Supporting Information

Spectroscopic and Reactivity Comparisons of a Pair of bTAML Complexes with Fe^{V}=O and Fe^{IV}=O Units

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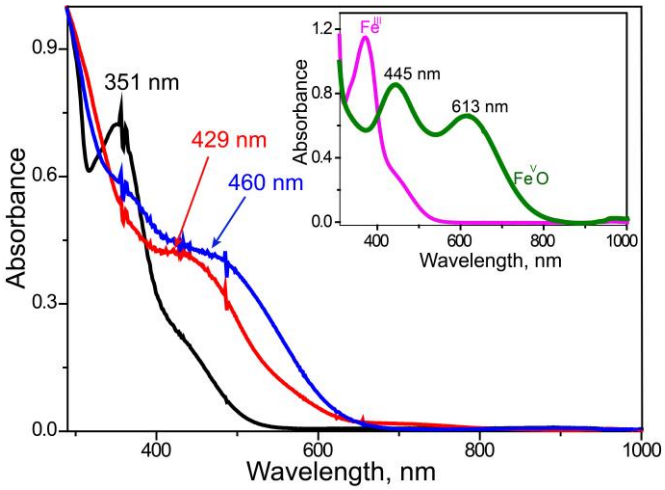


Figure S1: UV-vis absorption spectra of **2 (**1.8×10^{-4} M) synthesized in acetonitrile (red) and UV-vis and in pH 12 water (blue). Both samples were prepared via oxidation of **1** (1.8×10^{-4} M; black). Please note: the red shift in UV-Vis spectrum for $Fe^{IV}(O)$ in the water/acetonitrile solvent mixture compared to MeCN may be due to the difference in solvent polarity in the two solvents or to possible coordination of the solvent to the available sixth site. For example, $[Fe^{IV}(O)N_4Py]$ exhibits an absorption maxima at 695 in MeCN (*J. Am. Chem. Soc.*, **2004**, *126*,472–473) and at 670 nm in water (*Angew. Chem. Int. Ed.*, **2015**, *54*, 4357). This example shows that solvent can affect the absorbance max even when there are no available coordination sites in the Fe(IV)=O center. Inset: UV-vis absorption spectra of 2.8×10^{-4} M of **1** (pink) and **3** (green) in acetonitrile.

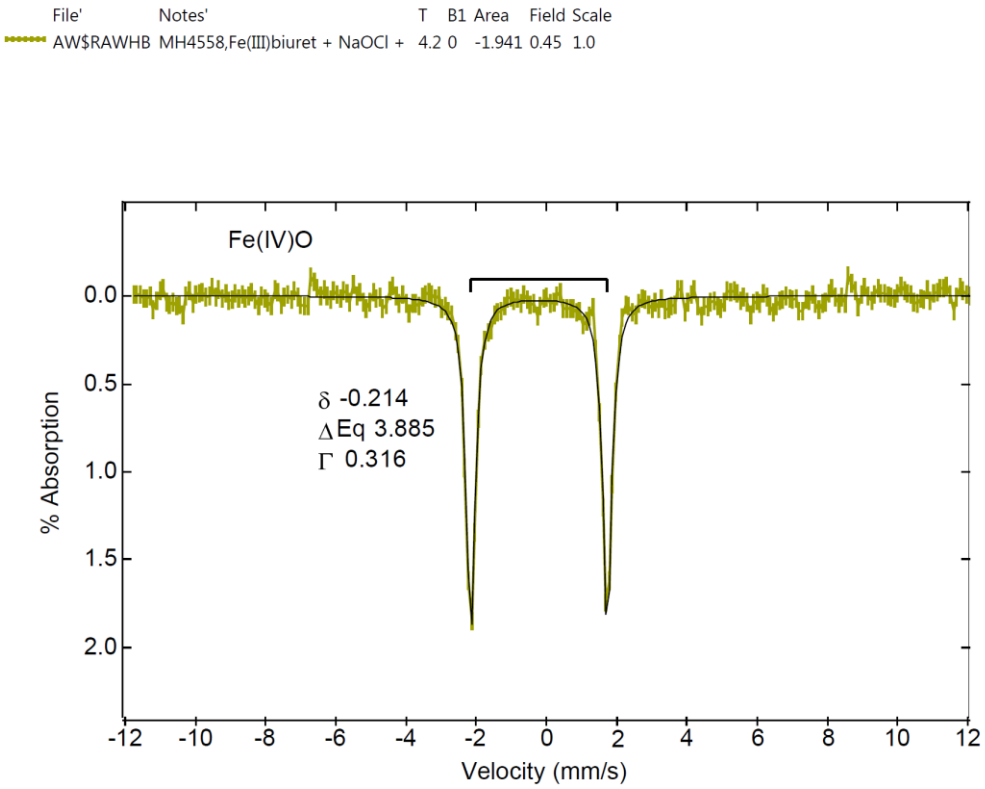
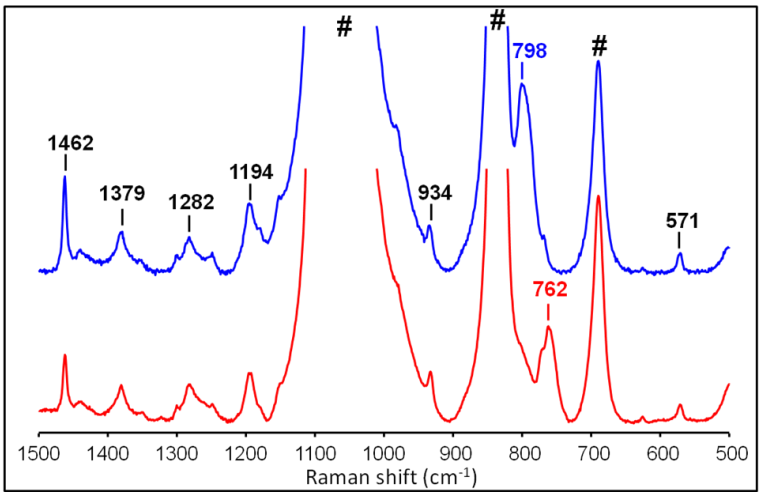


Figure S2a. Mossbauer spectra of $[Fe^{IV}(O)]^{2-}$ (**2**) synthesized in water (pH 12).



