Supporting Information

for

A Mononuclear Nonheme Iron(IV)-Oxo Complex of a Substituted N4Py Ligand: Effect of Ligand Field on Oxygen Atom Transfer and C-H Bond Cleavage Reactivity

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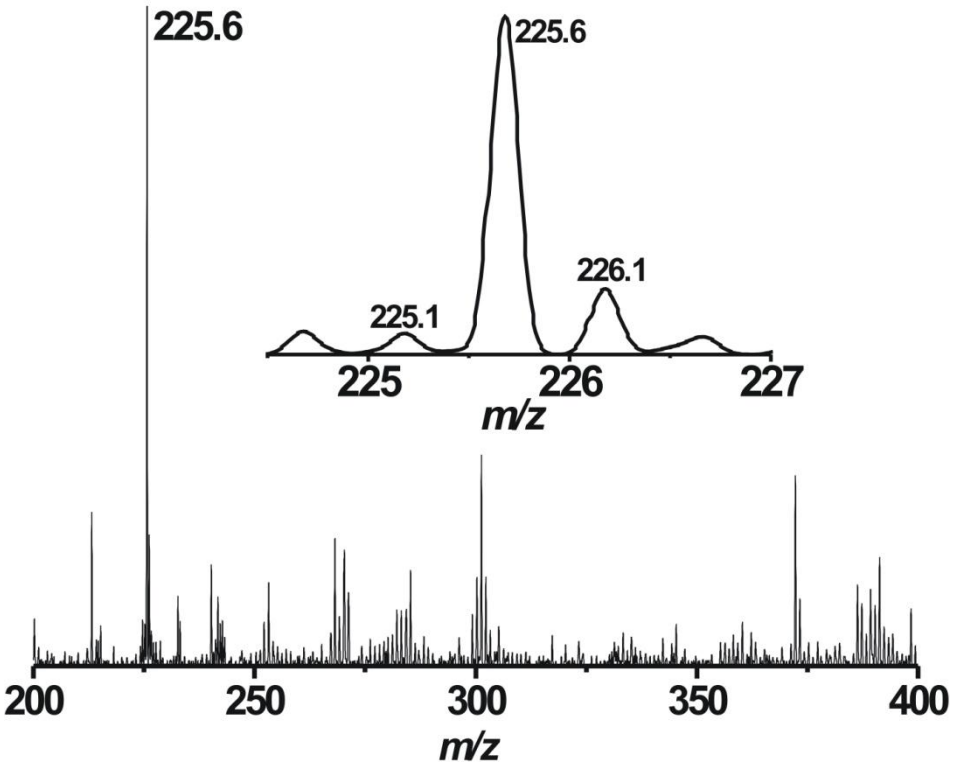


Figure S1 ESI-mass spectrum (positive ion mode in acetonitrile) of [Fe^{II}(N4Py^{Me2})(OTf)](OTf) (**1**).

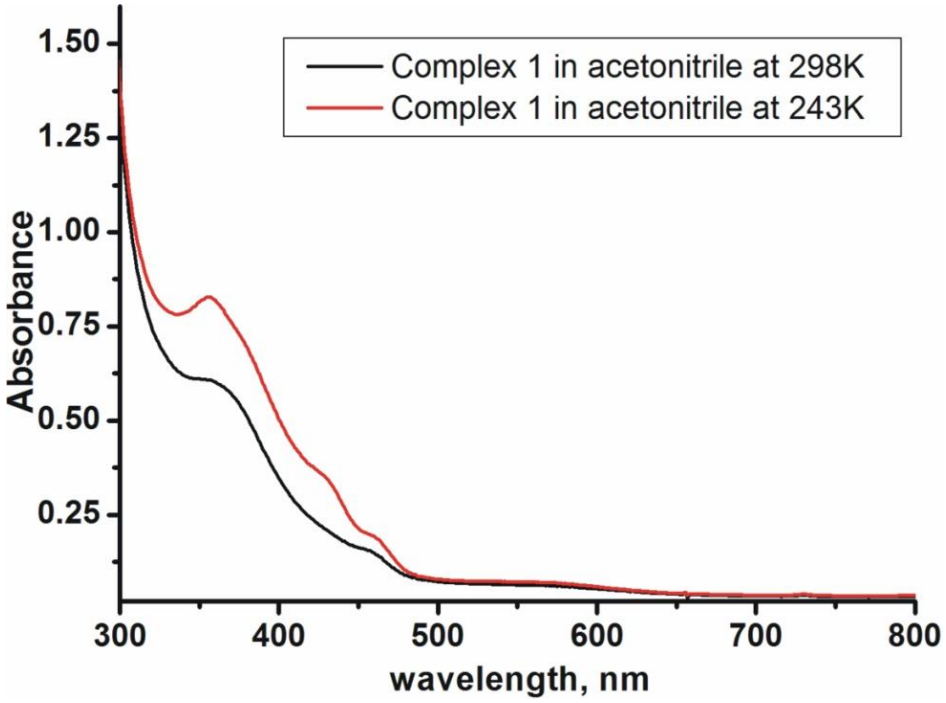


Figure S2 Optical spectrum of **1** (0.5 mM) in acetonitrile.

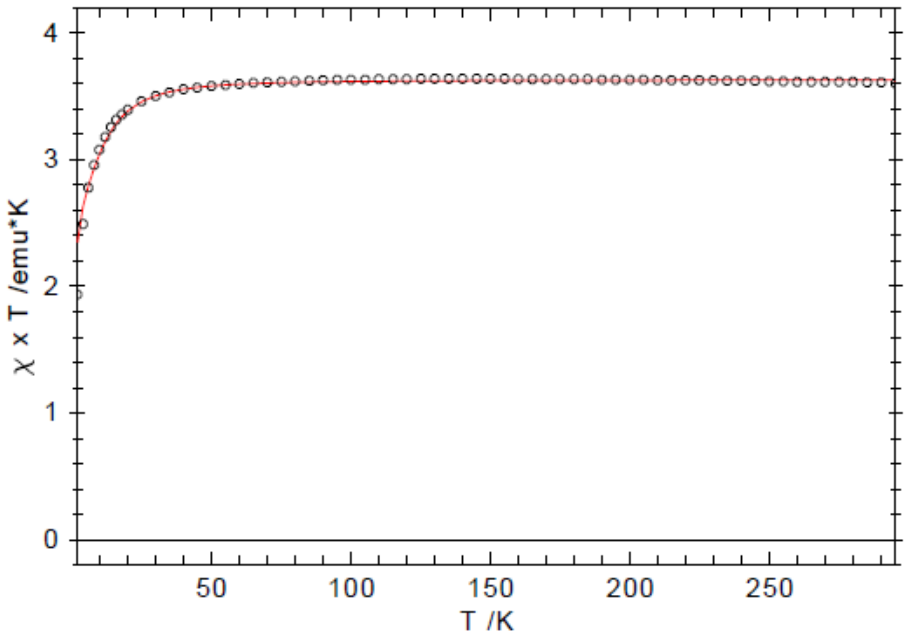


Figure S3 Variable-temperature magnetic data for a solid sample of **1**. The solid line represents the best curve fit with parameters g = 2.20 and $|D|$ = 8.3 cm^{-1}.

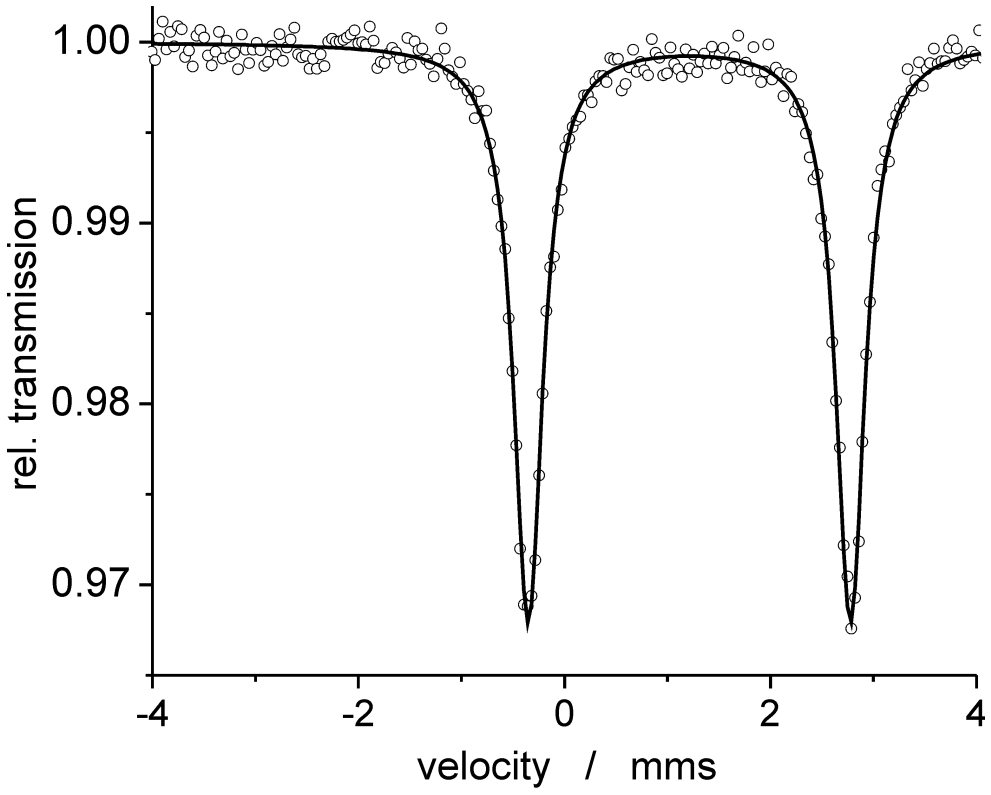


Figure S4 Zero-field ^{57}Fe Mössbauer spectrum of a solid sample of **1** measured at 10 K. Mössbauer parameters are δ = 1.21 mm/s and ΔE_Q = 3.13 mm/s.

