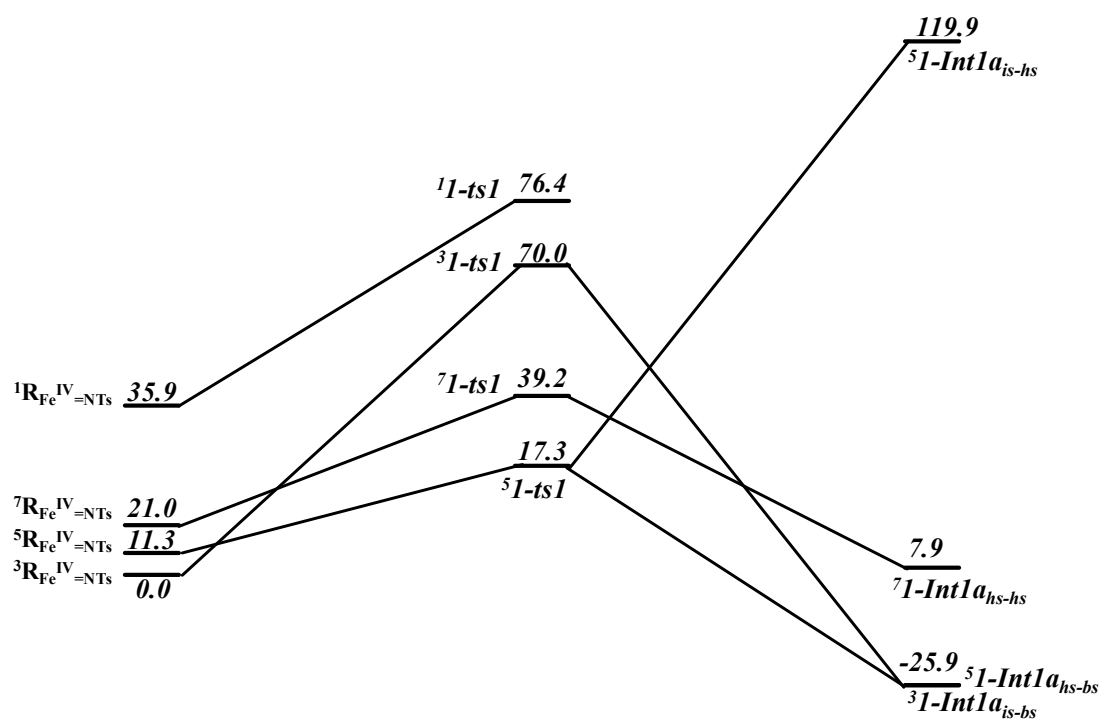


Figure S25. B3LYP-D3 (with D3-gcp scheme) computed free energy profile (ΔG in kJ/mol) for the formation of *1-Int1a* of intramolecular *ortho*-amination by $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{NTs}]^{2+}$.

Supporting Information

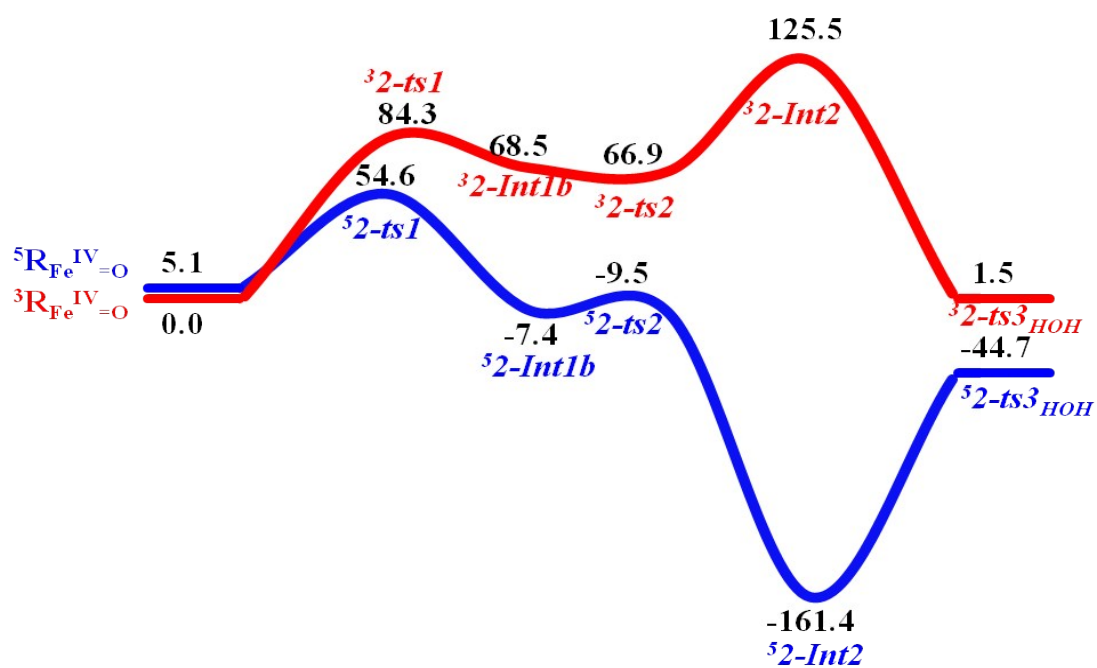


Figure S26. B3LYP computed free energy profile (ΔG in kJ/mol) of intramolecular *ortho*-hydroxylation by $[(6\text{-PhTPA})Fe^{IV}=O]^{2+}$.

Supporting Information

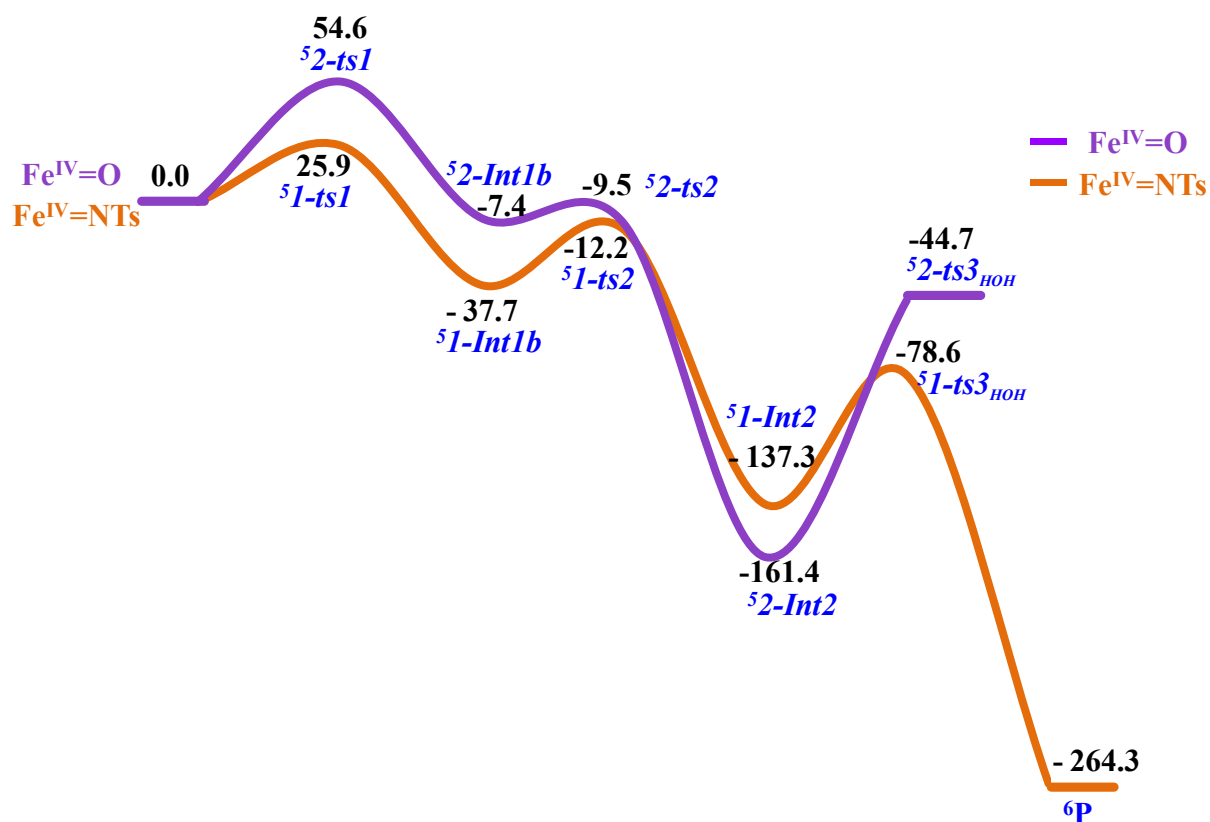


Figure S27. B3LYP computed free energy profile (ΔG in kJ/mol) of intramolecular *ortho*-amination and *ortho*-hydroxylation by $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{NTs}]^{2+}$ and $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$.

Supporting Information

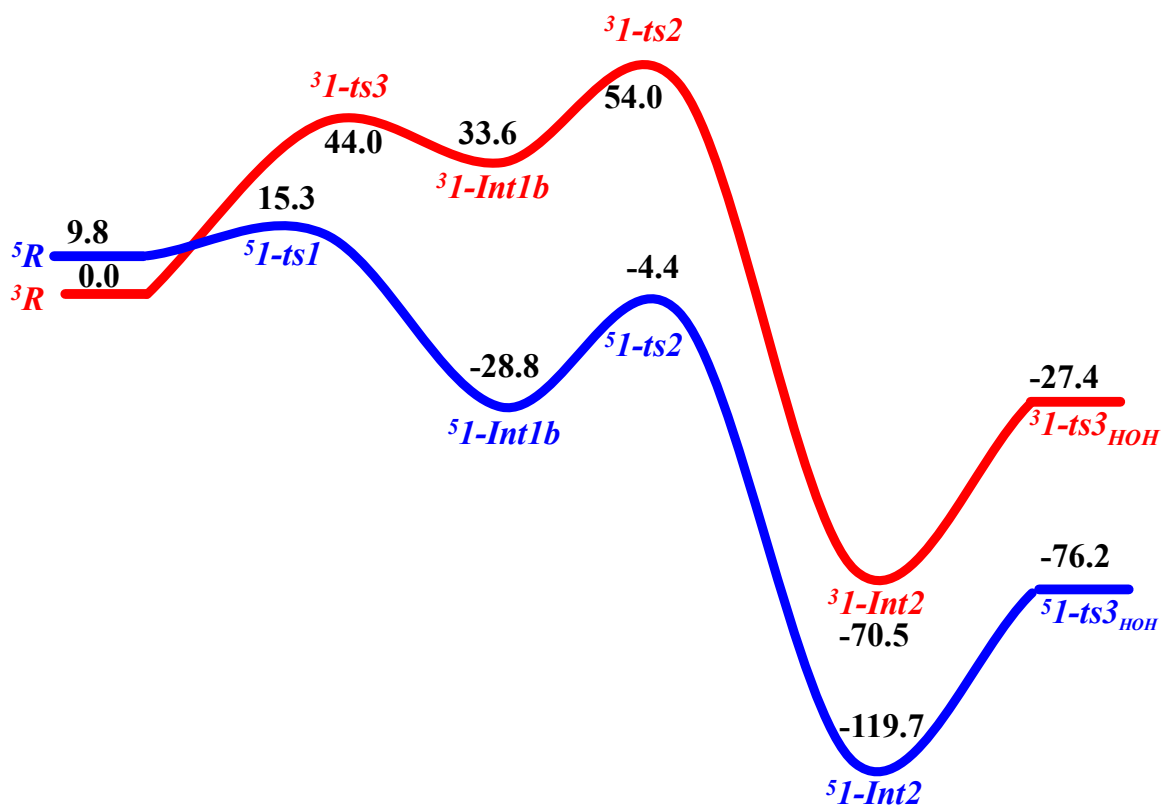


Figure S28. B3LYP-D3 computed free energy profile (ΔG in kJ/mol) of intramolecular *ortho*-amination by $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{NTs}]^{2+}$

Supporting Information

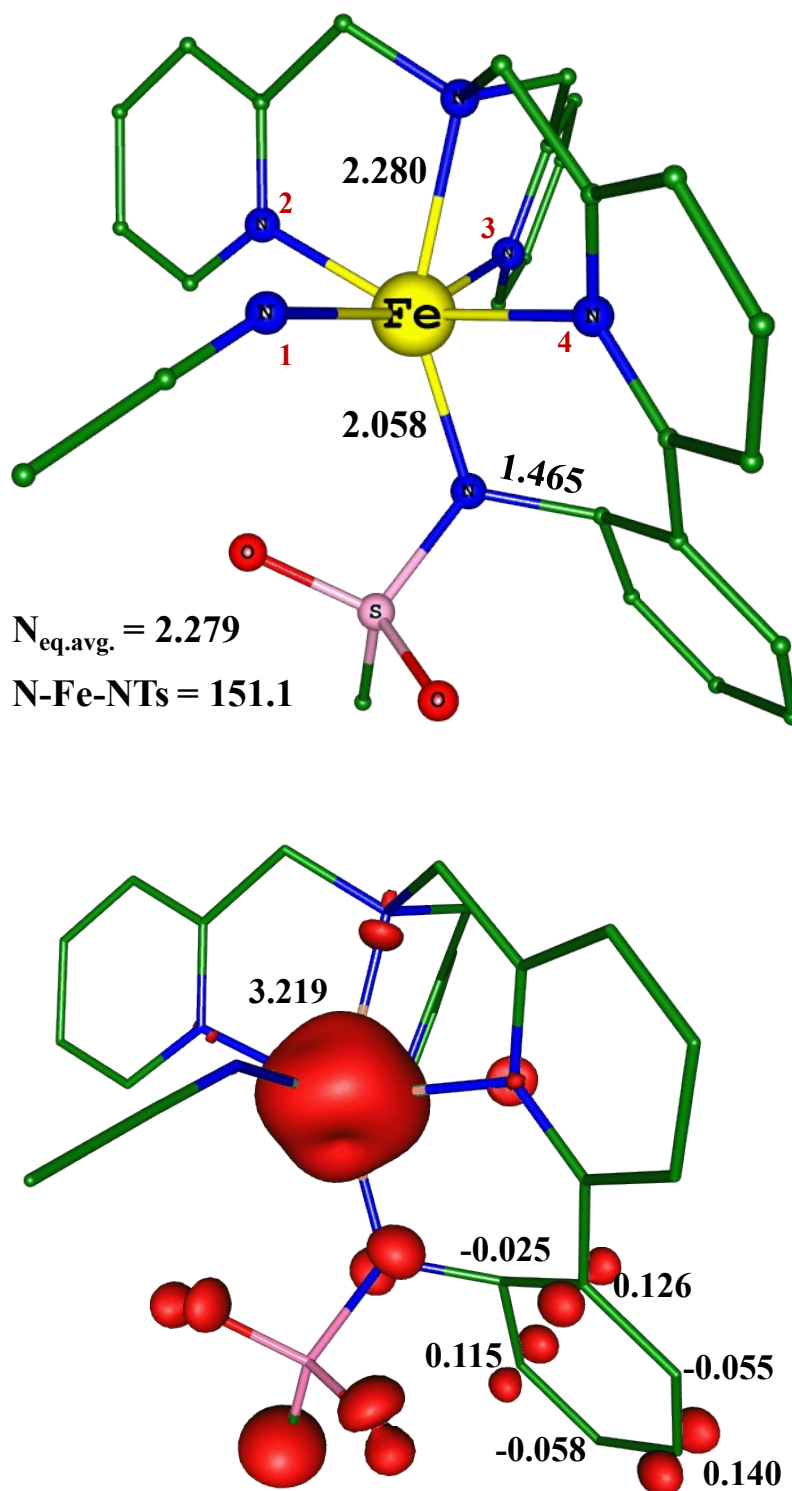


Figure S29. a) B3LYP optimized structure of *⁵I-Int1a* with selected structural parameters and b) Spin density plot of *⁵I-Int1a*.

Supporting Information

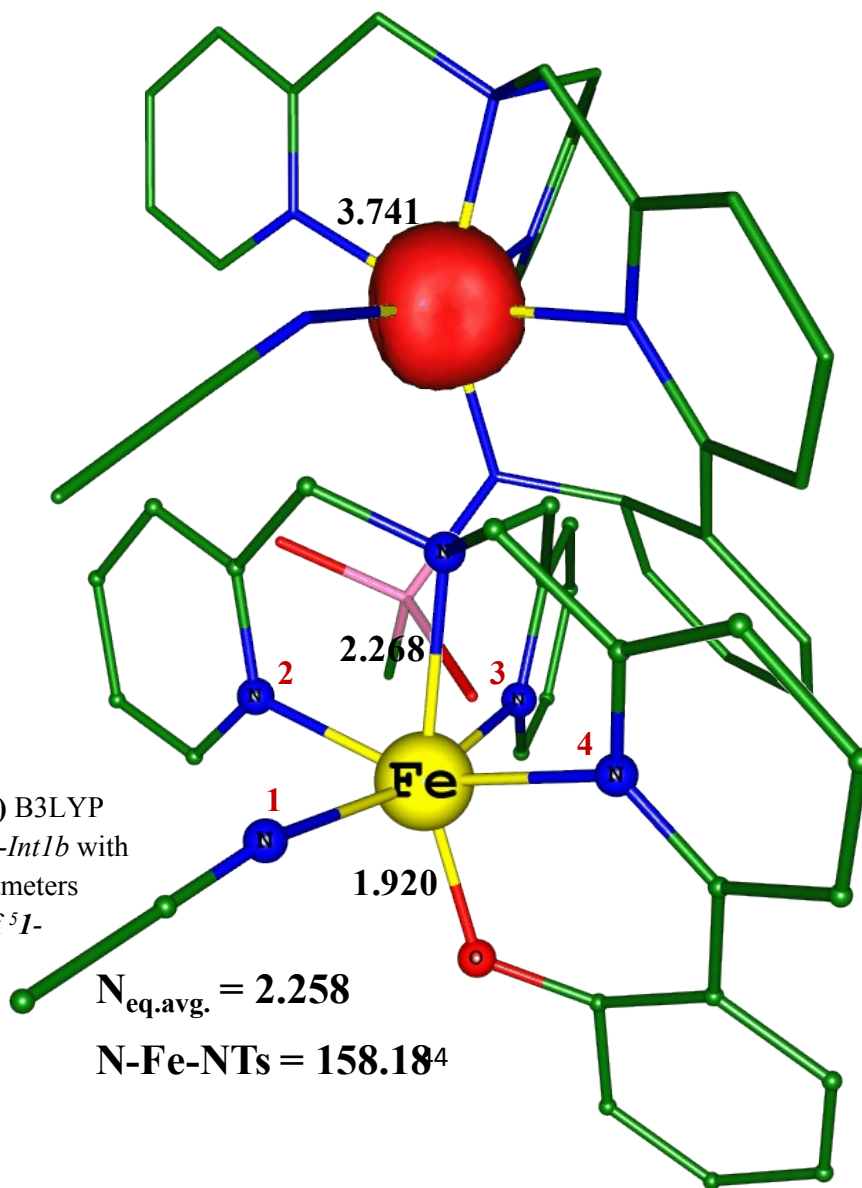
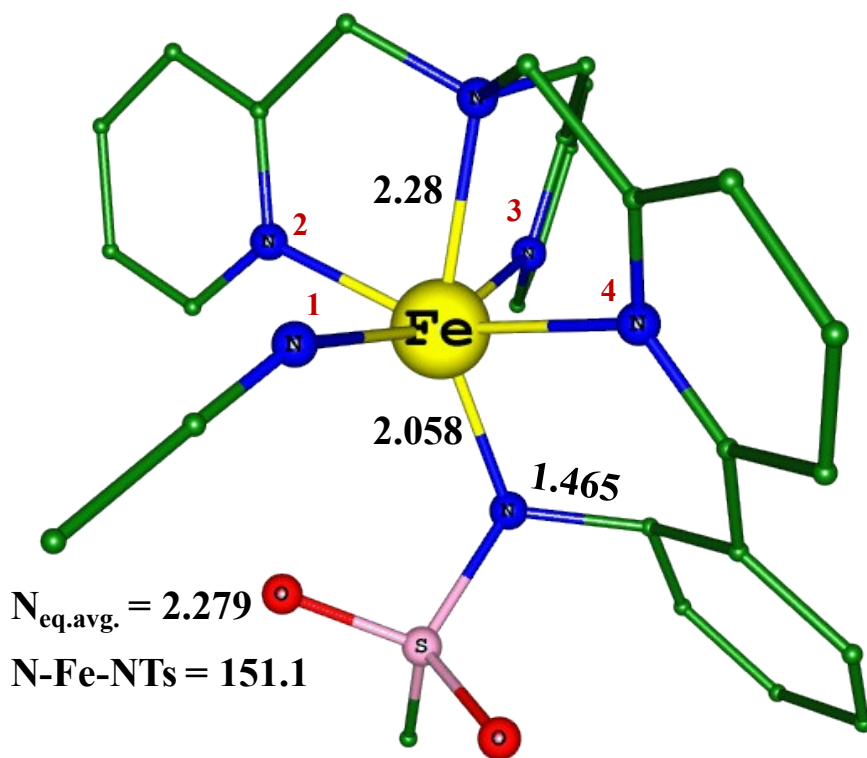


Figure S30. a) B3LYP structure of ${}^5I\text{-Int1b}$ with structural parameters density plot of ${}^5I\text{-}$

optimized selected and b) Spin $Int1b$.

Supporting Information

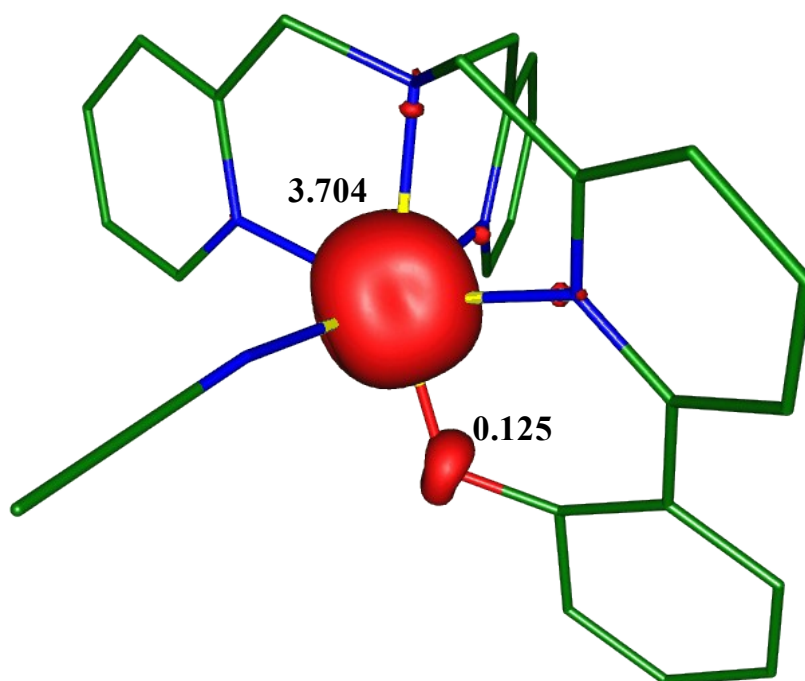


Figure S31. *a)* B3LYP optimized structure of $^5\mathbf{2-Int1b}$ with selected structural parameters and *b)* Spin density plot of $^5\mathbf{2-Int1b}$.