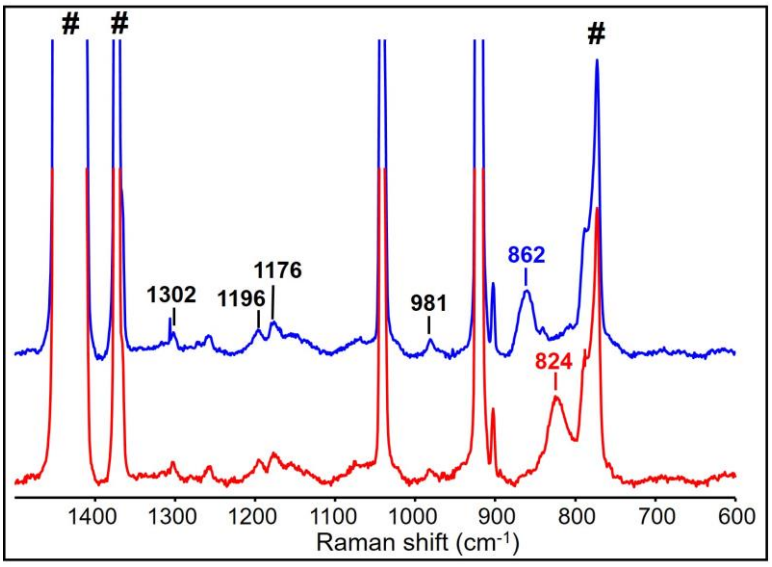


Figure S2b. Resonance Raman spectra of **2** (top) and **3** (bottom) at room temperature and 77 K, respectively**.** Blue and red lines represent ^{16}O-and ^{18}O-labelled samples, respectively. Conditions: **2**: λ_{ex} = 476.5 nm, power ~40 mW in CH_3CN; **3**: λ_{ex} = 476.5 nm, power ~40 mW in CD_3CN

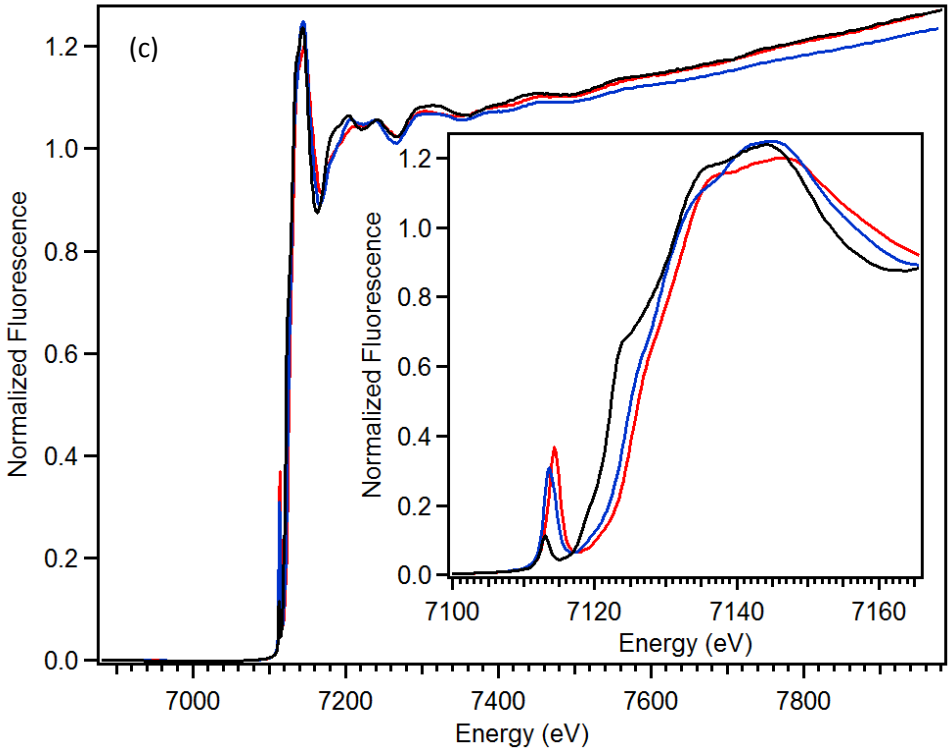


Figure S2c. Normalized Fe K-edge fluorescence spectra of **1** (black), **2** (blue) and **3** (red); inset – zoom in on the XANES region**.**

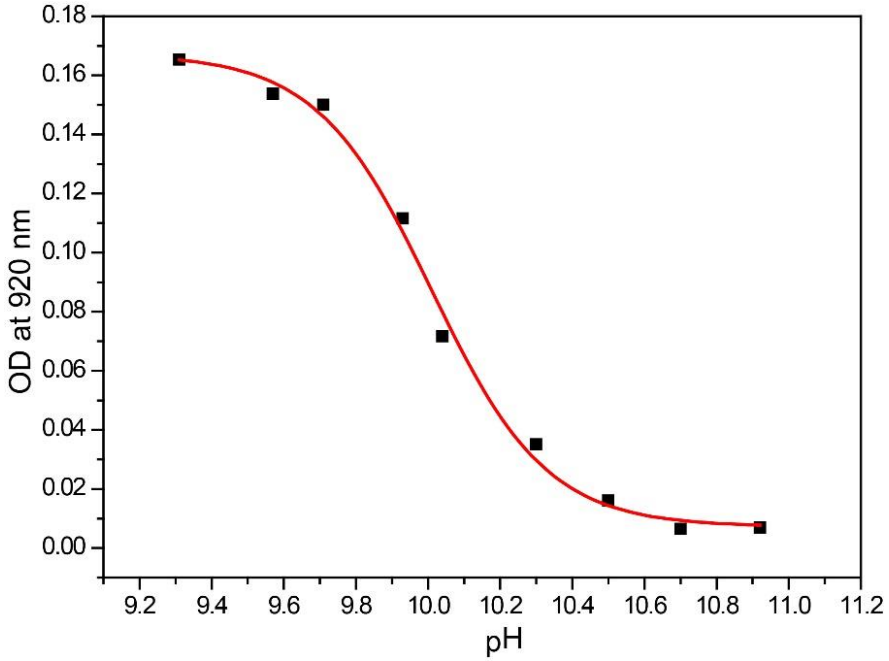


Figure S3. pK_a determination of **2** in water. The pK_a was determined by monitoring the increase in absorbance at 920 nm due to the formation of μ-O-Fe^{IV}_2 upon addition of acid. The following equilibrium takes place:

$$2\ Fe^{IV}(O)^{2-} + 2\ H^+ \rightleftharpoons Fe^{IV}(OH)^{1-} \xrightarrow{-\ H_2O} [Fe^{IV}_2O]^{1-}$$

