Supporting Information

Influence of ligand architecture in tuning reaction bifurcation pathways for chlorite oxidation by nonheme iron complexes.

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Full reference for Gaussian-09: *Gaussian* 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian*, Inc., Wallingford CT, 2013..

Part I: Experimental Data with Reaction Kinetics and Spectroscopic Characterization of Products and Intermediates.

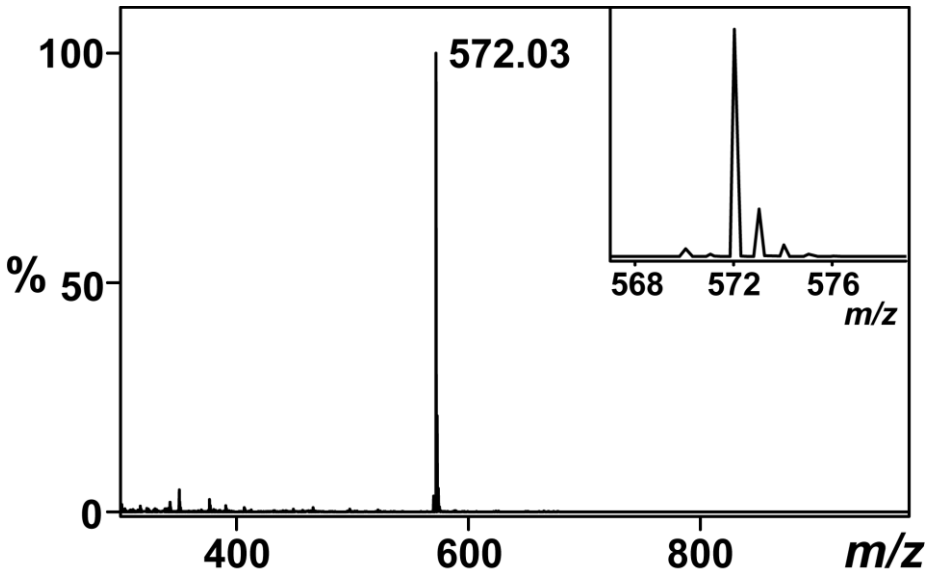


Figure S1. Electrospray ionization mass spectra of $[Fe^{II}(CH_3CN)(N4Py)](CF_3SO_3)_2$. The peak assigned for *m/z* = 572.03 corresponds to $[Fe^{II}(CF_3SO_3)(N4Py)]^+$ in CH_3CN at 298 K.

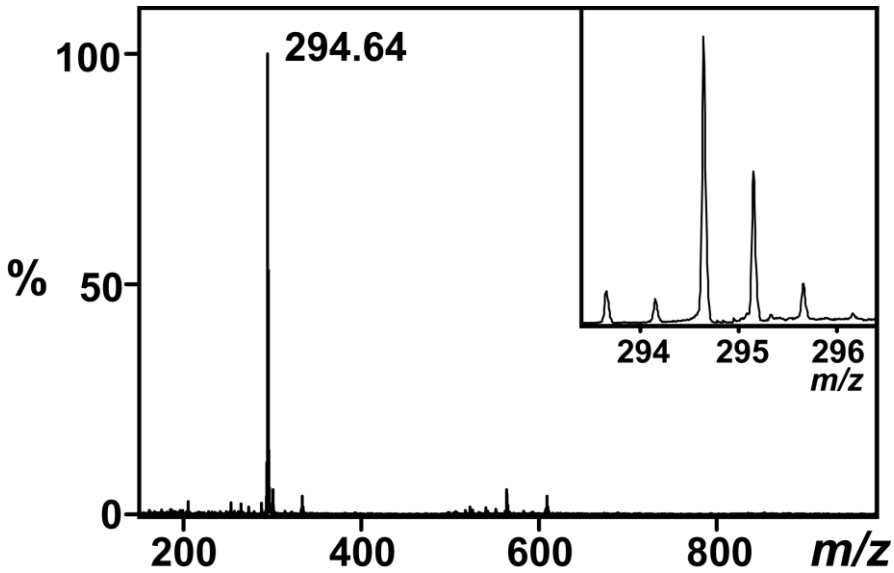


Figure S2. Electrospray ionization mass spectra of $[Fe^{II}(CH_3CN)(L^1)](BF_4)_2$. The peak assigned for *m/z* = 294.64 corresponds to $[Fe^{II}(L^1)]^{2+}$ in CH_3CN at 298 K.

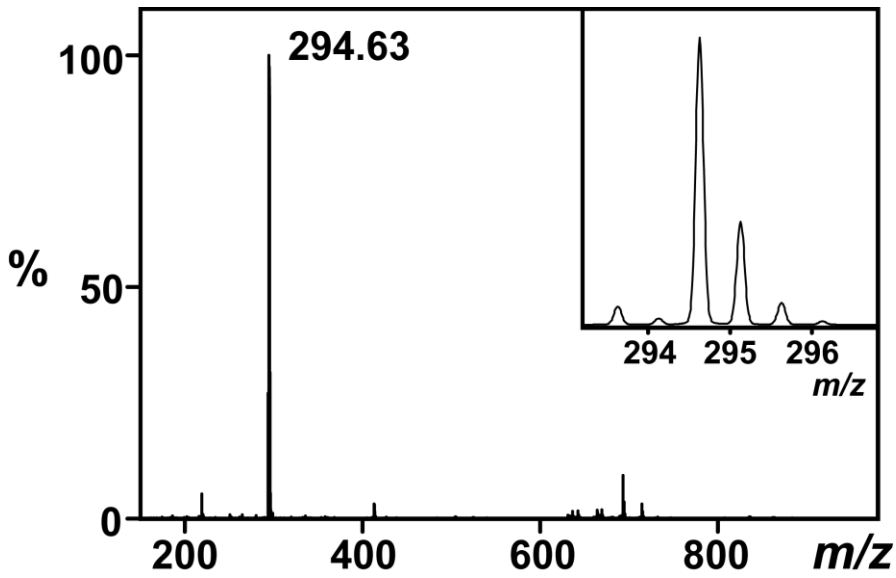


Figure S3. Electrospray ionization mass spectra of $[Fe^{II}(CH_3CN)(L^2)](BF_4)_2$. The peaks assigned for *m/z* = 294.63 correspond to $[Fe^{II}(L^2)]^{2+}$ in CH_3CN at 298 K.

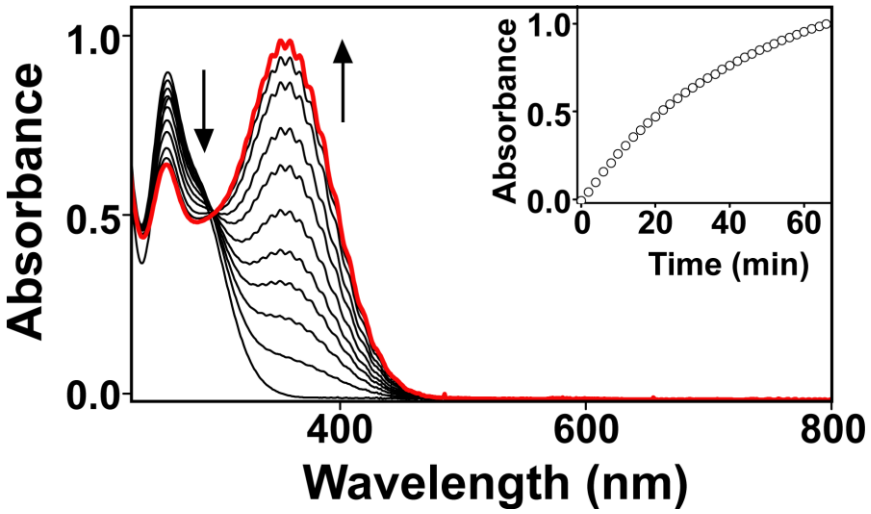


Figure S4. UV-vis spectral changes for the reaction of 10 μM $[Fe^{II}(L^2)]^{2+}$ with 8.0 mM $NaClO_2$. Inset shows the time trace for the formation of ClO_2 at 298 K and pH = 5.0 in acetate buffer. Scan interval was 120 s.

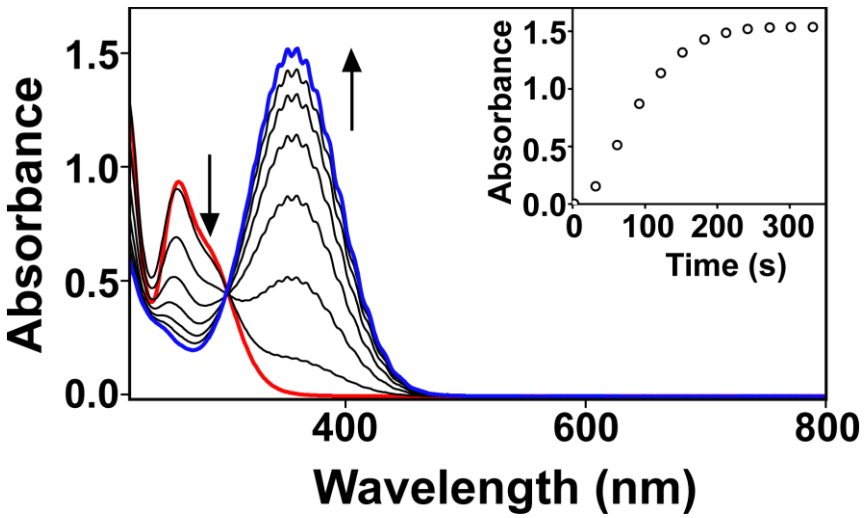


Figure S5. UV-vis spectral changes for the reaction of 10 μM $[Fe^{II}(N4Py)]^{2+}$ with 8.0 mM $NaClO_2$. Inset shows the time trace for the formation of ClO_2 at 298 K and pH = 5.0 in acetate buffer. Scan interval was 30 s.

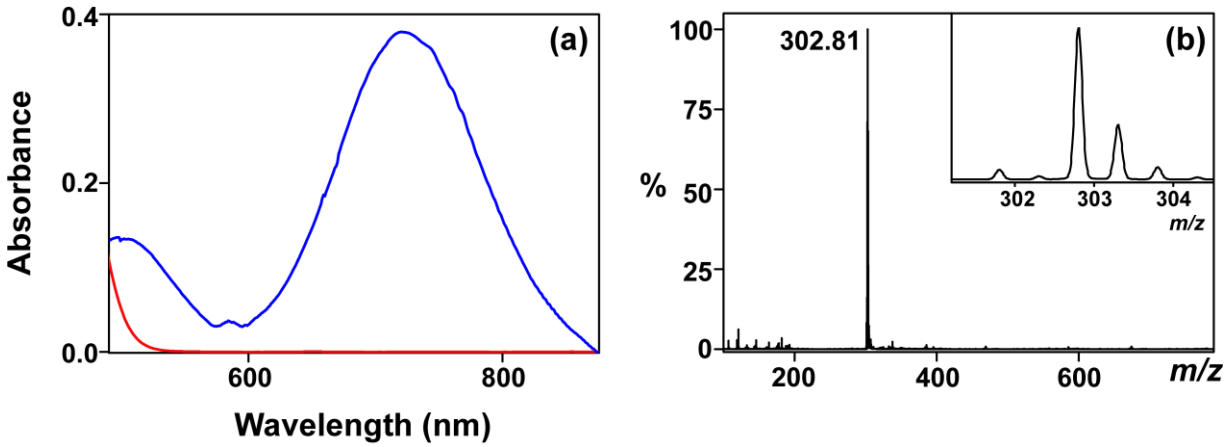


Figure S6. (a) UV-vis spectra of the iron(IV)-oxo formation for the reaction of 1 mM $[Fe^{II}(L^2)]^{2+}$with 1.2 equiv. of $NaClO_2$ at 298 K and pH = 5.0 in acetate buffer. **(b)** ESI-MS spectra of $[Fe^{IV}(O)(L^2)]^{2+}$.