Supporting Information

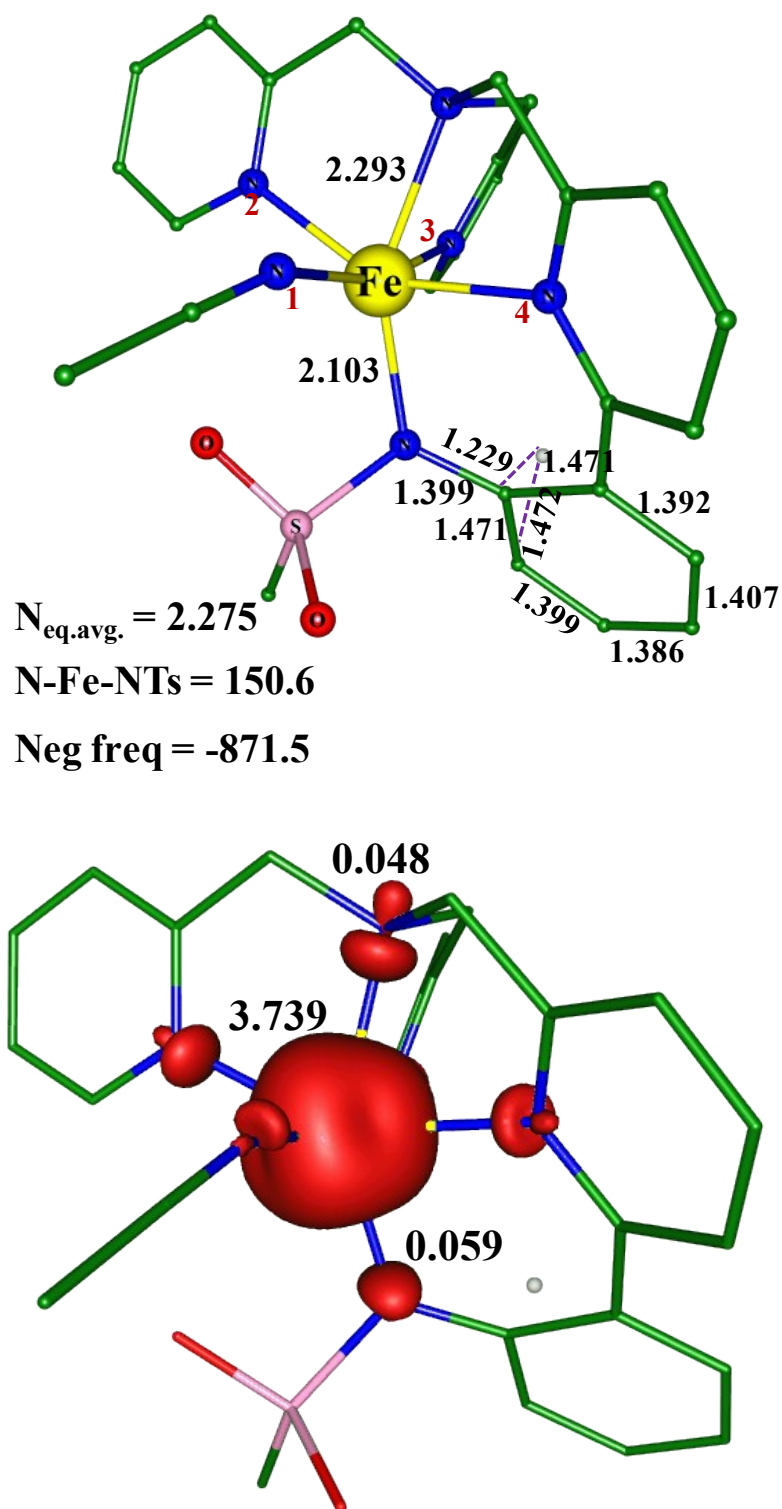


Figure S32. a) B3LYP optimized structure of $^5I\text{-ts2}$ with selected structural parameters and b) Spin density plot of $^5I\text{-ts2}$.

Supporting Information

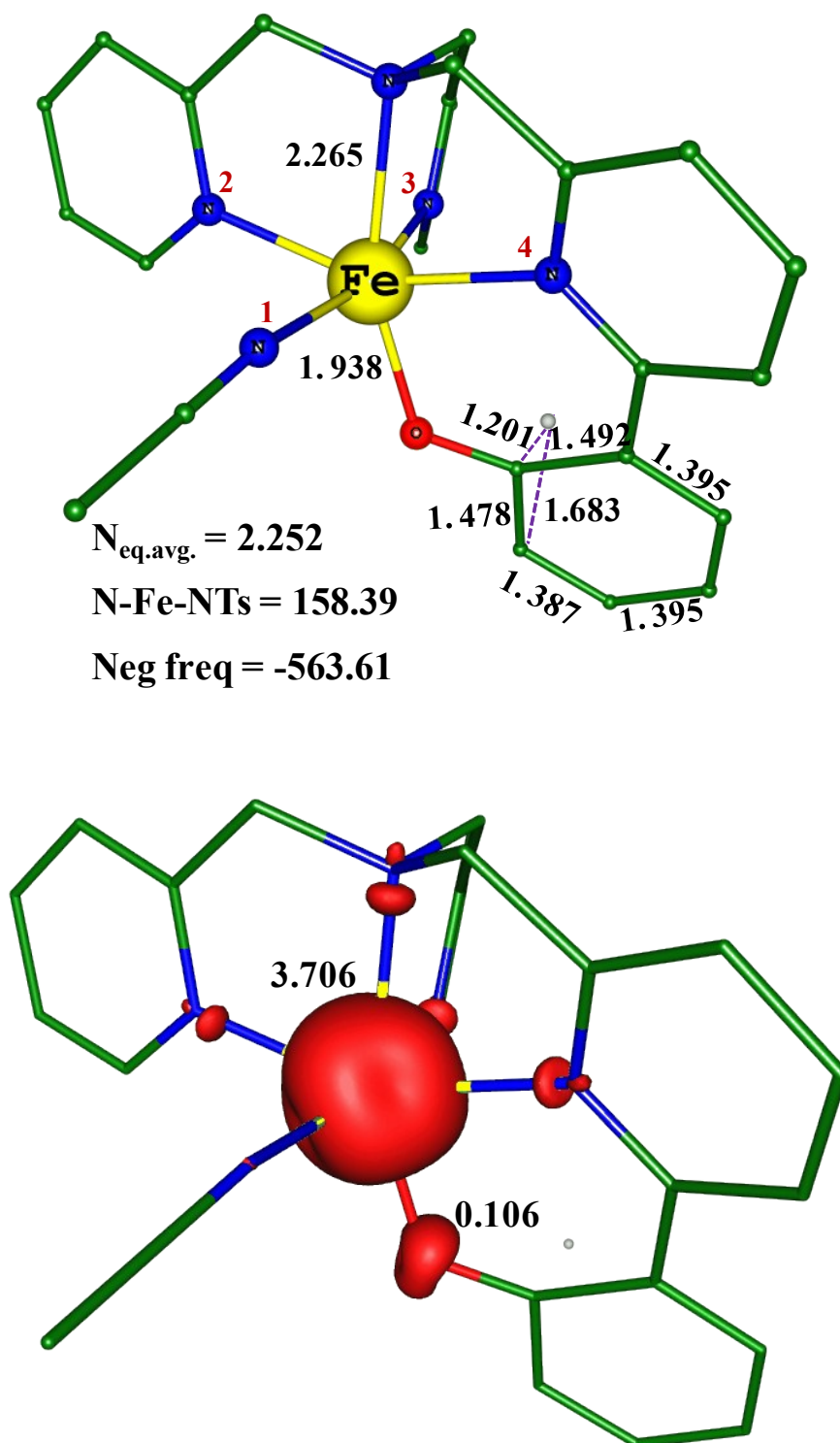


Figure S33. a) B3LYP optimized structure of $^{52}\text{-ts2}$ with selected structural parameters and b) Spin density plot of $^{52}\text{-ts2}$.

Supporting Information

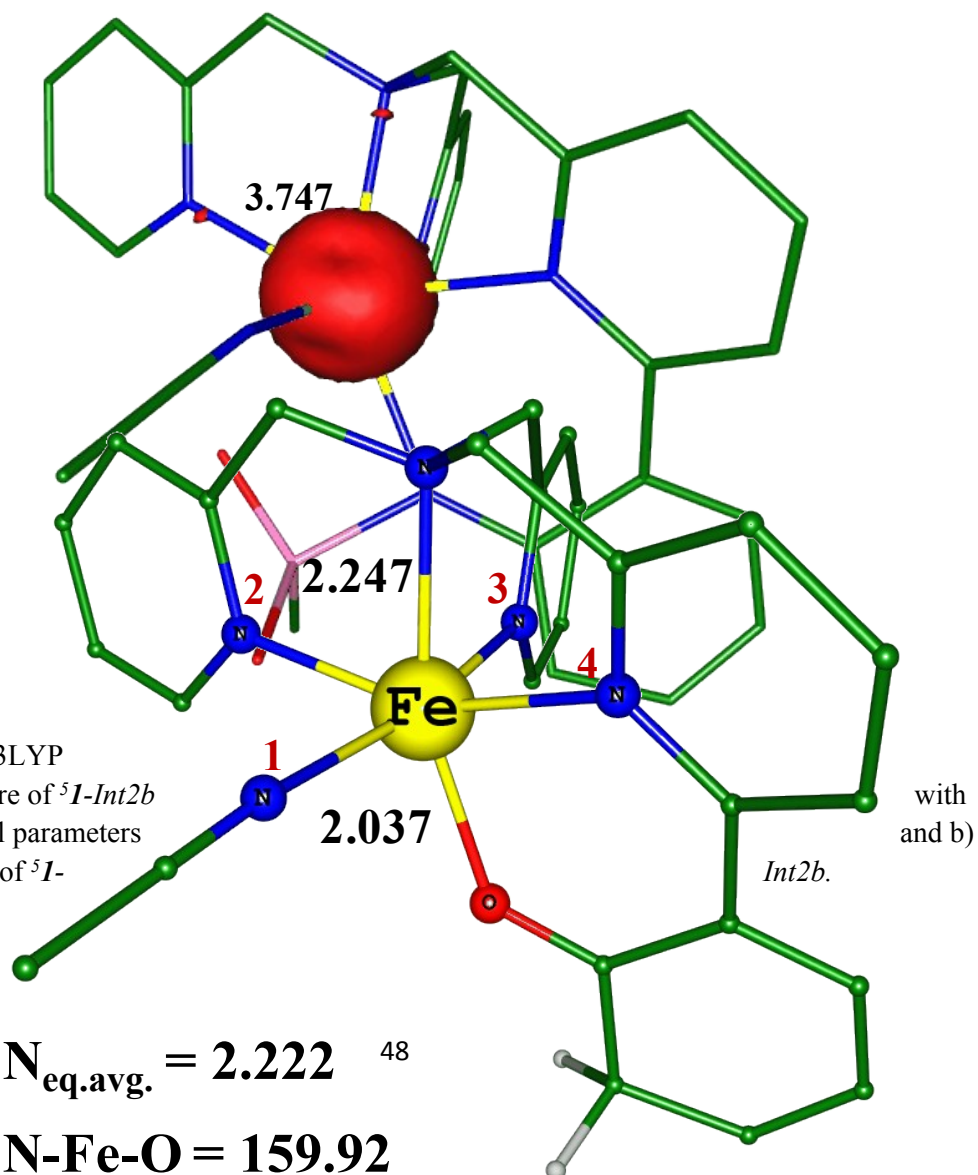
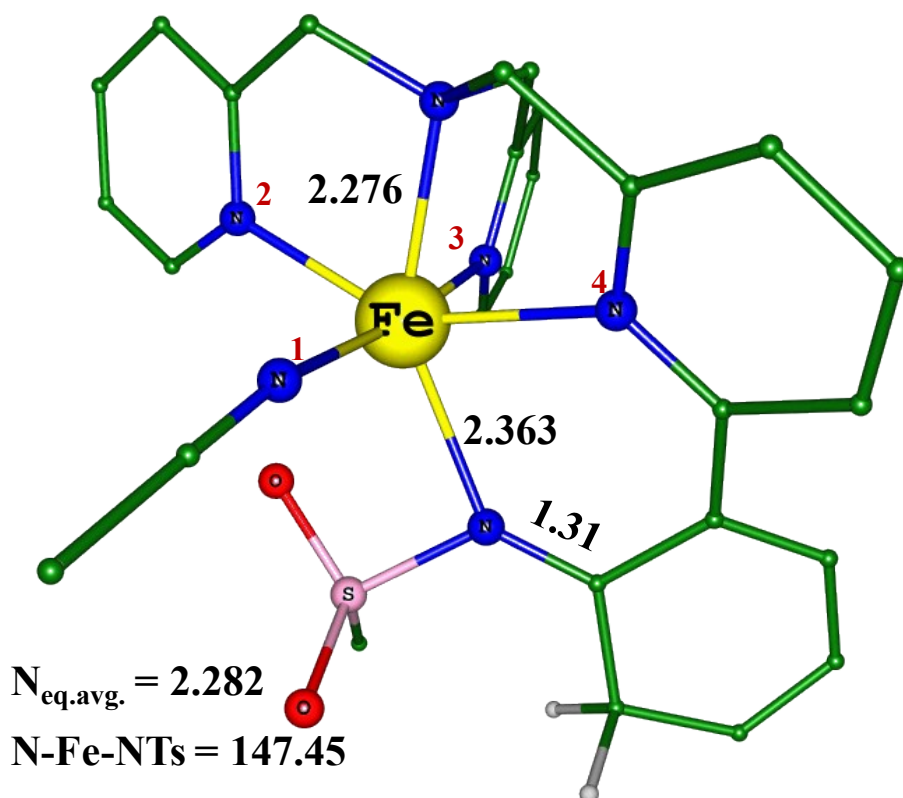


Figure S34. a) B3LYP
 optimized structure of $^5I\text{-Int2b}$
 selected structural parameters
 Spin density plot of $^5I\text{-}$

with
and b)

Int2b.

Supporting Information

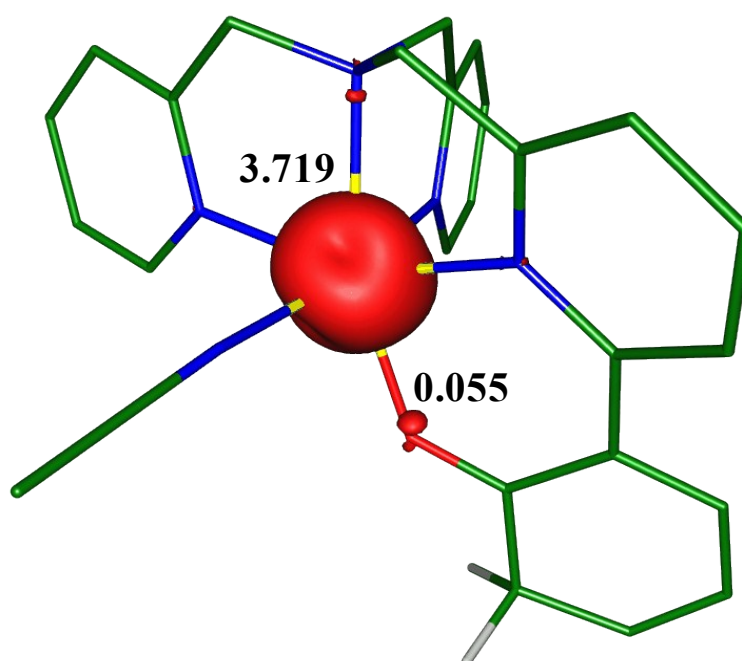


Figure S35. a) B3LYP optimized structure of $^5\mathbf{2-Int2b}$ with selected structural parameters and b) Spin density plot of $^5\mathbf{2-Int2b}$.

Supporting Information

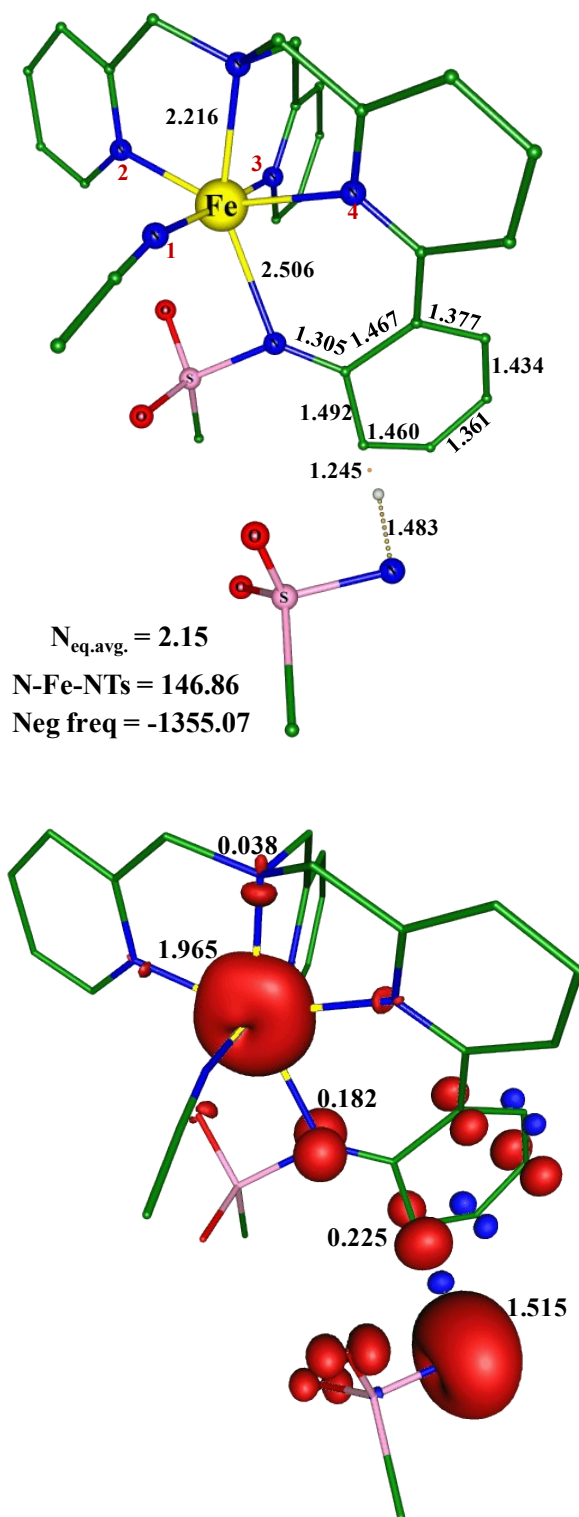


Figure S36. a) B3LYP optimized structure of ${}^5I\text{-ts3}$ with selected structural parameters and b) Spin density plot of ${}^5I\text{-ts3}$.

Supporting Information

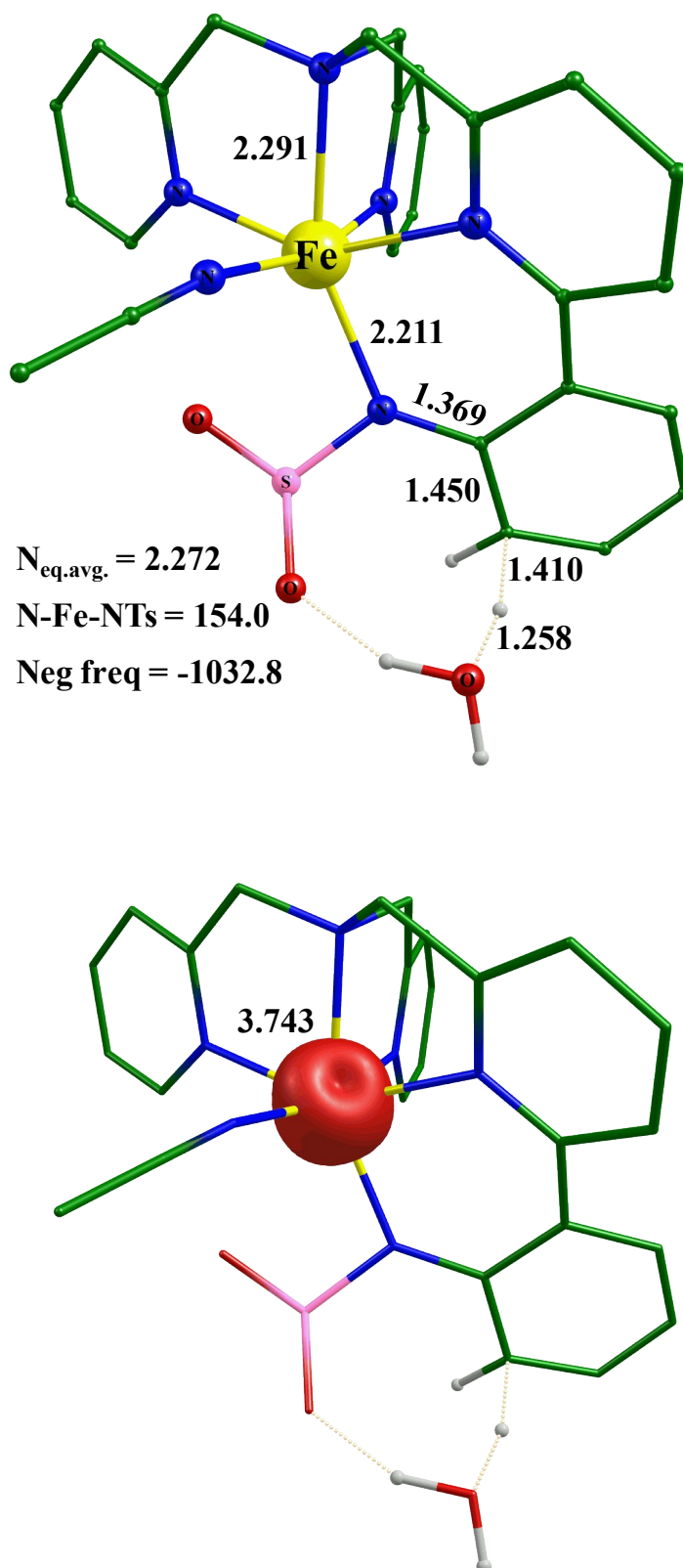


Figure S37. a) B3LYP optimized structure of ${}^5I\text{-}ts3_{HOH}$ with selected structural parameters and b) Spin density plot of ${}^5I\text{-}ts3_{HOH}$.