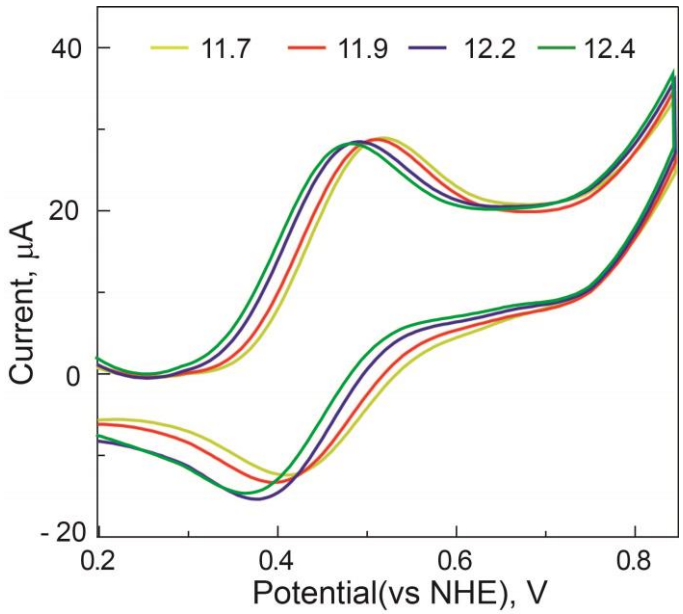


Figure S4: CVs of 2 mM of $[(bTAML)Fe^{III}(Cl)]^{2-}$ (scan rate 100 mV/s, 0.1 M KNO_3 as supporting electrolyte) in between pH 11.7 and 12.4. Scan window of 0.2 to 0.9 V.

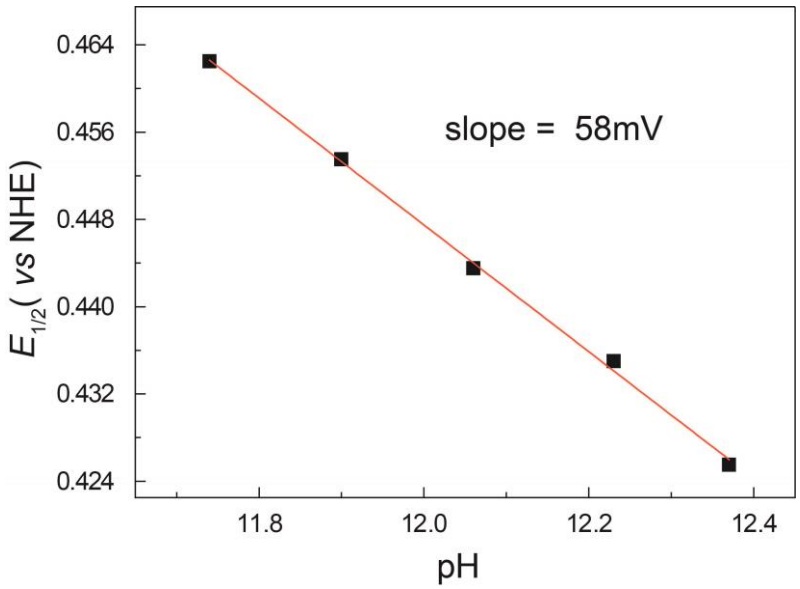


Figure S5: Plot of $E_{1/2}$ *vs* pH for [(bTAML) $Fe^{III}(Cl)]^{2-}$ (**1**) in water.

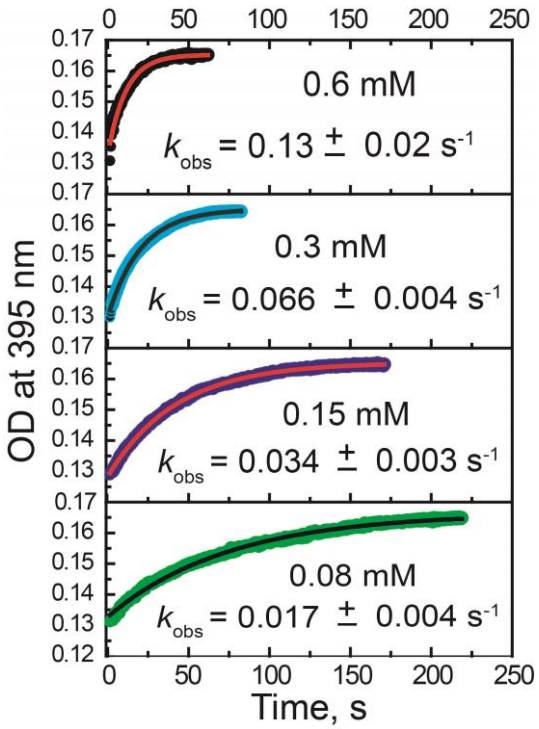


Figure S6: Kinetic traces for the reaction of **3** (5×10^{-5} M) with benzyl alcohol at various concentrations of benzyl alcohol. The kinetic traces were fitted to the equation, $[(A_t = A_\alpha - (A_\alpha - A_o)e^{(-k_{obs}t)}]$ for obtaining k_{obs} values.

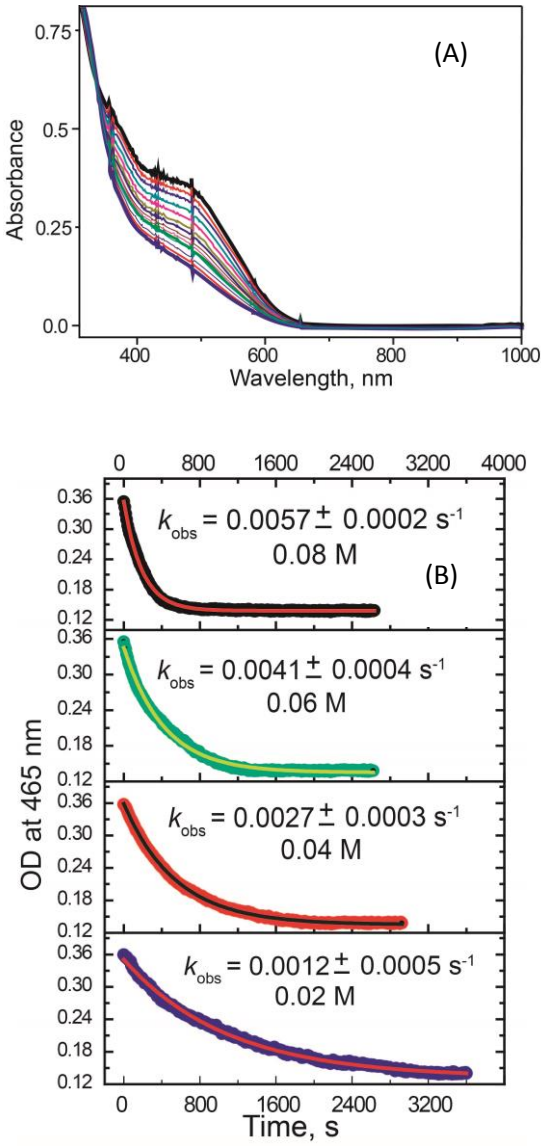


Figure S7: (A) Spectral scanning (B) Kinetic traces (The kinetic traces were fitted to the equation, $[(A_t = A_\alpha - (A_\alpha - A_o)e^{(-k_{obs}t)}]$ for obtaining k_{obs} values) for reaction with 1.5×10^{-4} M of **2** and benzyl alcohol.