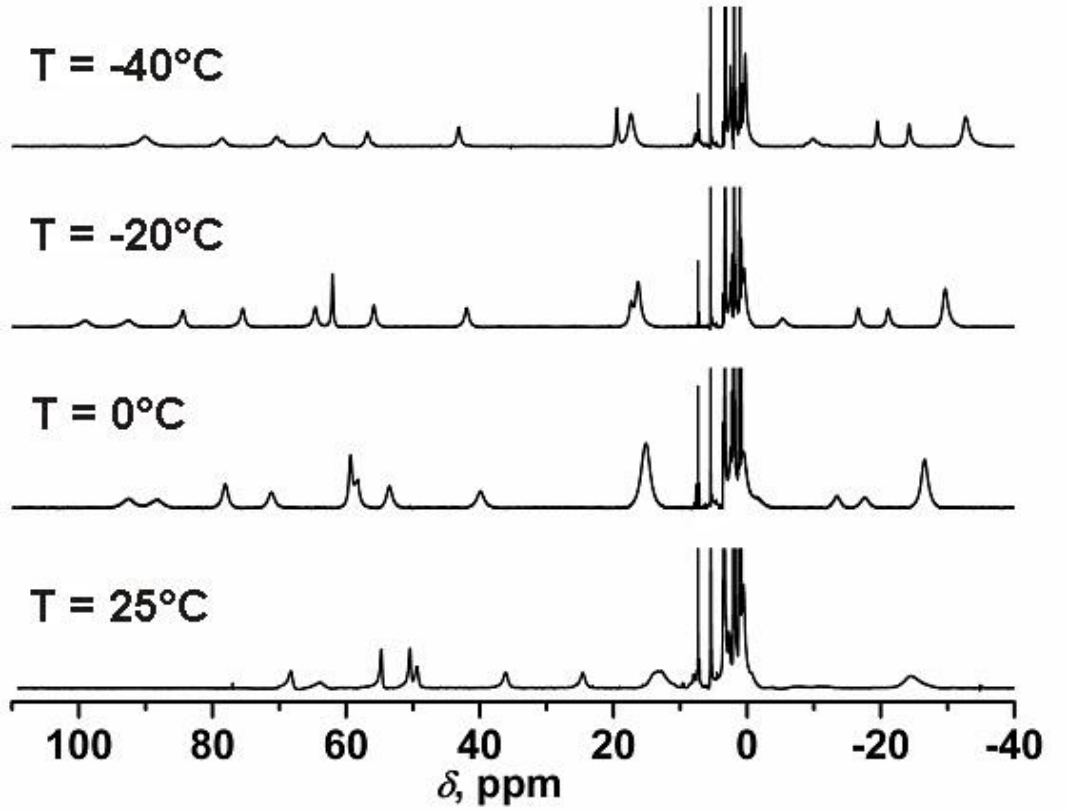


Figure S5 Variable temperature (VT) ^{1}H NMR (500 MHz) spectrum of **1** in CD_3CN.

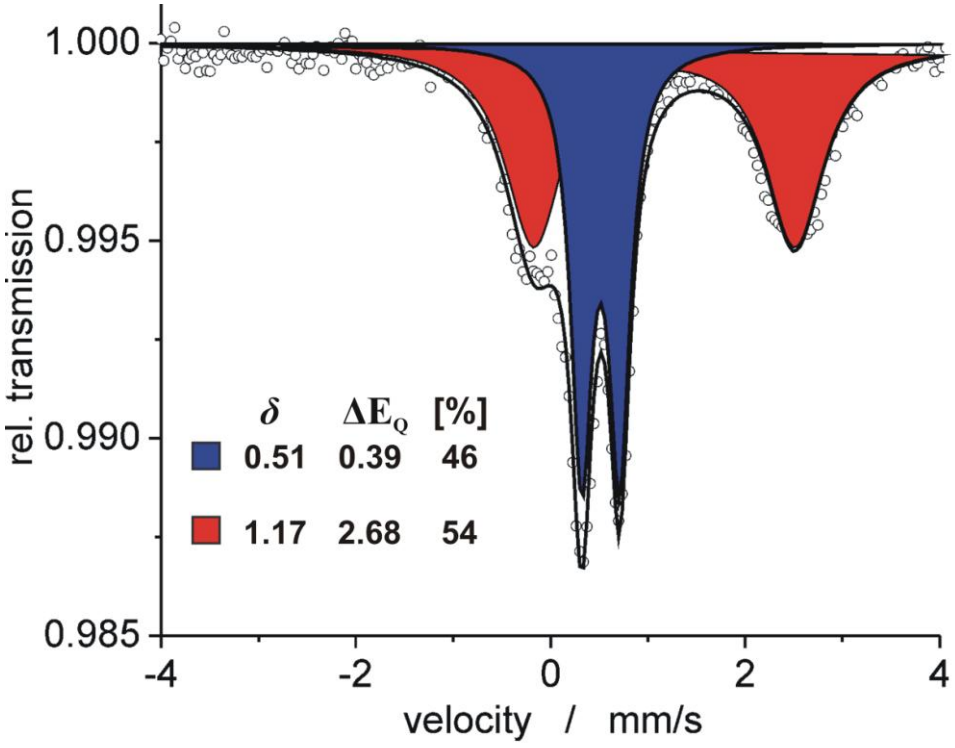


Figure S6 Zero-field ^{57}Fe Mössbauer spectrum of a frozen sample of **1** in acetonitrile measured at 10 K.

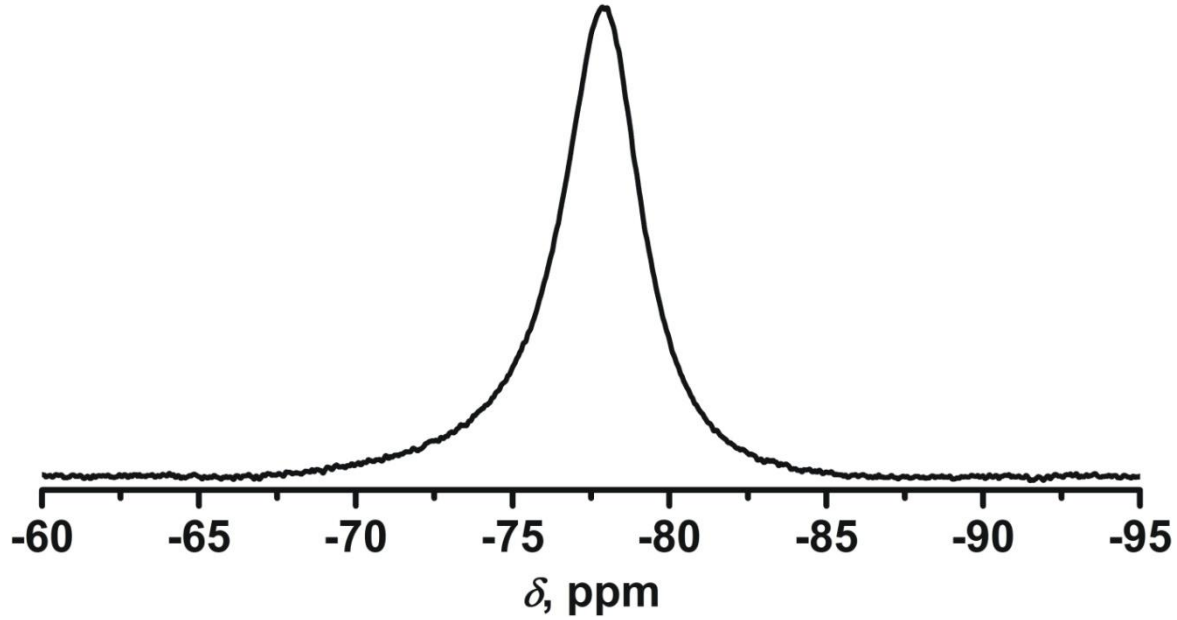


Figure S7 ^{19}F NMR spectrum (470 MHz, 298 K) of **1** in CD_3CN.

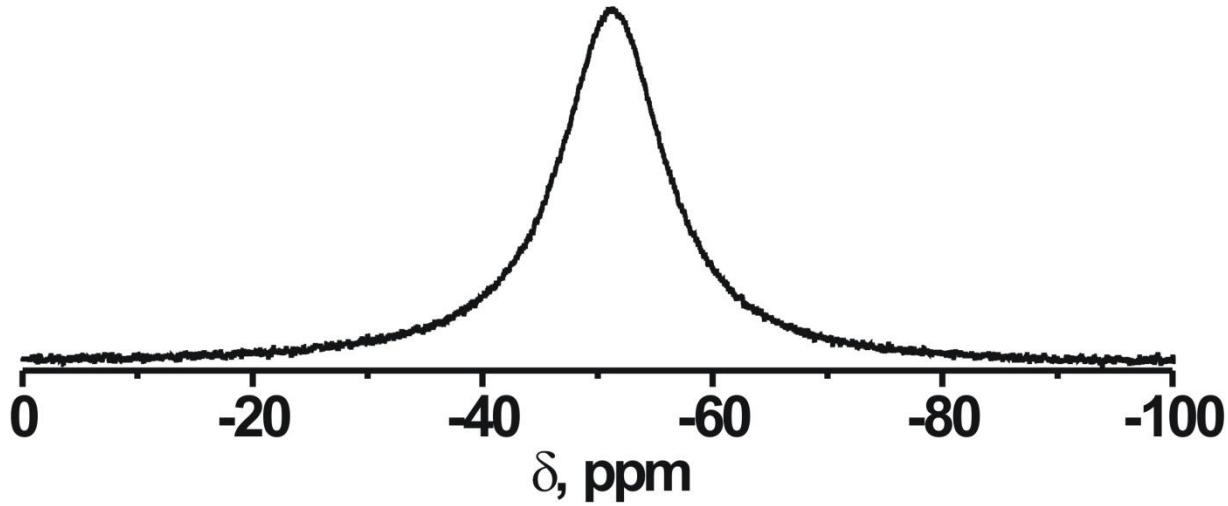


Figure S8 ^{19}F NMR spectrum (470 MHz, 298 K) of **1** in CD_2Cl_2.