Supporting Information

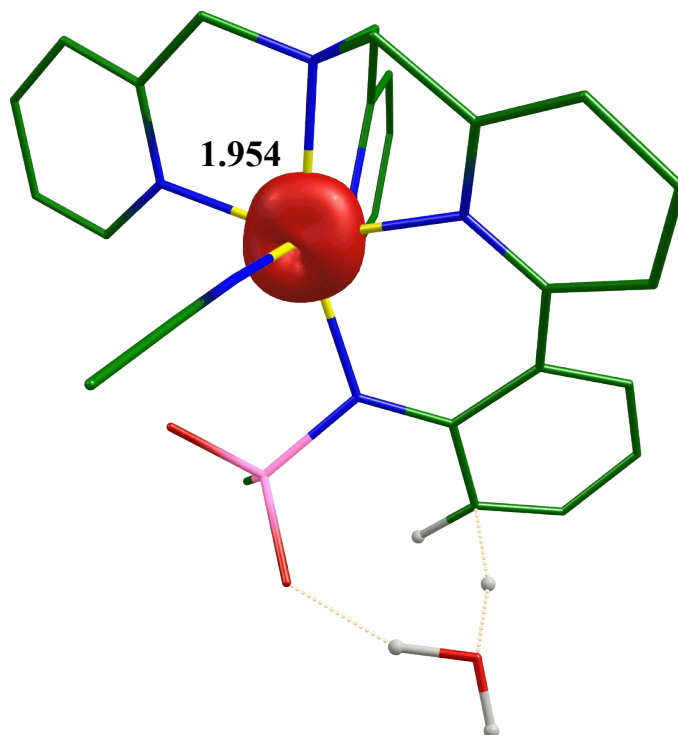
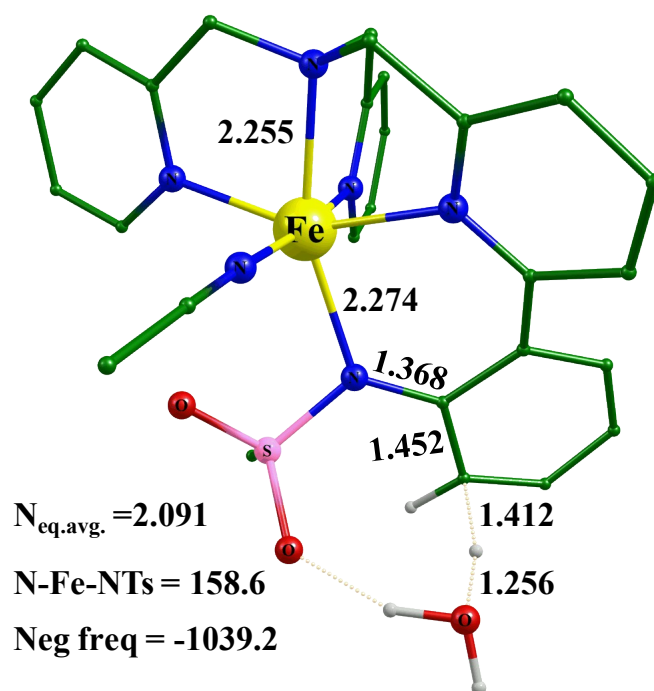


Figure S38. a) B3LYP optimized structure of ${}^3I\text{-}ts3_{HOH}$ with selected structural parameters and b) Spin density plot of ${}^3I\text{-}ts3_{HOH}$.

Supporting Information

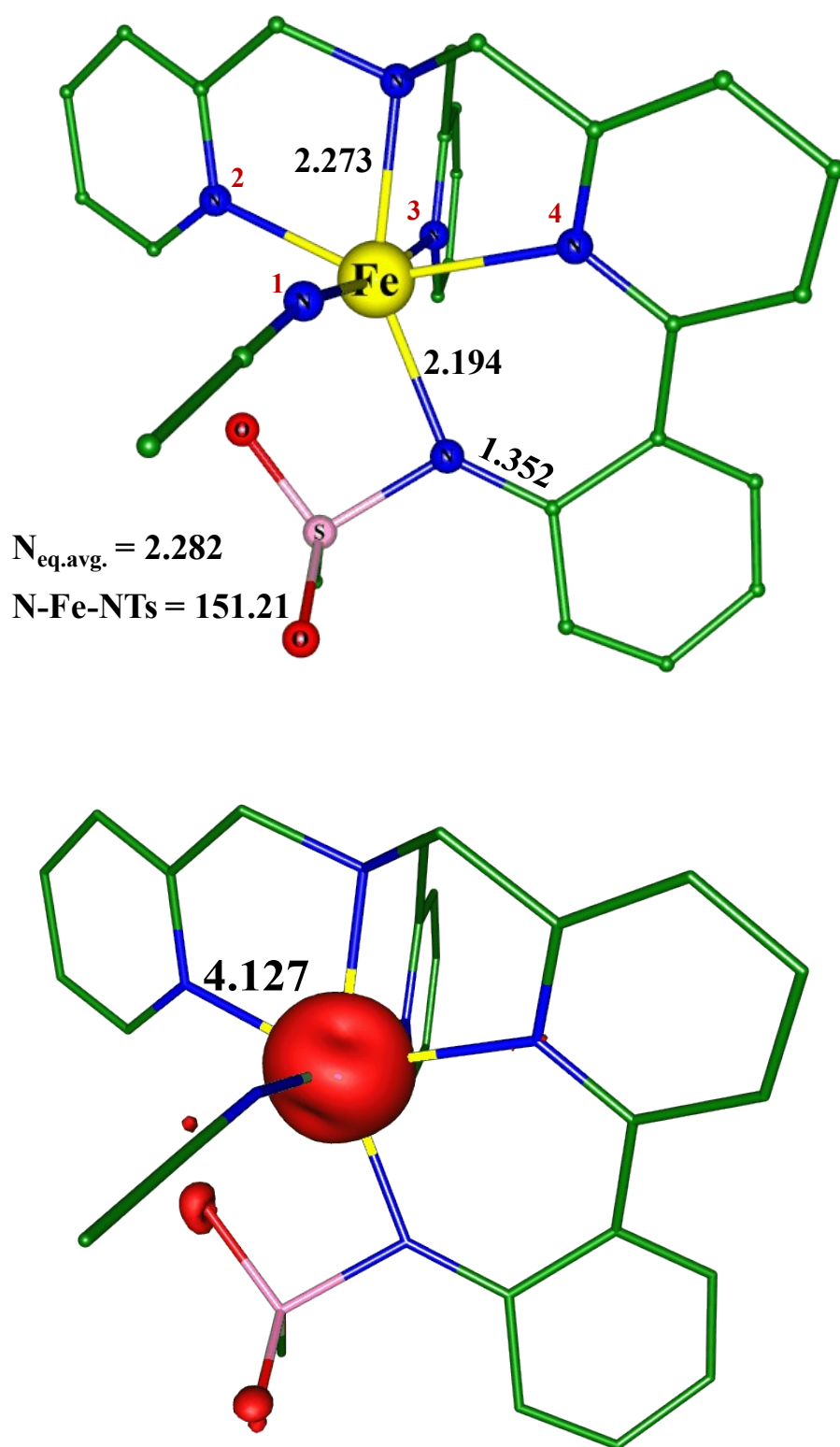


Figure S39. a) B3LYP optimized structure of ${}^6I\text{-}P$ with selected structural parameters and b) Spin density plot of ${}^6I\text{-}P$.

Supporting Information

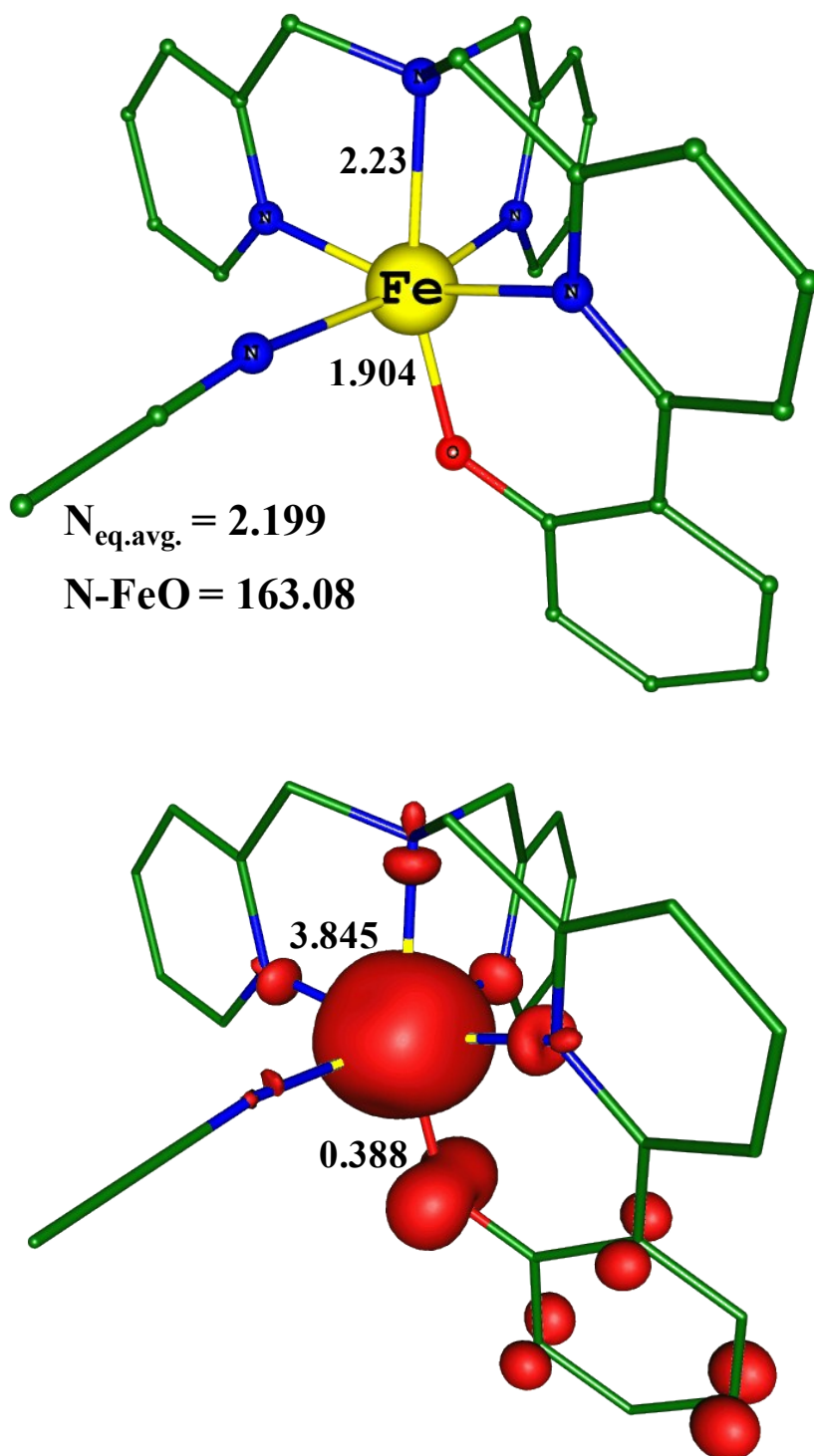


Figure S40. a) B3LYP optimized structure of **62-P** with selected structural parameters and b) Spin density plot of **62-P**.

Supporting Information

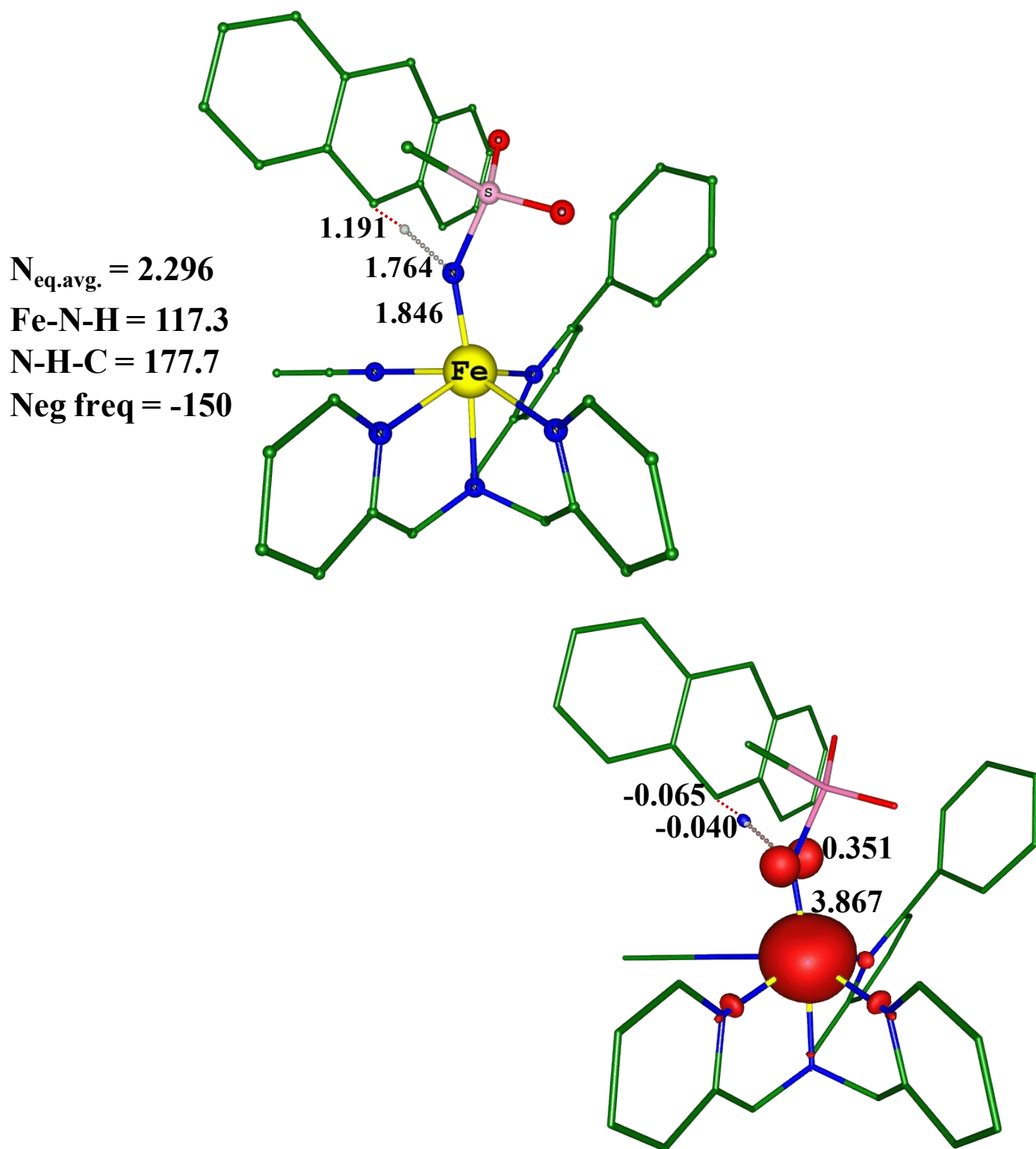


Figure S41. (a) B3LYP optimized structure of $^5\text{I-TS}_{\text{DHA}}$ with selected structural parameters and (b) Spin density plot of $^5\text{I-TS}_{\text{DHA}}$.

Supporting Information

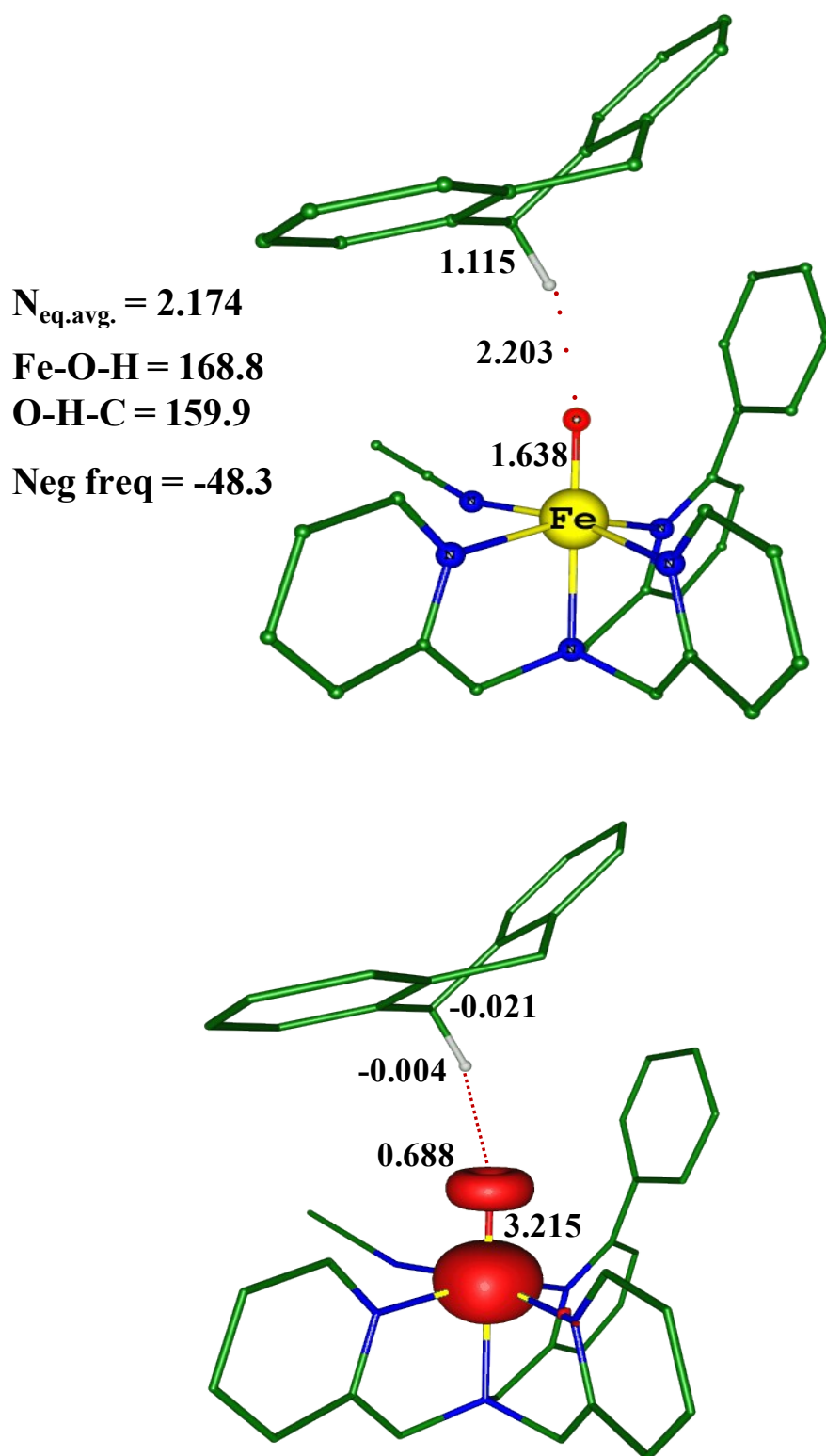
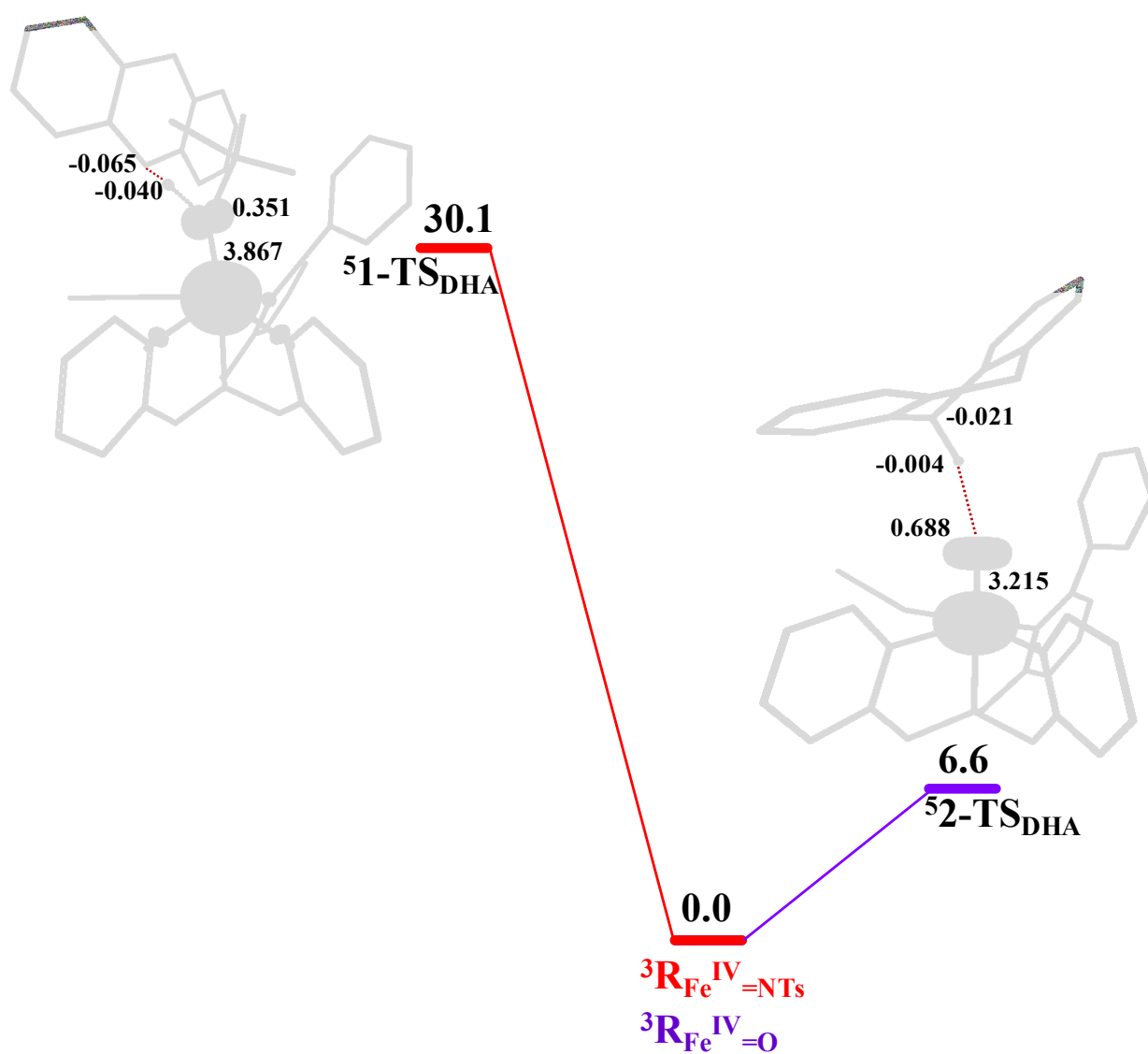


Figure S42. (a) B3LYP optimized structure of $^52\text{-TS}_{DHA}$ with selected structural parameters and (b) Spin density plot of $^52\text{-TS}_{DHA}$.

Supporting Information

Table S10. B3LYP computed structural parameters for *ortho*-hydroxylation reaction.