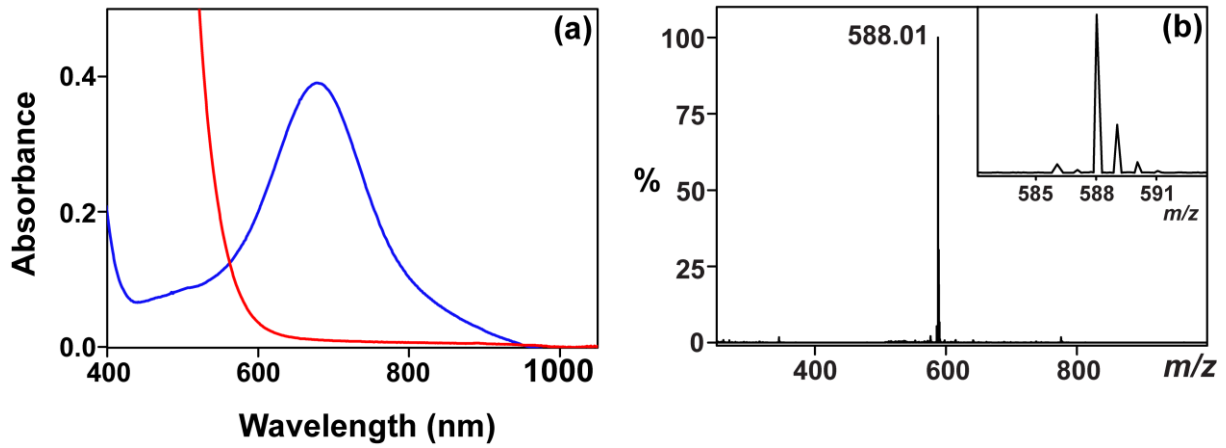


Figure S7. (a) UV-vis spectra of the iron(IV)-oxo formation for the reaction of 1 mM $[Fe^{II}(N4Py)]^{2+}$ with 1.2 equiv. of $NaClO_2$ at 298 K and pH = 5.0 in acetate buffer. **(b)** ESI-MS spectra of $[Fe^{IV}(O)(N4Py)]^{2+}$.

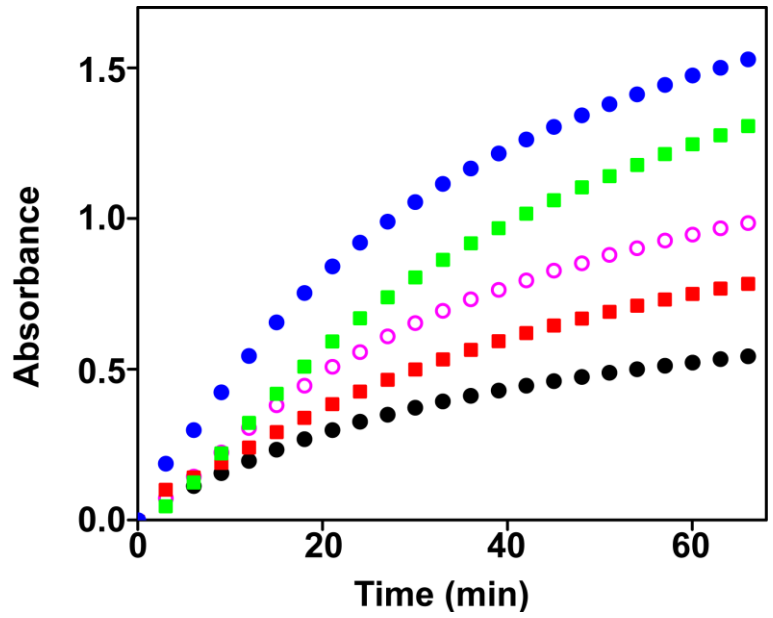


Figure S8. Formation of ClO_2 versus time. Experimental conditions: $[Fe^{II}(L^1)]^{2+}$ = 50 μM; $[ClO_2^-]$ = 10.0, 8.0, 6.0, 4.0, and 2.0 mM (top to bottom).

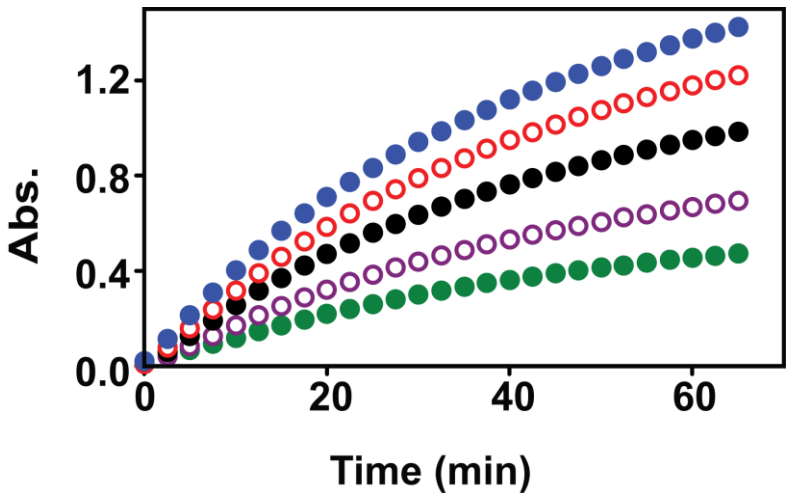


Figure S9. Absorbance changes at 360 nm as a function of time. Reaction conditions: $[Fe^{II}(L^2)]^{2+}$ = 10 μM; $[ClO_2^-]$ = 12.0, 10.0, 8.0, 6.0, 4.0 mM (top to bottom).

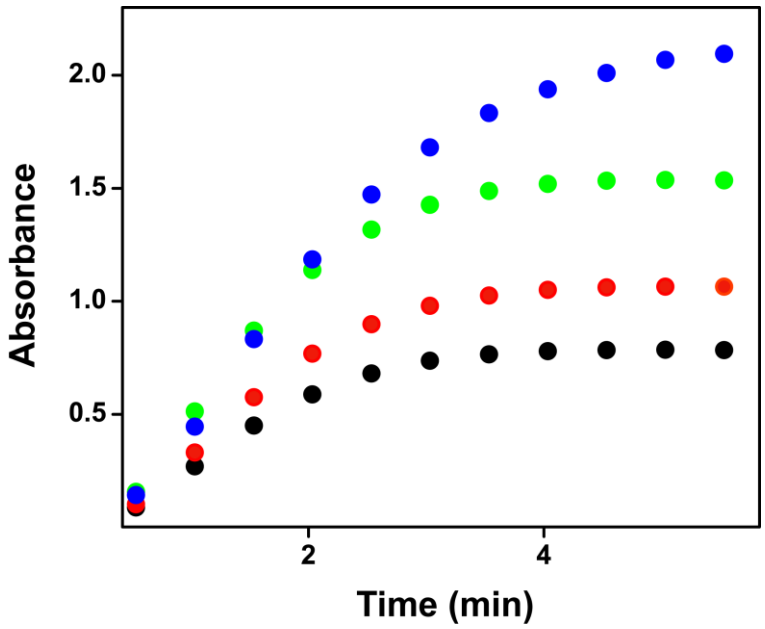


Figure S10. Formation of ClO_2 versus time. Experimental conditions: $[Fe^{II}(N4Py)]^{2+}$ = 10 μM; $[ClO_2^-]$ = 10.0, 8.0, 6.0, and 4.0 mM (top to bottom).

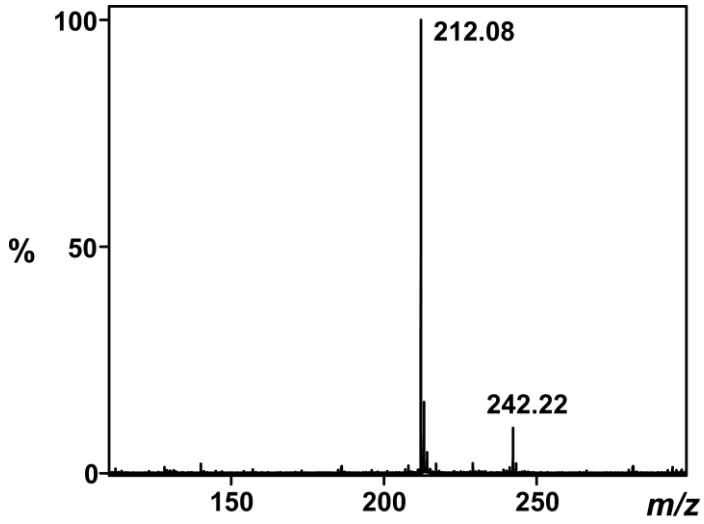


Figure S11. ESI-MS spectra of products obtained from the reaction of $NaClO_2$ with $[Fe^{II}(N4Py)]^{2+}$ in presence of o-tolidine.

Part II: Computational Data.

Table S1: Absolute energies, zero-point energies and free energies of structures. All calculations are the result of a B3LYP/BS1 geometry optimization + frequency followed by B3LYP/BS2 single point calculation in the gas phase and in solvent.

Structure	E (au)	ZPE (au)	G (au)	E2 (au)	E_{solv} (au)
	BS1	BS1	BS1	BS2	BS2
$^1O_2$	-150.20746	0.00323	-150.22324	-150.30261	-150.30353
$^3O_2$	-150.27026	0.00327	-150.28703	-150.36479	-150.36498
^1H_2O	-76.38612	0.02054	-76.38324	-76.44381	-76.45330
$^1H_3O^+$	-76.67873	0.03422	-76.66367	-76.71571	-76.83714
^2H	-0.50027	0.00000	-0.51093	-0.50216	-0.50218
$^1Cl^-$	-460.24873	0.00000	-460.26375	-460.30373	-460.41481
^1HOCl	-535.86670	0.01004	-535.87982	-535.92431	-535.93429
$^1ClO^-$	-535.32016	0.00125	-535.34041	-535.43276	-535.54132
^2ClO	-535.25301	0.00168	-535.27327	-535.34746	-535.34998
$^1ClO_2^-$	-610.39608	0.00326	-610.41877	-610.58651	-610.68895
$^2ClO_2$	-610.30071	0.00389	-610.32318	-610.48783	-610.49498
$^1ClO_3^-$	-685.47173	0.00641	-685.49298	-685.76712	-685.86328
$^2ClO_3$	-685.32274	0.00515	-685.34618	-685.60688	-685.61285
$^1CH_3COO^-$	-228.42964	0.04821	-228.40911	-228.59797	-228.70089
$^2CH_3COO$	-228.33579	0.04759	-228.31686	-228.47898	-228.48644
$^1CH_3COOO^-$	-303.51973	0.05145	-303.49712	-303.72841	-303.83767
$^2CH_3COOO$	-303.46008	0.05180	-303.43806	-303.64873	-303.81785

Table S2: Absolute energies, zero-point energies and free energies of structures. All calculations are the result of a B3LYP/BS1 geometry optimization + frequency followed by B3LYP/BS2 single point calculation in the gas phase and in solvent.