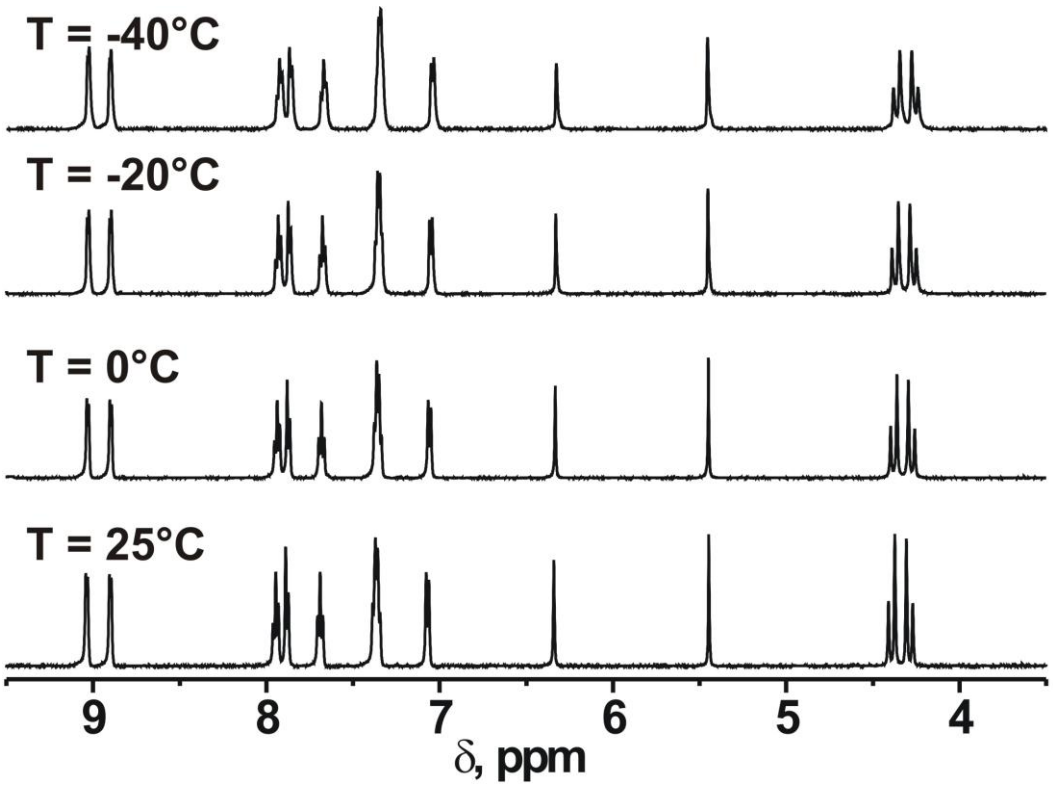


Figure S9 VT ^{1}H NMR (500 MHz) spectra of $[Fe^{II}(N4Py)(CH_3CN)]^{2+}$ in CD_3CN.

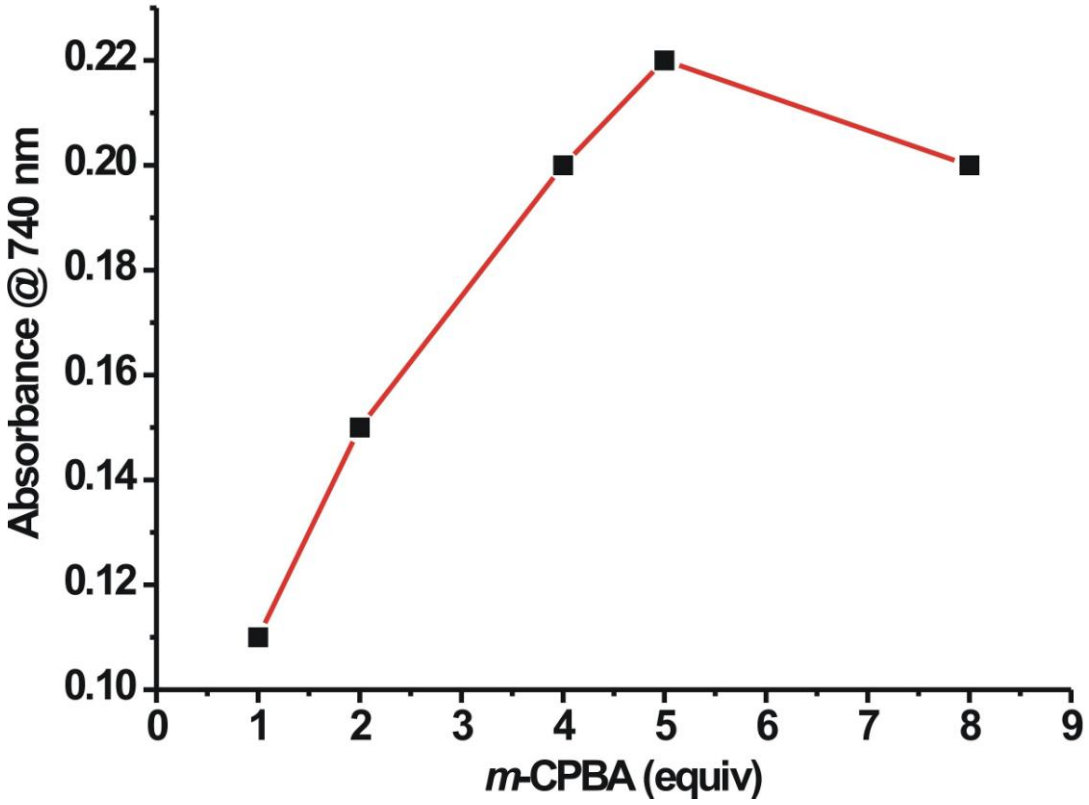


Figure S10 Titration of **1** with *m*-CPBA in acetonitrile at –40°C.

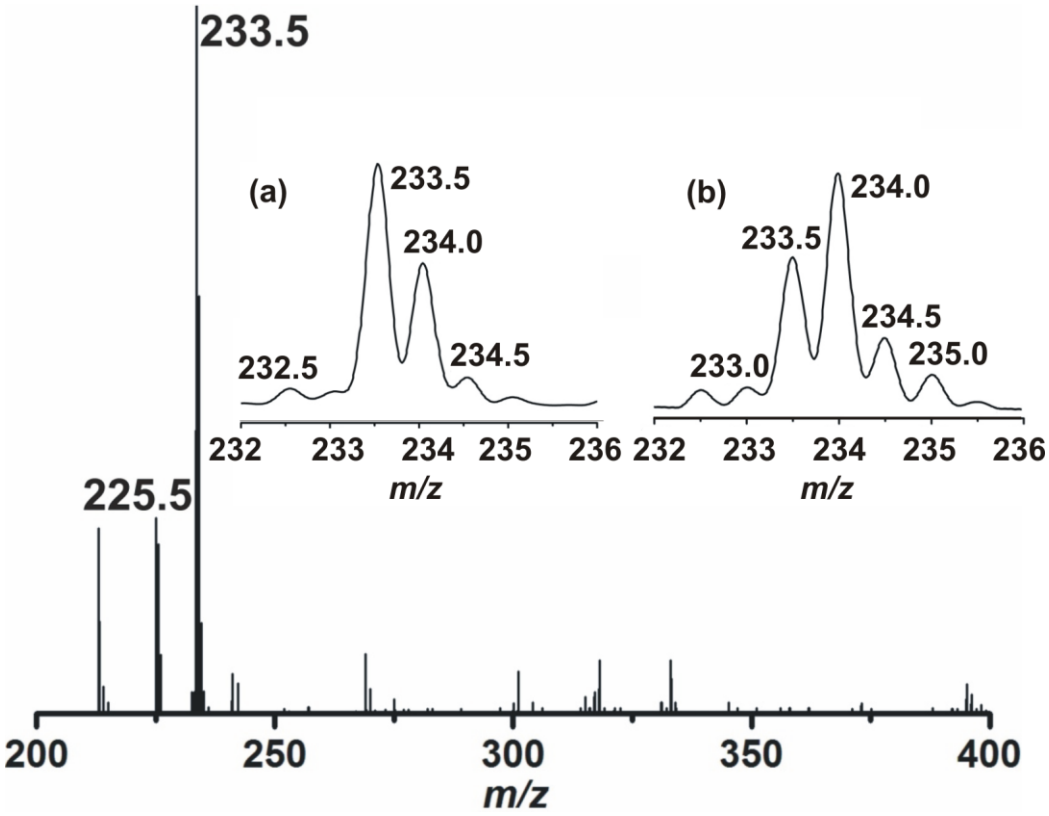


Figure S11 ESI-mass spectrum (positive ion, acetonitrile) of $[Fe^{IV}(O)(N4Py^{Me2})]^{2+}$ (**2**). Inset: isotope distribution patterns of the (a) peak at *m/z* 233.5 and (b) peak at *m/z* 234.0 appeared during the decay of **2**.