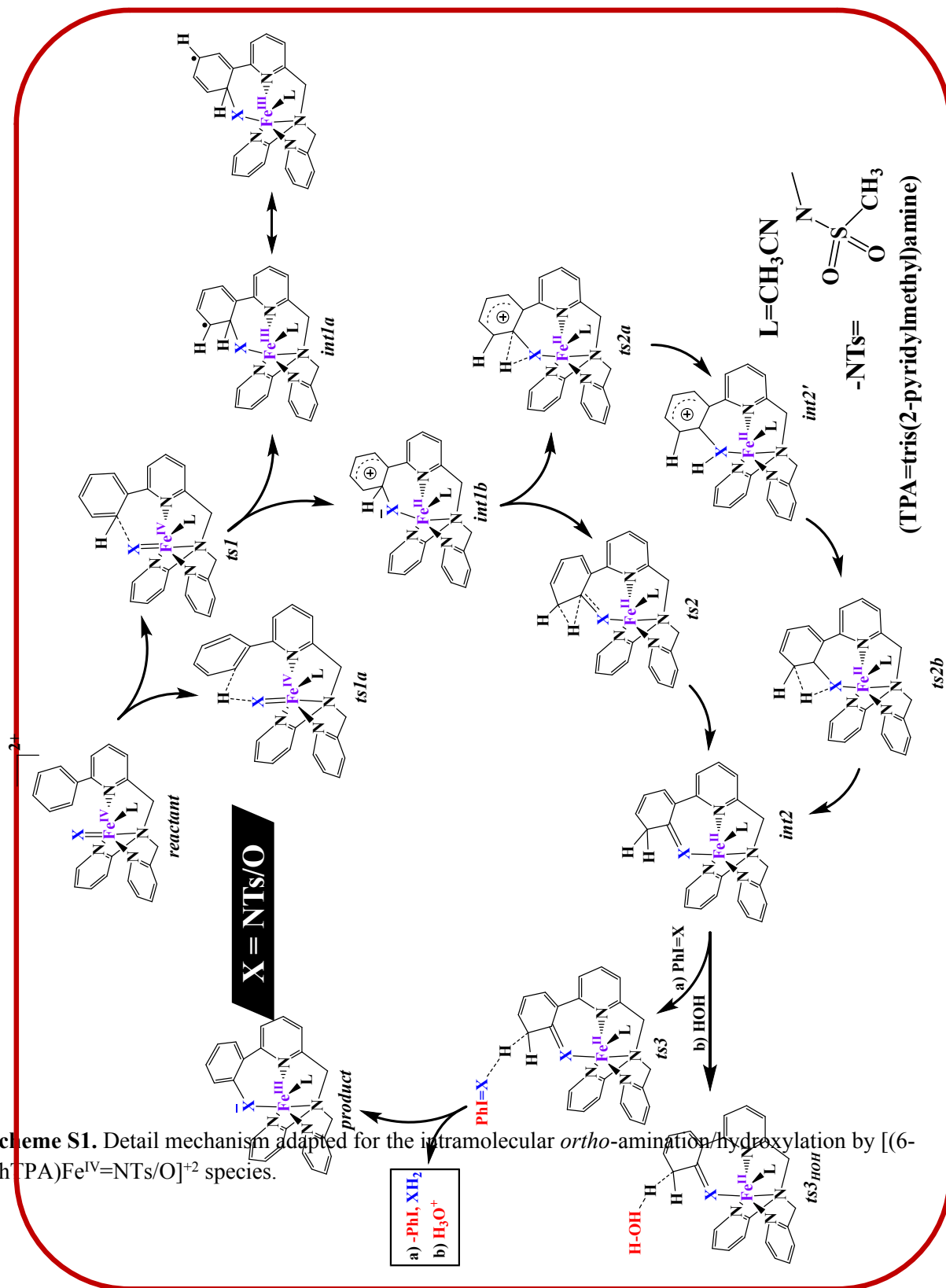
HAT TS1									
	Fe-N/O	N/O—H	H—C	N/O-H-C	Fe-N/O-H	N-Fe-NTs/O	Fe-N _{ax}	N _{eq} avg	Neg. Freq.
<i>⁵1-TS_{DHA}</i>	1.846	1.764	1.191	177.7	117.3	172.6	2.318	2.296	-149.96
<i>⁵2-TS_{DHA}</i>	1.638	2.203	1.115	159.9	168.75	175.6	2.162	2.174	-48.3



Supporting Information

Figure S43. B3LYP–D3 computed free energy profile (ΔG in kJ/mol) for transition state for HAT reaction by $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{NTs}]^{2+}$ and $[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$ species.

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Table S11: Relative energies of $\text{Fe}^{\text{IV}}=\text{NTs}$ and $\text{Fe}^{\text{IV}}=\text{O}$ spin state calculated in gas phase and solvent phase structure where structures are optimized explicitly.

	<i>Relative Energies (ΔE, kJ/mol)</i>	
	<i>In gas phase</i>	<i>In solvent phase</i>
$^3I_{(IS,S)}$	0.0	0.0
$^5I_{(HS,S)}$	6.8	12.2
$^32_{(IS)}$	0.0	0.0
$^52_{(HS)}$	13.0	14.3

Supporting Information

Table S12: Selected structural parameters obtained using gas phase vs. solvent phase optimization for $\text{Fe}^{\text{IV}}=\text{NTs}$ and $\text{Fe}^{\text{IV}}=\text{O}$ species (all bond lengths are given in Å).

	<i>In gas phase</i>		<i>In solvent phase</i>	
	Fe—X (X=NTs, O)	Fe-N_{ax}	Fe—X	Fe-N_{ax}
$^3I_{(IS,S)}$	1.767	2.055	1.764	2.043
$^5I_{(HS,S)}$	1.750	2.076	1.759	2.071
$^32_{(IS)}$	1.629	2.098	1.630	2.090
$^52_{(HS)}$	1.623	2.102	1.625	2.094

Supporting Information

Computational details:

All the calculations were carried out by using the Gaussian 09 suite of programs.¹ The geometry optimizations have been performed with B3LYP functional.² Single point calculations have been performed with the B3LYP-D3 functional.³ The B3LYP-D3 has a proven track record of predicting the structures and the energetics accurately for such metal mediated catalytic reactions. Earlier we have employed this functional along with a set of other modern functionals for predicting correct ground state for iron-oxo species where B3LYP-D3 is found to be superior compared to other functionals. The performance of B3LYP-D3 for reactivity studies has also been benchmarked against CCSD(T)/CBS level earlier.⁴ Due to these reasons, we have limited our calculations to B3LYP and B3LYP-D3 functionals. Here LACVP basis set comprising LanL2DZ - Los Alamos effective core potential⁵ for Fe and a 6-31G* basis set for the other atoms⁶ (B-I) has been employed for geometry optimization in gas phase and the optimized geometries were then used to perform single point energy calculations using a TZVP basis set (B-II) on all atoms with the incorporation of solvent.⁷ The solvation energies have been computed using PCM solvation model employing acetonitrile as the solvent.⁸ Frequency calculations were performed on the optimized structures at B-I level to verify that they are minima on the potential-energy surface (PES) and also to obtain free energy corrections. The quoted DFT energies are B3LYP-D3 solvation energies incorporating zero point energies correction at the B-I level computed at the temperature of 298.15 K, unless otherwise mentioned. The transition states were characterized by single negative frequency corresponding to the reaction coordinate and are verified by animating the frequency using visualization software such as Molden. The fragment approach available in Gaussian 09 is employed to aid smooth convergence in case of radical intermediates. The nature of all the spin-coupled states after convergence was verified by analyzing the computed spin densities and $\langle S^2 \rangle$ values. The involved spin states are represented by the notation $^M1_{(sFe,sN/O)}$, where superscript 'M' denotes the total multiplicities of the complexes and subscript '(sFe,sN/O)' denotes the spin multiplicity on Fe and N atoms. To get better insight into the electronic structure and nature of the bonding in species 1 and 2 (Fe=NTs and Fe=O, respectively), NBO, MO and EDA calculations have also been performed.⁹

Supporting Information

References:

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Supporting Information

Coordinates of the selected species at B3LYP level of theory

Reactant species

⁵¹

Fe	0.360774000	0.234091000	-0.321173000
N	1.331732000	2.069192000	-0.320834000
N	0.706195000	0.314300000	1.708106000
N	2.518052000	-0.434811000	-0.330601000
N	-1.357785000	1.694196000	-0.442974000
C	0.587455000	-0.710119000	2.577369000
H	0.155755000	-1.625143000	2.190441000
C	1.016981000	-0.605279000	3.895526000
H	0.904637000	-1.450709000	4.565576000
C	1.598318000	0.589293000	4.323038000
H	1.948639000	0.699439000	5.344749000
C	1.735324000	1.641700000	3.416031000
H	2.189274000	2.580796000	3.716419000
C	1.276648000	1.472078000	2.112666000
C	3.028543000	-1.651508000	-0.060743000
H	2.322406000	-2.464562000	0.057696000
C	4.397861000	-1.867006000	0.083041000
H	4.762484000	-2.867257000	0.290636000
C	5.268151000	-0.785107000	-0.032081000
H	6.339319000	-0.918195000	0.084491000
C	4.738716000	0.480522000	-0.293147000
H	5.385379000	1.347575000	-0.386339000
C	3.361346000	0.613448000	-0.444545000
C	-2.696940000	1.506212000	-0.275452000
C	-3.608888000	2.484669000	-0.705550000
H	-4.668033000	2.314915000	-0.550156000
C	-3.157446000	3.673676000	-1.263540000
H	-3.860611000	4.439956000	-1.575081000
C	-1.783404000	3.877163000	-1.385281000
H	-1.384769000	4.800449000	-1.793854000
C	-0.926373000	2.861039000	-0.979881000
C	1.307522000	2.581817000	1.094105000
H	0.396589000	3.178468000	1.209244000
H	2.155898000	3.254055000	1.262657000
C	2.727716000	1.919386000	-0.847580000
H	2.661651000	1.944338000	-1.939916000
H	3.338431000	2.776575000	-0.541455000
C	0.559910000	2.993151000	-1.204795000
H	0.788209000	2.724350000	-2.239630000
H	0.891994000	4.028386000	-1.053912000
C	0.476888000	-0.411228000	-3.456249000
N	0.446284000	0.112432000	-2.423362000
C	0.515587000	-1.092239000	-4.739311000
H	-0.336215000	-0.786415000	-5.355440000
H	1.445209000	-0.857013000	-5.267409000
H	0.464004000	-2.170427000	-4.551695000
S	-0.349922000	-2.880734000	-0.645761000
O	0.392473000	-3.445401000	0.493122000
O	0.206985000	-2.989854000	-2.001312000
C	-2.022759000	-3.522696000	-0.632400000
C	-3.236344000	0.306165000	0.411411000
C	-4.312177000	-0.394387000	-0.161367000

C	-2.795194000	-0.054071000	1.695043000
C	-4.922973000	-1.440825000	0.529588000
H	-4.671867000	-0.119142000	-1.149217000
C	-3.413955000	-1.094826000	2.388486000
H	-2.004797000	0.517399000	2.169828000
C	-4.478193000	-1.791185000	1.808205000
H	-5.756259000	-1.970832000	0.077916000
H	-3.087191000	-1.343422000	3.394117000
H	-4.972025000	-2.587491000	2.357267000
N	-0.564990000	-1.251048000	-0.302841000
H	-1.933862000	-4.601327000	-0.792364000
H	-2.474973000	-3.309446000	0.337163000
H	-2.586638000	-3.056787000	-1.441541000

³¹

Fe	0.486827000	0.231208000	-0.307404000
N	1.544285000	1.986602000	-0.461725000
N	0.637554000	0.534730000	1.643912000
N	2.353993000	-0.554575000	-0.099419000
N	-1.108858000	1.607196000	-0.638221000
C	0.357772000	-0.382654000	2.592746000
H	-0.101370000	-1.302468000	2.252509000
C	0.650948000	-0.165166000	3.934117000
H	0.409076000	-0.929117000	4.665028000
C	1.264136000	1.031425000	4.307904000
H	1.509892000	1.228010000	5.346873000
C	1.571068000	1.968628000	3.321752000
H	2.059013000	2.905017000	3.573549000
C	1.245343000	1.687446000	1.996875000
C	2.670455000	-1.786629000	0.350290000
H	1.853552000	-2.457213000	0.580103000
C	3.989462000	-2.194008000	0.529040000
H	4.187226000	-3.200360000	0.881833000
C	5.021859000	-1.298710000	0.260840000
H	6.059706000	-1.585868000	0.398183000
C	4.694782000	-0.015212000	-0.177244000
H	5.467206000	0.718602000	-0.385395000
C	3.356409000	0.322114000	-0.351630000
C	-2.457761000	1.478601000	-0.472371000
C	-3.334560000	2.435873000	-1.014611000
H	-4.398538000	2.306407000	-0.855638000
C	-2.853020000	3.550184000	-1.685058000
H	-3.533171000	4.296172000	-2.084261000
C	-1.473709000	3.703528000	-1.799181000
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C	-0.647710000	2.714350000	-1.281921000
C	1.495344000	2.664520000	0.878059000
H	0.670372000	3.384203000	0.856200000
H	2.413341000	3.237795000	1.046704000
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H	2.936145000	1.609004000	-1.989100000

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H	3.633875000	2.451768000	-0.608714000
C	0.842459000	2.815078000	-1.477795000
H	1.105421000	2.429706000	-2.466071000
H	1.178050000	3.858900000	-1.432855000
C	0.627888000	-0.593584000	-3.325473000
N	0.596465000	-0.077658000	-2.290516000
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H	1.629991000	-1.135398000	-5.093868000
H	0.506935000	-2.350073000	-4.418046000
S	-0.525343000	-2.867883000	-0.528744000
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H	-4.426121000	-0.173357000	-1.284376000
C	-3.525931000	-0.689497000	2.451896000
H	-2.013970000	0.807873000	2.141531000
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H	-3.299764000	-0.804111000	3.507985000
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H	-2.274622000	-4.390908000	-0.797783000
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52

Fe	-0.253877000	-0.275517000	-0.213288000
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N	-0.833698000	1.683671000	0.420668000
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C	-1.397194000	3.979134000	0.064553000
H	-1.355741000	4.854048000	-0.575199000
C	-2.039801000	4.016067000	1.303786000
H	-2.515056000	4.928278000	1.651322000
C	-2.068609000	2.864784000	2.094821000
H	-2.558649000	2.865983000	3.063419000
C	-1.446770000	1.712627000	1.621083000
C	-2.521226000	-0.094817000	-2.229304000
H	-1.714402000	0.211582000	-2.886518000
C	-3.849223000	-0.116817000	-2.639457000
H	-4.106769000	0.172908000	-3.652366000
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H	-5.874903000	-0.525894000	-2.008419000
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H	-5.187102000	-1.187550000	0.299821000
C	-3.096952000	-0.845818000	-0.090962000
C	2.723849000	-0.341824000	0.720436000
C	3.739132000	-0.886673000	1.522910000
H	4.769030000	-0.635781000	1.296085000

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H	4.206644000	-2.080632000	3.253202000
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C	1.109813000	-1.422521000	2.054139000
C	-1.318182000	0.448483000	2.435493000
H	-0.387859000	0.508168000	3.010980000
H	-2.136017000	0.346855000	3.157509000
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H	-2.490242000	-2.430635000	1.185882000
H	-3.298571000	-1.126501000	2.044807000
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C	0.495184000	-4.600790000	-2.284894000
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C	3.094475000	0.582510000	-0.376363000
C	4.006153000	0.164744000	-1.359472000
C	2.639798000	1.911882000	-0.377099000
C	4.425578000	1.052971000	-2.348653000
H	4.375625000	-0.857191000	-1.356977000
C	3.080087000	2.802227000	-1.355262000
H	1.979481000	2.254033000	0.414012000
C	3.965739000	2.372829000	-2.346820000
H	5.120333000	0.719159000	-3.113132000
H	2.750211000	3.836872000	-1.333192000
H	4.309993000	3.068238000	-3.106230000
O	0.440215000	0.199862000	-1.600735000

32

Fe	0.441150000	0.352429000	-0.057665000
N	1.535629000	-0.270544000	1.620661000
N	0.285082000	-1.572828000	-0.402882000
N	2.270492000	0.364365000	-0.860073000
N	-1.142563000	0.213771000	1.241914000
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H	-0.846855000	-1.355584000	-2.118665000
C	-0.479075000	-3.449189000	-1.674407000
H	-1.023541000	-3.819045000	-2.536310000
C	0.133895000	-4.319604000	-0.770974000
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C	0.819629000	-3.787924000	0.319224000
H	1.307467000	-4.435183000	1.041662000
C	0.878913000	-2.404135000	0.476212000
C	2.524107000	0.404356000	-2.180794000
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C	3.824750000	0.383187000	-2.675325000
H	3.992081000	0.419302000	-3.746285000
C	4.887713000	0.311340000	-1.774880000
H	5.912965000	0.285514000	-2.130916000
C	4.617696000	0.269477000	-0.404848000
H	5.422594000	0.213072000	0.321270000
C	3.294732000	0.305991000	0.023699000

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C	-2.470142000	0.110405000	0.958566000
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C	-2.947390000	-0.430420000	3.278152000
H	-3.652322000	-0.684311000	4.063816000
C	-1.586726000	-0.291052000	3.559751000
H	-1.203611000	-0.430439000	4.565414000
C	-0.720608000	0.032811000	2.525799000
C	1.617974000	-1.769278000	1.629537000
H	1.220129000	-2.148899000	2.576882000
H	2.670146000	-2.070943000	1.595116000
C	2.885896000	0.346894000	1.478148000
H	2.813808000	1.390006000	1.801988000
H	3.625053000	-0.143399000	2.122222000
C	0.754166000	0.245990000	2.777600000
H	0.954970000	1.318470000	2.860856000
H	1.068843000	-0.222332000	3.717410000
C	0.674889000	3.470851000	0.476266000
N	0.656166000	2.315919000	0.412748000
C	0.692176000	4.925976000	0.547896000
H	-0.048501000	5.274417000	1.275103000
H	1.684371000	5.277097000	0.849545000
H	0.451261000	5.342750000	-0.435950000
C	-3.009977000	0.368133000	-0.400743000
C	-2.888368000	1.632448000	-1.000611000
C	-3.766591000	-0.627126000	-1.041143000
C	-3.497860000	1.887735000	-2.228362000
H	-2.344207000	2.420886000	-0.490441000
C	-4.358974000	-0.372759000	-2.278553000
H	-3.889642000	-1.599927000	-0.571776000
C	-4.226341000	0.885239000	-2.872627000
H	-3.415017000	2.872930000	-2.677210000
H	-4.937780000	-1.149424000	-2.769242000
H	-4.703177000	1.088097000	-3.826732000
O	-0.298809000	0.739317000	-1.456270000

⁵¹-ts1

Fe	0.383288000	0.052488000	-0.255384000
N	1.802178000	1.745372000	-0.788005000
N	1.374060000	0.498608000	1.671263000
N	2.248030000	-1.032157000	-0.662562000
N	-0.949639000	1.848689000	-0.451975000
C	1.335664000	-0.327591000	2.734577000
H	0.621945000	-1.142137000	2.669390000
C	2.160314000	-0.157098000	3.841056000
H	2.094551000	-0.842420000	4.679220000
C	3.071830000	0.900297000	3.836993000
H	3.737311000	1.060357000	4.679781000
C	3.122875000	1.746712000	2.728996000
H	3.824040000	2.574711000	2.693399000
C	2.255114000	1.518760000	1.662154000
C	2.462297000	-2.333229000	-0.388730000
H	1.584993000	-2.913472000	-0.129737000
C	3.725780000	-2.911824000	-0.467715000
H	3.851755000	-3.965810000	-0.244858000
C	4.807406000	-2.112012000	-0.834374000
H	5.808575000	-2.527341000	-0.897804000

C	4.583520000	-0.765767000	-1.127402000
H	5.401166000	-0.119285000	-1.431147000
C	3.288205000	-0.259716000	-1.041973000
C	-2.257443000	1.944309000	-0.092024000
C	-3.011641000	3.082632000	-0.415334000
H	-4.040138000	3.157740000	-0.082928000
C	-2.420809000	4.129829000	-1.114495000
H	-2.990462000	5.022429000	-1.353867000
C	-1.084405000	4.017913000	-1.487969000
H	-0.586885000	4.812433000	-2.034998000
C	-0.387069000	2.857685000	-1.152050000
C	2.189102000	2.442593000	0.468756000
H	1.425798000	3.201408000	0.675774000
H	3.138580000	2.977216000	0.338137000
C	2.968204000	1.151030000	-1.492990000
H	2.719941000	1.103106000	-2.558898000
H	3.853022000	1.793887000	-1.403118000
C	1.026720000	2.656341000	-1.659545000
H	0.965431000	2.198079000	-2.651569000
H	1.527598000	3.626588000	-1.779962000
C	-0.627041000	-0.873588000	-3.229367000
N	-0.097128000	-0.234297000	-2.420003000
C	-1.308809000	-1.687220000	-4.222035000
H	-1.518125000	-1.098158000	-5.120450000
H	-0.685077000	-2.546846000	-4.486579000
H	-2.249013000	-2.045932000	-3.789348000
S	-1.632591000	-2.406015000	-0.215742000
O	-0.523885000	-2.977459000	-1.013758000
O	-2.866056000	-2.003507000	-0.902960000
C	-2.036671000	-3.645458000	1.027128000
C	-2.891496000	0.851900000	0.674677000
C	-4.230944000	0.529212000	0.461168000
C	-2.165501000	0.143914000	1.689768000
C	-4.880067000	-0.404884000	1.276431000
H	-4.783362000	0.997062000	-0.346818000
C	-2.869017000	-0.745371000	2.557189000
H	-1.248087000	0.583075000	2.060623000
C	-4.205524000	-1.024369000	2.345011000
H	-5.923712000	-0.639143000	1.090063000
H	-2.334061000	-1.195551000	3.387899000
H	-4.740351000	-1.702066000	3.003358000
N	-0.886366000	-1.119125000	0.544746000
H	-2.361132000	-4.528189000	0.469705000
H	-1.138197000	-3.873793000	1.602589000
H	-2.842106000	-3.288314000	1.666089000

³¹-ts1

Fe	0.458735000	0.172021000	-0.243558000
N	1.731640000	1.701068000	-0.822524000
N	1.204657000	0.592650000	1.597195000
N	2.125897000	-0.951383000	-0.422162000
N	-0.941726000	1.745687000	-0.418938000
C	1.100779000	-0.210150000	2.676909000
H	0.431166000	-1.054761000	2.570187000
C	1.814508000	0.014241000	3.847544000
H	1.688459000	-0.654962000	4.691726000
C	2.694591000	1.096070000	3.902821000