Structure	E (au)	ZPE (au)	G (au)	E2 (au)	E_{solv} (au)
	BS1	BS1	BS1	BS2	BS2
$^{1}[Fe^{II}(L^{1})]^{2+}$	-1933.27392	0.58030	-1932.75575	-1934.22736	-1934.43607
$^{3}[Fe^{II}(L^{1})]^{2+}$	-1933.26944	0.57940	-1932.75361	-1934.22456	-1934.43104
$^{5}[Fe^{II}(L^{1})]^{2+}$	-1933.27588	0.57778	-1932.76398	-1934.23549	-1934.44662
$^{2}[Fe^{I}(L^{1})]^{+}$	-1933.51555	0.57694	-1933.00194	-1934.47961	-1934.54152
$^{4}[Fe^{I}(L^{1})]^{+}$	-1933.52535	0.57412	-1933.01494	-1934.48988	-1934.55704
$^{6}[Fe^{I}(L^{1})]^{+}$	-1933.50305	0.57289	-1932.99435	-1934.47269	-1934.54322
$^{1}[Fe^{II}(L^{1})Ac]^{+}$	-2162.01375	0.63208	-2161.45061	-2163.11079	-2163.17993
$^{3}[Fe^{II}(L^{1})Ac]^{+}$	-2161.99816	0.62995	-2161.43981	-2163.09711	-2163.16530
$^{5}[Fe^{II}(L^{1})Ac]^{+}$	-2161.02375	0.62879	-2161.46863	-2163.12764	-2163.19422
$^{2}[Fe^{III}(OH)(L^{1})]^{2+}$	-2009.09422	0.59531	-2008.56237	-2010.09341	-2010.29391
$^{4}[Fe^{III}(OH)(L^{1})]^{2+}$	-2009.07285	0.59206	-2008.54761	-2010.07545	-2010.27598
$^{6}[Fe^{III}(OH)(L^{1})]^{2+}$	-2009.08833	0.59151	-2008.56430	-2010.09680	-2010.29694
$^{1}[Fe^{IV}(OH)(L^{1})]^{3+}$	-2008.56786	0.59397	-2008.03705	-2009.56239	-2009.99838
$^{3}[Fe^{IV}(OH)(L^{1})]^{3+}$	-2008.60655	0.59316	-2008.07793	-2009.60236	-2010.03838
$^{5}[Fe^{IV}(OH)(L^{1})]^{3+}$	-2008.60242	0.58818	-2008.08436	-2009.60207	-2010.02709
$^{1}[Fe^{II}(H_2O)(L^{1})]^{2+}$	-2009.70520	0.60571	-2009.16405	-2010.70588	-2010.91582
$^{3}[Fe^{II}(H_2O)(L^{1})]^{2+}$	-2009.68771	0.60354	-2009.15152	-2010.69068	-2010.89816
$^{5}[Fe^{II}(H_2O)(L^{1})]^{2+}$	-2009.70745	0.60209	-2009.17489	-2010.71303	-2010.92313
$^{2}[Fe^{III}(H_2O)(L^{1})]^{3+}$	-2009.26192	0.60614	-2008.72102	-2010.25606	-2010.70193
$^{4}[Fe^{III}(H_2O)(L^{1})]^{3+}$	-2009.24437	0.60369	-2008.70783		
$^{6}[Fe^{III}(H_2O)(L^{1})]^{3+}$	-2009.24333	0.60246	-2008.70980	-2010.24870	-2010.69371
$^{1}[Fe^{IV}(O)(L^{1})]^{2+}$	-2008.40393	0.58437	-2007.88222	-2009.39916	-2009.59983
$^{3}[Fe^{IV}(O)(L^{1})]^{2+}$	-2008.45211	0.58475	-2007.93075	-2009.44778	-2009.64843
$^{5}[Fe^{IV}(O)(L^{1})]^{2+}$	-2008.43387	0.58223	-2007.91783	-2009.43736	-2009.63742
$^{2}[Fe^{III}(O)(L^{1})]^{+}$	-2008.72649	0.58189	-2008.20811	-2009.72677	-2009.79724
$^{4}[Fe^{III}(O)(L^{1})]^{+}$	-2008.74214	0.58060	-2008.23022	-2009.75101	-2009.82006
$^{6}[Fe^{III}(O)(L^{1})]^{+}$	-2008.74033	0.57995	-2008.22822	-2009.75405	-2009.82838

Table S3: Absolute energies, zero-point energies and free energies of structures. All calculations are the result of a B3LYP/BS1 geometry optimization + frequency followed by B3LYP/BS2 single point calculation in the gas phase and in solvent.

Structure	E (au)	ZPE (au)	G (au)	E_{disp} (kcal/mol)	E_{solv} (kcal/mol)
$^{1}[Fe^{II}(H_2O)(N4Py)]^{2+}$	-1362.68259	0.42939	-1362.30584	-46.20674	-142.57320
$^{3}[Fe^{II}(H_2O)(N4Py)]^{2+}$	-1362.66828	0.42729	-1362.29652	-47.15309	-140.13070
$^{5}[Fe^{II}(H_2O)(N4Py)]^{2+}$	-1362.68870	0.42611	-1362.32158	-45.05719	-140.54800
$^{2}[Fe^{III}(OH)(N4Py)]^{2+}$	-1362.06347	0.41920	-1361.69554	-45.80631	-140.81570
$^{4}[Fe^{III}(OH)(N4Py)]^{2+}$	-1362.04417	0.41613	-1361.68228	-45.14647	-139.23060
$^{6}[Fe^{III}(OH)(N4Py)]^{2+}$	-1362.06655	0.41532	-1361.70669	-45.42371	-137.71250
$^{1}[Fe^{IV}(O)(N4Py)]^{2+}$	-1361.36135	0.40786	-1361.00417	-44.90958	-141.05360
$^{3}[Fe^{IV}(O)(N4Py)]^{2+}$	-1361.41053	0.40831	-1361.05353	-44.89556	-141.33110
$^{5}[Fe^{IV}(O)(N4Py)]^{2+}$	-1361.39819	0.40643	-1361.04585	-42.92293	-140.09780
$^{2}[Fe^{III}(O)(N4Py)]^{2+}$	-1361.69233	0.40550	-1361.33835	-42.86370	
$^{4}[Fe^{III}(O)(N4Py)]^{2+}$	-1361.71639	0.40430	-1361.36543	-42.66110	
$^{6}[Fe^{III}(O)(N4Py)]^{2+}$	-1361.72063	0.40388	-1361.37273	-42.29000	-52.62147

Table S4: DFT calculated reaction energies and free energies (in kcal mol^{-1}) for ligand system L^1.

Reaction	Rate	Structure L^1			
		gas-phase		solvent	
		ΔE+ZPE	ΔG	ΔE_{solv}+ZPE	ΔG_{solv}
$^5[Fe^{II}(H_2O)]^{2+} + ClO_2^- \rightarrow$ $^3[Fe^{IV}(O)]^{2+} + H_2O + OCl^-$	k_f	-14.82	-19.27	-18.69	-23.13
$^3[Fe^{IV}(O)]^{2+} + ClO_2^- \rightarrow$ $^4[Fe^{III}(O)]^{+} + ClO_2$	k_{ET}	-130.57	-134.13	11.80	8.24
$^4[Fe^{III}(O)]^{+} + H_3O^+ \rightarrow$ $^6[Fe^{III}(OH)]^{2+} + H_2O$	k_{PT}	-48.09	-46.41	-60.12	-58.43
$^3[Fe^{IV}(O)]^{2+} + ClO_2^- + H_3O^+$ $\rightarrow$ $^6[Fe^{III}(OH)]^{2+} + ClO_2 +$ H_2O	k_{ET+PT}	-178.66	-180.54	-48.31	-50.19
$^3[Fe^{IV}(O)]^{2+} + ClO_2^- + H_2O$ $\rightarrow$ $^5[Fe^{II}(H_2O)]^{2+} + ClO_3^-$	k_{OAT}	-1.32	4.85	2.64	8.81
$^5[Fe^{II}(H_2O)]^{2+} + H_2O + ClO_2$ $\rightarrow$ $^6[Fe^{III}(OH)]^{2+} + ClO_2^- +$ H_3O^+	k_{CT}	155.68	156.29	31.90	32.51
$^6[Fe^{III}(OH)]^{2+} + ClO_2^- +$ $H_3O^+ \rightarrow$ $^3[Fe^{IV}(O)]^{2+} + 2\ H_2O$ $+ ClO$	k_r	-179.03	-184.10	-52.37	-57.44

Table S5: DFT calculated reaction energies and free energies (in kcal mol^{-1}) for ligand system N4Py.

Reaction	Rate	Structure L^1			
		gas-phase		solvent	
		ΔE+ZPE	ΔG	ΔE_{solv}+ZPE	ΔG_{solv}
$^5[Fe^{II}(H_2O)]^{2+} + ClO_2^- \rightarrow$ $^3[Fe^{IV}(O)]^{2+} + H_2O + OCl^-$	k_f	-19.64	-23.12	-34.28	-37.75
$^3[Fe^{IV}(O)]^{2+} + ClO_2^- \rightarrow$ $^4[Fe^{III}(O)]^{+} + ClO_2$	k_{ET}	-137.13	-135.73	20.01	16.76
$^4[Fe^{III}(O)]^{+} + H_3O^+ \rightarrow$ $^6[Fe^{III}(OH)]^{2+} + H_2O$	k_{PT}	-34.85	-33.59	-59.19	-57.65
$^3[Fe^{IV}(O)]^{2+} + ClO_2^- + H_3O^+$ $\rightarrow$ $^6[Fe^{III}(OH)]^{2+} + ClO_2 +$ H_2O	k_{ET+PT}	-171.98	-169.32	-39.18	-40.89
$^3[Fe^{IV}(O)]^{2+} + ClO_2^- + H_2O$ $\rightarrow$ $^5[Fe^{II}(H_2O)]^{2+} + ClO_3^-$	k_{OAT}	20.52	25.72	40.13	45.33
$^5[Fe^{II}(H_2O)]^{2+} + H_2O + ClO_2$ $\rightarrow$ $^6[Fe^{III}(OH)]^{2+} + ClO_2^- +$ H_3O^+	k_{CT}	148.36	149.89	-18.47	-16.94
$^6[Fe^{III}(OH)]^{2+} + ClO_2^- +$ $H_3O^+ \rightarrow$ $^3[Fe^{IV}(O)]^{2+} + 2\ H_2O$ $+ ClO$	k_r	-159.87	-147.22	-61.50	-66.75

Table S6: DFT calculated electron affinities of selected structures. All values are in kcal mol^{-1}. Experimentally reported electron affinities from the NIST Database are also given.