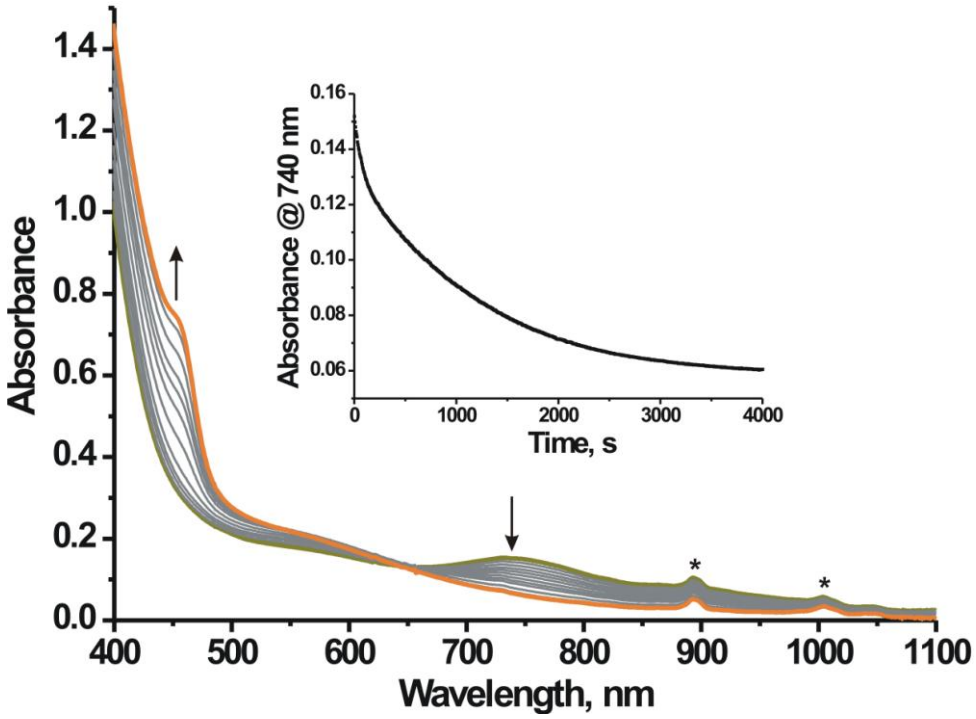


Figure S12 Self decay of **2**, generated from **1** (1 mM, CH_3CN) using *m*-CPBA (5 equiv), at 25°C. Inset: Absorbance vs time plot for 740 nm peak. Spikes marked with * likely arise from artifacts in the data collection process.

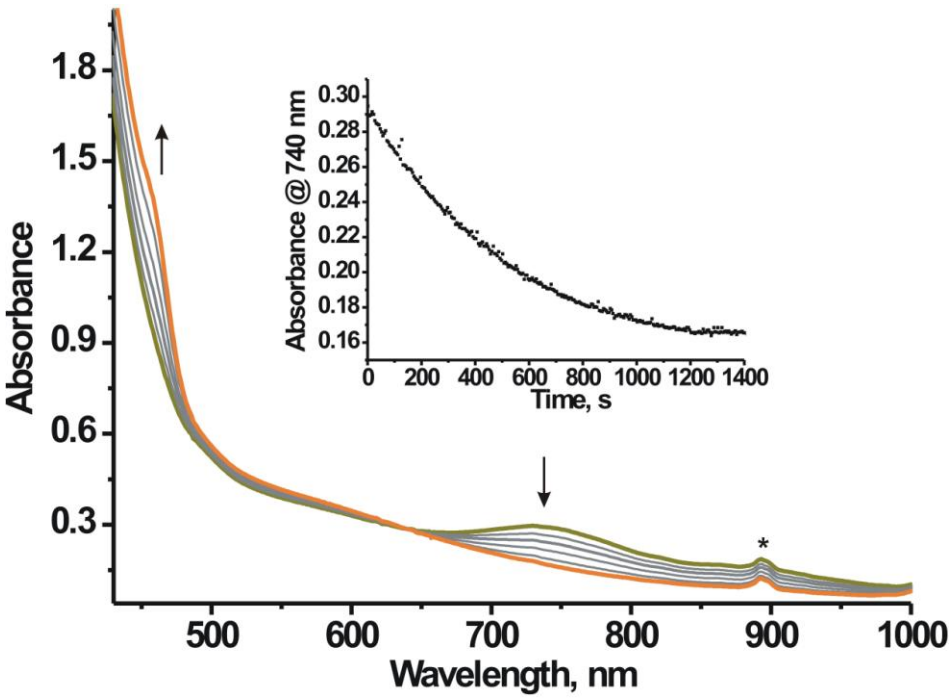


Figure S13 Decay kinetics of **2** (generated from 2 mM of **1** in CH_3CN) in the presence of 9,10-dihydroanthracene (5 equiv) at -10°C. Inset: Absorbance vs time plot for 740 nm peak. The spike marked with * likely arises from artifact in the data collection process.

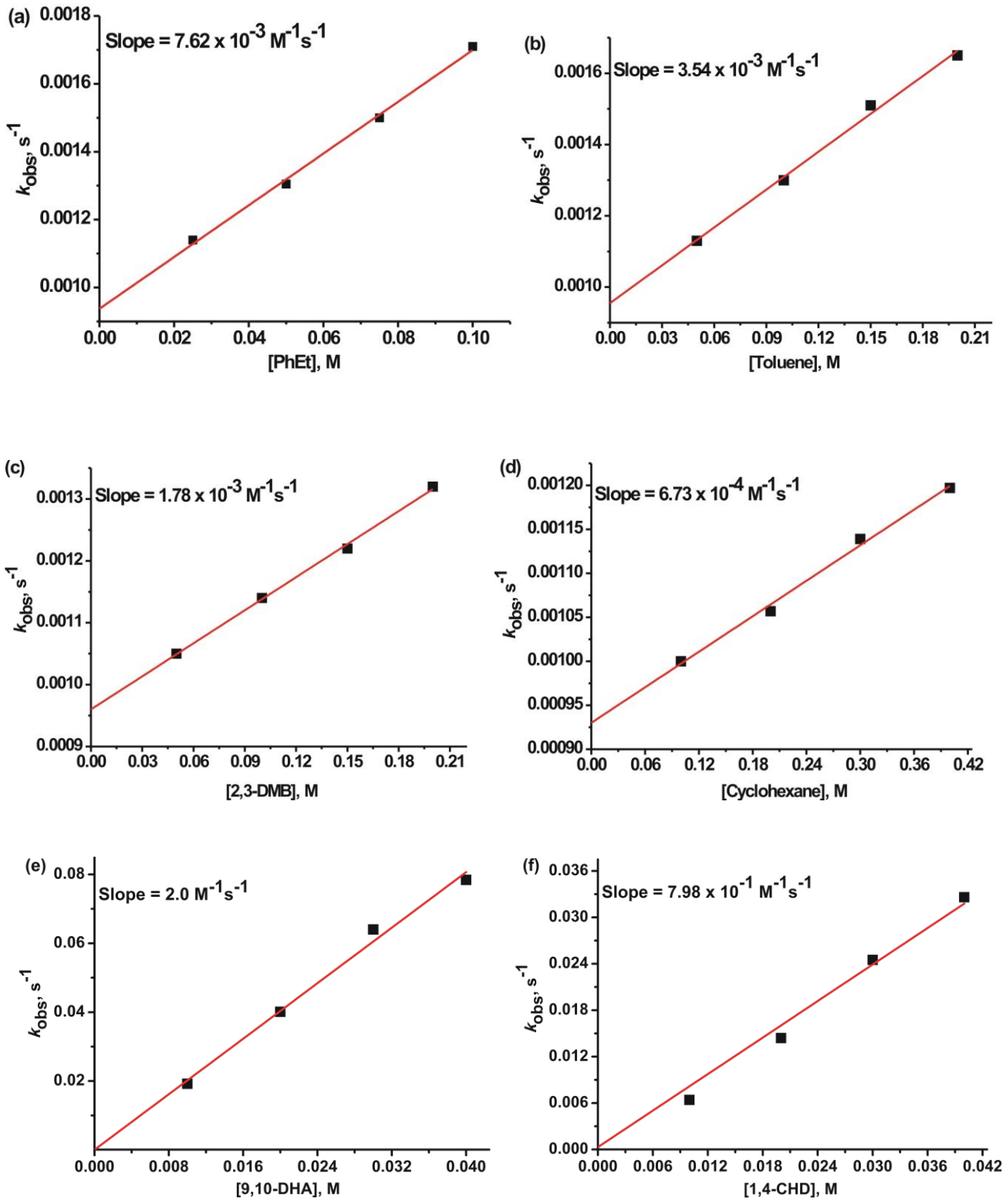


Figure S14 Plots of k_{obs} *vs* substrate concentration for the reaction of **2** with (a) PhEt, (b) $PhCH_3$, (c) 2,3-DMB, (d) *cyclo*-C_6H_{12}, (e) 9,10-DHA and (f) 1,4-CHD at 298 K.