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H	3.271759000	1.297794000	4.799800000	⁵¹-ts1a			
C	2.834909000	1.903297000	2.775592000	Fe	0.504317000	0.114427000	0.254352000
H	3.524835000	2.741319000	2.771551000	N	1.268776000	-0.825832000	1.912237000
C	2.076770000	1.621656000	1.640392000	N	0.453808000	-1.892570000	-0.498708000
C	2.302606000	-2.206185000	0.030590000	N	2.528380000	0.109338000	-0.347231000
H	1.431680000	-2.690178000	0.444883000	N	-1.322965000	-0.120449000	1.518969000
C	3.526762000	-2.861568000	-0.055066000	C	0.267169000	-2.278540000	-1.773366000
H	3.616669000	-3.877433000	0.313709000	H	-0.035156000	-1.500213000	-2.464483000
C	4.613068000	-2.193256000	-0.616349000	C	0.455905000	-3.594017000	-2.183470000
H	5.582817000	-2.675029000	-0.693402000	H	0.288629000	-3.868974000	-3.219209000
C	4.434497000	-0.888118000	-1.075914000	C	0.870678000	-4.536108000	-1.240828000
H	5.257038000	-0.333982000	-1.517215000	H	1.036529000	-5.569676000	-1.528808000
C	3.178105000	-0.298647000	-0.969041000	C	1.077196000	-4.132688000	0.079481000
C	-2.254724000	1.788701000	-0.055247000	H	1.402552000	-4.841703000	0.834377000
C	-3.050902000	2.904431000	-0.375748000	C	0.852050000	-2.799931000	0.415897000
H	-4.076209000	2.936890000	-0.028663000	C	3.021615000	0.392840000	-1.566704000
C	-2.519804000	3.970330000	-1.084459000	H	2.327174000	0.828114000	-2.272084000
H	-3.126940000	4.840232000	-1.314433000	C	4.356529000	0.170928000	-1.891946000
C	-1.187598000	3.900861000	-1.489242000	H	4.717796000	0.423085000	-2.882962000
H	-0.730055000	4.702349000	-2.060226000	C	5.203022000	-0.374392000	-0.927517000
C	-0.445851000	2.773412000	-1.156573000	H	6.247533000	-0.566958000	-1.152544000
C	2.139600000	2.467192000	0.399935000	C	4.690541000	-0.668458000	0.338159000
H	1.441384000	3.302798000	0.517112000	H	5.325668000	-1.085245000	1.113551000
H	3.135715000	2.902286000	0.261556000	C	3.349055000	-0.405390000	0.597010000
C	2.886516000	1.071808000	-1.527369000	C	-2.663146000	-0.053326000	1.258364000
H	2.608949000	0.963700000	-2.580989000	C	-3.561944000	0.275865000	2.286785000
H	3.772170000	1.716722000	-1.491679000	H	-4.608605000	0.418170000	2.048378000
C	0.946905000	2.598246000	-1.709233000	C	-3.120426000	0.417631000	3.595853000
H	0.878164000	2.127215000	-2.693329000	H	-3.818527000	0.666358000	4.389132000
H	1.449505000	3.564428000	-1.841940000	C	-1.773452000	0.201051000	3.873332000
C	-0.398018000	-0.692272000	-3.125974000	H	-1.393233000	0.237591000	4.889394000
N	0.014730000	-0.231153000	-2.149083000	C	-0.911191000	-0.043957000	2.810063000
C	-0.953217000	-1.322211000	-4.312315000	C	0.946767000	-2.294696000	1.833397000
H	-1.078422000	-0.593885000	-5.119302000	H	-0.027245000	-2.440015000	2.311094000
H	-0.292482000	-2.129016000	-4.644875000	H	1.679336000	-2.864256000	2.415528000
H	-1.927269000	-1.745479000	-4.042641000	C	2.746268000	-0.566751000	1.970738000
S	-1.402381000	-2.371709000	-0.470806000	H	2.891113000	0.371639000	2.515411000
O	-0.272197000	-2.951704000	-1.219829000	H	3.249916000	-1.353084000	2.543412000
O	-2.597009000	-1.941712000	-1.212953000	C	0.566341000	-0.222042000	3.086595000
C	-1.877188000	-3.622971000	0.735936000	H	1.020359000	0.750248000	3.284469000
C	-2.850339000	0.676722000	0.697944000	H	0.716737000	-0.845475000	3.977607000
C	-4.197823000	0.355600000	0.558912000	C	0.875262000	3.220440000	1.293386000
C	-2.034085000	-0.086337000	1.612326000	N	0.842017000	2.063381000	1.232625000
C	-4.794127000	-0.617062000	1.372645000	C	0.898669000	4.672281000	1.333712000
H	-4.805480000	0.856452000	-0.187392000	H	0.927915000	5.030354000	2.367401000
C	-2.695286000	-1.002220000	2.503403000	H	1.777687000	5.037727000	0.793018000
H	-1.173814000	0.429681000	2.016154000	H	-0.005138000	5.040376000	0.836389000
C	-4.042713000	-1.268969000	2.371380000	S	-0.242880000	2.496941000	-1.724302000
H	-5.847434000	-0.846909000	1.248900000	O	1.180848000	2.861521000	-1.762373000
H	-2.116849000	-1.473550000	3.292711000	O	-1.172227000	3.306516000	-0.927488000
H	-4.532845000	-1.962868000	3.048066000	C	-0.874070000	2.414602000	-3.407481000
N	-0.780007000	-1.044778000	0.400613000	C	-3.226065000	-0.419055000	-0.067834000
H	-2.099613000	-4.512017000	0.139312000	C	-4.472177000	-1.091035000	-0.115250000
H	-1.034808000	-3.824495000	1.400206000	C	-2.641861000	-0.181563000	-1.307452000
H	-2.757443000	-3.305415000	1.289376000	C	-5.059327000	-1.453418000	-1.325465000
				H	-4.970245000	-1.357441000	0.812024000
				C	-3.183917000	-0.519890000	-2.530709000

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H	-1.386693000	0.443823000	-1.298645000
C	-4.428238000	-1.167877000	-2.536760000
H	-6.014666000	-1.968632000	-1.319641000
H	-2.676932000	-0.296855000	-3.465173000
H	-4.887589000	-1.446701000	-3.480568000
N	-0.294607000	0.872298000	-1.211631000
H	-0.807143000	3.433396000	-3.799522000
H	-0.251166000	1.741060000	-3.998227000
H	-1.917121000	2.094636000	-3.386522000

³¹-ts1a

Fe	-0.559249000	-0.029018000	0.263831000
N	-1.282600000	0.964267000	1.896180000
N	-0.194878000	1.794166000	-0.437854000
N	-2.412280000	0.187767000	-0.436974000
N	1.174107000	-0.019192000	1.526644000
C	0.117156000	2.093942000	-1.713504000
H	0.280143000	1.249676000	-2.369929000
C	0.212069000	3.405405000	-2.163438000
H	0.473121000	3.600813000	-3.197718000
C	-0.044478000	4.445365000	-1.269631000
H	0.013829000	5.480562000	-1.591175000
C	-0.393560000	4.133786000	0.043991000
H	-0.614732000	4.915878000	0.763500000
C	-0.459044000	2.796749000	0.428020000
C	-2.818072000	-0.064540000	-1.695727000
H	-2.090762000	-0.524391000	-2.348478000
C	-4.110829000	0.223064000	-2.121529000
H	-4.400868000	-0.006741000	-3.140903000
C	-5.006335000	0.802034000	-1.223959000
H	-6.019110000	1.045321000	-1.529865000
C	-4.581708000	1.065032000	0.079284000
H	-5.253156000	1.510935000	0.806409000
C	-3.279555000	0.737595000	0.444490000
C	2.509913000	-0.185809000	1.286910000
C	3.361627000	-0.610839000	2.322046000
H	4.396483000	-0.829849000	2.090390000
C	2.894118000	-0.747232000	3.621203000
H	3.556658000	-1.073793000	4.416642000
C	1.568137000	-0.415704000	3.883846000
H	1.169753000	-0.432047000	4.893481000
C	0.746115000	-0.076578000	2.816030000
C	-0.773562000	2.375414000	1.838500000
H	0.147146000	2.423811000	2.428253000
H	-1.489976000	3.057191000	2.309361000
C	-2.776204000	0.882511000	1.859408000
H	-3.074638000	-0.007828000	2.422131000
H	-3.228469000	1.744594000	2.361578000
C	-0.704668000	0.261982000	3.077494000
H	-1.279935000	-0.649614000	3.247398000
H	-0.796964000	0.880641000	3.979637000
C	-1.371424000	-2.894953000	1.238816000
N	-1.138726000	-1.776199000	1.058828000
C	-1.630556000	-4.313727000	1.413122000
H	-1.795047000	-4.554755000	2.467772000
H	-2.511354000	-4.597468000	0.828106000
H	-0.759928000	-4.861558000	1.036190000

S	0.050221000	-2.549224000	-1.635228000
O	-1.390365000	-2.787829000	-1.816292000
O	0.807586000	-3.410791000	-0.716679000
C	0.855195000	-2.604948000	-3.243200000
C	3.146999000	0.162913000	-0.011453000
C	4.422312000	0.779000000	0.006759000
C	2.619085000	-0.065725000	-1.275579000
C	5.090366000	1.098214000	-1.173522000
H	4.881404000	1.030519000	0.958113000
C	3.245496000	0.227978000	-2.470916000
H	1.327870000	-0.587180000	-1.285947000
C	4.516178000	0.818804000	-2.414823000
H	6.066163000	1.570774000	-1.121319000
H	2.783004000	0.011420000	-3.429913000
H	5.041728000	1.059186000	-3.334408000
N	0.202786000	-0.920077000	-1.169272000
H	0.726615000	-3.629352000	-3.603512000
H	0.365454000	-1.904522000	-3.921993000
H	1.917239000	-2.384740000	-3.124691000

⁵²-ts1

Fe	0.182292000	0.253153000	-0.220454000
N	1.222764000	0.483779000	1.734317000
N	1.149605000	-1.689806000	0.014081000
N	2.079868000	0.905353000	-0.901783000
N	-1.477441000	0.073049000	1.214696000
C	1.238978000	-2.593678000	-0.980352000
H	0.654992000	-2.375052000	-1.867891000
C	2.036116000	-3.728455000	-0.878614000
H	2.078912000	-4.437602000	-1.698211000
C	2.777464000	-3.921587000	0.289015000
H	3.416363000	-4.792357000	0.400065000
C	2.692477000	-2.977090000	1.312973000
H	3.257854000	-3.099262000	2.231715000
C	1.860503000	-1.871708000	1.142772000
C	2.491745000	0.863770000	-2.183483000
H	1.740612000	0.589595000	-2.916908000
C	3.803019000	1.153035000	-2.545499000
H	4.098359000	1.115477000	-3.588417000
C	4.716238000	1.479015000	-1.541471000
H	5.750491000	1.700369000	-1.786726000
C	4.286476000	1.515580000	-0.213311000
H	4.975387000	1.768383000	0.586699000
C	2.953475000	1.231577000	0.075461000
C	-2.754475000	-0.313517000	0.948592000
C	-3.715367000	-0.345828000	1.969720000
H	-4.721032000	-0.679873000	1.740640000
C	-3.365005000	0.020371000	3.265024000
H	-4.096174000	-0.023663000	4.066402000
C	-2.061600000	0.447769000	3.517754000
H	-1.757166000	0.758815000	4.512020000
C	-1.151973000	0.479197000	2.464356000
C	1.627974000	-0.861147000	2.241717000
H	0.811337000	-1.235308000	2.869905000
H	2.509158000	-0.776266000	2.889364000
C	2.389834000	1.375847000	1.477252000
H	2.046316000	2.409927000	1.589890000

Supporting Information

H	3.177148000	1.221170000	2.225241000
C	0.224818000	1.090490000	2.651598000
H	0.154150000	2.155910000	2.410390000
H	0.541152000	1.014547000	3.699934000
C	-0.738743000	3.493097000	-0.660056000
N	-0.361905000	2.462023000	-0.289664000
C	-1.211743000	4.789633000	-1.127810000
H	-0.368494000	5.479025000	-1.237895000
H	-1.705412000	4.672865000	-2.098208000
H	-1.925752000	5.209769000	-0.412210000
C	-3.154837000	-0.644187000	-0.444018000
C	-4.276596000	-0.025509000	-0.993607000
C	-2.428872000	-1.573069000	-1.240713000
C	-4.674657000	-0.305614000	-2.310695000
H	-4.842164000	0.693522000	-0.408241000
C	-2.849192000	-1.859098000	-2.558495000
H	-1.683253000	-2.203695000	-0.772805000
C	-3.957156000	-1.216254000	-3.095923000
H	-5.550071000	0.190314000	-2.718981000
H	-2.303358000	-2.593847000	-3.141652000
H	-4.278305000	-1.432185000	-4.109788000
O	-0.695534000	-0.221148000	-1.578394000

³²-ts1

Fe	-0.205050000	-0.222501000	-0.143696000
N	-1.219381000	-1.195784000	1.401928000
N	-1.010176000	1.404852000	0.724341000
N	-1.948864000	-0.381915000	-1.098819000
N	1.389759000	-0.513080000	1.087050000
C	-1.069365000	2.617695000	0.134499000
H	-0.543267000	2.707970000	-0.806869000
C	-1.781548000	3.677078000	0.682380000
H	-1.790905000	4.636163000	0.176059000
C	-2.484723000	3.474966000	1.871012000
H	-3.053922000	4.280718000	2.323938000
C	-2.463131000	2.210017000	2.455101000
H	-3.018944000	2.004896000	3.364701000
C	-1.718353000	1.197335000	1.853263000
C	-2.264904000	0.226654000	-2.255257000
H	-1.468084000	0.803985000	-2.711716000
C	-3.530909000	0.111334000	-2.821053000
H	-3.751249000	0.611503000	-3.757867000
C	-4.496082000	-0.647551000	-2.158005000
H	-5.496752000	-0.747992000	-2.566910000
C	-4.160708000	-1.280283000	-0.959224000
H	-4.889120000	-1.882061000	-0.424614000
C	-2.869547000	-1.136788000	-0.457407000
C	2.654511000	-0.040020000	0.928992000
C	3.659285000	-0.384669000	1.850154000
H	4.649006000	0.041816000	1.734351000
C	3.373244000	-1.238342000	2.906596000
H	4.138190000	-1.489932000	3.634657000
C	2.090748000	-1.783445000	3.007892000
H	1.841545000	-2.490308000	3.792666000
C	1.135092000	-1.417300000	2.068148000
C	-1.619701000	-0.185262000	2.433099000
H	-0.852602000	-0.180024000	3.214942000

H	-2.558242000	-0.482685000	2.914173000
C	-2.385185000	-1.883043000	0.772164000
H	-2.053210000	-2.879599000	0.460927000
H	-3.199399000	-2.029669000	1.491206000
C	-0.210148000	-2.113617000	1.997594000
H	-0.115485000	-2.983938000	1.341199000
H	-0.526222000	-2.477789000	2.982786000
C	0.715416000	-2.779396000	-1.777899000
N	0.346100000	-1.939738000	-1.073400000
C	1.185426000	-3.825237000	-2.677294000
H	1.937488000	-4.443636000	-2.176973000
H	0.348792000	-4.459211000	-2.988115000
H	1.633525000	-3.366938000	-3.565357000
C	2.963881000	0.773253000	-0.258631000
C	4.136642000	0.547367000	-0.974480000
C	2.018315000	1.750738000	-0.736299000
C	4.427242000	1.290383000	-2.128196000
H	4.831310000	-0.222526000	-0.651491000
C	2.384258000	2.551285000	-1.870203000
H	1.393527000	2.218519000	0.015698000
C	3.546275000	2.297216000	-2.568792000
H	5.344308000	1.094437000	-2.674689000
H	1.722580000	3.354885000	-2.178530000
H	3.800847000	2.892059000	-3.440443000
O	0.586166000	0.698979000	-1.370533000

⁵²-ts1a

Fe	-0.416932000	-0.304989000	-0.235620000
N	-1.272546000	-0.621995000	1.606966000
N	-0.439376000	1.738421000	0.459393000
N	-2.337420000	-0.071906000	-0.848949000
N	1.340849000	-0.910832000	0.794171000
C	-0.208188000	2.835508000	-0.283046000
H	0.173654000	2.660154000	-1.282889000
C	-0.449526000	4.115705000	0.205943000
H	-0.245579000	4.981198000	-0.415095000
C	-0.963883000	4.254085000	1.496526000
H	-1.173304000	5.238433000	1.903896000
C	-1.210875000	3.111375000	2.261179000
H	-1.608964000	3.189399000	3.268137000
C	-0.926906000	1.865498000	1.708227000
C	-2.719791000	0.380310000	-2.057081000
H	-1.920420000	0.526881000	-2.775640000
C	-4.055079000	0.639475000	-2.346337000
H	-4.335064000	0.998967000	-3.330503000
C	-5.010040000	0.435766000	-1.348417000
H	-6.059143000	0.639503000	-1.540071000
C	-4.605380000	-0.033293000	-0.096126000
H	-5.329049000	-0.204829000	0.694547000
C	-3.254606000	-0.287682000	0.121426000
C	2.677928000	-0.756007000	0.548210000
C	3.615957000	-1.477079000	1.310969000
H	4.664614000	-1.413225000	1.050603000
C	3.213990000	-2.271908000	2.372881000
H	3.944815000	-2.819330000	2.960045000
C	1.856427000	-2.339277000	2.680129000
H	1.498448000	-2.914934000	3.527543000

Supporting Information

C	0.956627000	-1.667789000	1.863848000
C	-1.040130000	0.576787000	2.487653000
H	-0.092585000	0.414374000	3.012149000
H	-1.822542000	0.633718000	3.251902000
C	-2.732547000	-0.909344000	1.397736000
H	-2.849002000	-1.995345000	1.320135000
H	-3.317265000	-0.587142000	2.265675000
C	-0.526342000	-1.800707000	2.142788000
H	-0.909771000	-2.692552000	1.642403000
H	-0.705107000	-1.918430000	3.218563000
C	-0.692825000	-3.512739000	-1.498044000
N	-0.706026000	-2.589845000	-0.796533000
C	-0.674610000	-4.670994000	-2.382538000
H	-0.274795000	-4.381843000	-3.360053000
H	-0.043129000	-5.457952000	-1.957946000
H	-1.689584000	-5.059754000	-2.513260000
C	3.202632000	0.178533000	-0.478952000
C	4.448867000	0.819869000	-0.264853000
C	2.598831000	0.469679000	-1.696288000
C	5.013387000	1.646707000	-1.232577000
H	4.965647000	0.687571000	0.680878000
C	3.118483000	1.270622000	-2.690526000
H	1.244386000	0.072752000	-1.886706000
C	4.366502000	1.865687000	-2.451102000
H	5.967211000	2.124399000	-1.032122000
H	2.591794000	1.434468000	-3.626110000
H	4.816035000	2.499795000	-3.209735000
O	0.157141000	0.004227000	-1.859418000

³²-ts1a

Fe	-0.513268000	0.284817000	0.288749000
N	-1.343756000	0.841010000	-1.501725000
N	-0.209186000	-1.437534000	-0.616472000
N	-2.356825000	-0.320332000	0.716926000
N	1.198848000	1.146811000	-0.581704000
C	0.206380000	-2.559530000	0.005454000
H	0.459627000	-2.453307000	1.051536000
C	0.295899000	-3.775517000	-0.660882000
H	0.640718000	-4.654099000	-0.126788000
C	-0.072411000	-3.839191000	-2.005318000
H	-0.021578000	-4.776711000	-2.550203000
C	-0.517683000	-2.679676000	-2.639199000
H	-0.819905000	-2.693386000	-3.681726000
C	-0.571046000	-1.490995000	-1.915789000
C	-2.697931000	-1.068749000	1.780971000
H	-1.896084000	-1.281488000	2.478784000
C	-3.999204000	-1.526979000	1.962207000
H	-4.242553000	-2.124158000	2.834255000
C	-4.964907000	-1.209994000	1.006316000
H	-5.986059000	-1.562338000	1.114407000
C	-4.603579000	-0.431116000	-0.095099000
H	-5.333651000	-0.162917000	-0.852383000
C	-3.287468000	0.008106000	-0.206395000
C	2.537315000	1.020328000	-0.341223000
C	3.444057000	1.924104000	-0.928975000
H	4.490557000	1.865427000	-0.658635000
C	3.014104000	2.885793000	-1.829072000

H	3.719955000	3.575123000	-2.281831000
C	1.659946000	2.932517000	-2.152643000
H	1.278629000	3.635373000	-2.886491000
C	0.790998000	2.068178000	-1.500023000
C	-0.973476000	-0.179854000	-2.538494000
H	-0.123873000	0.209523000	-3.109258000
H	-1.795540000	-0.314245000	-3.249439000
C	-2.821803000	0.949974000	-1.294865000
H	-3.038527000	1.976344000	-0.980332000
H	-3.364953000	0.782821000	-2.231312000
C	-0.691845000	2.147094000	-1.802806000
H	-1.160845000	2.908870000	-1.175733000
H	-0.854332000	2.437353000	-2.848227000
C	-1.117948000	2.948406000	1.903328000
N	-0.962308000	2.072531000	1.164063000
C	-1.304093000	4.040851000	2.848595000
H	-0.795151000	4.941234000	2.489714000
H	-2.370561000	4.255293000	2.971767000
H	-0.882905000	3.755787000	3.818751000
C	3.111278000	-0.063116000	0.499625000
C	4.383333000	-0.595012000	0.170073000
C	2.537696000	-0.590898000	1.648504000
C	5.000973000	-1.546498000	0.978311000
H	4.880229000	-0.272647000	-0.740112000
C	3.112004000	-1.519322000	2.491203000
H	1.145333000	-0.307523000	1.881543000
C	4.383914000	-2.001048000	2.146387000
H	5.974531000	-1.933543000	0.694384000
H	2.609372000	-1.864082000	3.390382000
H	4.876452000	-2.729219000	2.784327000
O	0.067709000	-0.227907000	1.863298000

⁵¹-Int1b

Fe	0.449104000	-0.240080000	0.097835000
N	1.681678000	-0.907762000	-1.700300000
N	1.325181000	1.711216000	-0.734838000
N	2.408983000	-0.456726000	0.988108000
N	-1.083485000	-0.819281000	-1.558333000
C	1.453097000	2.857075000	-0.045739000
H	0.882615000	2.917067000	0.876841000
C	2.266092000	3.905291000	-0.470606000
H	2.337081000	4.814383000	0.117148000
C	2.988213000	3.748466000	-1.653936000
H	3.639046000	4.539153000	-2.014522000
C	2.870234000	2.552813000	-2.365162000
H	3.424046000	2.396421000	-3.285747000
C	2.024593000	1.558072000	-1.875810000
C	2.700455000	-0.105202000	2.254535000
H	1.851465000	0.142465000	2.884788000
C	4.004100000	-0.077815000	2.738050000
H	4.197115000	0.206614000	3.766788000
C	5.043113000	-0.421215000	1.871060000
H	6.074698000	-0.402880000	2.209152000
C	4.738650000	-0.796361000	0.562946000
H	5.524485000	-1.082498000	-0.129739000
C	3.403854000	-0.813514000	0.155803000
C	-2.437371000	-0.675245000	-1.472670000

Supporting Information

C	-3.300724000	-1.598959000	-2.083701000
H	-4.373236000	-1.532909000	-1.955642000
C	-2.770477000	-2.627286000	-2.861389000
H	-3.426990000	-3.340474000	-3.349536000
C	-1.393668000	-2.710773000	-3.008192000
H	-0.942557000	-3.480185000	-3.627803000
C	-0.579282000	-1.802306000	-2.311059000
C	1.784138000	0.261490000	-2.615429000
H	0.831325000	0.343156000	-3.149930000
H	2.563929000	0.093485000	-3.370560000
C	3.018062000	-1.355035000	-1.212474000
H	2.999433000	-2.446967000	-1.131246000
H	3.797772000	-1.113869000	-1.945759000
C	0.926838000	-1.999836000	-2.348973000
H	1.136960000	-2.926338000	-1.807784000
H	1.252831000	-2.154085000	-3.388652000
C	-0.122477000	-3.241679000	1.454388000
N	0.201248000	-2.492824000	0.630524000
C	-0.536422000	-4.145921000	2.516868000
H	-1.334412000	-4.808141000	2.167496000
H	0.311041000	-4.751303000	2.853133000
H	-0.906499000	-3.542945000	3.352668000
S	-1.817742000	0.135746000	2.248266000
O	-0.755288000	-0.713884000	2.823033000
O	-3.116867000	-0.448371000	1.853860000
C	-2.153261000	1.407132000	3.488936000
C	-2.964150000	0.514162000	-0.787006000
C	-4.285470000	0.916157000	-0.974939000
C	-2.028045000	1.439524000	-0.039333000
C	-4.768648000	2.115377000	-0.449679000
H	-4.974377000	0.311014000	-1.550618000
C	-2.647338000	2.694413000	0.478652000
H	-1.356871000	1.815610000	-0.846576000
C	-3.952786000	3.023999000	0.270664000
H	-5.812136000	2.368873000	-0.620153000
H	-1.979289000	3.349952000	1.029629000
H	-4.373448000	3.950884000	0.646880000
N	-1.103131000	0.831588000	0.920044000
H	-2.502544000	0.875926000	4.377989000
H	-1.226386000	1.939105000	3.709479000
H	-2.931934000	2.086245000	3.139896000