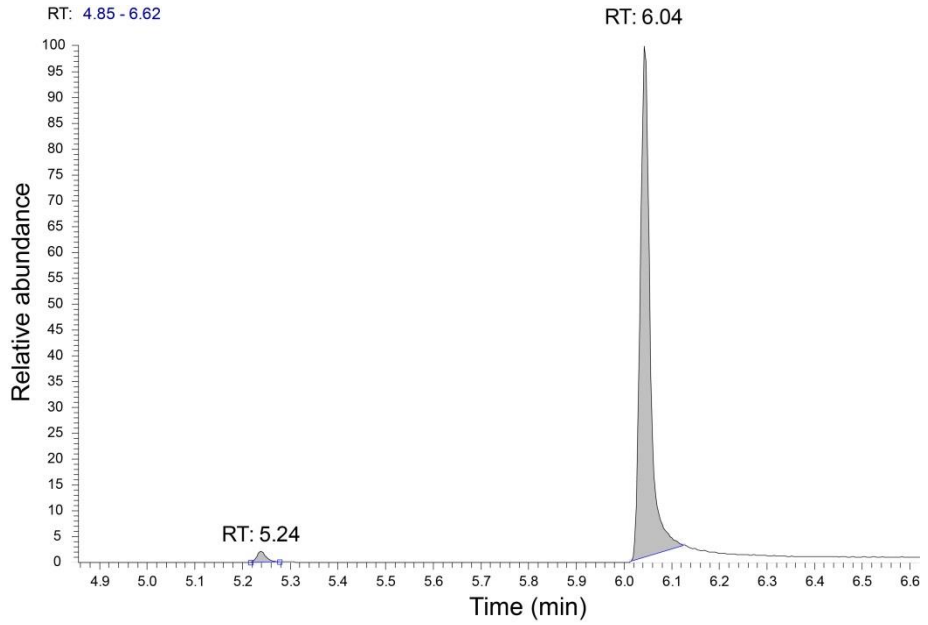


Figure S8: Gas chromatography traces for the reaction of benzyl alcohol with $[Fe^{IV}(O)]^{2-}$. Chromatogram at 5.24 min and 6.04 min retention time correspond to benzaldehyde and benzyl alcohol respectively.

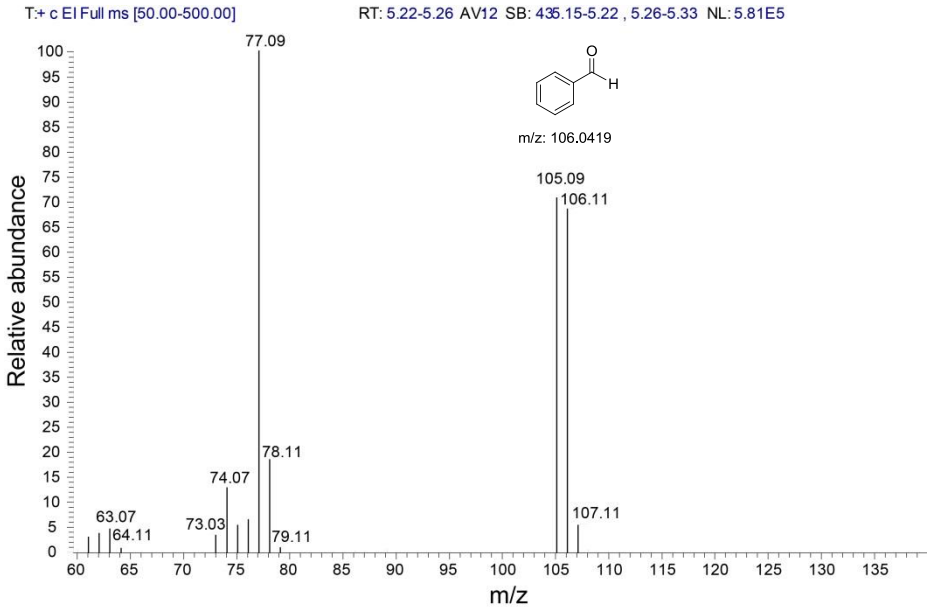


Figure S9: Mass spectra for benzaldehyde from the reaction of benzyl alcohol with $[Fe^{IV}(O)]^{2-}$ (106.1 molecular ion peak, 105.1 for $C_6H_5CO^+$ and 77.09 for $C_6H_5^+$).

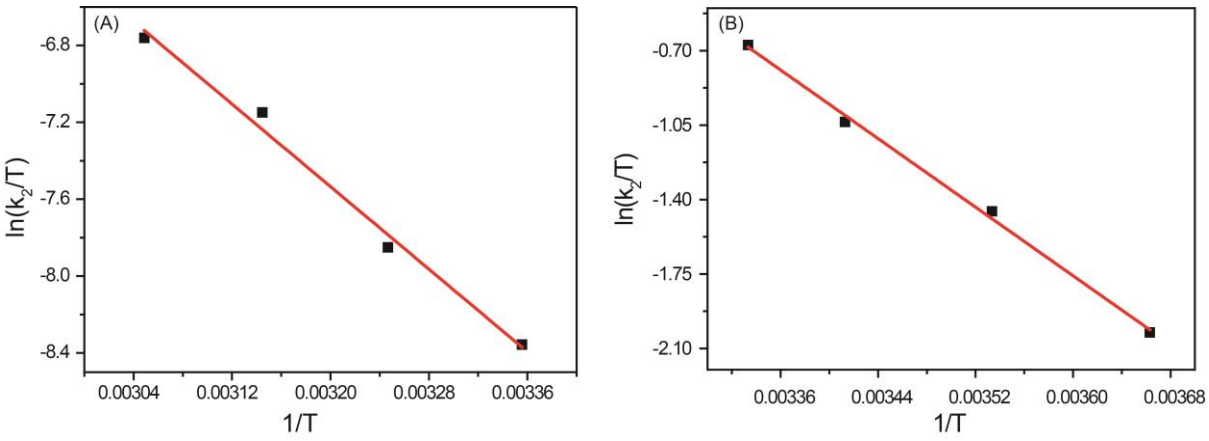


Figure S10: (A) Eyring plots for reaction of **2** with benzyl alcohol from 298 K to 328 K (B) Eyring plots for reaction of **3** with benzyl alcohol from 273 K to 300 K

Table S1. XAS Pre-edge Peak Analysis of 1, 2 and 3

Species	Peak Position (eV)	Area (units)	Relative Area
1	7113.0	14.1	1.0
2	7113.5	36.7	2.4
	7114.4	15.1	1.0
	Total	51.8	
3	7114.3	65.3	4.4

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Table S2. Fit Parameters of unfiltered XAS data for 1 from k = 2 – 15 Å^{-1}. Fit 8 is the most reasonable fit.