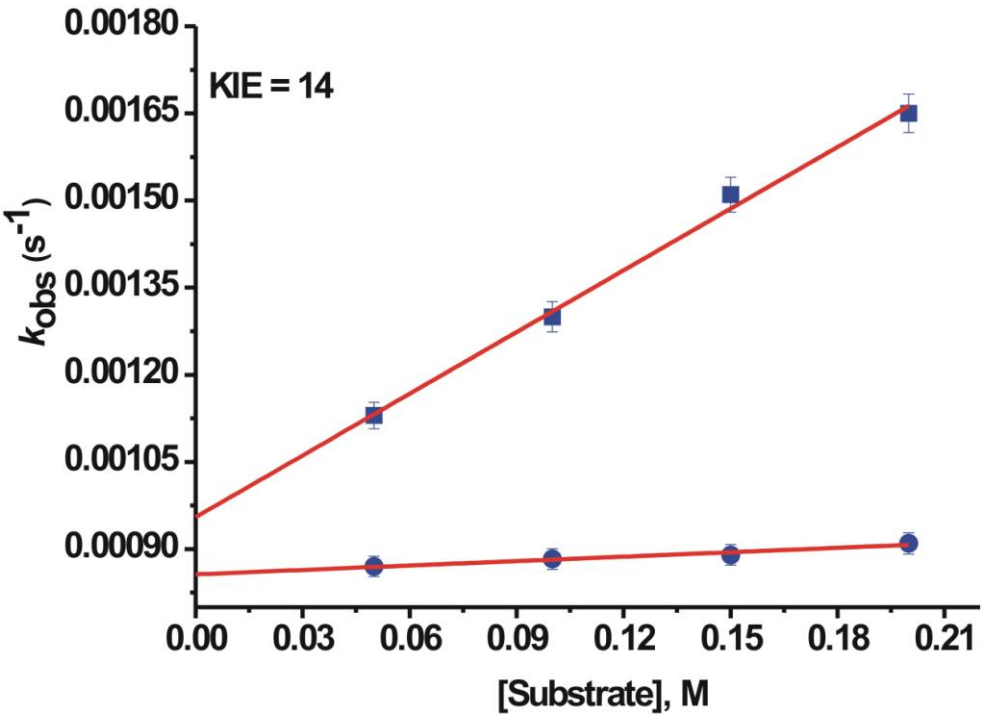


Figure S15 Kinetic isotope effect (observed rate constants) for **2** obtained from separate reaction with toluene (filled squares) and toluene-d_8 (filled circles).

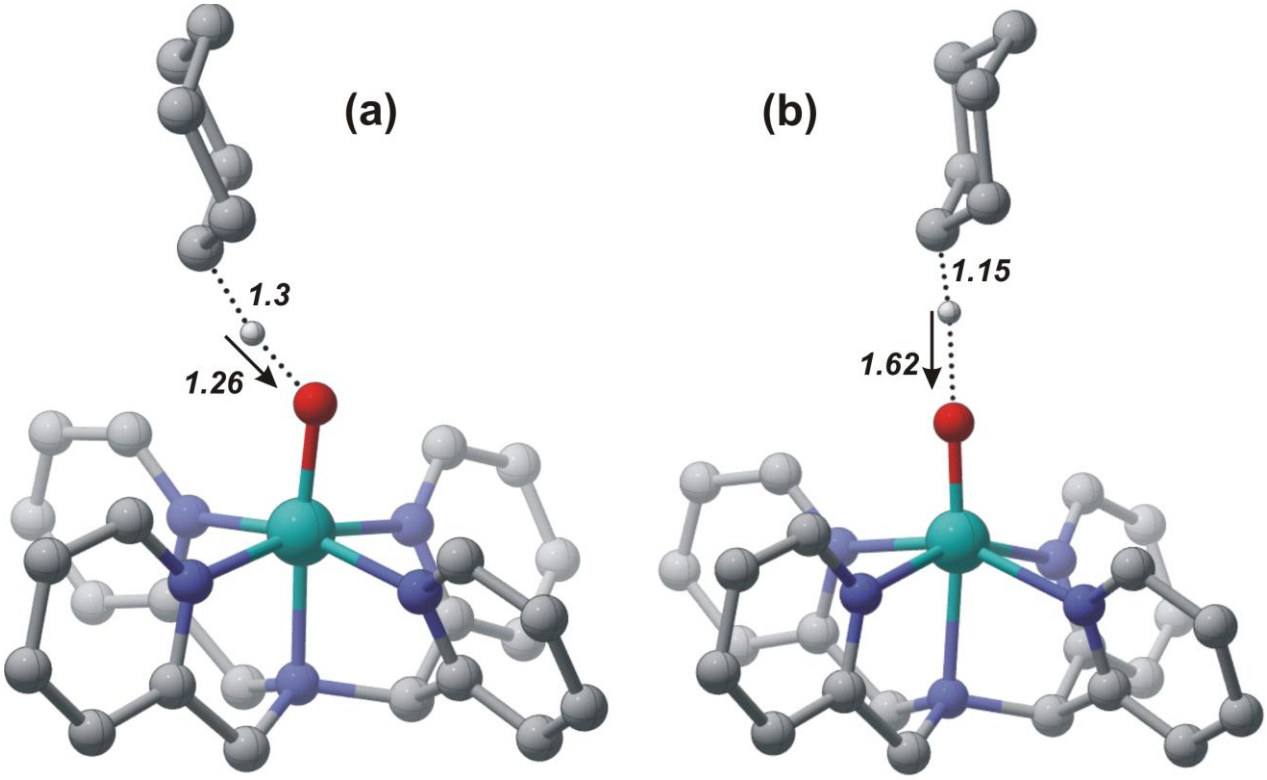


Figure S16 Energy optimized geometries of transition states of C-H bond activation of cyclohexane by $[Fe^{IV}(O)(N4Py)]^{2+}$ in (a) triplet spin state and (b) in quintet spin state at the UB3LYP/6-31++G(d,p)/Fe(SDD) level of theory.

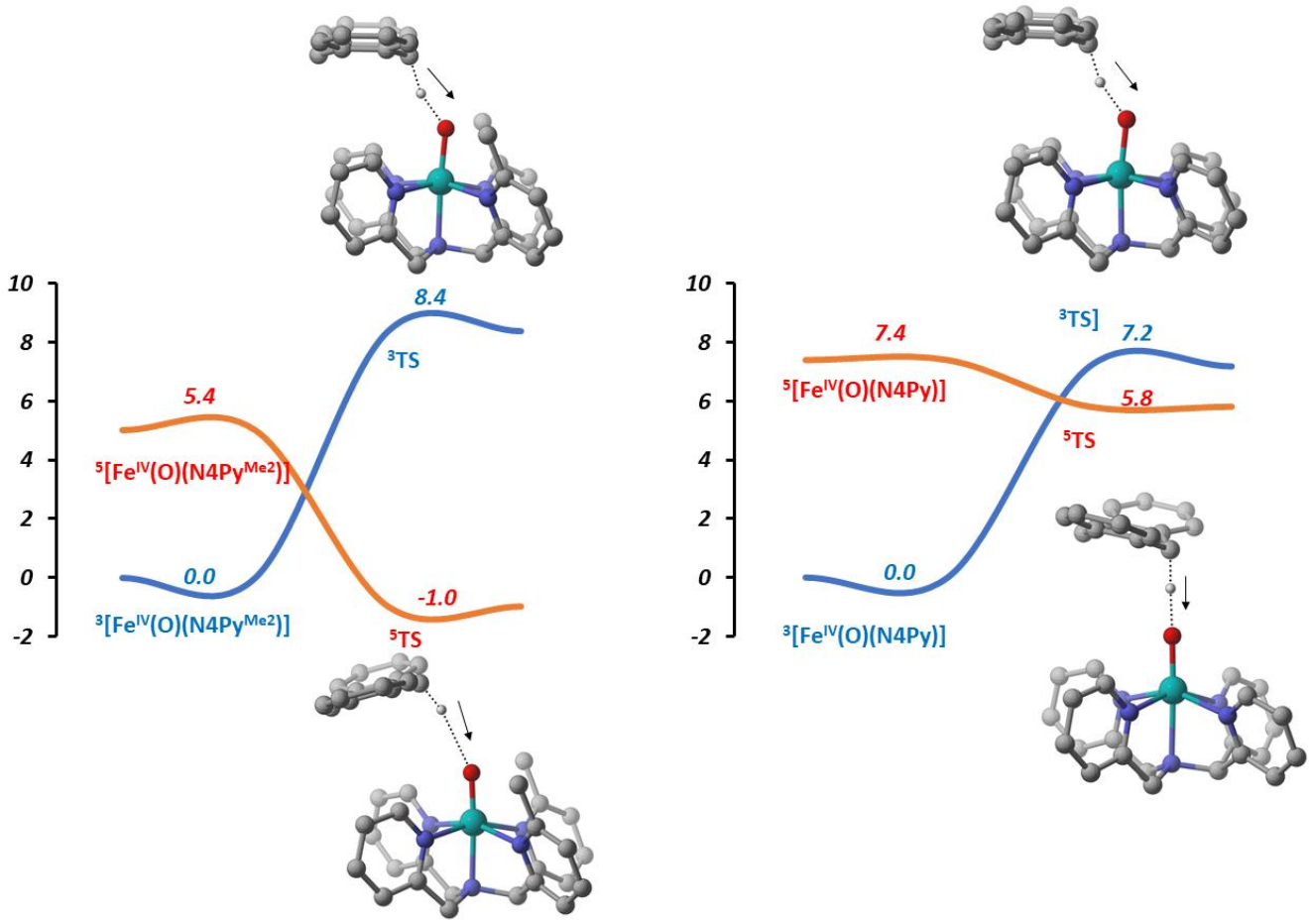
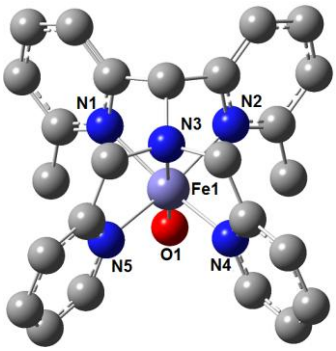


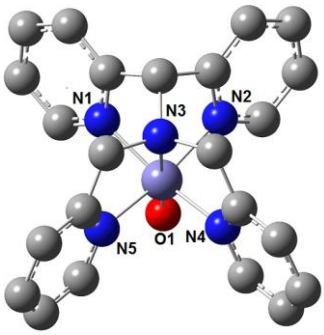
Figure S17 Relative condensed phase C-H activation barrier for the reaction of the iron oxo complexes (**2** and $[Fe^{IV}(O)(N4Py)]^{2+}$) with 9,10-DHA on triplet and quintet surfaces at the UB3LYP-D3(CPCM)/6-31++G(d,p)/Fe(SDD)//UB3LYP /6-31++G(d,p)/Fe(SDD) level of theory.