Reaction	EA		gas-phase		solvent	
		NIST	ΔE+ZPE	ΔG	ΔE_{solv}+ ZPE	ΔG_{solv}
$ClO + e^- \rightarrow ClO^-$	-EA(ClO)	-52.52	-53.80	-53.52	-120.33	-120.06
$ClO_2 + e^- \rightarrow ClO_2^-$	-EA(ClO_2)	-49.58	-62.32	-62.07	-122.11	-121.86
$ClO_3 + e^- \rightarrow ClO_3^-$	-EA(ClO_3)	-98.01	-99.76	-99.18	-156.36	-155.77
$CH_3COO + e^- \rightarrow CH_3COO^-$	-EA(CH_3COO)		-74.28	-73.66	-134.18	-133.56
$CH_3COOO + e^- \rightarrow CH_3COOO^-$	-EA(CH_3COOO)		-50.22	-49.63	-12.66	-12.07
$^3[Fe^{IV}(O)(L^1)]^{2+} + e^- \rightarrow {}^4[Fe^{III}(O)(L^1)]^+$			-192.89	-196.20	-110.31	-113.62
$^5[Fe^{II}(L^1)]^{2+} + e^- \rightarrow {}^4[Fe^{I}(L^1)]^+$	-EA($(L^1)Fe^{II}$)		-161.92	-160.56	-71.58	-70.22
$^3[Fe^{IV}(O)(N4Py)]^{2+} + e^- \rightarrow {}^4[Fe^{III}(O)(N4Py)]^+$			-197.37	-200.30	-108.66	-111.59

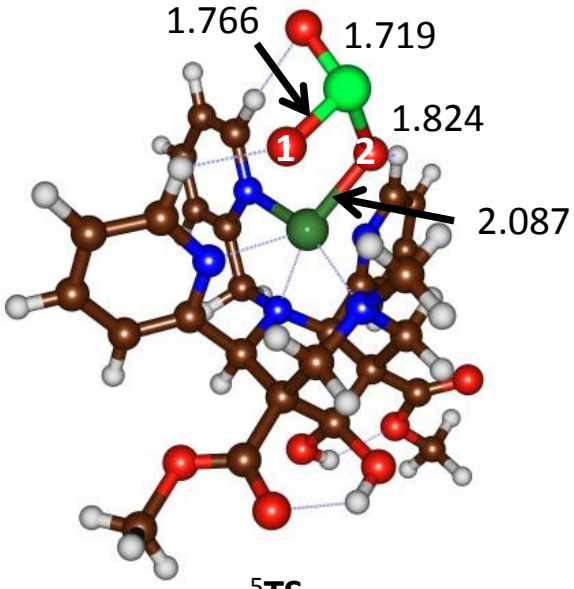


Figure S12: Optimized geometry of the oxygen addition transition state (^{5}TS$_{Add}$) for the reaction of ^{5}[Fe^{IV}(O)(L^1)]$^{2+}$ with ClO_2^- to form [Fe^{II}(ClO_3^-)(L^1)]$^+$ products. Bond lengths are given in angstroms. The imaginary frequency displays an Fe–O_1 bond formation and similtaneous Fe–O_2 bond breaking and elongation of the O_1–Cl bond.

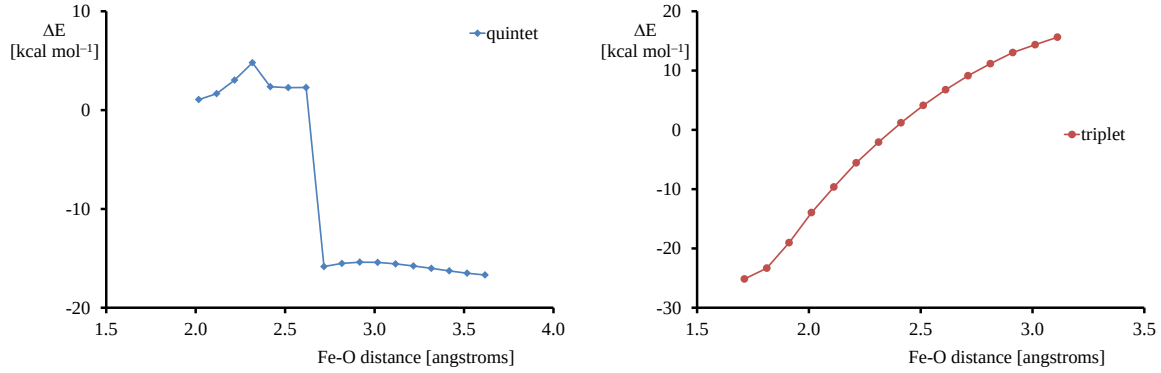


Figure S13: Geometry scans for the oxygen insertion into ClO_2^- starting from an iron(IV)-oxo species on the left-hand-side. Each data point corresponds to a full geometry optimization UB3LYP/BS1 with solvent model included and with fixed Fe–O distance. Calculations done in the quintet and triplet spin states. Energies are relative to the sum of ^{3}[Fe^{IV}(O)(L^1)]$^{2+}$ and ClO_2^-.

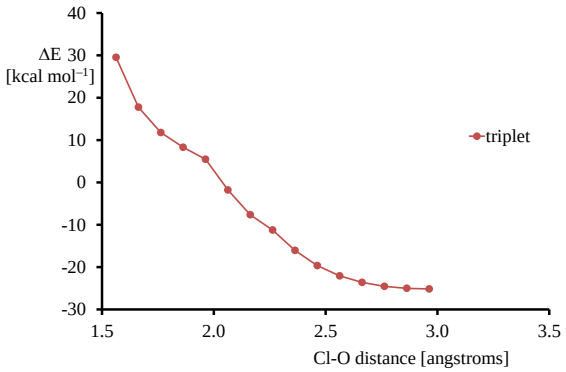


Figure S14: Geometry scan for the oxygen insertion into ClO_2^- starting from an iron(IV)-oxo species on the left-hand-side. Each data point corresponds to a full geometry optimization UB3LYP/BS1 with solvent model included and with fixed Cl–O distance. Calculations done in the quintet and triplet spin states. Energies are relative to the sum of $^3[Fe^{IV}(O)(L^1)]^{2+}$ and ClO_2^-.

Table S7: Absolute (in au) and relative (in kcal mol^{-1}) energies of the addition transition state relative to isolated reactants. Energies obtained in Gaussian at UB3LYP/BS2 in solvent.

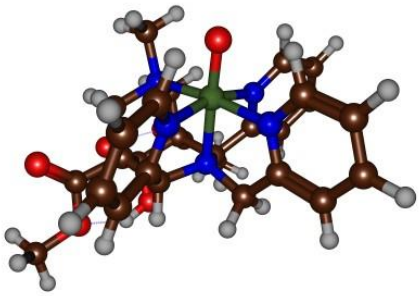
	E [au]	ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{5}**TS**$_{OAT}$	-2619.03535	0.58613	-2618.52115	2.05	0.87	11.80
ClO_2^-	-610.58651	0.00326	-610.60920			
$^5[Fe^{IV}(O)(L^1)]^{2+}$	-2008.45211	0.58475	-2007.93075			

Table S8: Calculated electron transfer free energies for the reactions of ClO_2^- with either $^3[Fe^{IV}(O)(L^1)]^{2+}$ or $^3[Fe^{IV}(O)(N4Py)]^{2+}$. All energies are in kcal mol^{-1} and calculated using Eq 1 and 2 above. Values for r_1 and r_2 taken from the solvent calculations in Gaussian, whereby r_1 refers to ClO_2^- and r_2 the oxidant.

	$^3[Fe^{IV}(O)(L^1)]^{2+}$	$^3[Fe^{IV}(O)(N4Py)]^{2+}$
r_1	3.66	3.66
r_2	7.39	5.84
λ	20.74	21.32
ΔG_{ET}	8.24 [a]	16.76 [b]
$\Delta G_{ET}^{\ddagger}$	10.10	17.04

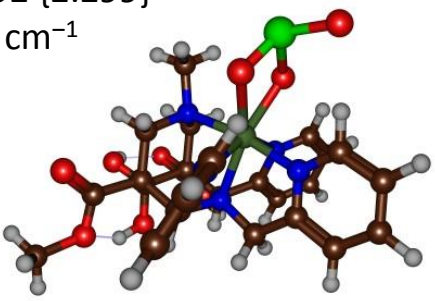
***a* Data taken from Table S4.**
***b* Data taken from Table S5.**

$r_{Fe\text{-}O}$ = 1.656 {1.650}
$r_{Fe\text{-}Naxial}$ = 2.054 {2.077}



$^{3}[Fe^{IV}(O)(L^{1})]^{2+}$ {$^{5}[Fe^{IV}(O)(L^{1})]^{2+}$}

$r_{Fe\text{-}O1}$ = 2.221 {2.131}
$r_{Fe\text{-}O2}$ = 2.407 {2.462}
$r_{Fe\text{-}Naxial}$ = 2.192 {2.299}
i72 {i17} cm^{-1}



^{3}**TS1** {^{5}**TS1**}

Figure S15: Optimized geometries of $^{3,5}[Fe^{IV}(O)(L^{1})]^{2+}$ as calculated with a solvent model included at UB3LYP/BS1 in Gaussian. Bond lengths are in angstroms.

Part III: Cartesian coordinates of all optimized geometries.

$^{3}[(L^{1})Fe^{II}]^{2+}$

26	0.777939000	3.852916000	2.403701000
8	3.983722000	4.418342000	-1.470424000
8	3.440771000	2.120052000	-1.301007000
8	0.792605000	5.195418000	-2.646139000
8	1.693058000	3.137371000	-3.103690000
8	5.999426000	3.727056000	0.168543000
8	5.536777000	1.782197000	1.261017000
7	1.361760000	2.265194000	1.101866000
7	2.068660000	5.139371000	1.377268000
7	2.236410000	3.139387000	3.581589000
7	-0.721905000	4.108172000	1.074359000
7	-0.391075000	2.473709000	3.281458000
6	0.874498000	2.782854000	-0.228694000
6	1.789566000	3.913065000	-0.812914000
6	1.682042000	5.268153000	-0.073510000
6	3.507833000	4.677091000	1.425140000
6	3.682894000	3.295552000	0.743515000
6	2.843695000	2.155868000	1.410506000
6	3.259655000	3.428391000	-0.761327000
6	0.617098000	1.034299000	1.524217000
6	-0.532562000	3.338039000	-0.040313000
6	-1.910211000	4.733548000	1.262986000
6	-2.955956000	4.618128000	0.346204000
6	-2.777455000	3.818341000	-0.786803000
6	-1.549693000	3.170204000	-0.978881000
6	1.374909000	4.180138000	-2.272444000
6	1.427893000	3.322882000	-4.561288000
1	0.378638000	3.577245000	-4.710104000
1	1.678338000	2.364555000	-5.008529000
1	2.067778000	4.121548000	-4.937218000
6	1.964887000	6.487400000	2.042165000
6	5.185560000	2.961102000	0.709738000
6	6.969783000	1.373691000	1.137023000
1	7.213213000	1.259012000	0.080807000
1	7.027461000	0.426054000	1.665490000
1	7.603797000	2.134101000	1.592602000
6	2.986396000	2.193598000	2.934975000
6	2.358170000	3.299829000	4.922782000
6	3.223261000	2.511928000	5.681628000
6	3.961976000	1.513749000	5.038703000
6	3.840734000	1.354984000	3.651877000
6	-0.316655000	1.240988000	2.711090000
6	-1.215543000	2.679824000	4.343109000
6	-1.998937000	1.660572000	4.875473000
6	-1.930356000	0.386271000	4.296649000
6	-1.080886000	0.178409000	3.207109000
1	4.955780000	4.342890000	-1.309246000
1	3.159217000	2.126988000	-2.245317000
1	0.862143000	1.966695000	-0.958741000
1	0.677293000	5.677030000	-0.140929000
1	2.361564000	5.970864000	-0.566601000
1	4.130923000	5.405110000	0.894443000
1	3.829534000	4.648640000	2.465821000
1	3.228618000	1.210393000	1.022983000
1	0.034577000	0.655861000	0.675692000
1	1.336693000	0.244933000	1.771492000
1	-2.013033000	5.330673000	2.160724000
1	-3.887481000	5.141455000	0.522561000
1	-3.576221000	3.702250000	-1.509937000
1	-1.383522000	2.549870000	-1.852103000
1	2.624738000	7.213077000	1.551029000
1	0.935464000	6.844882000	1.971866000
1	2.256306000	6.400127000	3.091733000
1	1.741482000	4.062642000	5.381784000
1	3.301775000	2.670666000	6.750025000
1	4.623727000	0.868909000	5.605337000
1	4.415515000	0.605899000	3.125966000
1	-1.232567000	3.679824000	4.759641000
1	-2.644442000	1.859562000	5.721881000
1	-2.527572000	-0.429058000	4.688156000
1	-1.009796000	-0.799442000	2.743456000