	Fe-N			Fe-Cl			Fe•••C				GOF	
Fit	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**E_o**	**F**	**F'**
1	6	1.86	3.17							-1.36	1722	675
2	5	1.86	2.31							-0.95	1579	647
3	4	1.87	1.43							-0.10	1516	633
4	3	1.87	0.46							0.63	1566	644
5	4	1.87	1.45	1	2.38	3.54				-0.62	1224	569
6	4	1.87	1.34	1	2.37	3.10	6	2.83	1.00	-0.03	761	449
7	4	1.87	1.26	1	2.37	3.00	6	2.83	1.21	0.11	620	405
							4	3.99	0.00			
8	**4**	**1.87**	**1.29**	**1**	**2.37**	**3.06**	**6**	**2.83**	**1.15**	**0.06**	**641**	**411**
							5	**3.99**	**1.19**			
9	4	1.87	1.32	1	2.37	3.07	6	2.83	1.02	1.69	673	422
							6	3.83	1.44			

Scale Factor S_0^2=0.9. GOF= Goodness-of-fit calculated as $F = \sqrt{\sum k^6 \left(\chi_{\exp} - \chi_{calc}\right)^2}$

$$F' = \sqrt{\sum k^6 \left(\chi_{\exp} - \chi_{calc}\right)^2 / \sum k^6 \chi_{\exp}{}^2}$$

Fit 8 gives the most reasonable fit of the experimental data

Table S3. Fit Parameters of unfiltered XAS data for 2 from k = 2 – 15 Å^{-1}

	Fe-N			Fe-O			Fe•••C				GOF	
Fit	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**E_o**	**F**	**F'**
1	6	1.86	6.04							5.00	1051	702
2	5	1.86	4.48							5.38	903	650
3	4	1.87	3.15							6.70	795	610
4	3	1.87	1.87							8.01	768	599
5	4	1.87	3.06				6	2.83	2.78	5.77	519	493
6	4	1.86	2.69	1	1.64	6.19	6	2.82	2.66	3.39	409	437
7	**4**	**1.86**	**2.67**	**1**	**1.64**	**5.95**	**6**	**2.82**	**2.67**	**3.22**	**345**	**402**
							5	**4.01**	**5.14**			

Scale Factor S_0^2=0.9. GOF= Goodness-of-fit calculated as $F = \sqrt{\sum k^6 \left(\chi_{\exp} - \chi_{calc}\right)^2}$

$$F' = \sqrt{\sum k^6 \left(\chi_{\exp} - \chi_{calc}\right)^2 / \sum k^6 \chi_{\exp}{}^2}$$

Fit 7 gives the most reasonable fit of the experimental data

Table S4. Fit Parameters of unfiltered XAS data for 3 from k = 2 – 15 Å^{-1}.

	Fe-N			Fe-O			Fe•••C				GOF	
Fit	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**N**	**R(Å)**	**$\sigma^2(10^{-3})$**	**E_o**	**F**	**F'**
1	6	1.87	4.85							0.31	1796	853
2	5	1.87	3.06							0.56	1457	769
3	4	1.87	1.82							1.61	1163	687
4	3	1.87	0.58							2.64	957	623
5	4	1.86	2.11	1	1.59	1.56				-0.40	677	524
6	5	1.86	3.41	1	1.60	0.93				-0.95	789	565
7	**4**	**1.86**	**2.19**	**1**	**1.59**	**1.34**	**6**	**2.82**	**2.18**	**-1.63**	**295**	**346**
8	4	1.86	2.17	1	1.59	1.33	5	2.82	1.42	-1.52	291	343
9	4	1.86	2.15	1	1.59	1.32	4	2.83	0.66	-1.25	298	347

Scale Factor S_0^2=0.9. GOF= Goodness-of-fit calculated as $F = \sqrt{\sum k^6 \left(\chi_{\exp} - \chi_{calc}\right)^2}$

$$F' = \sqrt{\sum k^6 \left(\chi_{\exp} - \chi_{calc}\right)^2 / \sum k^6 \chi_{\exp}{}^2}$$

Fit 7 gives the most reasonable fit of the experimental data

Table S5a. The relative energies of $[Fe^{V}(O)(bTAML)]^{-}$ (**3**) in doublet and quartet electronic states in kcal/mol using UBP86 or UB3LYP functionals and the 6-311+G* basis set in acetonitrile solvent.

	ΔE(kCal) UBP86(UB3LYP)	Δ(E+ZPE)(kCal) UBP86(UB3LYP)	ΔG(kCal) UBP86(UB3LYP)
S=1/2	0.0(0.0)	0.0(0.0)	0.0(0.0)
S=3/2	14.1(10.4)	13.1(9.3)	11.7(7.3)

Table S5b. The relative energies of $[Fe^{IV}(O)(bTAML)]^{2-}$ (**2**) in triplet and quintet electronic states in kcal/mol using UBP86 or UB3LYP functionals and the 6-311+G* basis set in acetonitrile solvent.

	ΔE(kCal) UBP86(UB3LYP)	Δ(E+ZPE)(kCal) UBP86(UB3LYP)	ΔG(kCal) UBP86(UB3LYP)
S=1	0.0(0.0)	0.0(0.0)	0.0(0.0)
S=2	26.0(19.5)	24.8(18.2)	23.0(16.5)

XYZ Coordinates for the optimized geometries in Gas Phase

Fe^{V}(O)_(S = ½) (BP86)