³¹-Int1b

Fe	-0.564378000	0.164788000	0.101317000
N	-1.721613000	1.235775000	-1.496719000
N	-1.172793000	-1.415586000	-0.979152000
N	-2.508466000	0.138939000	0.951143000
N	1.024527000	1.200603000	-1.345001000
C	-1.200464000	-2.675099000	-0.497785000
H	-0.702023000	-2.817050000	0.454491000
C	-1.823026000	-3.719778000	-1.172779000
H	-1.821450000	-4.716513000	-0.744743000
C	-2.454133000	-3.453082000	-2.388315000
H	-2.956213000	-4.242877000	-2.938468000
C	-2.442416000	-2.147474000	-2.879806000
H	-2.933021000	-1.900506000	-3.815999000
C	-1.794071000	-1.151535000	-2.152125000

C	-2.798472000	-0.475766000	2.113707000
H	-1.949933000	-0.848290000	2.680553000
C	-4.104098000	-0.607637000	2.574212000
H	-4.299437000	-1.105121000	3.518027000
C	-5.141570000	-0.089136000	1.796433000
H	-6.174080000	-0.181700000	2.119045000
C	-4.834448000	0.560064000	0.601187000
H	-5.618482000	0.989062000	-0.015929000
C	-3.498080000	0.666540000	0.212770000
C	2.374430000	1.099535000	-1.207576000
C	3.216370000	2.191745000	-1.469791000
H	4.281851000	2.132377000	-1.287075000
C	2.666974000	3.379344000	-1.950500000
H	3.304698000	4.229611000	-2.170530000
C	1.294077000	3.450724000	-2.143714000
H	0.830212000	4.352427000	-2.533035000
C	0.502187000	2.344457000	-1.795032000
C	-1.696662000	0.274901000	-2.631865000
H	-0.741100000	0.400389000	-3.151844000
H	-2.490366000	0.499785000	-3.356754000
C	-3.105062000	1.488123000	-1.006245000
H	-3.178201000	2.543462000	-0.722022000
H	-3.834868000	1.338653000	-1.811939000
C	-1.011243000	2.479280000	-1.852771000
H	-1.293241000	3.249012000	-1.128099000
H	-1.315312000	2.851394000	-2.843365000
C	0.036198000	2.568431000	2.005761000
N	-0.193931000	1.778732000	1.192673000
C	0.354477000	3.491877000	3.084882000
H	1.132254000	4.195353000	2.772602000
H	-0.535904000	4.050692000	3.389131000
H	0.721750000	2.905351000	3.934209000
S	1.785546000	-0.576073000	2.190993000
O	0.704889000	-0.083581000	3.061722000
O	2.977000000	0.263317000	1.923020000
C	2.373966000	-2.087764000	2.998247000
C	2.924844000	-0.208569000	-0.826783000
C	4.252172000	-0.522730000	-1.112192000
C	2.006837000	-1.302257000	-0.324303000
C	4.760521000	-1.805968000	-0.906624000
H	4.919205000	0.221983000	-1.529103000
C	2.657420000	-2.632619000	-0.134291000
H	1.357282000	-1.486029000	-1.211283000
C	3.965511000	-2.877943000	-0.429676000
H	5.804651000	-1.992384000	-1.145942000
H	2.009275000	-3.417687000	0.243456000
H	4.403151000	-3.862447000	-0.299236000
N	1.054558000	-0.971727000	0.742465000
H	2.712403000	-1.772108000	3.988363000
H	1.540256000	-2.784950000	3.096617000
H	3.207179000	-2.530208000	2.452798000

⁵²-Int1b

Fe	-0.213646000	-0.279913000	-0.419589000
N	-1.147694000	-0.900059000	1.551694000
N	-0.841675000	1.703990000	0.477221000
N	-2.350136000	-0.390840000	-0.939272000

Supporting Information

N	1.545845000	-0.730999000	0.949867000	N	1.196882000	-1.127387000	-1.406545000
C	-0.958211000	2.863621000	-0.191834000	N	0.654541000	1.464747000	-0.594409000
H	-0.513044000	2.886082000	-1.183081000	N	2.466537000	-0.123558000	0.861574000
C	-1.617640000	3.973868000	0.328792000	N	-1.471564000	-0.957889000	-0.822064000
H	-1.681699000	4.891380000	-0.246426000	C	0.612087000	2.691433000	-0.034907000
C	-2.199922000	3.866129000	1.592222000	H	0.265708000	2.722314000	0.992857000
H	-2.732955000	4.704714000	2.029718000	C	1.007303000	3.838322000	-0.713338000
C	-2.095375000	2.658770000	2.284192000	H	0.954576000	4.803989000	-0.222156000
H	-2.542722000	2.541676000	3.266547000	C	1.484499000	3.711574000	-2.019156000
C	-1.401180000	1.600330000	1.697507000	H	1.810691000	4.583453000	-2.577582000
C	-2.888579000	0.069438000	-2.082951000	C	1.550953000	2.441850000	-2.590882000
H	-2.187134000	0.378950000	-2.852748000	H	1.930060000	2.306028000	-3.599006000
C	-4.262492000	0.151165000	-2.285550000	C	1.126121000	1.336221000	-1.853718000
H	-4.653054000	0.523715000	-3.226383000	C	3.017540000	0.556849000	1.882448000
C	-5.111365000	-0.248718000	-1.252395000	H	2.327008000	0.975230000	2.609417000
H	-6.189350000	-0.191227000	-1.368212000	C	4.392822000	0.722433000	2.015794000
C	-4.555144000	-0.724188000	-0.064801000	H	4.794944000	1.273601000	2.859035000
H	-5.189412000	-1.046704000	0.755359000	C	5.226950000	0.171685000	1.041789000
C	-3.166734000	-0.790601000	0.054484000	H	6.304464000	0.288059000	1.105435000
C	2.855321000	-0.443615000	0.722240000	C	4.655656000	-0.533185000	-0.017894000
C	3.867485000	-1.103294000	1.442493000	H	5.277054000	-0.978846000	-0.788848000
H	4.912897000	-0.933531000	1.220152000	C	3.268447000	-0.669851000	-0.070138000
C	3.525544000	-2.009497000	2.442703000	C	-2.782936000	-0.693935000	-0.596815000
H	4.299765000	-2.517291000	3.009118000	C	-3.784479000	-1.519940000	-1.136295000
C	2.181361000	-2.243291000	2.706480000	H	-4.829335000	-1.353803000	-0.906895000
H	1.875445000	-2.927529000	3.492014000	C	-3.427965000	-2.587707000	-1.957444000
C	1.219587000	-1.597679000	1.919972000	H	-4.193094000	-3.227508000	-2.385737000
C	-1.166648000	0.297733000	2.435951000	C	-2.082449000	-2.814348000	-2.220124000
H	-0.186012000	0.363696000	2.920087000	H	-1.766618000	-3.627393000	-2.866930000
H	-1.906962000	0.171541000	3.237090000	C	-1.132949000	-1.983273000	-1.611966000
C	-2.512071000	-1.421389000	1.271924000	C	1.112271000	-0.056557000	-2.440197000
H	-2.423712000	-2.495648000	1.075215000	H	0.166984000	-0.183654000	-2.979031000
H	-3.162234000	-1.316615000	2.150264000	H	1.912355000	-0.168039000	-3.183334000
C	-0.251025000	-1.938904000	2.100396000	C	2.595887000	-1.535233000	-1.120524000
H	-0.442278000	-2.868276000	1.553464000	H	2.568747000	-2.560041000	-0.733366000
H	-0.458118000	-2.141470000	3.161307000	H	3.198092000	-1.562636000	-2.038259000
C	0.045285000	-3.345027000	-1.908839000	C	0.348562000	-2.278207000	-1.779072000
N	-0.068680000	-2.417363000	-1.223599000	H	0.602484000	-3.110980000	-1.114784000
C	0.187796000	-4.509395000	-2.775482000	H	0.549904000	-2.617159000	-2.805992000
H	0.805670000	-5.270084000	-2.288095000	C	0.114849000	-2.721132000	2.299642000
H	-0.796101000	-4.936124000	-2.994657000	N	0.199895000	-1.857954000	1.532623000
H	0.663671000	-4.214146000	-3.716188000	C	0.006093000	-3.797566000	3.277717000
C	3.211002000	0.565932000	-0.297171000	H	-0.573230000	-4.629155000	2.864083000
C	4.478835000	1.154597000	-0.290807000	H	1.002260000	-4.159354000	3.551794000
C	2.210925000	1.096099000	-1.291608000	H	-0.496828000	-3.428384000	4.177473000
C	4.892040000	2.058929000	-1.274283000	C	-3.151577000	0.464795000	0.244502000
H	5.189887000	0.905551000	0.487710000	C	-4.433188000	1.014933000	0.153238000
C	2.761528000	1.980653000	-2.349694000	C	-2.159773000	1.151433000	1.145735000
H	1.961236000	2.014129000	-0.617890000	C	-4.870481000	2.045628000	0.991222000
C	4.039552000	2.479335000	-2.311858000	H	-5.135150000	0.629812000	-0.577323000
H	5.902190000	2.455991000	-1.221077000	C	-2.731478000	2.182431000	2.048927000
H	2.048076000	2.273517000	-3.114743000	H	-1.961764000	1.982216000	0.339897000
H	4.394295000	3.167981000	-3.071807000	C	-4.024207000	2.636660000	1.945223000
O	1.107949000	0.419796000	-1.623913000	H	-5.889726000	2.406479000	0.884125000
				H	-2.024828000	2.614093000	2.752138000
				H	-4.389970000	3.427345000	2.592368000
				O	-1.039015000	0.573338000	1.560586000

³²-Int1b

Fe	0.344306000	-0.208844000	0.433272000
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Supporting Information

⁵1-ts2

Fe	0.429442000	-0.295972000	0.040572000
N	1.596832000	-0.525217000	-1.919434000
N	1.133357000	1.822324000	-0.434401000
N	2.494262000	-0.533169000	0.748777000
N	-1.131754000	-0.570356000	-1.663194000
C	1.214224000	2.833826000	0.445838000
H	0.725276000	2.667556000	1.402048000
C	1.888343000	4.021645000	0.174567000
H	1.926098000	4.811334000	0.917511000
C	2.521262000	4.157077000	-1.061649000
H	3.066345000	5.062928000	-1.308832000
C	2.452604000	3.103623000	-1.974234000
H	2.940015000	3.174227000	-2.941757000
C	1.744824000	1.952280000	-1.627543000
C	2.868431000	-0.398705000	2.036034000
H	2.060829000	-0.350207000	2.758551000
C	4.203271000	-0.349356000	2.424298000
H	4.459569000	-0.246117000	3.473215000
C	5.189136000	-0.433961000	1.440240000
H	6.241460000	-0.389342000	1.703857000
C	4.802456000	-0.585541000	0.109391000
H	5.544660000	-0.670725000	-0.678721000
C	3.442804000	-0.642868000	-0.199574000
C	-2.475516000	-0.450030000	-1.532624000
C	-3.356459000	-1.252176000	-2.269745000
H	-4.425226000	-1.205120000	-2.096935000
C	-2.842337000	-2.128559000	-3.224874000
H	-3.508682000	-2.754283000	-3.810301000
C	-1.468141000	-2.173176000	-3.422544000
H	-1.031751000	-2.818272000	-4.179184000
C	-0.643167000	-1.396081000	-2.600077000
C	1.563910000	0.800210000	-2.592336000
H	0.582189000	0.905124000	-3.066072000
H	2.314539000	0.846070000	-3.392918000
C	2.987565000	-0.958635000	-1.613567000
H	3.037220000	-2.046460000	-1.732767000
H	3.693978000	-0.538366000	-2.340555000
C	0.864370000	-1.532650000	-2.714921000
H	1.132273000	-2.521753000	-2.333038000
H	1.159172000	-1.505377000	-3.774968000
C	-0.005638000	-3.527872000	0.815400000
N	0.234568000	-2.574837000	0.201282000
C	-0.313704000	-4.701367000	1.620184000
H	0.575145000	-5.330912000	1.727257000
H	-0.641445000	-4.370099000	2.611165000
H	-1.113476000	-5.284891000	1.154153000
S	-1.474694000	-0.413542000	2.523454000
O	-0.176326000	-1.090077000	2.714788000
O	-2.713850000	-1.190761000	2.409181000
C	-1.664989000	0.699477000	3.937181000
C	-3.007156000	0.622635000	-0.659639000
C	-4.196139000	1.249769000	-1.022052000
C	-2.304285000	1.108156000	0.538426000
C	-4.786576000	2.281905000	-0.269487000
H	-4.697214000	0.937222000	-1.931521000
C	-2.946986000	2.215920000	1.261990000

H	-1.952872000	2.228750000	0.176984000
C	-4.158705000	2.787338000	0.858377000
H	-5.726253000	2.709011000	-0.606828000
H	-2.397430000	2.608996000	2.110267000
H	-4.581683000	3.610522000	1.424372000
N	-1.209628000	0.459331000	1.119315000
H	-1.625217000	0.056121000	4.820252000
H	-0.836173000	1.409815000	3.959307000
H	-2.634220000	1.199058000	3.904771000

³1-ts2

Fe	-0.542547000	0.217770000	0.091096000
N	-1.666669000	1.234596000	-1.569597000
N	-1.020934000	-1.393727000	-0.996074000
N	-2.537511000	0.103897000	0.832976000
N	1.042455000	1.189076000	-1.326968000
C	-0.981315000	-2.653445000	-0.515758000
H	-0.530714000	-2.760507000	0.465206000
C	-1.496632000	-3.739447000	-1.215046000
H	-1.445237000	-4.734096000	-0.785122000
C	-2.092997000	-3.514995000	-2.456784000
H	-2.514920000	-4.336781000	-3.027000000
C	-2.153601000	-2.210997000	-2.946445000
H	-2.623097000	-1.997270000	-3.901533000
C	-1.608769000	-1.170925000	-2.193761000
C	-2.879728000	-0.553031000	1.958080000
H	-2.055470000	-0.896722000	2.574934000
C	-4.207770000	-0.754930000	2.321258000
H	-4.443153000	-1.283752000	3.238569000
C	-5.212782000	-0.266194000	1.485565000
H	-6.259651000	-0.413948000	1.732562000
C	-4.853728000	0.426359000	0.329458000
H	-5.611377000	0.835551000	-0.332310000
C	-3.500824000	0.604194000	0.039783000
C	2.382689000	1.040125000	-1.216246000
C	3.265063000	2.080488000	-1.533543000
H	4.331138000	1.971082000	-1.371426000
C	2.753232000	3.271706000	-2.047654000
H	3.419514000	4.089062000	-2.305189000
C	1.380982000	3.387819000	-2.233902000
H	0.947655000	4.289771000	-2.655986000
C	0.556075000	2.329284000	-1.834578000
C	-1.595038000	0.256315000	-2.685791000
H	-0.652611000	0.423654000	-3.217628000
H	-2.404126000	0.423440000	-3.409396000
C	-3.061343000	1.481397000	-1.120404000
H	-3.126360000	2.520772000	-0.780513000
H	-3.765499000	1.386626000	-1.957078000
C	-0.953880000	2.480834000	-1.912481000
H	-1.249639000	3.248023000	-1.190707000
H	-1.240311000	2.853806000	-2.907759000
C	0.027447000	2.653003000	1.959015000
N	-0.239764000	1.850599000	1.169819000
C	0.407361000	3.604365000	2.992589000
H	-0.355236000	3.626707000	3.777461000
H	1.358585000	3.274867000	3.424506000
H	0.523734000	4.609032000	2.575000000

Supporting Information

S	1.460434000	-0.437710000	2.485294000
O	0.133513000	-0.269747000	3.098203000
O	2.435090000	0.666202000	2.533181000
C	2.231493000	-1.840251000	3.331568000
C	2.908926000	-0.292358000	-0.838546000
C	4.090900000	-0.730058000	-1.428549000
C	2.205856000	-1.202702000	0.083510000
C	4.673303000	-1.981915000	-1.154248000
H	4.590873000	-0.083737000	-2.142014000
C	2.847281000	-2.512429000	0.301497000
H	1.835800000	-2.082080000	-0.686607000
C	4.046292000	-2.888728000	-0.312865000
H	5.605160000	-2.248615000	-1.644054000
H	2.300270000	-3.200419000	0.936901000
H	4.462875000	-3.873088000	-0.126581000
N	1.121650000	-0.844243000	0.891990000
H	2.314679000	-1.521444000	4.373947000
H	1.581336000	-2.714760000	3.268090000
H	3.230680000	-2.037778000	2.940084000

⁵¹I-ts2a

26	0.480281000	-0.345168000	0.174856000
7	1.700899000	-0.984863000	-1.634540000
7	1.281805000	1.626022000	-0.639026000
7	2.535093000	-0.488326000	0.996070000
7	-1.043537000	-0.856617000	-1.541516000
6	1.380262000	2.787339000	0.031480000
1	0.862152000	2.830029000	0.985901000
6	2.106344000	3.877142000	-0.440188000
1	2.152385000	4.794708000	0.136625000
6	2.777698000	3.748191000	-1.656407000
1	3.362829000	4.570699000	-2.056223000
6	2.696146000	2.538857000	-2.347780000
1	3.215254000	2.403668000	-3.291642000
6	1.934615000	1.499806000	-1.812192000
6	2.893240000	-0.085311000	2.231587000
1	2.078247000	0.156603000	2.902946000
6	4.221323000	0.002569000	2.635646000
1	4.459869000	0.326233000	3.643076000
6	5.222580000	-0.329397000	1.722615000
1	6.270564000	-0.264793000	1.999011000
6	4.854723000	-0.751090000	0.445906000
1	5.606870000	-1.027996000	-0.286711000
6	3.500288000	-0.828084000	0.120420000
6	-2.383595000	-0.641201000	-1.557457000
6	-3.253301000	-1.521116000	-2.220361000
1	-4.325823000	-1.384547000	-2.153248000
6	-2.730828000	-2.580773000	-2.956963000
1	-3.391137000	-3.264516000	-3.481284000
6	-1.351333000	-2.732668000	-3.021003000
1	-0.900228000	-3.522272000	-3.614339000
6	-0.545637000	-1.865911000	-2.277057000
6	1.746418000	0.189444000	-2.546745000
1	0.790567000	0.233807000	-3.078414000
1	2.530253000	0.059499000	-3.304907000
6	3.060838000	-1.411405000	-1.208454000
1	3.054702000	-2.501458000	-1.098913000

1	3.801242000	-1.185550000	-1.986197000
6	0.951730000	-2.101353000	-2.246961000
1	1.135916000	-2.994859000	-1.642659000
1	1.312151000	-2.320586000	-3.263396000
6	-0.380038000	-3.267750000	1.547232000
7	0.040185000	-2.442784000	0.850579000
6	-0.923069000	-4.276938000	2.445444000
1	-1.271908000	-5.146089000	1.879374000
1	-0.155111000	-4.596101000	3.157062000
1	-1.764627000	-3.842794000	2.995947000
16	-1.455233000	0.181749000	2.605969000
8	-0.095228000	-0.309359000	2.898065000
8	-2.610413000	-0.716707000	2.673034000
6	-1.752230000	1.566078000	3.727342000
6	-2.945214000	0.580579000	-0.934704000
6	-4.053628000	1.177416000	-1.543496000
6	-2.406436000	1.233437000	0.240604000
6	-4.705563000	2.290576000	-1.002191000
1	-4.427522000	0.767053000	-2.474831000
6	-3.106628000	2.372593000	0.776747000
1	-1.335196000	1.819072000	0.114560000
6	-4.235985000	2.890039000	0.168877000
1	-5.571599000	2.699022000	-1.514038000
1	-2.681564000	2.873802000	1.638434000
1	-4.729095000	3.762796000	0.583992000
7	-1.252166000	0.686818000	0.980157000
1	-1.603371000	1.150701000	4.728263000
1	-1.019959000	2.354331000	3.542239000
1	-2.778677000	1.919724000	3.629860000

³¹I-ts2a

26	0.584763000	-0.298271000	0.121127000
7	1.723880000	-1.063308000	-1.655429000
7	1.232880000	1.449860000	-0.617419000
7	2.557355000	-0.452655000	0.939922000
7	-0.987545000	-0.855963000	-1.534816000
6	1.269836000	2.598183000	0.091724000
1	0.814688000	2.558277000	1.075604000
6	1.870675000	3.757894000	-0.384142000
1	1.872510000	4.655443000	0.224881000
6	2.480620000	3.728102000	-1.638839000
1	2.966984000	4.611356000	-2.041006000
6	2.473229000	2.535162000	-2.360347000
1	2.956250000	2.469829000	-3.330233000
6	1.841496000	1.412632000	-1.825226000
6	2.903533000	-0.022974000	2.169666000
1	2.084497000	0.274488000	2.814073000
6	4.226416000	0.017118000	2.598477000
1	4.458759000	0.364393000	3.599459000
6	5.229223000	-0.393266000	1.719685000
1	6.273157000	-0.367284000	2.016753000
6	4.868419000	-0.845330000	0.451234000
1	5.621384000	-1.185369000	-0.253594000
6	3.519176000	-0.871564000	0.097543000
6	-2.319148000	-0.607497000	-1.512201000
6	-3.234345000	-1.485772000	-2.112699000
1	-4.299787000	-1.312146000	-2.020015000

Supporting Information

6	-2.764776000	-2.590995000	-2.817926000
1	-3.459832000	-3.275675000	-3.293899000
6	-1.392468000	-2.789181000	-2.912095000
1	-0.982306000	-3.618605000	-3.480561000
6	-0.541288000	-1.911994000	-2.234102000
6	1.761669000	0.104294000	-2.573907000
1	0.836634000	0.103213000	-3.159099000
1	2.591693000	0.018202000	-3.287651000
6	3.077929000	-1.486181000	-1.218730000
1	3.064729000	-2.573133000	-1.082187000
1	3.822732000	-1.284740000	-1.999345000
6	0.952771000	-2.176483000	-2.239507000
1	1.142720000	-3.068207000	-1.634488000
1	1.285245000	-2.408824000	-3.262774000
6	-0.267858000	-2.978117000	1.476043000
7	0.097932000	-2.061709000	0.872056000
6	-0.763049000	-4.088288000	2.276573000
1	-1.018461000	-4.940852000	1.639820000
1	-0.003285000	-4.396116000	3.001924000
1	-1.658206000	-3.753290000	2.811693000
16	-1.424976000	0.151048000	2.617435000
8	-0.069531000	-0.160166000	3.095600000
8	-2.451828000	-0.896259000	2.540284000
6	-2.062669000	1.448819000	3.702240000
6	-2.823260000	0.649889000	-0.912566000
6	-3.904730000	1.279355000	-1.534696000
6	-2.260393000	1.290198000	0.260456000
6	-4.515668000	2.425540000	-1.012988000
1	-4.291889000	0.866255000	-2.459806000
6	-2.924576000	2.465197000	0.775301000
1	-1.192878000	1.872074000	0.156645000
6	-4.028336000	3.020448000	0.152474000
1	-5.361885000	2.861305000	-1.535377000
1	-2.481916000	2.962908000	1.630121000
1	-4.486049000	3.919468000	0.552116000
7	-1.131163000	0.716433000	1.016614000
1	-2.030591000	1.001821000	4.700010000
1	-1.404359000	2.318937000	3.670232000
1	-3.093145000	1.694087000	3.445960000