$^{2}[(L^{1})Fe^{I}]^{+}$

26	0.780656000	3.859597000	2.405791000
8	4.012265000	4.421521000	-1.485785000
8	3.457922000	2.131379000	-1.325847000
8	0.864157000	5.225533000	-2.676758000
8	1.670921000	3.125650000	-3.098956000
8	6.024896000	3.707028000	0.149406000
8	5.550587000	1.781574000	1.260616000
7	1.385146000	2.267098000	1.079213000
7	2.113365000	5.159584000	1.364255000
7	2.215219000	3.158517000	3.556512000
7	-0.691535000	4.103354000	1.111566000
7	-0.378612000	2.511179000	3.250563000
6	0.888243000	2.800901000	-0.230633000
6	1.808310000	3.928093000	-0.815507000
6	1.712690000	5.283802000	-0.074723000
6	3.536717000	4.682907000	1.414890000
6	3.698921000	3.298281000	0.730696000
6	2.853655000	2.164177000	1.401828000
6	3.275448000	3.436696000	-0.769944000
6	0.633073000	1.053132000	1.506873000
6	-0.517102000	3.351924000	-0.027456000
6	-1.905860000	4.688795000	1.318190000
6	-2.966482000	4.543151000	0.425154000
6	-2.793375000	3.765691000	-0.725227000
6	-1.545298000	3.162244000	-0.945419000
6	1.398149000	4.196854000	-2.270189000
6	1.374985000	3.307064000	-4.541117000
1	0.321005000	3.555019000	-4.670226000
1	1.619179000	2.349955000	-4.995679000
1	1.997470000	4.109346000	-4.939216000
6	2.025700000	6.504567000	2.018406000
6	5.195303000	2.956899000	0.696321000
6	6.979939000	1.390288000	1.160742000
1	7.245535000	1.266638000	0.110381000
1	7.041997000	0.449120000	1.700923000
1	7.603777000	2.159557000	1.616610000
6	2.984699000	2.206513000	2.926271000
6	2.317175000	3.288007000	4.910676000
6	3.143745000	2.470364000	5.678457000
6	3.894912000	1.474108000	5.045146000
6	3.808664000	1.348421000	3.650319000
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6	-1.217912000	2.707867000	4.306804000
6	-2.009632000	1.689549000	4.832270000
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6	-1.084246000	0.211159000	3.172097000
1	4.977114000	4.347414000	-1.286695000
1	3.117537000	2.141971000	-2.250120000
1	0.860429000	1.995791000	-0.976255000
1	0.700403000	5.677736000	-0.123793000
1	2.375929000	5.990631000	-0.586902000
1	4.183796000	5.402191000	0.897132000
1	3.844086000	4.631961000	2.459205000
1	3.250481000	1.215705000	1.028381000
1	0.053500000	0.668742000	0.657705000
1	1.346414000	0.261506000	1.767585000
1	-2.004157000	5.273077000	2.224036000
1	-3.911635000	5.030889000	0.632518000
1	-3.603690000	3.629980000	-1.431467000
1	-1.375097000	2.549793000	-1.824487000
1	2.679497000	7.234207000	1.517442000
1	0.993473000	6.855857000	1.967707000
1	2.323022000	6.412590000	3.064870000
1	1.702876000	4.056735000	5.361843000
1	3.188377000	2.608835000	6.752333000
1	4.531338000	0.810185000	5.618346000

1	4.385432000	0.599562000	3.124595000
1	-1.234687000	3.709370000	4.717717000
1	-2.661626000	1.893259000	5.673354000
1	-2.548191000	-0.398692000	4.641360000
1	-1.011686000	-0.765264000	2.704101000

$^{3}[(L^{1})Fe^{II}Ac]^{+}$

26	0.719462000	3.926463000	2.551185000
8	4.003357000	4.354189000	-1.514753000
8	3.408261000	2.085835000	-1.231904000
8	0.858646000	5.169749000	-2.678545000
8	1.606574000	3.032141000	-3.014621000
8	6.043505000	3.674851000	0.104661000
8	5.552816000	1.785345000	1.269661000
7	1.379144000	2.359271000	1.212851000
7	2.196253000	5.237127000	1.333371000
7	2.203149000	3.208998000	3.657347000
7	-0.725223000	4.172299000	1.155942000
7	-0.529212000	2.253513000	3.257020000
6	0.885744000	2.848911000	-0.128797000
6	1.807404000	3.940477000	-0.774021000
6	1.748436000	5.322053000	-0.084964000
6	3.604923000	4.753689000	1.389849000
6	3.727408000	3.343711000	0.760025000
6	2.874334000	2.259258000	1.495343000
6	3.266659000	3.423413000	-0.735934000
6	0.728030000	1.039253000	1.545755000
6	-0.520666000	3.393531000	0.049421000
6	-1.908926000	4.818462000	1.301143000
6	-2.941223000	4.672873000	0.369190000
6	-2.755908000	3.842026000	-0.736872000
6	-1.521269000	3.199786000	-0.901197000
6	1.375247000	4.149712000	-2.233046000
6	1.297679000	3.158127000	-4.460861000
1	0.249491000	3.429832000	-4.589269000
1	1.510203000	2.175706000	-4.875595000
1	1.936856000	3.924808000	-4.900414000
6	2.091303000	6.583777000	1.979101000
6	5.212183000	2.960842000	0.693448000
6	6.966445000	1.349600000	1.123406000
1	7.189645000	1.208064000	0.065573000
1	7.020135000	0.411940000	1.670665000
1	7.628363000	2.104513000	1.548362000
6	3.023671000	2.323825000	3.016127000
6	2.290734000	3.370436000	4.999319000
6	3.194447000	2.632250000	5.764846000
6	4.008864000	1.691096000	5.129448000
6	3.920338000	1.535295000	3.740132000
6	-0.415332000	1.118517000	2.538956000
6	-1.478926000	2.356260000	4.216656000
6	-2.360962000	1.310745000	4.487712000
6	-2.260518000	0.132803000	3.735767000
6	-1.275905000	0.033739000	2.748321000
1	4.970834000	4.284613000	-1.327233000
1	3.063525000	2.065409000	-2.154575000
1	0.870589000	2.007266000	-0.829572000
1	0.736811000	5.722331000	-0.105494000
1	2.390885000	6.007824000	-0.651221000
1	4.269042000	5.440817000	0.848104000
1	3.919272000	4.731913000	2.434864000
1	3.236397000	1.295856000	1.130473000
1	0.386890000	0.557231000	0.621170000
1	1.495592000	0.381056000	1.968168000
1	-1.970865000	5.491439000	2.147627000
1	-3.869142000	5.211610000	0.516803000
1	-3.546027000	3.704700000	-1.466269000
1	-1.334736000	2.566571000	-1.761460000
1	2.704944000	7.321898000	1.441941000
1	1.046684000	6.900864000	1.987534000
1	2.435488000	6.507833000	3.012121000
1	1.595940000	4.092010000	5.410218000
1	3.242181000	2.784094000	6.836369000
1	4.701041000	1.083815000	5.701888000
1	4.545690000	0.824489000	3.219378000
1	-1.499243000	3.298715000	4.748814000
1	-3.110246000	1.418051000	5.262685000
1	-2.938127000	-0.694285000	3.915824000
1	-1.174956000	-0.868737000	2.154561000
8	0.162974000	5.094974000	4.100210000
8	-0.971441000	6.884352000	3.248577000
6	-0.493704000	6.243480000	4.222679000
6	-0.618816000	6.763898000	5.641695000
1	0.373742000	7.012022000	6.036340000
1	-1.244815000	7.656483000	5.662249000
1	-1.045499000	5.996097000	6.296329000

$^{2}[(L^{1})Fe^{III}(OH)]^{2+}$

26	1.462456000	4.203572000	2.794300000
8	5.349318000	6.180634000	0.158212000
8	5.663107000	3.837980000	0.317118000
8	2.695345000	5.798072000	-2.043938000
8	4.349047000	4.208279000	-2.025889000
8	6.828221000	6.187872000	2.410099000
8	6.772890000	4.141839000	3.414107000
8	0.018257000	5.009472000	3.552688000
7	2.950858000	3.126103000	1.934262000
7	2.485549000	5.979206000	2.177048000
7	2.601159000	4.031243000	4.409872000
7	0.559136000	3.927349000	1.046887000
7	0.679867000	2.432324000	3.257655000
6	2.842890000	3.449224000	0.443747000
6	3.409608000	4.862727000	0.104241000
6	2.567695000	6.024482000	0.669205000
6	3.892725000	6.082079000	2.720288000
6	4.774595000	4.912534000	2.232920000
6	4.230718000	3.524734000	2.681368000
6	4.849648000	4.958356000	0.666551000
6	2.698380000	1.635611000	2.142712000
6	1.370488000	3.390921000	0.091593000
6	-0.768197000	4.063157000	0.830507000
6	-1.339553000	3.656675000	-0.377866000
6	-0.524466000	3.083612000	-1.359749000
6	0.851943000	2.947519000	-1.122238000
6	3.433204000	5.035035000	-1.427192000
6	4.535116000	4.352534000	-3.501415000
1	3.571931000	4.248500000	-4.000477000
1	5.218458000	3.551305000	-3.770172000
1	4.964146000	5.333352000	-3.707822000
6	1.735494000	7.207501000	2.627637000
6	6.219458000	5.148282000	2.708529000
6	8.215410000	4.283521000	3.785792000
1	8.809678000	4.345619000	2.874305000
1	8.439483000	3.381358000	4.348370000
1	8.346566000	5.182831000	4.387321000
6	3.843904000	3.522601000	4.154984000
6	2.147312000	4.132459000	5.681901000
6	2.928841000	3.727038000	6.763805000
6	4.190935000	3.176826000	6.517192000
6	4.652476000	3.071286000	5.197459000
6	1.396835000	1.355753000	2.853636000
6	-0.498170000	2.269420000	3.910763000
6	-0.995901000	0.997630000	4.187217000
6	-0.265001000	-0.124967000	3.777575000
6	0.945723000	0.056670000	3.101063000
1	6.171381000	6.462611000	0.628852000
1	5.731885000	3.790188000	-0.664823000
1	3.426472000	2.717367000	-0.120316000
1	1.559425000	6.021138000	0.261854000
1	3.046773000	6.960439000	0.365318000
1	4.336969000	7.021100000	2.373315000
1	3.841224000	6.112277000	3.808771000
1	5.008868000	2.789538000	2.472501000
1	2.712356000	1.134036000	1.169596000
1	3.531372000	1.218933000	2.717829000
1	-1.333328000	4.496311000	1.645732000
1	-2.402894000	3.783383000	-0.538722000
1	-0.949457000	2.750198000	-2.299334000
1	1.504720000	2.515658000	-1.871793000