Fe	0.03811100	0.07370500	-0.00044800
O	-0.00935100	-0.00176800	3.97117600
O	4.04984600	0.14101500	0.71339300
O	2.05855000	1.39252600	-3.20596200
O	-3.00301000	1.60191000	-2.14596600
N	-0.60797300	0.25567000	1.73388300
N	1.73443500	0.27503400	0.81852100
N	0.52352100	1.00968800	-1.51227100
N	-1.71383900	0.67542400	-0.43369100
C	-2.00427400	0.39776700	1.86927600
C	0.29181600	0.08415900	2.77019800
C	1.74867200	-0.02902800	2.26994200
C	2.93549900	0.33514400	0.17879400
C	1.80937100	1.04831000	-2.03084300
C	-0.59035200	1.30433700	-2.46880400
C	-1.91930300	1.21409500	-1.67371500
C	-2.64001000	0.63693600	0.61330300
C	-4.03227100	0.84630800	0.54990600
H	-4.48885900	1.04701800	-0.42110600
C	-4.78108300	0.80126100	1.73717900
H	-5.86658200	0.95453100	1.69304000
C	-4.15585900	0.55930000	2.97402500
H	-4.75429800	0.52053000	3.89257600
C	-2.76671400	0.36231500	3.05402600
H	-2.26060500	0.18046300	4.00311500
C	2.58453300	0.97989400	3.09214700
H	3.65467300	0.84979300	2.87869200
H	2.37766600	0.81643400	4.16381400
H	2.29251500	2.01433400	2.83531400
C	2.20810500	-1.48619300	2.53034800
H	3.26981400	-1.58561000	2.25509100

H	1.60877500	-2.17744800	1.91203600
H	2.06505800	-1.73894800	3.59585000
C	4.19357300	0.73047500	-1.90188300
H	4.39732300	1.75359200	-2.26242800
H	4.18777300	0.06031700	-2.77788800
H	4.95235000	0.41985800	-1.17227700
C	-0.66557000	0.23227000	-3.58373400
H	0.21240600	0.30882700	-4.24335500
H	-1.59218200	0.38239100	-4.16555200
H	-0.69260600	-0.77329100	-3.12717500
C	-0.51046800	2.73346500	-3.04834600
H	0.32368400	2.81621800	-3.75850900
H	-0.36177800	3.46512900	-2.23368700
H	-1.47174100	2.95797700	-3.54174200
O	-0.01536700	-1.47477800	-0.37488700
N	2.89705800	0.67660300	-1.21375900

Fe^{V}(O) (S = 3/2) (BP86)

Fe	0.09085700	0.23822200	0.02084100
O	-0.01233600	-0.06292300	4.02006300
O	4.04445900	0.22336700	0.71805600
O	2.10163000	1.30066800	-3.28059700
O	-3.00606000	1.63046800	-2.11710800
N	-0.63169800	0.14389600	1.77430100
N	1.73939500	0.41573400	0.88070100
N	0.53720400	1.09421400	-1.57521500
N	-1.69151200	0.74268400	-0.39789500
C	-2.01441600	0.32786100	1.89547200
C	0.26971700	0.02346700	2.81340600
C	1.74738300	0.03229800	2.32024100
C	2.92365300	0.37892500	0.18687400
C	1.80170000	1.00158900	-2.10480900
C	-0.60324800	1.35065500	-2.49804000
C	-1.91313400	1.25570000	-1.66108200

C	-2.62530600	0.67373900	0.64298900
C	-4.01439600	0.91359500	0.57556600
H	-4.45339900	1.19003000	-0.38468900
C	-4.78199300	0.79986900	1.74428800
H	-5.86265200	0.98240900	1.69597500
C	-4.18219700	0.45995900	2.97413000
H	-4.79841700	0.37916700	3.87814800
C	-2.80164900	0.22654100	3.06236400
H	-2.31296800	-0.02280600	4.00590100
C	2.52280200	1.05171900	3.18102100
H	3.59431700	1.00634600	2.93644000
H	2.35636900	0.81964600	4.24689900
H	2.15402300	2.07477400	2.98546600
C	2.28786800	-1.40787500	2.51454200
H	3.35851800	-1.44159500	2.26115200
H	1.73743000	-2.09571100	1.84886000
H	2.13712800	-1.71904500	3.56311200
C	4.16349300	0.52431900	-1.91624900
H	4.55655800	1.53602600	-2.12916500
H	4.03806500	0.00325300	-2.87700200
H	4.85907700	-0.00302000	-1.25163100
C	-0.69573000	0.25653600	-3.59285900
H	0.17376200	0.32771400	-4.26424100
H	-1.62951200	0.38815100	-4.16719400
H	-0.70133200	-0.73793800	-3.11318100
C	-0.53415900	2.76438500	-3.11203100
H	0.32860600	2.83046000	-3.79141600
H	-0.42162000	3.52154900	-2.31526700
H	-1.47382000	2.96634400	-3.65412400
O	0.28503700	-1.30854000	-0.50167400
N	2.86353600	0.59112700	-1.23372300

Fe^{IV}(O)_(S = 1) (BP86)

Fe	0.06225900	0.24826400	0.03785000
O	0.03211900	-0.04473700	4.05282400
O	4.07726200	0.24381200	0.72601700
O	2.13182600	1.35498400	-3.28427600
O	-3.00162700	1.65514300	-2.16221700
N	-0.62073700	0.23291400	1.81486900
N	1.75686200	0.41587800	0.86182000
N	0.55974200	1.09142700	-1.57411100
N	-1.69711500	0.83510800	-0.39004000
C	-2.00812800	0.40035800	1.91687000
C	0.27502300	0.05982500	2.82588000
C	1.74605900	-0.03043400	2.28385500
C	2.94588700	0.45534400	0.20696600
C	1.81697900	1.09250400	-2.09109400
C	-0.58955500	1.28700100	-2.50022800
C	-1.91332900	1.28686300	-1.65715700
C	-2.62259700	0.74397600	0.65785400
C	-4.01350300	0.97345000	0.59913800
H	-4.44597900	1.24684000	-0.36692000
C	-4.79195000	0.85880400	1.76796000
H	-5.87629900	1.03489700	1.71396800
C	-4.19297900	0.52369900	2.99556100
H	-4.80816500	0.43719500	3.90320500
C	-2.80459200	0.29725100	3.07695600
H	-2.30737100	0.05040000	4.01871000
C	2.62355700	0.84902200	3.20166100
H	3.68759600	0.70099400	2.96478400
H	2.40418900	0.59031700	4.25320700
H	2.37382800	1.91627300	3.04929100
C	2.15150500	-1.52395500	2.37425200
H	3.21165600	-1.63568400	2.08965400
H	1.51975000	-2.08977200	1.66610900
H	1.99075900	-1.90197100	3.40178900

C	4.21284000	0.87069700	-1.85861500
H	4.38552500	1.87566500	-2.28807900
H	4.26916300	0.14929700	-2.69501000
H	4.96432900	0.63799900	-1.09096800
C	-0.68981700	0.08944700	-3.47994300
H	0.18125300	0.09784900	-4.15730300
H	-1.62798200	0.14812600	-4.06408100
H	-0.68049900	-0.84033600	-2.88308900
C	-0.52805000	2.63019600	-3.25977400
H	0.31456700	2.62168400	-3.96736900
H	-0.37898500	3.46054600	-2.54363900
H	-1.49069900	2.79008700	-3.77806500
O	-0.00255300	-1.34302100	-0.36381700
N	2.90901100	0.80372800	-1.19763900