Table S1 Comparative Fe=O stretching frequencies and their corresponding IR intensity and Raman activity of $[Fe^{IV}(O)(N4Py^{Me2})]^{2+}$ **(2)** and $[Fe^{IV}(O)(N4Py)]^{2+}$ species at the B3LYP/6-31++G(d,p)/LANL2DZ(Fe) level of theory.

Fe(IV)=O intermediates	**Spin**	**Fe=O stretching (symmetrical) frequency (cm^{-1})**	**IR intensity**	**Raman activity**
$[Fe^{IV}(O)(N4Py)]^{2+}$	*S*=1 (triplet)	938.45	9.156	9.189
$[Fe^{IV}(O)(N4Py^{Me2})]^{2+}$	*S*=1(triplet)	919.35	9.574	9.325

Table S2 Calculated bond parameters for $[Fe^{IV}(O)(N4Py^{Me2})]^{2+}$ (**2**) and $[Fe^{IV}(O)(N4Py)]^{2+}$.





Distances/Angles (Å)/(°)	$[Fe^{IV}(O)(N4Py^{Me2})]^{2+}$		$[Fe^{IV}(O)(N4Py)]^{2+}$	
	Calculated (*S*=1) ublyp/ 6-311++g(d,p)	Calculated (*S*=2) ublyp/ 6-311++g(d,p)	Calculated (*S*=1) ublyp/ 6-311++g(d,p)	Calculated (*S*=2) ublyp/ 6-311++g(d,p)
Fe1-N1	2.053	2.189	2.006	2.155
Fe1-N2	2.053	2.189	2.006	2.155
Fe1-N3	2.090	2.116	2.093	2.124
Fe1-N4	2.000	2.110	1.993	2.103
Fe1-N5	2.000	2.110	1.993	2.103
Fe1-O1	1.619	1.612	1.618	1.610
N1-Fe1-N2	85.9	83.1	85.3	82.0
N1-Fe1-N3	81.7	79.0	81.4	78.6
N1-Fe1-N4	164.1	159.6	164.3	159.4
N1-Fe1-N5	91.0	90.7	90.8	90.6
N2-Fe1-N3	81.7	79.0	81.4	78.6
N2-Fe1-N4	91.0	90.7	90.8	90.6
N2-Fe1-N5	164.1	159.6	164.3	159.4
N3-Fe1-N4	82.4	80.8	82.9	81.1
N3-Fe1-N5	82.4	80.8	82.9	81.1
N4-Fe1-N5	87.7	88.5	88.9	89.7
O1-Fe1-N1	100.4	103.3	98.4	101.7
O1-Fe1-N2	100.4	103.3	98.4	101.7
O1-Fe1-N3	177.2	176.8	179.7	179.5
O1-Fe1-N4	95.6	97.0	97.2	98.5
O1-Fe1-N5	95.6	97.0	97.2	98.5

Table S3 Distances between the nitrogen atom of coordinated acetonitrile and the hydrogen atoms of the 6-methyl substituents and the 6-H hydrogens of the non-substituted pyridyl groups in iron(II) complexes of 6-methyl substituted N4Py-type ligands.

Complex	**N_{MeCN}–H**
$[Fe^{II}(N2Py)(N2CH_2Py^{Me})(MeCN)]^{2+}$ [a]	2.727 (N6–H11) 2.732 (N6–H1) 2.529 (N6–H27A_{Me}) 2.960 (N6–H27C_{Me}) 2.599 (N6–H26A_{Me}) 2.940 (N6–H26C_{Me})
$[Fe^{II}(N4Py^{Me2})(MeCN)]^{2+}$ (**1b**)	2.674 (N6–H20) 2.672 (N6–H19) 2.691 (N6–H1C_{Me}) 2.812 (N6–H1A_{Me}) 2.669 (N6–H13C_{Me}) 2.793 (N6–H13A_{Me})

[a] Spek, A. L.; Schoondergang, M. F. J.; Feringa, B. L., CSD Communication. *Private Communication* **2004**.

Optimized Cartesian Coordinates, Gas Phase (E(gas)), Solvent Phase (CPCM) (E(sol)) Abbsolute Energies, Enthalpy (H(corr)) and Free Energy (G(corr)) Correction at uB3LYP-D3/6-31++G(d,p)/Fe(SDD)

Quintet (*S*=2) $[Fe^{IV}(O)(N4Py)]^{2+}$

E(gas) = -1361.59761 Eh
E(sol) = -1361.869735 Eh
H(corr) = 0.43234 Eh
G(corr) = 0.35297 Eh

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N -1.30499000 0.08279200 0.00000000
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H 2.28087200 -2.25873500 1.71129300
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C -0.66107000 2.11047800 1.22390400
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H 2.28087200 -2.25873500 -1.71129300
C 0.85676500 -3.39190200 -2.89885900
H 1.59756700 -4.06686000 -3.31315900
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H -2.47056800 -2.67736200 -2.91072900
H 2.29075100 1.37858400 -2.48977200
H 2.29075100 1.37858400 2.48977200

Triplet (*S*=1) [Fe^{IV}(O)(N4Py)]$^{2+}$

E(gas) = -1361.608056 Eh
E(sol) = -1361.884637 Eh
H(corr) = 0.43335 Eh
G(corr) = 0.35808 Eh

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H -2.39601700 -2.62277700 -3.01446500
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H 2.28602800 1.15743300 2.36503900

***S*=2, ^{5}TS{[Fe^{IV}(O)(N4Py)(C$_6$H$_{12}$)]$^{2+}$}**

E(gas) = -1597.493642 Eh
E(sol) = -1597.77669 Eh
H(corr) = 0.606085 Eh

G(corr) = 0.506802 Eh

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C -1.52957900 2.15702300 1.40572300
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H -4.14457700 -0.47400100 -0.97101600
C -3.01412100 -0.34519100 1.30767500
H -4.06237600 -0.62197000 1.15233600
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C 0.24409100 2.69534000 3.43269700
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N -1.02323500 -1.39261300 -1.57546100
N -0.40316500 1.41959700 1.51625000
N -0.90974900 -1.59113300 1.39177200
C -0.12312900 -2.59650500 1.82693500
H 0.91018100 -2.56447400 1.49799400
C -0.60893000 -3.61181400 2.64364500
H 0.05421000 -4.40181600 2.97845600
C -1.95758000 -3.59005300 3.00719200
H -2.37249600 -4.37231400 3.63521800
C -2.77024300 -2.55008900 2.55087400
H -3.82141900 -2.50877600 2.81901500
C 4.11681900 -0.81752800 -0.23154000

C 4.71090600 -0.55733100 1.14796800
C 4.70744600 0.07746000 -1.31534200
H 4.47919100 0.46920400 1.46503500
H 4.28622400 -1.23737300 1.89614300
H 4.47450800 1.12904400 -1.09776100
H 4.28174300 -0.15897900 -2.29795700
H 4.20761600 -1.87862700 -0.50485000
H 2.97915100 -0.63614800 -0.18097800
C 6.25350500 -0.72783700 1.10019800
C 6.25069400 -0.09354400 -1.35856600
C 6.87605000 0.16357000 0.01818400
H 6.49181300 -1.78010100 0.89642700
H 6.66889900 -0.49428600 2.08732900
H 7.95778700 -0.01187000 -0.02854000
H 6.74373500 1.21994800 0.29083300
H 6.48965200 -1.11256200 -1.69042800
H 6.66347200 0.58920600 -2.11027900
H 1.17330200 1.40856200 -2.51489100
H 1.35853100 1.05816900 2.53602700

***S*=1, ^{3}TS{[Fe^{IV}(O)(N4Py)(C$_6$H$_{12}$)]$^{2+}$}**

E(gas) = -1597.480485 Eh
E(sol) = -1597.751977 Eh
H(corr) = 0.51017 Eh
G(corr) = 0.604448 Eh

Fe 0.01664200 -0.38681900 0.00000000
N 1.25047900 -1.22787400 1.35555100
N -0.77670300 -2.30950900 0.00000000
O 0.87912800 1.12440500 0.00000000
C 0.53400500 -3.05897400 0.00000000
H 0.40607700 -4.14689100 0.00000000
C -1.73065600 1.13905100 1.91330200
H -1.14022000 1.98225700 1.57927500
C 1.95943800 -0.61893800 -2.31723000
C 1.31355500 -2.57184200 -1.21554500
C 1.31355500 -2.57184200 1.21554500
C -3.14802500 -1.08104000 2.67568900
H -3.68910000 -1.97920000 2.95680100
C -2.08392100 -1.15974600 1.77854200
C 1.95943800 -0.61893800 2.31723000
C 2.75989400 -1.34775200 3.19827500
H 3.32759300 -0.82915100 3.96297500
C -2.08392100 -1.15974600 -1.77854200
C -2.77087800 1.28881700 2.82468000