1	2.230370000	8.107341000	2.244926000
1	0.714765000	7.171258000	2.248764000
1	1.733348000	7.252989000	3.718553000
1	1.143864000	4.518241000	5.800785000
1	2.546363000	3.826690000	7.772043000
1	4.808103000	2.830340000	7.338107000
1	5.628195000	2.662287000	4.978261000
1	-1.002993000	3.186559000	4.183600000
1	-1.938311000	0.891632000	4.710049000
1	-0.631996000	-1.124725000	3.979287000
1	1.529448000	-0.795588000	2.771397000
1	0.117508000	5.875284000	3.994224000

$^3[(L^1)Fe^{IV}(OH)]^{3+}$

26	1.443089000	4.201917000	2.791117000
8	5.344148000	6.193436000	0.193549000
8	5.654392000	3.840280000	0.319062000
8	2.662362000	5.807163000	-2.031408000
8	4.380660000	4.280186000	-2.037068000
8	6.807384000	6.171209000	2.461608000
8	6.765346000	4.080528000	3.386326000
8	0.125029000	5.048410000	3.575867000
7	2.915172000	3.136217000	1.922130000
7	2.480850000	5.979866000	2.170210000
7	2.583547000	3.986897000	4.390508000
7	0.543892000	3.897286000	1.038255000
7	0.689622000	2.422814000	3.310965000
6	2.836005000	3.473806000	0.422691000
6	3.415860000	4.878037000	0.096355000
6	2.569244000	6.031121000	0.659782000
6	3.889016000	6.053710000	2.739933000
6	4.767507000	4.892691000	2.241965000
6	4.217017000	3.507300000	2.672172000
6	4.852816000	4.962083000	0.672197000
6	2.652293000	1.628658000	2.105674000
6	1.371406000	3.408598000	0.063607000
6	-0.793909000	3.988012000	0.827009000
6	-1.352059000	3.609267000	-0.394509000
6	-0.519856000	3.100501000	-1.398935000
6	0.860169000	2.994384000	-1.162892000
6	3.441465000	5.063119000	-1.441566000
6	4.599648000	4.450209000	-3.517905000
1	3.639384000	4.407252000	-4.030282000
1	5.247530000	3.622017000	-3.791416000
1	5.082178000	5.413549000	-3.682802000
6	1.738263000	7.216892000	2.638255000
6	6.217428000	5.115989000	2.729362000
6	8.226487000	4.185376000	3.746287000
1	8.803688000	4.267320000	2.825789000
1	8.439546000	3.259428000	4.272747000
1	8.375506000	5.062012000	4.375889000
6	3.832220000	3.482574000	4.139997000
6	2.118336000	4.122388000	5.657794000
6	2.905467000	3.744495000	6.745671000
6	4.170112000	3.190675000	6.511406000
6	4.639096000	3.060578000	5.194015000
6	1.400100000	1.346737000	2.890248000
6	-0.451232000	2.273696000	4.033931000
6	-0.921768000	1.003361000	4.358637000
6	-0.203930000	-0.122788000	3.931299000
6	0.970652000	0.051922000	3.189543000
1	6.188806000	6.463279000	0.630878000
1	5.782326000	3.820252000	-0.658458000
1	3.435695000	2.736802000	-0.117671000
1	1.565274000	6.044107000	0.240889000
1	3.056222000	6.970834000	0.378785000
1	4.334578000	6.994203000	2.399020000
1	3.821753000	6.085828000	3.827113000
1	4.975896000	2.762966000	2.425847000
1	2.591617000	1.169796000	1.114429000
1	3.521501000	1.190702000	2.604720000
1	-1.398812000	4.356802000	1.644011000
1	-2.420016000	3.707773000	-0.547656000
1	-0.935560000	2.789367000	-2.350646000
1	1.523303000	2.603135000	-1.925578000
1	2.309307000	8.104512000	2.347070000
1	0.765443000	7.271204000	2.146737000
1	1.638473000	7.203893000	3.723572000
1	1.121889000	4.527418000	5.770837000
1	2.525297000	3.873510000	7.751950000
1	4.787082000	2.865207000	7.341503000
1	5.621135000	2.659819000	4.986955000
1	-0.958074000	3.180675000	4.332977000
1	-1.833891000	0.902749000	4.934499000
1	-0.552606000	-1.120681000	4.172487000
1	1.543817000	-0.804208000	2.850856000
1	-0.269615000	5.934493000	3.446751000

$^3[(L^1)Fe^{II}(H_2O)]^{2+}$

26	0.742106000	3.944740000	2.480341000
8	3.977975000	4.456712000	-1.445347000
8	3.462876000	2.153275000	-1.282463000
8	0.778229000	5.185682000	-2.633803000
8	1.689190000	3.129766000	-3.076570000
8	5.998262000	3.779826000	0.205579000
8	5.541631000	1.810238000	1.254659000
8	0.079275000	5.520649000	3.912682000
7	1.363448000	2.326861000	1.156161000
7	2.074706000	5.199717000	1.386539000
7	2.304065000	3.101891000	3.635279000
7	-0.788711000	4.083334000	1.020880000
7	-0.434291000	2.519229000	3.301607000
6	0.889302000	2.789151000	-0.197482000
6	1.786760000	3.923538000	-0.790788000
6	1.667646000	5.280595000	-0.065119000
6	3.504816000	4.706522000	1.446700000
6	3.682143000	3.327244000	0.767770000
6	2.847296000	2.185899000	1.426910000
6	3.262416000	3.457284000	-0.738911000
6	0.634803000	1.085092000	1.580182000
6	-0.541302000	3.292539000	-0.060636000
6	-2.011051000	4.647337000	1.170663000
6	-3.034171000	4.449305000	0.241946000
6	-2.792219000	3.626538000	-0.862920000
6	-1.529378000	3.038448000	-1.012540000
6	1.366430000	4.177250000	-2.251041000
6	1.411285000	3.302074000	-4.532511000
1	0.357046000	3.538781000	-4.675550000
1	1.673665000	2.345175000	-4.976047000
1	2.035016000	4.108613000	-4.918723000
6	2.060852000	6.599464000	1.935416000
6	5.186116000	3.000385000	0.731098000
6	6.973911000	1.408233000	1.117752000
1	7.215068000	1.317359000	0.058641000
1	7.035482000	0.449249000	1.624944000
1	7.608319000	2.159266000	1.588149000
6	3.017442000	2.165971000	2.946197000
6	2.448202000	3.197603000	4.979126000
6	3.291155000	2.350040000	5.697166000
6	3.992383000	1.358025000	5.003551000
6	3.853951000	1.267769000	3.613148000
6	-0.312976000	1.281418000	2.748578000
6	-1.321862000	2.698362000	4.316403000
6	-2.091773000	1.662367000	4.834070000
6	-1.954107000	0.382042000	4.283138000
6	-1.060386000	0.197802000	3.227415000
1	4.950100000	4.388495000	-1.283139000
1	3.171349000	2.156395000	-2.223781000
1	0.922941000	1.951538000	-0.902910000
1	0.653429000	5.667817000	-0.122740000
1	2.326435000	5.985101000	-0.583203000
1	4.146863000	5.424527000	0.924488000
1	3.809232000	4.672265000	2.492506000
1	3.208503000	1.246467000	1.001590000
1	0.065560000	0.691636000	0.729070000
1	1.363802000	0.307699000	1.836665000
1	-2.155551000	5.258746000	2.052637000
1	-3.996486000	4.924716000	0.386543000

1	-3.570236000	3.445568000	-1.595395000
1	-1.314034000	2.398958000	-1.861152000
1	2.756601000	7.240230000	1.380046000
1	1.057029000	7.017611000	1.822241000
1	2.361618000	6.583844000	2.984679000
1	1.870575000	3.968023000	5.473557000
1	3.385195000	2.458783000	6.770695000
1	4.638143000	0.667876000	5.534170000
1	4.400306000	0.526803000	3.046669000
1	-1.424124000	3.704248000	4.697190000
1	-2.784156000	1.854708000	5.644311000
1	-2.536358000	-0.449421000	4.662858000
1	-0.942200000	-0.778705000	2.770469000
1	0.186290000	6.470956000	3.725153000
1	-0.209096000	5.393712000	4.834593000

$^{2}[(L^{1})Fe^{III}(H_2O)]^{3+}$

26	0.751473000	3.811693000	2.431331000
8	3.973149000	4.418558000	-1.458548000
8	3.432875000	2.113857000	-1.263514000
8	0.748321000	5.165007000	-2.618207000
8	1.696464000	3.124978000	-3.085071000
8	6.001516000	3.753977000	0.197985000
8	5.527562000	1.761682000	1.211910000
8	0.104639000	5.265925000	3.708537000
7	1.344791000	2.374639000	1.209248000
7	2.061945000	5.142695000	1.387868000
7	2.190350000	3.096101000	3.597665000
7	-0.731117000	4.044580000	1.129935000
7	-0.451883000	2.450833000	3.286994000
6	0.881274000	2.805953000	-0.187061000
6	1.789544000	3.910099000	-0.801008000
6	1.670383000	5.258564000	-0.074291000
6	3.511613000	4.679827000	1.440805000
6	3.692680000	3.310851000	0.761129000
6	2.855140000	2.196497000	1.442300000
6	3.261942000	3.429856000	-0.747378000
6	0.642526000	1.065221000	1.586652000
6	-0.528609000	3.330294000	-0.021976000
6	-1.922327000	4.660527000	1.347430000
6	-2.951028000	4.600072000	0.408996000
6	-2.759505000	3.860627000	-0.765626000
6	-1.532618000	3.213651000	-0.979357000
6	1.359711000	4.158928000	-2.266511000
6	1.446391000	3.291404000	-4.559435000
1	0.411394000	3.592530000	-4.716921000
1	1.655589000	2.312102000	-4.980890000
1	2.130219000	4.050266000	-4.939675000
6	2.023274000	6.539849000	1.966285000
6	5.197590000	2.966782000	0.715954000
6	6.955364000	1.313225000	1.038189000
1	7.167228000	1.240827000	-0.028188000
1	6.991954000	0.340812000	1.521040000
1	7.617009000	2.035633000	1.515066000
6	3.010926000	2.205600000	2.952557000
6	2.295361000	3.261827000	4.942582000
6	3.210705000	2.536016000	5.700593000
6	4.020973000	1.591696000	5.057834000
6	3.919321000	1.428078000	3.668606000
6	-0.316977000	1.213816000	2.737485000
6	-1.349802000	2.639293000	4.293943000
6	-2.113386000	1.595763000	4.804368000
6	-1.962069000	0.312578000	4.257989000
6	-1.058847000	0.125960000	3.208052000
1	4.951679000	4.341395000	-1.343911000
1	3.198145000	2.105012000	-2.221130000
1	0.924305000	1.936509000	-0.847607000
1	0.666007000	5.670000000	-0.146234000
1	2.352485000	5.962651000	-0.560635000
1	4.123972000	5.415158000	0.909157000
1	3.831337000	4.662905000	2.482902000
1	3.165409000	1.245984000	1.005645000
1	0.108319000	0.692159000	0.707101000
1	1.404572000	0.318126000	1.826938000
1	-2.035566000	5.194088000	2.280931000
1	-3.884347000	5.116065000	0.598913000
1	-3.550397000	3.788428000	-1.503585000
1	-1.361804000	2.638110000	-1.881571000
1	2.722956000	7.182794000	1.421881000
1	1.025524000	6.966965000	1.830979000
1	2.322203000	6.522931000	3.015272000
1	1.639280000	3.983172000	5.408335000
1	3.277632000	2.699972000	6.769265000
1	4.723019000	0.993100000	5.627317000
1	4.548936000	0.724948000	3.142647000
1	-1.475759000	3.641670000	4.675492000
1	-2.815253000	1.784538000	5.607630000
1	-2.543553000	-0.520245000	4.636851000
1	-0.934084000	-0.851578000	2.755255000
1	0.157560000	6.215271000	3.492365000
1	-0.132835000	5.137574000	4.644177000