⁵¹1-ts2b

Fe	0.512528000	-0.220233000	0.144358000
N	1.677340000	-0.958378000	-1.646529000
N	1.300002000	1.681453000	-0.750167000
N	2.499983000	-0.385844000	0.978459000
N	-1.065057000	-0.862851000	-1.397050000
C	1.434167000	2.865137000	-0.127218000
H	0.978174000	2.938410000	0.856542000
C	2.130701000	3.936310000	-0.678544000
H	2.211903000	4.872897000	-0.137187000
C	2.730239000	3.764256000	-1.927180000
H	3.289471000	4.572163000	-2.389040000
C	2.613883000	2.530625000	-2.568039000
H	3.079996000	2.360668000	-3.533670000
C	1.888398000	1.510668000	-1.951325000
C	2.823249000	-0.004943000	2.230429000
H	1.992486000	0.269145000	2.873699000

C	4.137103000	0.016099000	2.682942000
H	4.357316000	0.325094000	3.698992000
C	5.151271000	-0.367077000	1.802379000
H	6.190311000	-0.355863000	2.117257000
C	4.812835000	-0.772491000	0.512298000
H	5.579053000	-1.089073000	-0.189125000
C	3.469585000	-0.779627000	0.132728000
C	-2.403979000	-0.634971000	-1.359685000
C	-3.304502000	-1.499703000	-1.987321000
H	-4.373295000	-1.343299000	-1.899499000
C	-2.813428000	-2.570841000	-2.732289000
H	-3.497409000	-3.247783000	-3.234702000
C	-1.437883000	-2.745294000	-2.840275000
H	-1.020804000	-3.545316000	-3.444155000
C	-0.593784000	-1.881978000	-2.136611000
C	1.675829000	0.166788000	-2.617661000
H	0.696997000	0.179688000	-3.108442000
H	2.426725000	0.005696000	-3.402895000
C	3.053912000	-1.333420000	-1.222863000
H	3.109093000	-2.425783000	-1.159272000
H	3.785584000	-1.037517000	-1.984834000
C	0.908269000	-2.112092000	-2.162775000
H	1.126967000	-2.969815000	-1.520060000
H	1.220180000	-2.383342000	-3.182425000
C	-0.084795000	-3.219906000	1.602969000
N	0.242755000	-2.334418000	0.932274000
C	-0.527280000	-4.306671000	2.464434000
H	-0.471911000	-5.263234000	1.935754000
H	0.101508000	-4.353784000	3.359043000
H	-1.563611000	-4.118122000	2.763565000
S	-1.692662000	-0.138522000	2.496082000
O	-0.456399000	-0.413361000	3.231629000
O	-2.519049000	-1.227363000	1.967620000
C	-2.748100000	0.900032000	3.533045000
C	-2.840701000	0.640260000	-0.742184000
C	-4.022714000	1.299826000	-1.139706000
C	-2.106325000	1.310671000	0.241306000
C	-4.430791000	2.549606000	-0.634249000
H	-4.668449000	0.816783000	-1.866790000
C	-2.373101000	2.675426000	0.599828000
H	-1.634291000	2.190233000	1.661001000
C	-3.602277000	3.276512000	0.207115000
H	-5.370782000	2.970796000	-0.975434000
H	-1.500482000	3.346336000	0.577550000
H	-3.838838000	4.298824000	0.485456000
N	-1.139831000	0.832382000	1.158585000
H	-3.059015000	0.248674000	4.354482000
H	-2.173783000	1.740607000	3.926943000
H	-3.625268000	1.228777000	2.973481000

³¹1-ts2b

Fe	0.596386000	-0.230599000	0.141287000
N	1.682582000	-1.011162000	-1.648515000
N	1.231427000	1.498581000	-0.638155000
N	2.533083000	-0.402842000	0.948219000
N	-1.034297000	-0.887695000	-1.417481000
C	1.319843000	2.646572000	0.063538000

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H	0.915087000	2.615603000	1.069295000
C	1.911252000	3.795966000	-0.447750000
H	1.962299000	4.694259000	0.158244000
C	2.448833000	3.756108000	-1.735577000
H	2.923047000	4.632452000	-2.166380000
C	2.386171000	2.562262000	-2.452183000
H	2.813062000	2.487633000	-3.447336000
C	1.773674000	1.449307000	-1.876194000
C	2.856896000	-0.029295000	2.201983000
H	2.028714000	0.259862000	2.842252000
C	4.170280000	-0.034671000	2.657762000
H	4.392513000	0.270036000	3.674708000
C	5.179611000	-0.439073000	1.781404000
H	6.217504000	-0.449174000	2.099834000
C	4.836495000	-0.840471000	0.491294000
H	5.597400000	-1.176300000	-0.207131000
C	3.494643000	-0.819690000	0.107192000
C	-2.369806000	-0.660154000	-1.356490000
C	-3.286738000	-1.544683000	-1.932402000
H	-4.353112000	-1.381675000	-1.827351000
C	-2.814046000	-2.644488000	-2.646679000
H	-3.509485000	-3.337918000	-3.109267000
C	-1.440951000	-2.828230000	-2.772876000
H	-1.037158000	-3.653859000	-3.351181000
C	-0.583463000	-1.937165000	-2.121440000
C	1.645709000	0.130794000	-2.598216000
H	0.678900000	0.111344000	-3.110944000
H	2.421899000	0.031842000	-3.368669000
C	3.068614000	-1.369687000	-1.247728000
H	3.139294000	-2.461653000	-1.193434000
H	3.786358000	-1.059011000	-2.017163000
C	0.918972000	-2.165075000	-2.167205000
H	1.154551000	-3.029076000	-1.538624000
H	1.222749000	-2.423147000	-3.192934000
C	-0.074347000	-2.968325000	1.501570000
N	0.194103000	-2.003530000	0.923059000
C	-0.463171000	-4.144899000	2.264920000
H	-0.423869000	-5.042617000	1.640255000
H	0.207006000	-4.273467000	3.120794000
H	-1.486235000	-4.000202000	2.628065000
S	-1.639526000	-0.032222000	2.497886000
O	-0.416106000	-0.272035000	3.267359000
O	-2.474087000	-1.144300000	2.032775000
C	-2.700982000	1.066857000	3.466312000
C	-2.786219000	0.634055000	-0.768169000
C	-3.970426000	1.290188000	-1.162816000
C	-2.030320000	1.321187000	0.188023000
C	-4.361842000	2.556227000	-0.685139000
H	-4.632117000	0.790184000	-1.863737000
C	-2.282331000	2.699259000	0.510595000
H	-1.542193000	2.238865000	1.576779000
C	-3.513335000	3.299191000	0.120733000
H	-5.305379000	2.974182000	-1.020522000
H	-1.405644000	3.362843000	0.455662000
H	-3.737706000	4.330341000	0.375688000
N	-1.064252000	0.857556000	1.113207000
H	-3.022747000	0.458408000	4.315972000
H	-2.128985000	1.924720000	3.824504000

H	-3.570866000	1.369634000	2.881565000
⁵²-ts2			
Fe	-0.223157000	-0.282928000	-0.412565000
N	-1.163580000	-0.886240000	1.557711000
N	-0.825365000	1.705967000	0.469367000
N	-2.358934000	-0.377395000	-0.935315000
N	1.527988000	-0.744313000	0.948115000
C	-0.922490000	2.865460000	-0.203062000
H	-0.485284000	2.874969000	-1.198192000
C	-1.554540000	3.991173000	0.317707000
H	-1.604003000	4.907628000	-0.260621000
C	-2.129808000	3.900096000	1.585810000
H	-2.642184000	4.751189000	2.023829000
C	-2.045295000	2.693524000	2.281591000
H	-2.487629000	2.589439000	3.267666000
C	-1.377579000	1.618362000	1.694250000
C	-2.891105000	0.078242000	-2.083979000
H	-2.185657000	0.376450000	-2.854601000
C	-4.263659000	0.168708000	-2.290855000
H	-4.649006000	0.537029000	-3.235490000
C	-5.118119000	-0.217131000	-1.256851000
H	-6.195343000	-0.152496000	-1.375933000
C	-4.568550000	-0.687981000	-0.064441000
H	-5.207344000	-0.999894000	0.756301000
C	-3.180938000	-0.763970000	0.059281000
C	2.837318000	-0.469933000	0.713170000
C	3.845653000	-1.142368000	1.425075000
H	4.891115000	-0.987015000	1.191818000
C	3.499811000	-2.040102000	2.431391000
H	4.272088000	-2.555828000	2.993371000
C	2.154651000	-2.258601000	2.705828000
H	1.846572000	-2.937469000	3.495082000
C	1.196989000	-1.607502000	1.921772000
C	-1.163912000	0.314795000	2.437403000
H	-0.182389000	0.367473000	2.921260000
H	-1.906166000	0.203393000	3.238872000
C	-2.535012000	-1.390916000	1.283456000
H	-2.462646000	-2.468505000	1.098624000
H	-3.183673000	-1.267324000	2.160403000
C	-0.276406000	-1.934752000	2.105239000
H	-0.479754000	-2.861884000	1.558942000
H	-0.483911000	-2.134408000	3.166545000
C	0.022287000	-3.351387000	-1.897966000
N	-0.089000000	-2.413134000	-1.226934000
C	0.161699000	-4.529425000	-2.746418000
H	0.776713000	-5.284354000	-2.246593000
H	-0.823425000	-4.956291000	-2.959763000
H	0.639331000	-4.250460000	-3.691192000
C	3.199569000	0.549785000	-0.300354000
C	4.460551000	1.144774000	-0.269255000
C	2.242901000	1.020812000	-1.344467000
C	4.903854000	2.053497000	-1.243410000
H	5.147941000	0.901734000	0.532387000
C	2.792172000	1.943437000	-2.359552000
H	2.054154000	2.101734000	-0.855770000
C	4.073725000	2.467948000	-2.284587000

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H	5.908150000	2.458538000	-1.160333000
H	2.080108000	2.253275000	-3.118997000
H	4.418127000	3.179890000	-3.027449000
O	1.115729000	0.401981000	-1.635591000

³²-ts2

Fe	0.350199000	-0.215125000	0.427151000
N	1.211918000	-1.115188000	-1.416584000
N	0.640250000	1.464469000	-0.593735000
N	2.464508000	-0.109950000	0.860936000
N	-1.452689000	-0.968478000	-0.816372000
C	0.578584000	2.688285000	-0.030093000
H	0.239443000	2.709403000	1.000414000
C	0.948888000	3.844361000	-0.706775000
H	0.881864000	4.807401000	-0.212187000
C	1.420718000	3.730232000	-2.015827000
H	1.727740000	4.609634000	-2.573325000
C	1.506914000	2.463857000	-2.591907000
H	1.882512000	2.338079000	-3.602647000
C	1.106654000	1.348120000	-1.855885000
C	3.005581000	0.570104000	1.887511000
H	2.308788000	0.976981000	2.615007000
C	4.378620000	0.749027000	2.025715000
H	4.772614000	1.299509000	2.873221000
C	5.221117000	0.212234000	1.051088000
H	6.297200000	0.339180000	1.118570000
C	4.660083000	-0.492390000	-0.014167000
H	5.288237000	-0.927366000	-0.785735000
C	3.274520000	-0.642863000	-0.071818000
C	-2.763863000	-0.713208000	-0.584053000
C	-3.761441000	-1.546489000	-1.118575000
H	-4.805749000	-1.389866000	-0.879791000
C	-3.402478000	-2.606588000	-1.948081000
H	-4.16557000	-3.250678000	-2.373662000
C	-2.056900000	-2.821662000	-2.221794000
H	-1.739200000	-3.628974000	-2.874778000
C	-1.110828000	-1.988634000	-1.613710000
C	1.115211000	-0.042794000	-2.446993000
H	0.173894000	-0.181702000	-2.989880000
H	1.919522000	-0.139939000	-3.187562000
C	2.614584000	-1.508623000	-1.130167000
H	2.598860000	-2.536467000	-0.750553000
H	3.219624000	-1.522110000	-2.046306000
C	0.372054000	-2.272740000	-1.788009000
H	0.636482000	-3.104572000	-1.126732000
H	0.571464000	-2.607582000	-2.816576000
C	0.138602000	-2.738316000	2.280162000
N	0.218114000	-1.869019000	1.519492000
C	0.036784000	-3.823150000	3.249613000
H	-0.545672000	-4.650922000	2.832715000
H	1.034875000	-4.187376000	3.513285000
H	-0.459624000	-3.461879000	4.156179000
C	-3.138536000	0.451253000	0.251648000
C	-4.418137000	0.997094000	0.146794000
C	-2.174643000	1.109185000	1.188853000
C	-4.877903000	2.029186000	0.977980000
H	-5.106076000	0.609258000	-0.595710000

C	-2.749465000	2.159693000	2.060281000
H	-2.017999000	2.068727000	0.490015000
C	-4.047105000	2.621999000	1.931816000
H	-5.895777000	2.386853000	0.852617000
H	-2.043580000	2.606763000	2.754404000
H	-4.408615000	3.425986000	2.564655000
O	-1.038855000	0.566129000	1.572582000

⁵¹-Int2

Fe	0.479410000	-0.064670000	-0.372198000
N	1.664373000	1.864927000	-0.606214000
N	0.972540000	0.386999000	1.725048000
N	2.691153000	-0.735737000	-0.427633000
N	-1.097640000	1.725750000	-0.549258000
C	0.854752000	-0.459928000	2.762970000
H	0.296346000	-1.370441000	2.570866000
C	1.415209000	-0.215003000	4.011397000
H	1.290066000	-0.929986000	4.817436000
C	2.145917000	0.960727000	4.188568000
H	2.607949000	1.187529000	5.144549000
C	2.281423000	1.838337000	3.113937000
H	2.848291000	2.758431000	3.217933000
C	1.677360000	1.524125000	1.895456000
C	3.163438000	-1.946565000	-0.075552000
H	2.422650000	-2.723705000	0.058426000
C	4.520116000	-2.206375000	0.101782000
H	4.846891000	-3.203058000	0.378443000
C	5.431515000	-1.167730000	-0.078606000
H	6.496169000	-1.330272000	0.058918000
C	4.948823000	0.089253000	-0.442612000
H	5.626589000	0.922572000	-0.600608000
C	3.576873000	0.262948000	-0.616904000
C	-2.425452000	1.760509000	-0.270266000
C	-3.241451000	2.791797000	-0.769060000
H	-4.313129000	2.756726000	-0.615870000
C	-2.682222000	3.844786000	-1.482807000
H	-3.306166000	4.648754000	-1.860739000
C	-1.310098000	3.840808000	-1.699686000
H	-0.821766000	4.649526000	-2.234149000
C	-0.563742000	2.755866000	-1.239289000
C	1.720234000	2.501982000	0.736862000
H	0.848723000	3.158612000	0.832223000
H	2.605921000	3.145015000	0.822198000
C	3.013861000	1.561812000	-1.140578000
H	2.923022000	1.467132000	-2.228709000
H	3.708716000	2.391502000	-0.952682000
C	0.911710000	2.698432000	-1.562647000
H	1.029810000	2.248614000	-2.554283000
H	1.318190000	3.718940000	-1.621246000
C	-0.075249000	-0.959826000	-3.542644000
N	0.171253000	-0.426749000	-2.544055000
C	-0.395856000	-1.655355000	-4.781427000
H	-0.950628000	-0.994783000	-5.455042000
H	0.523980000	-1.981275000	-5.277265000
H	-1.009384000	-2.532215000	-4.548923000
S	-1.147255000	-2.674703000	-0.293623000
O	0.318205000	-2.457053000	-0.370377000

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O	-1.891889000	-3.135889000	-1.464242000
C	-1.375948000	-3.856581000	1.060178000
C	-3.100624000	0.719153000	0.554754000
C	-4.146495000	1.102339000	1.367883000
C	-2.792215000	-0.701205000	0.497274000
C	-5.054925000	0.201329000	2.026443000
H	-4.320112000	2.164880000	1.511811000
C	-3.892346000	-1.664411000	0.896885000
C	-4.981228000	-1.116469000	1.761145000
H	-5.828137000	0.610925000	2.667472000
H	-4.335814000	-2.055856000	-0.037948000
H	-5.708765000	-1.822947000	2.150024000
N	-1.602915000	-1.079110000	0.097414000
H	-0.650077000	-4.648468000	0.853777000
H	-1.144457000	-3.382999000	2.016601000
H	-2.383272000	-4.271577000	1.037717000
H	-3.472344000	-2.542462000	1.393316000

³¹I-Int2

Fe	0.560523000	0.000191000	-0.337494000
N	1.673317000	1.921431000	-0.351711000
N	0.794883000	0.173406000	1.624577000
N	2.732183000	-0.649444000	-0.270668000
N	-1.059514000	1.760484000	-0.427036000
C	0.529101000	-0.809698000	2.507025000
H	0.088341000	-1.706908000	2.090751000
C	0.822099000	-0.705303000	3.860393000
H	0.588302000	-1.525299000	4.530649000
C	1.433069000	0.461184000	4.323157000
H	1.685453000	0.577242000	5.372569000
C	1.727942000	1.470959000	3.410319000
H	2.215144000	2.385959000	3.732742000
C	1.395246000	1.301082000	2.065808000
C	3.199713000	-1.872495000	0.039521000
H	2.462581000	-2.661834000	0.100363000
C	4.550855000	-2.128768000	0.262467000
H	4.875352000	-3.135660000	0.502581000
C	5.458910000	-1.075321000	0.175659000
H	6.518084000	-1.236179000	0.351613000
C	4.978973000	0.194684000	-0.143506000
H	5.652900000	1.041834000	-0.227897000
C	3.613661000	0.363637000	-0.368112000
C	-2.396662000	1.739780000	-0.209422000
C	-3.220686000	2.786345000	-0.660774000
H	-4.296261000	2.712743000	-0.553599000
C	-2.660830000	3.905541000	-1.266026000
H	-3.289792000	4.721633000	-1.607898000
C	-1.280767000	3.951937000	-1.420272000
H	-0.791902000	4.812053000	-1.867308000
C	-0.526920000	2.852354000	-1.008479000
C	1.643053000	2.401653000	1.058476000
H	0.831329000	3.130871000	1.153607000
H	2.569771000	2.935309000	1.304368000
C	3.052440000	1.682679000	-0.840194000
H	3.009873000	1.655502000	-1.934817000
H	3.717489000	2.512657000	-0.566282000
C	0.965589000	2.854251000	-1.249668000

H	1.157086000	2.532845000	-2.278626000
H	1.357631000	3.877543000	-1.155774000
C	0.287963000	-0.483520000	-3.406726000
N	0.434565000	-0.164815000	-2.303654000
C	0.081775000	-0.929610000	-4.777229000
H	-0.405033000	-0.145997000	-5.366151000
H	1.040276000	-1.184567000	-5.240334000
H	-0.557963000	-1.818638000	-4.759969000
S	-1.047894000	-2.623279000	-0.728779000
O	0.406102000	-2.458553000	-0.496272000
O	-1.568101000	-2.808406000	-2.083422000
C	-1.522538000	-4.059603000	0.267402000
C	-3.069565000	0.619330000	0.505970000
C	-4.129716000	0.916190000	1.333409000
C	-2.748630000	-0.786535000	0.299953000
C	-5.036420000	-0.051852000	1.894282000
H	-4.319992000	1.960325000	1.565392000
C	-3.839049000	-1.795601000	0.611236000
C	-4.944379000	-1.337552000	1.508795000
H	-5.822318000	0.288187000	2.560119000
H	-4.272583000	-2.124507000	-0.351362000
H	-5.666768000	-2.085184000	1.823321000
N	-1.560045000	-1.106501000	-0.144711000
H	-0.820358000	-4.838715000	-0.044063000
H	-1.386533000	-3.848774000	1.330355000
H	-2.539909000	-4.368848000	0.029724000
H	-3.404595000	-2.696853000	1.050402000

⁵²I-Int2

Fe	-0.259695000	-0.302123000	-0.346437000
N	-1.280208000	-0.797491000	1.593575000
N	-0.742971000	1.724479000	0.419947000
N	-2.361956000	-0.330582000	-0.951056000
N	1.426497000	-0.752800000	1.010458000
C	-0.700171000	2.869875000	-0.283885000
H	-0.212628000	2.815181000	-1.252921000
C	-1.246433000	4.061980000	0.180749000
H	-1.183459000	4.962605000	-0.420491000
C	-1.880959000	4.060257000	1.423702000
H	-2.329555000	4.967072000	1.817705000
C	-1.936020000	2.872465000	2.153408000
H	-2.423229000	2.838874000	3.123108000
C	-1.347658000	1.723454000	1.624331000
C	-2.834928000	0.116219000	-2.129584000
H	-2.092302000	0.375252000	-2.879049000
C	-4.194604000	0.245720000	-2.390056000
H	-4.532316000	0.605690000	-3.355836000
C	-5.098850000	-0.089647000	-1.380822000
H	-6.168169000	0.006872000	-1.542192000
C	-4.610475000	-0.550206000	-0.157993000
H	-5.289590000	-0.821753000	0.644412000
C	-3.232331000	-0.667601000	0.022015000
C	2.740206000	-0.482909000	0.805362000
C	3.716118000	-1.069667000	1.630670000
H	4.769247000	-0.928316000	1.420590000
C	3.332391000	-1.854710000	2.711073000
H	4.082333000	-2.296752000	3.359742000

Supporting Information

C	1.975585000	-2.069964000	2.945230000
H	1.638623000	-2.667991000	3.785939000
C	1.055106000	-1.525444000	2.053799000
C	-1.277398000	0.436829000	2.424952000
H	-0.337062000	0.452606000	2.987384000
H	-2.086112000	0.404201000	3.166432000
C	-2.650560000	-1.278326000	1.285730000
H	-2.598928000	-2.362494000	1.133761000
H	-3.328888000	-1.114262000	2.133084000
C	-0.424106000	-1.846493000	2.191873000
H	-0.620999000	-2.779913000	1.653438000
H	-0.670107000	-2.024590000	3.248277000
C	-0.060063000	-3.401078000	-1.782036000
N	-0.139908000	-2.404897000	-1.195430000
C	0.039409000	-4.653347000	-2.522931000
H	0.713104000	-5.343916000	-2.005807000
H	-0.948669000	-5.116696000	-2.608831000
H	0.429209000	-4.461181000	-3.527725000
C	3.162706000	0.424551000	-0.296381000
C	4.349934000	1.126076000	-0.188099000
C	2.378177000	0.659350000	-1.500249000
C	4.923523000	1.958730000	-1.208315000
H	4.898744000	1.065924000	0.747444000
C	3.032800000	1.361062000	-2.669979000
C	4.315741000	2.067926000	-2.409239000
H	5.856024000	2.470577000	-0.995878000
H	3.210040000	0.584765000	-3.437431000
H	4.747489000	2.654012000	-3.215590000
H	2.294866000	2.026729000	-3.137216000
O	1.182676000	0.312639000	-1.647174000