H -3.00525400 2.27219900 3.21708300
C 2.81692000 -2.73596900 3.07199400
H 3.42818000 -3.32581600 3.74781500
C -1.58912400 -2.48781800 1.24282800
H -0.96290700 -2.95810500 2.00726000
H -2.42571500 -3.16998800 1.06224400
C -1.58912400 -2.48781800 -1.24282800
H -2.42571500 -3.16998800 -1.06224400
H -0.96290700 -2.95810500 -2.00726000
C 2.75989400 -1.34775200 -3.19827500
H 3.32759300 -0.82915100 -3.96297500
C 2.08165200 -3.36459900 -2.05877300
H 2.11170700 -4.44193600 -1.93076700
C -3.49765400 0.16048300 3.20846300
H -4.32160300 0.24395400 3.91008500
C 2.08165200 -3.36459900 2.05877300
H 2.11170700 -4.44193600 1.93076700
C 2.81692000 -2.73596900 -3.07199400
H 3.42818000 -3.32581600 -3.74781500
N -1.39509600 -0.05949000 1.39691700
N 1.25047900 -1.22787400 -1.35555100
N -1.39509600 -0.05949000 -1.39691700
C -1.73065600 1.13905100 -1.91330200
H -1.14022000 1.98225700 -1.57927500
C -2.77087800 1.28881700 -2.82468000
H -3.00525400 2.27219900 -3.21708300
C -3.49765400 0.16048300 -3.20846300
H -4.32160300 0.24395400 -3.91008500
C -3.14802500 -1.08104000 -2.67568900
H -3.68910000 -1.97920000 -2.95680100
C 0.38728600 3.62579700 0.00000000
C 1.05698600 4.11263700 -1.27158800
C 1.05698600 4.11263700 1.27158800
H 2.07806900 3.71225100 -1.32396000
H 0.52426900 3.76635600 -2.16602100
H 2.07806900 3.71225100 1.32396000
H 0.52426900 3.76635600 2.16602100
H -0.69960200 3.79421700 0.00000000
H 0.50916700 2.32595900 0.00000000
C 1.12733900 5.66454000 -1.27001700
C 1.12733900 5.66454000 1.27001700
C 1.81203300 6.18801700 0.00000000
H 0.11009900 6.07292800 -1.33816800
H 1.66176700 5.99668000 -2.16712600
H 1.80572200 7.28385200 0.00000000
H 2.86754800 5.88290200 0.00000000
H 0.11009900 6.07292800 1.33816800
H 1.66176700 5.99668000 2.16712600
H 1.88346000 0.46194300 2.35149300
H 1.88346000 0.46194300 -2.35149300

##

Quintet (*S*=2) [Fe^{IV}(O)($N4Py^{Me2}$)]$^{2+}$

E(gas) = -1440.24741 Eh
E(sol) = -1440.52624 Eh
H(corr) = 0.490628 Eh
G(corr) = 0.404121 Eh

Fe -0.65584000 0.14405900 0.00000000
N -0.29324100 -1.45337100 1.45160800
N 1.45846400 0.07098800 0.00000000
O -2.26174500 0.28849600 0.00000000
C 1.63686000 -1.42955300 0.00000000
H 2.69671700 -1.70736900 0.00000000
C -1.19428800 2.43701500 1.98751300
H -2.21852500 2.25783700 1.67717000
C -1.06309700 -1.92236500 -2.46245600
C 0.93138100 -1.99074900 -1.22655100
C 0.93138100 -1.99074900 1.22655100
C 1.45108800 2.77679700 2.65438300
H 2.50257800 2.89086100 2.89886000
C 1.03468800 1.75984700 1.79711500
C -1.06309700 -1.92236500 2.46245600
C -0.58717200 -2.97081200 3.26891600
H -1.21613700 -3.34559600 4.06895600
C 1.03468800 1.75984700 -1.79711500
C -0.85182400 3.46352200 2.86118400
H -1.62286900 4.11251800 3.26161700
C 0.67156900 -3.51553600 3.04579000
H 1.04197500 -4.32019100 3.67339800
C 1.98889500 0.72302400 1.24506600
H 2.13278900 -0.05101000 2.00507600
H 2.97294800 1.16156700 1.05393300
C 1.98889500 0.72302400 -1.24506600
H 2.97294800 1.16156700 -1.05393300
H 2.13278900 -0.05101000 -2.00507600
C -0.58717200 -2.97081200 -3.26891600
H -1.21613700 -3.34559600 -4.06895600
C 1.45683000 -3.01415100 -2.00026400
H 2.44386900 -3.41543300 -1.79501100
C 0.49352000 3.63797400 3.19620600
H 0.79511800 4.43534800 3.86835000
C -2.40678900 -1.30306800 -2.71596500
H -2.96679000 -1.17086800 -1.78811900
H -2.98898400 -1.91942400 -3.40286300
H -2.29116600 -0.31316600 -3.17263500
C -2.40678900 -1.30306800 2.71596500
H -2.29116600 -0.31316600 3.17263500
H -2.98898400 -1.91942400 3.40286300
H -2.96679000 -1.17086800 1.78811900
C 1.45683000 -3.01415100 2.00026400

H 2.44386900 -3.41543300 1.79501100
C 0.67156900 -3.51553600 -3.04579000
H 1.04197500 -4.32019100 -3.67339800
N -0.26737000 1.60418400 1.47272700
N -0.29324100 -1.45337100 -1.45160800
N -0.26737000 1.60418400 -1.47272700
C -1.19428800 2.43701500 -1.98751300
H -2.21852500 2.25783700 -1.67717000
C -0.85182400 3.46352200 -2.86118400
H -1.62286900 4.11251800 -3.26161700
C 0.49352000 3.63797400 -3.19620600
H 0.79511800 4.43534800 -3.86835000
C 1.45108800 2.77679700 -2.65438300
H 2.50257800 2.89086100 -2.89886000

Triplet (*S*=1) $[Fe^{IV}(O)(N4Py^{Me2})]^{2+}$

E(gas) = -1440.253749 Eh
E(sol) = -1440.537219 Eh
H(corr) = 0.491667 Eh
G(corr) = 0.409071 Eh

Fe -0.53163200 0.11309200 0.00000000
N -0.28643800 -1.37025800 1.39870800
N 1.55732100 0.04088000 0.00000000
O -2.14500500 0.24937100 0.00000000
C 1.67078100 -1.45948300 0.00000000
H 2.71083000 -1.80315400 0.00000000
C -1.18203000 2.33483700 1.86216400
H -2.18397000 2.14468000 1.49426900
C -1.10074700 -1.78413000 -2.40183000
C 0.92010400 -1.96969500 -1.21813900
C 0.92010400 -1.96969500 1.21813900
C 1.41467800 2.69831800 2.68122400
H 2.45059300 2.81980500 2.98203400
C 1.06312600 1.69139700 1.78377700
C -1.10074700 -1.78413000 2.40183000
C -0.68246200 -2.83282600 3.24050500
H -1.34690000 -3.16128400 4.03191700
C 1.06312600 1.69139700 -1.78377700
C -0.90074800 3.35127500 2.76830200
H -1.70340900 3.98331100 3.13207500
C 0.55510400 -3.43730900 3.06418500
H 0.87475400 -4.24096300 3.72019700
C 2.06667800 0.69500700 1.24530900
H 2.24004600 -0.07523000 2.00324800
H 3.03241000 1.17542100 1.06134100
C 2.06667800 0.69500700 -1.24530900
H 3.03241000 1.17542100 -1.06134100
H 2.24004600 -0.07523000 -2.00324800
C -0.68246200 -2.83282600 -3.24050500

H -1.34690000 -3.16128400 -4.03191700
C 1.38326800 -2.99473800 -2.02672400
H 2.35768700 -3.43886800 -1.85216800
C 0.41956900 3.53822300 3.18403100
H 0.67214000 4.32758600 3.88502400
C -2.43433900 -1.13173400 -2.61807500
H -3.02142200 -1.11174900 -1.69772000
H -2.99226200 -1.66443100 -3.38947500
H -2.31199900 -0.09449200 -2.94542800
C -2.43433900 -1.13173400 2.61807500
H -2.31199900 -0.09449200 2.94542800
H -2.99226200 -1.66443100 3.38947500
H -3.02142200 -1.11174900 1.69772000
C 1.38326800 -2.99473800 2.02672400
H 2.35768700 -3.43886800 1.85216800
C 0.55510400 -3.43730900 -3.06418500
H 0.87475400 -4.24096300 -3.72019700
N -0.21756500 1.52079200 1.38631800
N -0.28643800 -1.37025800 -1.39870800
N -0.21756500 1.52079200 -1.38631800
C -1.18203000 2.33483700 -1.86216400
H -2.18397000 2.14468000 -1.49426900
C -0.90074800 3.35127500 -2.76830200
H -1.70340900 3.98331100 -3.13207500
C 0.41956900 3.53822300 -3.18403100
H 0.67214000 4.32758600 -3.88502400
C 1.41467800 2.69831800 -2.68122400
H 2.45059300 2.81980500 -2.98203400

S=2, ^{5}TS{[Fe^{IV}(O)(N4Py^{Me2}) (C_6H_{12})]$^{2+}$}

E(gas) = -1676.14089 Eh
E(sol) = -1676.433613 Eh
H(corr) = 0.663847 Eh
G(corr) = 0.557241 Eh

Fe -0.29509700 0.09424500 -0.03041100
N -0.86632200 -1.21309400 1.68190400
N -2.52051200 0.31186200 0.06414200
O 1.38743300 0.08618200 -0.11835500
C -2.85728600 -1.13035800 0.30053800
H -3.93914800 -1.28814100 0.38700100
C 0.50319200 2.62704000 1.57941900
H 1.48751400 2.28337600 1.28033900
C -0.42009300 -2.36371100 -2.18432600
C -2.30239400 -1.95871400 -0.85116200
C -2.16157700 -1.59451200 1.57375500
C -2.05430600 3.37008800 2.23831400
H -3.07714000 3.64048200 2.48176400
C -1.78668100 2.18577400 1.55128000