$^{3}[(L1)Fe^{IV}=O]^{2+}$

26	0.746488000	3.844650000	2.443125000
8	3.981275000	4.422864000	-1.453397000
8	3.432696000	2.124895000	-1.278501000
8	0.799140000	5.204633000	-2.630540000
8	1.679238000	3.134603000	-3.079025000
8	6.000139000	3.726810000	0.186457000
8	5.524165000	1.769710000	1.254419000
8	0.220230000	5.004972000	3.496730000
7	1.342330000	2.338823000	1.173803000
7	2.064827000	5.138917000	1.402205000
7	2.206183000	3.130079000	3.571911000
7	-0.713010000	4.058135000	1.108601000
7	-0.401706000	2.438837000	3.258498000
6	0.878273000	2.799280000	-0.203645000
6	1.787482000	3.921812000	-0.794045000
6	1.672042000	5.266939000	-0.048455000
6	3.504102000	4.675780000	1.450109000
6	3.684246000	3.303873000	0.762161000
6	2.843455000	2.176721000	1.433254000
6	3.257867000	3.436924000	-0.742418000
6	0.629179000	1.044577000	1.537657000
6	-0.530654000	3.330399000	-0.031182000
6	-1.881600000	4.702579000	1.333345000
6	-2.926921000	4.636810000	0.410098000
6	-2.763586000	3.874983000	-0.751647000
6	-1.547697000	3.211965000	-0.975300000
6	1.371765000	4.185630000	-2.254325000
6	1.417242000	3.315077000	-4.539095000
1	0.373000000	3.588255000	-4.689418000
1	1.649920000	2.349209000	-4.979588000
1	2.072224000	4.099247000	-4.919482000
6	2.001167000	6.515949000	2.026887000
6	5.184013000	2.960300000	0.721924000
6	6.952856000	1.346177000	1.117609000
1	7.191570000	1.251572000	0.058389000
1	7.000207000	0.386692000	1.625284000
1	7.596579000	2.089229000	1.587921000
6	2.992974000	2.203273000	2.948647000
6	2.304946000	3.340276000	4.905897000
6	3.194790000	2.600272000	5.685443000
6	3.972189000	1.612395000	5.072315000
6	3.872969000	1.414006000	3.687571000
6	-0.322711000	1.207413000	2.697075000
6	-1.232486000	2.663499000	4.309557000
6	-2.019640000	1.643268000	4.836673000
6	-1.949293000	0.365293000	4.266496000
6	-1.091180000	0.146382000	3.184627000
1	4.953743000	4.352050000	-1.291540000
1	3.160714000	2.131662000	-2.225696000
1	0.909959000	1.952314000	-0.893947000
1	0.666059000	5.674563000	-0.108714000
1	2.345925000	5.977836000	-0.536547000
1	4.123379000	5.411085000	0.925806000
1	3.822043000	4.647421000	2.491687000
1	3.180377000	1.227713000	1.014099000

1	0.087250000	0.678518000	0.659216000
1	1.378932000	0.283363000	1.776743000
1	-1.949493000	5.262367000	2.256897000
1	-3.848751000	5.170689000	0.604530000
1	-3.565763000	3.800600000	-1.476554000
1	-1.393175000	2.624413000	-1.872688000
1	2.671530000	7.192243000	1.484702000
1	0.979144000	6.886635000	1.974378000
1	2.299606000	6.453745000	3.072184000
1	1.654729000	4.099987000	5.319584000
1	3.263440000	2.789871000	6.749424000
1	4.651579000	1.006003000	5.660199000
1	4.482429000	0.677456000	3.184167000
1	-1.240217000	3.672087000	4.701013000
1	-2.673289000	1.848231000	5.675349000
1	-2.552342000	-0.445936000	4.657662000
1	-1.018090000	-0.833079000	2.725322000

^{2}[(L^{1})Fe^{III}=O]$^{+}$

26	0.758919000	3.832924000	2.423815000
8	3.997849000	4.409719000	-1.478708000
8	3.435416000	2.122208000	-1.298422000
8	0.853403000	5.220395000	-2.666832000
8	1.656127000	3.116118000	-3.079318000
8	6.014980000	3.700522000	0.152125000
8	5.535441000	1.779948000	1.272020000
8	0.127723000	5.055711000	3.559493000
7	1.356106000	2.320609000	1.141977000
7	2.094488000	5.149193000	1.384845000
7	2.205638000	3.146372000	3.560488000
7	-0.695545000	4.082569000	1.097877000
7	-0.375274000	2.431047000	3.236614000
6	0.879611000	2.803219000	-0.214492000
6	1.794495000	3.929389000	-0.800377000
6	1.694137000	5.280037000	-0.052818000
6	3.522378000	4.686448000	1.429640000
6	3.691848000	3.304438000	0.747240000
6	2.848192000	2.177871000	1.426264000
6	3.261726000	3.435450000	-0.753243000
6	0.640672000	1.037908000	1.507783000
6	-0.530723000	3.345187000	-0.034658000
6	-1.857183000	4.729476000	1.333799000
6	-2.921055000	4.646393000	0.430917000
6	-2.776364000	3.869438000	-0.723330000
6	-1.561605000	3.208583000	-0.962373000
6	1.385916000	4.193124000	-2.256734000
6	1.370386000	3.293970000	-4.524951000
1	0.319889000	3.552245000	-4.661607000
1	1.607829000	2.332480000	-4.973735000
1	2.003672000	4.088204000	-4.922032000
6	2.009111000	6.500301000	2.039146000
6	5.185605000	2.957135000	0.706480000
6	6.962537000	1.378463000	1.164320000
1	7.221417000	1.255099000	0.112333000
1	7.021041000	0.435766000	1.702246000
1	7.593392000	2.142938000	1.618469000
6	2.993333000	2.216102000	2.948672000
6	2.275247000	3.344540000	4.895891000
6	3.142390000	2.590431000	5.689402000
6	3.925360000	1.600889000	5.085305000
6	3.851187000	1.410500000	3.697534000
6	-0.310945000	1.201083000	2.674262000
6	-1.190223000	2.658589000	4.296776000
6	-1.983894000	1.643062000	4.827366000
6	-1.931772000	0.367017000	4.251790000
6	-1.083619000	0.142805000	3.162809000
1	4.962909000	4.343931000	-1.276620000
1	3.110439000	2.132267000	-2.228330000
1	0.890515000	1.971869000	-0.926878000
1	0.683637000	5.678298000	-0.097688000
1	2.356165000	5.990668000	-0.560497000
1	4.160203000	5.411377000	0.909393000
1	3.834682000	4.644056000	2.472723000
1	3.206506000	1.226565000	1.027645000

1	0.092395000	0.671214000	0.632178000
1	1.385349000	0.270177000	1.746629000
1	-1.872809000	5.297686000	2.257203000
1	-3.843184000	5.177613000	0.633277000
1	-3.592249000	3.780403000	-1.431551000
1	-1.421331000	2.608616000	-1.854612000
1	2.611668000	7.229984000	1.480254000
1	0.964570000	6.801317000	2.085443000
1	2.370874000	6.418016000	3.063583000
1	1.597826000	4.104457000	5.269970000
1	3.188233000	2.765919000	6.757475000
1	4.585987000	0.982647000	5.682769000
1	4.458528000	0.664946000	3.203775000
1	-1.150532000	3.675838000	4.672255000
1	-2.627754000	1.848982000	5.673786000
1	-2.539352000	-0.440356000	4.644985000
1	-1.021530000	-0.836584000	2.700662000

^{3}[(N4Py)$Fe^{II}H_2O$]$^{2+}$

26	-0.125661000	0.009041000	-0.013520000
7	-0.052560000	-0.001124000	2.080947000
7	0.481480000	0.000335000	-1.995409000
7	0.320124000	1.968532000	0.131659000
7	-0.044339000	-1.995885000	-0.062932000
6	1.166152000	0.423925000	2.514049000
6	1.487597000	0.469075000	3.869138000
1	2.466620000	0.805689000	4.190656000
6	0.522309000	0.069018000	4.804959000
1	0.746091000	0.096146000	5.865089000
6	-0.727618000	-0.370292000	4.354646000
1	-1.492535000	-0.688512000	5.052177000
6	-0.980584000	-0.399523000	2.981106000
1	-1.926316000	-0.742763000	2.581332000
6	1.827145000	-0.003890000	-2.189822000
6	2.369101000	-0.113169000	-3.474725000
1	3.445328000	-0.125663000	-3.607700000
6	1.515667000	-0.200292000	-4.578453000
1	1.921835000	-0.283789000	-5.579826000
6	0.130952000	-0.179401000	-4.370669000
1	-0.562234000	-0.241912000	-5.200380000
6	-0.348614000	-0.083244000	-3.066818000
1	-1.410714000	-0.068691000	-2.857386000
6	1.492877000	2.157097000	0.806589000
6	2.043690000	3.426564000	0.970600000
1	2.977313000	3.552124000	1.507010000
6	1.374333000	4.533058000	0.428219000
1	1.783824000	5.529786000	0.543988000
6	0.178752000	4.333051000	-0.270228000
1	-0.359686000	5.165043000	-0.706994000
6	-0.317617000	3.035184000	-0.406258000
1	-1.227735000	2.827518000	-0.954678000
6	1.175849000	-2.526950000	0.242373000
6	1.399423000	-3.905064000	0.162996000
1	2.379138000	-4.305317000	0.399347000
6	0.358705000	-4.756913000	-0.217981000
1	0.520718000	-5.826673000	-0.280693000
6	-0.891641000	-4.205788000	-0.521448000
1	-1.723215000	-4.830576000	-0.822848000
6	-1.051891000	-2.825295000	-0.437601000
1	-1.998578000	-2.357904000	-0.673834000
6	2.089775000	0.876538000	1.387536000
1	3.099815000	1.064769000	1.771712000
6	2.725704000	0.183199000	-0.974939000
1	3.031044000	1.234923000	-0.930387000
1	3.646318000	-0.399025000	-1.104880000
6	2.272481000	-1.588992000	0.728718000
1	2.305414000	-1.631302000	1.822929000
1	3.246300000	-1.951982000	0.377888000
7	2.059710000	-0.176880000	0.305709000
8	-2.311210000	0.361408000	-0.120051000
1	-2.672395000	1.108245000	0.392461000
1	-3.034819000	-0.133838000	-0.546053000