Fe^{IV}(O)_(S = 2) (BP86)

Fe	0.06761200	-0.17136700	-0.09604900
O	-0.01010600	-0.01384000	3.99242200
O	4.07696300	0.36610600	0.70509300
O	2.15972400	1.21949100	-3.33985600
O	-2.92475100	1.86103900	-2.07461400
N	-0.64032900	-0.17941100	1.74091700
N	1.74255700	0.23434900	0.80571100
N	0.57761800	0.83119800	-1.67050900
N	-1.63101200	1.01900400	-0.30144800
C	-2.01537300	0.10906500	1.85079400
C	0.25111400	-0.05329600	2.76673900
C	1.73619200	0.07012800	2.27872000
C	2.93553000	0.36825000	0.16650300
C	1.83424500	0.87594400	-2.17100800
C	-0.56827000	1.31823700	-2.47952900
C	-1.85563300	1.43061900	-1.56843700
C	-2.56704800	0.77400400	0.69051400
C	-3.94089800	1.11496600	0.68483900

H	-4.33524000	1.60490400	-0.20999300
C	-4.74464200	0.83128000	1.80406900
H	-5.81024300	1.10548200	1.78715000
C	-4.19766600	0.21051700	2.94145200
H	-4.82910500	0.00439800	3.81787400
C	-2.83543300	-0.15143200	2.96468100
H	-2.38107200	-0.61446300	3.84451800
C	2.34314100	1.29874700	2.99796600
H	3.41498300	1.37355800	2.75500000
H	2.18740100	1.20092500	4.08671200
H	1.83418700	2.21801100	2.65452400
C	2.47167100	-1.22444200	2.71089800
H	3.53949200	-1.14816900	2.44889000
H	2.03358300	-2.09345600	2.18554500
H	2.34646300	-1.37353200	3.79962400
C	4.23693500	0.46045000	-1.87710100
H	4.82063300	1.37466000	-1.64458100
H	4.09423200	0.39455300	-2.96484300
H	4.80769300	-0.39837900	-1.48560900
C	-0.89324100	0.30024500	-3.59904900
H	-0.05373000	0.26417700	-4.31550200
H	-1.82685800	0.58864200	-4.11611700
H	-1.02348900	-0.69041600	-3.12781100
C	-0.32216000	2.73105800	-3.05832100
H	0.47340100	2.70564800	-3.81850300
H	-0.01513500	3.42046500	-2.24910400
H	-1.27287600	3.09701500	-3.48552300
O	-0.68612100	-1.50223900	-0.74887500
N	2.90609200	0.48526200	-1.27115700

Fe^{V}(O)_(S = ½) (B3LYP)

Fe	0.02380000	-0.06578700	-0.01563400
O	0.00800400	0.20511000	3.92521500
O	4.03573500	-0.07048900	0.71407700
O	2.04556000	1.40262200	-3.15583400
O	-2.99619700	1.42523400	-2.17741000
N	-0.59046600	0.25387100	1.70106200
N	1.75635900	0.09501000	0.79222400
N	0.51459600	0.79470500	-1.58748900
N	-1.70931900	0.57586400	-0.45930300
C	-1.98578100	0.38511100	1.83712800
C	0.30633100	0.16996900	2.74087000
C	1.75555100	0.01106900	2.26834800
C	2.94234700	0.03833200	0.14872300
C	2.92900000	0.05821800	-1.39853000
C	1.79252300	0.83948900	-2.09294100
C	-0.59805600	1.26445400	-2.46667700
C	-1.92061000	1.08334300	-1.69903700
C	-2.62737900	0.55781700	0.58837300
C	-4.01295700	0.73275000	0.52434800
H	-4.48046000	0.88030100	-0.43841100
C	-4.74996500	0.72188900	1.70728800
H	-5.82802700	0.84974200	1.66330700
C	-4.11872000	0.54690800	2.93871700
H	-4.70479200	0.53703800	3.85337500
C	-2.73586300	0.38289800	3.01747600
H	-2.23513900	0.25743600	3.96514400
C	2.56203200	1.15277100	2.92025900
H	3.62083600	1.03618800	2.70414600
H	2.39245100	1.14196300	3.99880300
H	2.22933000	2.11882000	2.52922500
C	2.24600300	-1.36727200	2.76063200
H	3.29722700	-1.49266300	2.50689500
H	1.66982400	-2.16351500	2.28187700

H	2.11321400	-1.44359900	3.84223000
C	4.27228600	0.63020000	-1.88522600
H	4.38065000	1.67997300	-1.60166500
H	4.33480300	0.57072400	-2.97104000
H	5.08997700	0.07503700	-1.42935300
C	2.82063900	-1.41718100	-1.87426100
H	1.89648500	-1.88825500	-1.53955300
H	3.66307900	-1.98573600	-1.47184600
H	2.86348600	-1.46118700	-2.96630600
C	-0.68717000	0.43042000	-3.75750300
H	0.17278000	0.61794100	-4.39782300
H	-1.60500200	0.69379600	-4.28737200
H	-0.72471500	-0.63530300	-3.51508400
C	-0.49076000	2.77224400	-2.77394200
H	0.36163200	2.97230300	-3.41765800
H	-0.36990900	3.33659400	-1.84479600
H	-1.41440500	3.09974800	-3.25521900
O	-0.11401200	-1.60857900	-0.28057500

Fe^{V}(O) (S = 3/2) (B3LYP)

Fe	0.08621500	0.20425900	0.01281100
O	0.00310800	0.08648000	4.00150300
O	4.02303600	0.19883000	0.68083900
O	2.09620300	1.26813400	-3.26693000
O	-2.95750900	1.74076000	-2.06134400
N	-0.62156300	0.18517500	1.77531700
N	1.74253400	0.41932600	0.85806200
N	0.55572500	1.08560400	-1.57031000
N	-1.67929100	0.77728200	-0.38988800
C	-2.01719400	0.30638800	1.88122000
C	0.27787700	0.12482000	2.80245100
C	1.74694600	0.10164500	2.30988900
C	2.91290000	0.35156800	0.15775700
C	1.80791200	0.96660100	-2.10278000