³²-Int2

Fe	0.362896000	-0.225031000	0.370421000
N	1.373268000	-1.099466000	-1.407820000
N	0.570676000	1.447528000	-0.688141000
N	2.390397000	0.037227000	0.921813000
N	-1.315534000	-1.005599000	-0.825967000
C	0.326079000	2.676077000	-0.186682000
H	-0.107458000	2.703521000	0.806111000
C	0.617318000	3.842232000	-0.882877000
H	0.400197000	4.806615000	-0.436655000
C	1.199816000	3.739113000	-2.146966000
H	1.449160000	4.628126000	-2.717859000
C	1.465858000	2.471973000	-2.661456000
H	1.924632000	2.353848000	-3.638298000
C	1.136416000	1.343521000	-1.910431000
C	2.823233000	0.796447000	1.944904000
H	2.057545000	1.216396000	2.590801000
C	4.173526000	1.038988000	2.175536000
H	4.479008000	1.653642000	3.015339000
C	5.108724000	0.482323000	1.301982000
H	6.170821000	0.656894000	1.443653000
C	4.659113000	-0.302313000	0.239746000
H	5.361366000	-0.751611000	-0.455880000
C	3.289760000	-0.513443000	0.082236000
C	-2.634576000	-0.740069000	-0.657406000
C	-3.600030000	-1.503492000	-1.338859000

H	-4.654593000	-1.350700000	-1.144396000
C	-3.204365000	-2.475485000	-2.249500000
H	-3.946625000	-3.054994000	-2.789649000
C	-1.844112000	-2.699772000	-2.449482000
H	-1.495248000	-3.445820000	-3.156594000
C	-0.933559000	-1.963725000	-1.695064000
C	1.337444000	-0.050776000	-2.460594000
H	0.498272000	-0.269490000	-3.130669000
H	2.243260000	-0.087979000	-3.079033000
C	2.746486000	-1.451843000	-0.981920000
H	2.712962000	-2.459354000	-0.551863000
H	3.434878000	-1.497691000	-1.836101000
C	0.553340000	-2.269244000	-1.783898000
H	0.783167000	-3.077423000	-1.081481000
H	0.800256000	-2.638780000	-2.789165000
C	0.241376000	-2.761530000	2.219248000
N	0.287238000	-1.868681000	1.483008000
C	0.182607000	-3.881159000	3.151934000
H	-0.635379000	-4.555825000	2.879601000
H	1.125347000	-4.437417000	3.132542000
H	0.012967000	-3.508862000	4.167594000
C	-3.083865000	0.338785000	0.264512000
C	-4.291421000	0.972095000	0.043502000
C	-2.306659000	0.810557000	1.406346000
C	-4.897103000	1.941352000	0.916756000
H	-4.834727000	0.741219000	-0.868617000
C	-3.012156000	1.624694000	2.471180000
C	-4.310325000	2.249391000	2.092336000
H	-5.841139000	2.386256000	0.620770000
H	-3.194447000	0.935308000	3.317091000
H	-4.771318000	2.934604000	2.798066000
H	-2.308141000	2.362552000	2.876490000
O	-1.087490000	0.592815000	1.573310000

⁵¹-ts₃HOH

C	-3.397233000	2.059879000	2.877079000
C	-3.087711000	3.317735000	2.423601000
C	-2.243419000	3.427433000	1.304985000
C	-1.648719000	2.341200000	0.651731000
C	-1.808684000	1.035896000	1.232634000
C	-2.852673000	0.902676000	2.229996000
C	-0.965008000	2.635299000	-0.638574000
N	0.154000000	1.976933000	-1.022069000
C	0.797040000	2.374182000	-2.140415000
C	0.341220000	3.413140000	-2.948643000
C	-0.859045000	4.033330000	-2.616292000
C	-1.515900000	3.639196000	-1.457171000
Fe	0.882151000	-0.047699000	-0.294054000
N	-1.044374000	-0.010307000	0.790268000
S	-1.431511000	-1.597711000	1.087657000
C	-1.108222000	-2.065305000	2.806245000
C	2.046728000	1.614620000	-2.533618000
N	2.653098000	0.917581000	-1.381630000
C	3.594639000	-0.137839000	-1.820640000
C	3.690442000	-1.280199000	-0.834424000
N	2.551276000	-1.611717000	-0.194346000
C	2.556735000	-2.700927000	0.595529000

Supporting Information

C	3.688636000	-3.487732000	0.791338000
C	4.871809000	-3.129837000	0.146690000
C	4.870094000	-2.007604000	-0.681370000
N	2.078422000	0.848390000	1.404896000
C	1.902066000	0.619375000	2.717322000
C	2.810039000	1.020691000	3.691504000
C	3.968368000	1.682842000	3.283406000
C	4.156665000	1.929335000	1.924562000
C	3.185557000	1.508558000	1.013665000
C	3.288977000	1.884747000	-0.450448000
O	-0.431536000	-2.326650000	0.288500000
O	-2.870391000	-1.873199000	0.846498000
N	0.185023000	-0.993781000	-2.230333000
C	-0.288309000	-1.714136000	-3.004000000
C	-0.886280000	-2.633699000	-3.963868000
H	0.988557000	0.101230000	2.989406000
H	2.615998000	0.813400000	4.738452000
H	4.710029000	2.003101000	4.008734000
H	5.042028000	2.449968000	1.572573000
H	1.610767000	-2.949111000	1.060444000
H	3.637465000	-4.359072000	1.435460000
H	5.777448000	-3.713449000	0.281032000
H	5.768263000	-1.704085000	-1.210481000
H	-2.460676000	4.097564000	-1.192022000
H	-1.274143000	4.814998000	-3.245053000
H	0.904391000	3.710418000	-3.827780000
H	2.779090000	2.846764000	-0.571504000
H	4.338853000	2.050996000	-0.725723000
H	3.216293000	-0.548136000	-2.763646000
H	4.589097000	0.277692000	-2.032026000
H	1.773350000	0.857118000	-3.274444000
H	2.760352000	2.297045000	-3.018314000
H	-1.656294000	-2.121333000	-4.549014000
H	-0.119642000	-3.018074000	-4.644119000
H	-1.340890000	-3.474360000	-3.429761000
H	-2.040775000	4.422793000	0.922540000
H	-3.493157000	4.207693000	2.891751000
H	-3.916240000	0.562440000	1.368652000
H	-4.084510000	1.913777000	3.705892000
H	-1.370784000	-3.124577000	2.873784000
H	-0.044701000	-1.930481000	3.007666000
H	-1.713113000	-1.490367000	3.507277000
H	-2.882521000	-0.012236000	2.814847000
O	-4.676953000	0.016530000	0.528338000
H	-5.562822000	-0.178299000	0.891419000
H	-4.183862000	-0.846992000	0.422544000

³¹I-ts₃HOH

C	-3.182952000	1.993339000	2.944788000
C	-2.832913000	3.245665000	2.507346000
C	-2.026593000	3.336926000	1.358786000
C	-1.497106000	2.237570000	0.674530000
C	-1.684322000	0.923875000	1.239254000
C	-2.713417000	0.824835000	2.259311000
C	-0.872851000	2.535355000	-0.645203000
N	0.252454000	1.915748000	-1.066957000
C	0.845935000	2.324615000	-2.207190000

C	0.328157000	3.341018000	-3.005789000
C	-0.879810000	3.924011000	-2.633778000
C	-1.481975000	3.517512000	-1.449035000
Fe	1.025809000	-0.001663000	-0.334141000
N	-0.960575000	-0.135590000	0.765146000
S	-1.440567000	-1.709172000	1.046228000
C	-1.105150000	-2.198001000	2.759383000
C	2.118453000	1.608936000	-2.618155000
N	2.738856000	0.926512000	-1.468585000
C	3.664781000	-0.151436000	-1.867706000
C	3.709411000	-1.278887000	-0.857472000
N	2.566357000	-1.540337000	-0.191365000
C	2.524832000	-2.618374000	0.613475000
C	3.617242000	-3.459608000	0.804535000
C	4.808184000	-3.172624000	0.139255000
C	4.850752000	-2.065515000	-0.707356000
N	1.967686000	0.854107000	1.218985000
C	1.658271000	0.643759000	2.513825000
C	2.422640000	1.132144000	3.565710000
C	3.570488000	1.868409000	3.271479000
C	3.895588000	2.090429000	1.935769000
C	3.073053000	1.578315000	0.931246000
C	3.350986000	1.891394000	-0.522586000
O	-0.544882000	-2.538681000	0.232764000
O	-2.906493000	-1.868238000	0.853264000
N	0.254974000	-0.883367000	-1.930920000
C	-0.240373000	-1.534700000	-2.748641000
C	-0.879311000	-2.386389000	-3.743410000
H	0.759444000	0.068301000	2.691364000
H	2.124791000	0.932916000	4.589417000
H	4.199788000	2.259903000	4.064654000
H	4.779478000	2.660565000	1.666880000
H	1.571779000	-2.819154000	1.085979000
H	3.528730000	-4.318662000	1.460886000
H	5.684572000	-3.799868000	0.270234000
H	5.754495000	-1.817693000	-1.255780000
H	-2.428132000	3.950237000	-1.147395000
H	-1.341226000	4.688669000	-3.251087000
H	0.851687000	3.651709000	-3.904688000
H	2.935319000	2.883817000	-0.730182000
H	4.432938000	1.969081000	-0.690952000
H	3.302662000	-0.568898000	-2.814024000
H	4.675445000	0.234053000	-2.059054000
H	1.872566000	0.849670000	-3.366915000
H	2.807750000	2.319943000	-3.096927000
H	-1.628543000	-1.819975000	-4.305295000
H	-0.134260000	-2.782235000	-4.440786000
H	-1.369176000	-3.223164000	-3.234118000
H	-1.806012000	4.327634000	0.972973000
H	-3.186012000	4.143242000	3.002487000
H	-3.817461000	0.568562000	1.417904000
H	-3.853756000	1.859993000	3.789292000
H	-1.429345000	-3.239520000	2.832488000
H	-0.030359000	-2.131704000	2.936776000
H	-1.653273000	-1.589634000	3.478426000
H	-2.783933000	-0.099852000	2.823381000
O	-4.622608000	0.085657000	0.584224000
H	-5.504711000	-0.082256000	0.969215000

Supporting Information

H -4.163391000 -0.795574000 0.456965000

⁵²-ts₃HOH

C	-3.227015000	1.871610000	2.878515000
C	-3.267516000	3.123570000	2.295946000
C	-2.503068000	3.365321000	1.146097000
C	-1.712551000	2.395475000	0.506505000
C	-1.640545000	1.106027000	1.118112000
C	-2.449537000	0.845004000	2.282544000
C	-1.014147000	2.752641000	-0.756672000
N	0.106854000	2.081663000	-1.119260000
C	0.805773000	2.470965000	-2.204496000
C	0.412837000	3.542355000	-3.001358000
C	-0.779048000	4.194517000	-2.688551000
C	-1.498234000	3.794673000	-1.568834000
Fe	0.794406000	0.158270000	-0.279298000
C	2.030850000	1.647686000	-2.566368000
N	2.599116000	0.955431000	-1.386338000
C	3.463420000	-0.190938000	-1.757679000
C	3.408634000	-1.328017000	-0.752680000
N	2.242570000	-1.508123000	-0.101053000
C	2.117200000	-2.557537000	0.731190000
C	3.140071000	-3.474828000	0.946425000
C	4.351629000	-3.285813000	0.279470000
C	4.487760000	-2.195223000	-0.578874000
N	1.999324000	1.018658000	1.391412000
C	1.797077000	0.814147000	2.704680000
C	2.716461000	1.190747000	3.678682000
C	3.908089000	1.789917000	3.268684000
C	4.126269000	1.996448000	1.906653000
C	3.144265000	1.606715000	0.994841000
C	3.283272000	1.920515000	-0.482868000
N	-0.032605000	-0.970623000	-2.117751000
C	-0.498056000	-1.560258000	-3.000592000
C	-1.083176000	-2.301355000	-4.113132000
H	0.861892000	0.331269000	2.972820000
H	2.505674000	1.011306000	4.727480000
H	4.656739000	2.089226000	3.995804000
H	5.042803000	2.460869000	1.555695000
H	1.162223000	-2.654959000	1.240151000
H	2.991610000	-4.308723000	1.623954000
H	5.178323000	-3.973820000	0.427673000
H	5.417491000	-2.020381000	-1.111664000
H	-2.435547000	4.283159000	-1.333728000
H	-1.141866000	5.008463000	-3.308654000
H	1.011681000	3.844256000	-3.854880000
H	2.831983000	2.904690000	-0.650670000
H	4.343470000	2.012660000	-0.752789000
H	3.106539000	-0.580957000	-2.717675000
H	4.502725000	0.126370000	-1.915424000
H	1.730525000	0.879773000	-3.286810000
H	2.776289000	2.283282000	-3.065071000
H	-0.519088000	-2.107125000	-5.031014000
H	-1.058316000	-3.375469000	-3.903691000
H	-2.121705000	-1.990440000	-4.265075000
H	-2.521809000	4.370374000	0.737360000
H	-3.855280000	3.924852000	2.730025000

H	-3.280071000	-0.098338000	1.468514000
H	-3.772850000	1.665994000	3.794914000
H	-2.135614000	0.007069000	2.909884000
O	-3.398665000	-0.985681000	0.676913000
H	-3.635222000	-1.822389000	1.123346000
H	-2.423630000	-0.998735000	0.423694000
O	-0.998178000	0.071380000	0.606818000

³²-ts₃HOH

C	-3.113087000	1.876533000	2.891032000
C	-3.112781000	3.134099000	2.321936000
C	-2.338695000	3.361590000	1.174336000
C	-1.576516000	2.375275000	0.527565000
C	-1.531966000	1.079033000	1.132873000
C	-2.359648000	0.832938000	2.291124000
C	-0.899518000	2.719461000	-0.751308000
N	0.212867000	2.048073000	-1.136855000
C	0.876592000	2.425251000	-2.246811000
C	0.460190000	3.486205000	-3.046292000
C	-0.722246000	4.140999000	-2.707053000
C	-1.407474000	3.751611000	-1.562495000
Fe	0.901832000	0.119523000	-0.332775000
C	2.097540000	1.604648000	-2.631523000
N	2.663442000	0.899747000	-1.462824000
C	3.504685000	-0.261204000	-1.825555000
C	3.437164000	-1.377679000	-0.797767000
N	2.281654000	-1.506498000	-0.116811000
C	2.139092000	-2.532715000	0.741060000
C	3.137094000	-3.478017000	0.953518000
C	4.339442000	-3.342752000	0.257939000
C	4.491168000	-2.275503000	-0.626819000
N	1.867289000	0.947361000	1.198302000
C	1.524003000	0.754941000	2.487980000
C	2.296828000	1.213963000	3.547248000
C	3.484558000	1.889803000	3.264975000
C	3.849456000	2.076713000	1.933457000
C	3.018797000	1.597539000	0.920309000
C	3.340105000	1.845884000	-0.536867000
N	0.052192000	-0.809905000	-1.873161000
C	-0.465010000	-1.372253000	-2.744181000
C	-1.116764000	-2.079933000	-3.841249000
H	0.601991000	0.210699000	2.652310000
H	1.975170000	1.037468000	4.567852000
H	4.118263000	2.257866000	4.065835000
H	4.770201000	2.591487000	1.676744000
H	1.192816000	-2.586629000	1.271834000
H	2.976201000	-4.291962000	1.652164000
H	5.146812000	-4.053668000	0.404050000
H	5.414087000	-2.141312000	-1.182882000
H	-2.339544000	4.239502000	-1.306274000
H	-1.104862000	4.946924000	-3.325739000
H	1.034254000	3.776776000	-3.920689000
H	3.005104000	2.859663000	-0.782946000
H	4.426446000	1.833266000	-0.692937000
H	3.131908000	-0.659534000	-2.776027000
H	4.548762000	0.033341000	-1.997116000
H	1.797747000	0.848420000	-3.364270000

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H	2.841656000	2.247919000	-3.122750000
H	-2.153837000	-1.743724000	-3.941229000
H	-0.590526000	-1.883828000	-4.781118000
H	-1.107252000	-3.158068000	-3.650971000
H	-2.330275000	4.369147000	0.770959000
H	-3.678681000	3.948743000	2.760156000
H	-3.192656000	-0.098781000	1.473907000
H	-3.671378000	1.677419000	3.801439000
H	-2.067326000	-0.010598000	2.921812000
O	-3.292335000	-0.993738000	0.680254000
H	-3.519565000	-1.828299000	1.134628000
H	-2.303510000	-0.983152000	0.454639000
O	-0.909449000	0.037539000	0.624907000

⁶P

Fe	-0.417158000	-0.145632000	0.351428000
N	-1.652277000	1.679206000	0.909168000
N	-0.803879000	0.718995000	-1.632966000
N	-2.647519000	-0.790621000	0.164729000
N	1.098511000	1.610614000	0.745718000
C	-0.495454000	0.146202000	-2.811494000
H	0.181807000	-0.700214000	-2.764773000
C	-0.993369000	0.596159000	-4.028048000
H	-0.713407000	0.099740000	-4.950901000
C	-1.860193000	1.690382000	-4.023225000
H	-2.280791000	2.068692000	-4.949895000
C	-2.175979000	2.293683000	-2.807571000
H	-2.839813000	3.152174000	-2.771431000
C	-1.623621000	1.788092000	-1.628905000
C	-3.121640000	-1.850260000	-0.514717000
H	-2.380464000	-2.545480000	-0.886918000
C	-4.481741000	-2.068667000	-0.721452000
H	-4.810533000	-2.942926000	-1.273014000
C	-5.394494000	-1.149258000	-0.207922000
H	-6.462100000	-1.285436000	-0.350725000
C	-4.909379000	-0.045335000	0.494270000
H	-5.587314000	0.692394000	0.912301000
C	-3.533461000	0.095219000	0.662308000
C	2.406255000	1.709555000	0.390063000
C	3.200966000	2.762456000	0.886140000
H	4.261326000	2.788654000	0.673540000
C	2.642896000	3.752354000	1.684728000
H	3.254598000	4.566553000	2.060565000
C	1.290982000	3.670598000	1.993335000
H	0.804490000	4.424246000	2.604305000
C	0.565184000	2.576035000	1.521834000
C	-1.854507000	2.507691000	-0.313271000
H	-1.146146000	3.343448000	-0.277176000
H	-2.855702000	2.955360000	-0.306254000
C	-2.938049000	1.210651000	1.481890000
H	-2.727779000	0.826941000	2.486434000
H	-3.647757000	2.041645000	1.593404000
C	-0.880447000	2.418276000	1.928246000
H	-0.921644000	1.842846000	2.858856000
H	-1.323957000	3.402025000	2.136813000
C	0.038881000	-1.349413000	3.445541000

N	-0.189498000	-0.696275000	2.516000000
C	0.336393000	-2.192128000	4.595416000
H	0.912422000	-1.630184000	5.337385000
H	-0.593141000	-2.544183000	5.053898000
H	0.922800000	-3.055541000	4.263224000
S	1.029596000	-2.728860000	-0.010175000
O	-0.422182000	-2.497083000	0.217406000
O	1.825223000	-3.437074000	0.988122000
C	1.137201000	-3.575858000	-1.603014000
C	3.083180000	0.701645000	-0.465943000
C	4.213184000	1.100016000	-1.191408000
C	2.749921000	-0.710916000	-0.488912000
C	5.097071000	0.183256000	-1.765650000
H	4.426469000	2.156825000	-1.303184000
C	3.756297000	-1.633317000	-0.937154000
C	4.898973000	-1.195985000	-1.567814000
H	5.959574000	0.540402000	-2.319024000
H	3.616792000	-2.692866000	-0.768075000
H	5.633625000	-1.912322000	-1.921283000
N	1.498428000	-1.091526000	-0.147018000
H	0.623026000	-4.528637000	-1.445019000
H	0.612289000	-2.987595000	-2.357187000
H	2.172915000	-3.754651000	-1.887460000

⁴P

Fe	-0.506416000	0.095326000	-0.367445000
N	-1.583815000	-1.868274000	-0.695841000
N	-0.821553000	-0.534256000	1.698833000
N	-2.712887000	0.665923000	-0.268646000
N	1.148138000	-1.577964000	-0.764458000
C	-0.693710000	0.243407000	2.789054000
H	-0.224618000	1.208767000	2.628931000
C	-1.148632000	-0.137060000	4.046763000
H	-1.021070000	0.524226000	4.897030000
C	-1.780392000	-1.374619000	4.176191000
H	-2.158856000	-1.705726000	5.138451000
C	-1.929714000	-2.177768000	3.046106000
H	-2.424832000	-3.141685000	3.112757000
C	-1.434457000	-1.729982000	1.820891000
C	-3.210743000	1.838300000	0.168460000
H	-2.491049000	2.633601000	0.314847000
C	-4.566089000	2.034986000	0.419552000
H	-4.917029000	3.002154000	0.763141000
C	-5.444735000	0.970250000	0.226670000
H	-6.506855000	1.082546000	0.421836000
C	-4.934072000	-0.246503000	-0.225427000
H	-5.588065000	-1.096262000	-0.395758000
C	-3.566604000	-0.357178000	-0.472574000
C	2.491539000	-1.558904000	-0.554443000
C	3.346689000	-2.423702000	-1.255533000
H	4.418871000	-2.346226000	-1.120406000
C	2.819341000	-3.367706000	-2.132433000
H	3.473765000	-4.040087000	-2.678425000
C	1.440312000	-3.441990000	-2.271831000
H	0.978287000	-4.188490000	-2.910490000
C	0.644948000	-2.523182000	-1.581050000
C	-1.495779000	-2.614278000	0.589590000

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H	-0.577438000	-3.210386000	0.567029000
H	-2.327697000	-3.324711000	0.679960000
C	-2.986763000	-1.603498000	-1.100325000
H	-2.994157000	-1.455858000	-2.186175000
H	-3.626527000	-2.472598000	-0.897113000
C	-0.856191000	-2.568277000	-1.773026000
H	-1.098942000	-2.068919000	-2.716845000
H	-1.182900000	-3.614333000	-1.870880000
C	-0.144229000	1.269293000	-3.449714000
N	-0.334691000	0.645587000	-2.492312000
C	0.112759000	2.080207000	-4.630709000
H	0.678268000	1.504570000	-5.370176000
H	-0.831546000	2.407276000	-5.077179000
H	0.696180000	2.957199000	-4.331212000
S	1.096514000	2.722416000	-0.225561000
O	-0.323194000	2.370651000	0.079454000
O	1.446487000	3.232280000	-1.548447000
C	1.544190000	3.977802000	0.994294000
C	3.121202000	-0.672487000	0.461949000
C	4.136818000	-1.212594000	1.249680000
C	2.808781000	0.739074000	0.619683000
C	4.888592000	-0.429138000	2.134324000
H	4.350796000	-2.273839000	1.182484000
C	3.635844000	1.526612000	1.492046000
C	4.648478000	0.954674000	2.228407000
H	5.665706000	-0.890554000	2.735280000
H	3.466586000	2.589917000	1.575287000
H	5.255482000	1.569671000	2.885102000
N	1.752328000	1.183791000	-0.071204000
H	0.815620000	4.777567000	0.830746000
H	1.443674000	3.582241000	2.006029000
H	2.547636000	4.351286000	0.786102000