^{3}[(N4Py)Fe^{IV}O]$^{2+}$

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.989754000
7	0.479503000	0.000000000	-1.916064000
7	0.433187000	1.937274000	0.136846000
7	0.038037000	-1.974558000	-0.030383000
6	1.200313000	0.405594000	2.494035000
6	1.430047000	0.458017000	3.864217000
1	2.390650000	0.776217000	4.252576000
6	0.386133000	0.093870000	4.731325000
1	0.536023000	0.126937000	5.804249000
6	-0.845567000	-0.304397000	4.201120000
1	-1.669798000	-0.576838000	4.848285000
6	-1.012396000	-0.345209000	2.813223000
1	-1.942619000	-0.634735000	2.342937000
6	1.813283000	0.021162000	-2.187460000
6	2.276579000	-0.050813000	-3.501991000
1	3.341668000	-0.041003000	-3.704153000
6	1.351108000	-0.130930000	-4.549250000
1	1.693750000	-0.186643000	-5.575996000
6	-0.017916000	-0.138650000	-4.255213000
1	-0.759833000	-0.196466000	-5.041757000
6	-0.425388000	-0.076075000	-2.924038000
1	-1.466552000	-0.082152000	-2.630021000
6	1.590697000	2.147856000	0.826329000
6	2.096004000	3.428628000	1.019575000
1	3.020498000	3.582659000	1.564014000
6	1.376696000	4.516701000	0.497043000
1	1.745627000	5.526570000	0.634077000
6	0.181943000	4.287851000	-0.193545000
1	-0.397550000	5.110272000	-0.593824000
6	-0.269950000	2.975358000	-0.363357000
1	-1.189887000	2.734221000	-0.879005000
6	1.240111000	-2.542673000	0.262114000
6	1.411114000	-3.926281000	0.199589000
1	2.375785000	-4.365495000	0.427337000
6	0.323995000	-4.733797000	-0.155066000
1	0.439281000	-5.810215000	-0.207684000
6	-0.909643000	-4.136005000	-0.440533000
1	-1.771148000	-4.731878000	-0.714752000
6	-1.021927000	-2.748563000	-0.373926000
1	-1.944687000	-2.225451000	-0.586861000
6	2.157204000	0.853996000	1.396887000
1	3.182966000	0.970522000	1.758845000
6	2.737754000	0.190460000	-1.001324000
1	3.052803000	1.237136000	-0.933315000
1	3.648136000	-0.404616000	-1.125680000
6	2.335358000	-1.601467000	0.714393000
1	2.405148000	-1.625134000	1.807052000
1	3.309769000	-1.919001000	0.329667000
7	2.039401000	-0.185592000	0.282988000
8	-1.628736000	0.153320000	-0.220944000

^{6}[(N4Py)Fe^{IV}O]$^{+}$

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	2.228682000
7	1.138798000	0.000000000	-1.874443000
7	0.707451000	2.072300000	0.365523000
7	0.383999000	-2.152044000	0.067160000
6	1.180338000	0.378129000	2.778241000
6	1.359348000	0.424545000	4.161073000
1	2.311905000	0.726299000	4.582578000
6	0.283674000	0.075366000	4.990443000
1	0.396771000	0.102542000	6.068441000
6	-0.933264000	-0.304272000	4.414987000
1	-1.783493000	-0.572373000	5.030086000
6	-1.041202000	-0.331983000	3.020635000
1	-1.955562000	-0.608662000	2.510409000
6	2.490548000	-0.034269000	-1.839035000
6	3.236710000	-0.198657000	-3.011509000
1	4.320092000	-0.234863000	-2.968268000
6	2.566787000	-0.311785000	-4.234603000
1	3.128600000	-0.437632000	-5.153682000
6	1.167361000	-0.265203000	-4.258929000
1	0.619502000	-0.350488000	-5.189392000
6	0.480957000	-0.114037000	-3.053836000
1	-0.600142000	-0.084915000	-2.981769000
6	1.784941000	2.152870000	1.184212000
6	2.362965000	3.380514000	1.508564000
1	3.227345000	3.426207000	2.161893000
6	1.802053000	4.549872000	0.974634000
1	2.232392000	5.516575000	1.211019000
6	0.683799000	4.457567000	0.139643000
1	0.224508000	5.343769000	-0.280840000
6	0.158521000	3.193463000	-0.147342000
1	-0.709437000	3.049812000	-0.779088000
6	1.591518000	-2.605294000	0.474000000
6	1.920603000	-3.961751000	0.373174000
1	2.896166000	-4.311897000	0.693169000
6	0.974596000	-4.855141000	-0.141465000
1	1.211310000	-5.910169000	-0.225009000
6	-0.275469000	-4.374077000	-0.550355000
1	-1.027934000	-5.040907000	-0.953405000
6	-0.537433000	-3.008289000	-0.438008000
1	-1.470111000	-2.550388000	-0.746091000
6	2.242597000	0.816234000	1.769789000
1	3.202008000	0.956024000	2.289333000
6	3.164909000	0.191060000	-0.494074000
1	3.398149000	1.258942000	-0.410130000
1	4.128683000	-0.337482000	-0.474806000
6	2.541912000	-1.603677000	1.114245000
1	2.397289000	-1.650471000	2.199972000
1	3.579795000	-1.914683000	0.928065000
7	2.329445000	-0.200832000	0.670897000
8	-1.626475000	0.036680000	-0.584222000

^{6}[(N4Py)Fe^{III}OH]$^{2+}$

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	2.185680000
7	0.944842000	0.000000000	-1.919733000
7	0.623875000	2.066776000	0.294334000
7	0.288959000	-2.116190000	0.034460000
6	1.182744000	0.410481000	2.716824000
6	1.386023000	0.459649000	4.093668000
1	2.337578000	0.784348000	4.499268000
6	0.334779000	0.079805000	4.942862000
1	0.467340000	0.107913000	6.018326000
6	-0.881549000	-0.334329000	4.389100000
1	-1.711078000	-0.629152000	5.019679000
6	-1.017368000	-0.365337000	2.998491000
1	-1.934664000	-0.678933000	2.517284000
6	2.302808000	-0.000305000	-1.946065000
6	2.997138000	-0.144950000	-3.149913000
1	4.081381000	-0.152330000	-3.155372000
6	2.277464000	-0.274962000	-4.343276000
1	2.800964000	-0.386765000	-5.285916000
6	0.877050000	-0.262099000	-4.305635000
1	0.291054000	-0.359641000	-5.211027000
6	0.240237000	-0.128550000	-3.074129000
1	-0.837470000	-0.124678000	-2.976628000
6	1.715742000	2.185763000	1.096286000
6	2.271804000	3.428442000	1.389628000
1	3.145429000	3.505177000	2.026983000
6	1.678114000	4.577211000	0.843070000
1	2.091853000	5.556359000	1.055252000
6	0.551078000	4.446680000	0.024335000
1	0.070127000	5.315371000	-0.407791000
6	0.046236000	3.169607000	-0.234134000
1	-0.821689000	3.009786000	-0.860658000
6	1.507779000	-2.572638000	0.422060000
6	1.822959000	-3.931709000	0.342772000
1	2.803003000	-4.281927000	0.647121000
6	0.859236000	-4.830707000	-0.128140000
1	1.087379000	-5.888414000	-0.194373000
6	-0.398866000	-4.349697000	-0.514533000
1	-1.165953000	-5.019926000	-0.881970000
6	-0.650825000	-2.982598000	-0.426336000
1	-1.596315000	-2.546783000	-0.720998000
6	2.199496000	0.861122000	1.675046000

1	3.192034000	0.974851000	2.126042000
6	3.021527000	0.238100000	-0.633989000
1	3.252610000	1.305973000	-0.554413000
1	3.982265000	-0.289662000	-0.626327000
6	2.474614000	-1.564473000	1.010088000
1	2.390980000	-1.600026000	2.101863000
1	3.506350000	-1.845014000	0.768457000
7	2.197043000	-0.160442000	0.555784000
8	-1.728082000	0.123623000	-0.441063000
1	-2.673814000	0.313229000	-0.539779000

^{5}[(N4Py)Fe^{II}]$^{2+}$

6	-1.950367000	-2.482521000	1.270250000
6	-2.995916000	-3.318048000	0.870019000
6	-3.604130000	-3.094170000	-0.369258000
6	-3.155317000	-2.036313000	-1.174090000
6	-2.114625000	-1.233091000	-0.711010000
7	-1.520718000	-1.457121000	0.496660000
6	-1.604770000	-0.000011000	-1.459104000
6	-2.114643000	1.233061000	-0.711010000
6	-3.155346000	2.036269000	-1.174092000
6	-3.604175000	3.094119000	-0.369261000
6	-2.995965000	3.318006000	0.870017000
6	-1.950404000	2.482494000	1.270249000
7	-1.520740000	1.457100000	0.496660000
7	-0.087758000	0.000000000	-1.418317000
6	0.560352000	1.254657000	-1.924291000
6	0.560370000	-1.254649000	-1.924290000
6	1.632778000	-1.808711000	-0.995376000
6	1.632749000	1.808738000	-0.995377000
6	2.636308000	2.648201000	-1.488057000
6	3.554757000	3.218853000	-0.600301000
6	3.454350000	2.931609000	0.766522000
6	2.442945000	2.076673000	1.197100000
7	1.547488000	1.525029000	0.335600000
7	1.547512000	-1.525004000	0.335601000
6	2.442979000	-2.076633000	1.197100000
6	3.454400000	-2.931550000	0.766521000
6	3.554811000	-3.218792000	-0.600302000
6	2.636353000	-2.648155000	-1.488057000
26	0.096839000	0.000001000	0.722984000
1	-1.445242000	-2.626147000	2.217393000
1	-3.320948000	-4.124317000	1.515788000
1	-4.413592000	-3.730738000	-0.707477000
1	-3.610182000	-1.844898000	-2.139422000
1	-3.610207000	1.844847000	-2.139424000
1	-4.413645000	3.730676000	-0.707481000
1	-3.321009000	4.124271000	1.515786000
1	-1.445283000	2.626127000	2.217393000
1	0.987161000	1.084063000	-2.919257000
1	-0.216448000	2.017787000	-2.045249000
1	-0.216418000	-2.017792000	-2.045244000
1	0.987174000	-1.084051000	-2.919257000
1	2.696859000	2.856336000	-2.550508000
1	4.336013000	3.873559000	-0.969009000
1	4.147525000	3.355889000	1.482164000
1	2.335089000	1.817352000	2.243486000
1	2.335119000	-1.817315000	2.243487000
1	4.147582000	-3.355819000	1.482163000
1	4.336079000	-3.873483000	-0.969010000
1	2.696907000	-2.856288000	-2.550508000
1	-1.985877000	-0.000015000	-2.487062000