C	-0.58658700	1.39925200	-2.46824600
C	-1.88305500	1.33141600	-1.62251200
C	-2.62185300	0.64516100	0.64334600
C	-4.00714900	0.82431100	0.56110600
H	-4.44807700	1.09645700	-0.38853000
C	-4.78039700	0.66194300	1.71464300
H	-5.85792100	0.79923700	1.65532900
C	-4.18493000	0.32822600	2.93370700
H	-4.79888900	0.20567000	3.82335100
C	-2.80159500	0.14872100	3.02913300
H	-2.32060000	-0.09555800	3.96682700
C	2.53053300	1.15490700	3.11226300
H	3.59294400	1.09559900	2.87259700
H	2.36929500	0.97885700	4.18005000
H	2.16796900	2.16048600	2.87008800
C	2.27605700	-1.32581900	2.57546800
H	3.33544100	-1.38655400	2.32082200
H	1.72020900	-2.04334600	1.96186700
H	2.13044600	-1.57554300	3.63161000
C	4.14659500	0.36210500	-1.93303100
H	4.67682300	1.32098100	-1.98959200
H	3.97038500	0.00695500	-2.94696000
H	4.75514000	-0.33889700	-1.36564000
C	-0.73635900	0.34185700	-3.58502200
H	0.11625100	0.39035200	-4.26446500
H	-1.66433100	0.52627000	-4.13631900
H	-0.78135300	-0.65804600	-3.13961000
C	-0.47118500	2.82093600	-3.04479000
H	0.37379600	2.87917000	-3.73203900
H	-0.32105400	3.54491800	-2.23572700
H	-1.40255300	3.07076800	-3.56179600
O	0.18746300	-1.34253600	-0.46279200
N	2.85267600	0.50282800	-1.25612000

Fe^{IV}(O)_(S = 1) (B3LYP)

Fe	0.05803100	0.20579800	0.02887600
O	0.03488700	-0.03150600	4.02844500
O	4.05569200	0.24155400	0.71536900
O	2.12593200	1.33352900	-3.26474300
O	-2.97566900	1.66465100	-2.14490000
N	-0.62080400	0.22337700	1.81049600
N	1.75649400	0.39316800	0.85470900
N	0.56200000	1.06756100	-1.57904800
N	-1.69521700	0.82516600	-0.39205700
C	-2.00500600	0.38609200	1.90627300
C	0.27175200	0.06485200	2.81114300
C	1.74192300	-0.01530400	2.28096300
C	2.93258300	0.43515000	0.19927300
C	1.81157900	1.06429100	-2.08490300
C	-0.58494100	1.29713400	-2.48930200
C	-1.90127100	1.28753400	-1.64440700
C	-2.61560900	0.72831300	0.65429200
C	-3.99818700	0.94949400	0.59539100
H	-4.43284800	1.22022300	-0.35922700
C	-4.77435100	0.83054600	1.75647600
H	-5.84979100	1.00204800	1.70118500
C	-4.17998200	0.49730300	2.97534300
H	-4.78983800	0.40771300	3.87484300
C	-2.79808600	0.27673900	3.05647000
H	-2.31142900	0.03084800	3.99254300
C	2.59514100	0.90577100	3.17450500
H	3.65316300	0.78866600	2.93670700
H	2.39975800	0.66544800	4.22492500
H	2.31350000	1.95327400	3.00517300
C	2.17525300	-1.49240700	2.42335300
H	3.22849900	-1.59608500	2.14758600
H	1.56411000	-2.09630100	1.74377300
H	2.02201300	-1.83467500	3.45453500

C	4.19583700	0.79625300	-1.87076500
H	4.40035000	1.79786100	-2.26971100
H	4.21655200	0.10381200	-2.71975400
H	4.94671700	0.52280900	-1.13274000
C	-0.70753300	0.13939400	-3.50675300
H	0.15309800	0.15131800	-4.18160600
H	-1.63701600	0.23555200	-4.08207000
H	-0.71734200	-0.80606100	-2.95357100
C	-0.51119100	2.66005000	-3.20402700
H	0.33032500	2.67362700	-3.89812900
H	-0.36814700	3.46031500	-2.46627000
H	-1.45573200	2.84287400	-3.72733500
O	-0.00167500	-1.36391500	-0.37035700
N	2.89750900	0.75410500	-1.20335300

Fe^{IV}(O)_(S = 2) (B3LYP)

Fe	0.05413700	-0.19599800	-0.10599900
O	0.00447700	-0.02011900	3.97960400
O	4.05869600	0.37820200	0.68652300
O	2.16308400	1.23357700	-3.30857500
O	-2.91040100	1.85480000	-2.06360200
N	-0.64540600	-0.16633100	1.75257100
N	1.74994500	0.19988600	0.80393600
N	0.57529300	0.83713400	-1.67199300
N	-1.65141100	0.94126900	-0.32731700
C	-2.01583300	0.11690100	1.85553700
C	0.24869800	-0.05800700	2.76083500
C	1.73292400	0.06435000	2.27377300
C	2.92515100	0.35299200	0.15996500
C	1.82623600	0.87189200	-2.16134200
C	-0.56726700	1.33285400	-2.46998500
C	-1.85811800	1.40226500	-1.56961300

C	-2.57547000	0.73253700	0.68188400
C	-3.94044500	1.06705400	0.67128300
H	-4.34134600	1.52782400	-0.22396900
C	-4.73543500	0.81697300	1.79588900
H	-5.79254900	1.08538200	1.77425100
C	-4.18541900	0.23592500	2.94069300
H	-4.80753100	0.05350600	3.81737300
C	-2.82850400	-0.11481200	2.97056400
H	-2.37573400	-0.54525600	3.85587500
C	2.32209700	1.30954300	2.97099000
H	3.38272400	1.40132700	2.72735800
H	2.17713800	1.22942900	4.05294800
H	1.80150300	2.20881800	2.61949400
C	2.47443400	-1.21095200	2.73369400
H	3.53566700	-1.13500400	2.48426900
H	2.05359100	-2.08684000	2.22411400
H	2.34455600	-1.34345100	3.81448500
C	4.20472900	0.40479600	-1.89782200
H	4.74020200	1.36293200	-1.81834900
H	4.07277700	0.17423100	-2.95409300
H	4.80949300	-0.35274800	-1.39654600
C	-0.87186600	0.35787300	-3.62714800
H	-0.03197400	0.34861600	-4.32920000
H	-1.79151800	0.65677000	-4.14352500
H	-1.00263500	-0.64557900	-3.20758900
C	-0.32881200	2.76377100	-2.99458000
H	0.47747000	2.77364000	-3.72981600
H	-0.05071400	3.42298500	-2.16217200
H	-1.26129500	3.13601600	-3.43148800
O	-0.53951900	-1.58321000	-0.73036400
N	2.88520900	0.45019400	-1.27520700