C -0.13188500 -1.62539900 2.74230800
C -0.70969900 -2.45476700 3.71750900
H -0.10540800 -2.78372400 4.55579600
C -1.98728400 1.65284800 -1.98032100
C 0.31303600 3.81416600 2.27820800
H 1.16597800 4.42705600 2.54816800
C -2.03993000 -2.84253000 3.60899400
H -2.49210200 -3.47766200 4.36444900
C -2.88464300 1.19922100 1.20563600
H -3.06846000 0.57789800 2.08775500
H -3.82112300 1.72917200 1.00071800
C -3.02402000 0.83169900 -1.23957100
H -3.93952400 1.41553000 -1.09560800
H -3.29616600 -0.01769000 -1.87407200
C -1.09098800 -3.43370300 -2.80002400
H -0.58034700 -4.00425700 -3.56816300
C -3.01904700 -2.99373900 -1.43475000
H -4.03545300 -3.20838700 -1.12119400
C -0.99008400 4.19368800 2.60985100
H -1.17605600 5.11855000 3.14702600
C 0.96938900 -1.98387400 -2.60726000
H 1.57562800 -1.68137500 -1.75262200
H 1.45432300 -2.81465500 -3.12346400
H 0.93340000 -1.13767500 -3.30466500
C 1.29262300 -1.16795200 2.86427400
H 1.32983400 -0.11192300 3.15618800
H 1.81782400 -1.74441000 3.62775600
H 1.81851800 -1.25971300 1.91239900
C -2.78920500 -2.40046600 2.51326600
H -3.83124500 -2.67916600 2.39539000
C -2.39226900 -3.75083000 -2.43084100
H -2.91635500 -4.57258500 -2.90898100
N -0.52612300 1.83033500 1.22744200
N -1.03433500 -1.64694100 -1.21368400
N -0.69293200 1.38465800 -1.71037500
C 0.27743600 2.02419400 -2.39429600
H 1.29473500 1.76610100 -2.12068600
C -0.00894200 2.95724400 -3.38485600
H 0.79844100 3.44794300 -3.91717800
C -1.34692100 3.24722700 -3.66395400
H -1.60682800 3.97738000 -4.42410400
C -2.34929900 2.58866600 -2.94950300
H -3.39725000 2.79476800 -3.14412000
C 4.10305300 0.20140700 -0.31719600
C 4.62921100 -0.96482500 -1.14300500
C 4.71711800 0.28076900 1.07383200
H 4.36643100 -1.91534000 -0.65920500
H 4.18834200 -0.97118300 -2.14646500
H 4.46182800 -0.61996000 1.64800200
H 4.33492700 1.14557500 1.62922000
H 4.21750800 1.15349200 -0.85563800
H 2.94340600 0.09187700 -0.20742200

C 6.17704600 -0.87073000 -1.25246200
C 6.26418800 0.37434600 0.95767500
C 6.82665100 -0.79070200 0.13404300
H 6.44223300 0.01844800 -1.83950000
H 6.54478300 -1.74004900 -1.80952100
H 7.91238800 -0.67749800 0.02761900
H 6.66354100 -1.73479100 0.67209200
H 6.53268700 1.32815400 0.48460900
H 6.69461300 0.38742200 1.96557600

S=1, ^{3}TS{[Fe^{IV}(O)(N4Py^{Me2})(C$_6$H$_{12}$)]$^{2+}$}

E(gas) = -1676.120978 Eh
E(sol) = -1676.421071 Eh
H(corr) = 0.662896 Eh
G(corr) = 0.561609 Eh

Fe -0.05234700 -0.40749100 0.00000000
N 1.13872300 -1.37394000 1.42380300
N -0.97659400 -2.26764400 0.00000000
O 0.84883300 1.08242000 0.00000000
C 0.26751200 -3.10795400 0.00000000
H 0.04842200 -4.18168300 0.00000000
C -1.73415500 1.22837200 1.88620700
H -1.09593100 2.03405800 1.55024600
C 1.87967300 -0.89593100 -2.45520300
C 1.08079100 -2.71481100 -1.21891200
C 1.08079100 -2.71481100 1.21891200
C -3.28328500 -0.89775000 2.65374100
H -3.87787100 -1.76134700 2.93493900
C -2.21526200 -1.04595200 1.76954100
C 1.87967300 -0.89593100 2.45520300
C 2.59165100 -1.78844000 3.27635200
H 3.18909900 -1.38542200 4.08650900
C -2.21526200 -1.04595200 -1.76954100
C -2.77561900 1.44728300 2.78151800
H -2.95962400 2.44739700 3.15827300
C 2.52970400 -3.15873400 3.06229800
H 3.07463400 -3.84404700 3.70395800
C -1.79866100 -2.39988700 1.24099400
H -1.20071800 -2.90316000 2.00688100
H -2.67257200 -3.03348800 1.06005700
C -1.79866100 -2.39988700 -1.24099400
H -2.67257200 -3.03348800 -1.06005700
H -1.20071800 -2.90316000 -2.00688100
C 2.59165100 -1.78844000 -3.27635200
H 3.18909900 -1.38542200 -4.08650900
C 1.74658300 -3.63932500 -2.00848400
H 1.65938500 -4.70182500 -1.80670300
C -3.56854800 0.36607900 3.17044000
H -4.39433300 0.50358900 3.86131600

C 1.93566500 0.57713500 -2.73002600
H 2.19902800 1.13014700 -1.82760800
H 2.65930400 0.78570000 -3.51957000
H 0.95855500 0.94489100 -3.06026900
C 1.93566500 0.57713500 2.73002600
H 0.95855500 0.94489100 3.06026900
H 2.65930400 0.78570000 3.51957000
H 2.19902800 1.13014700 1.82760800
C 1.74658300 -3.63932500 2.00848400
H 1.65938500 -4.70182500 1.80670300
C 2.52970400 -3.15873400 -3.06229800
H 3.07463400 -3.84404700 -3.70395800
N -1.45669500 0.00700500 1.38787800
N 1.13872300 -1.37394000 -1.42380300
N -1.45669500 0.00700500 -1.38787800
C -1.73415500 1.22837200 -1.88620700
H -1.09593100 2.03405800 -1.55024600
C -2.77561900 1.44728300 -2.78151800
H -2.95962400 2.44739700 -3.15827300
C -3.56854800 0.36607900 -3.17044000
H -4.39433300 0.50358900 -3.86131600
C -3.28328500 -0.89775000 -2.65374100
H -3.87787100 -1.76134700 -2.93493900
C 0.41024000 3.60815800 0.00000000
C 1.07357500 4.10695900 -1.27007800
C 1.07357500 4.10695900 1.27007800
H 2.10482600 3.73375700 -1.31912300
H 0.55414400 3.74825400 -2.16698200
H 2.10482600 3.73375700 1.31912300
H 0.55414400 3.74825400 2.16698200
H -0.67759700 3.77034200 0.00000000
H 0.52491100 2.28937100 0.00000000
C 1.10643700 5.66057000 -1.26952500
C 1.10643700 5.66057000 1.26952500
C 1.77778200 6.20123200 0.00000000
H 0.07970100 6.04415100 -1.33896200
H 1.63335500 6.00397500 -2.16681500
H 1.74409500 7.29651800 0.00000000
H 2.84055700 5.92278000 0.00000000
H 0.07970100 6.04415100 1.33896200
H 1.63335500 6.00397500 2.16681500

S=1, ^{3}{[Fe(OH)(N4Py^{Me2})(·C_6H_{11})]$^{2+}$]}

E(gas) = -1676.138018 Eh
E(sol) = -1676.436014 Eh
H(corr) = 0.667906 Eh
G(corr) = 0.562885 Eh

Fe 0.04051300 -0.50417300 0.00000000
N -1.13981300 -1.47755500 -1.41611900
N 0.99611200 -2.31044100 0.00000000
O -0.89263800 1.01518800 0.00000000
C -0.22434400 -3.19103300 0.00000000
H 0.03002500 -4.25656400 0.00000000
C 1.66622800 1.20209400 -1.87900900
H 1.01273100 1.99855000 -1.54308700
C -1.89818100 -1.01006200 2.43994000
C -1.04901700 -2.81799200 1.21761600
C -1.04901700 -2.81799200 -1.21761600
C 3.26998500 -0.88264400 -2.65487800
H 3.88615700 -1.72963300 -2.93996900
C 2.20845900 -1.06009800 -1.76894100
C -1.89818100 -1.01006200 -2.43994000
C -2.59518000 -1.91679100 -3.25924000
H -3.20853500 -1.52446500 -4.06271800
C 2.20845900 -1.06009800 1.76894100
C 2.70035700 1.44895900 -2.77594100
H 2.85722600 2.45444900 -3.15052700
C -2.49860500 -3.28617100 -3.05302500
H -3.03184600 -3.98077100 -3.69453400
C 1.82408000 -2.42393100 -1.24272700
H 1.23672700 -2.94058200 -2.00778100
H 2.71086800 -3.03796800 -1.05895400
C 1.82408000 -2.42393100 1.24272700
H 2.71086800 -3.03796800 1.05895400
H 1.23672700 -2.94058200 2.00778100
C -2.59518000 -1.91679100 3.25924000
H -3.20853500 -1.52446500 4.06271800
C -1.69691100 -3.75445900 2.00709500
H -1.58417200 -4.81566800 1.81124900
C 3.52020300 0.38981200 -3.16924100
H 4.34016100 0.55068100 -3.86202300
C -1.98945700 0.46238900 2.71234500
H -2.24151100 1.01318400 1.80526000
H -2.73397000 0.65488700 3.48635500
H -1.02744000 0.84772800 3.06719100
C -1.98945700 0.46238900 -2.71234500
H -1.02744000 0.84772800 -3.06719100
H -2.73397000 0.65488700 -3.48635500
H -2.24151100 1.01318400 -1.80526000
C -1.69691100 -3.75445900 -2.00709500
H -1.58417200 -4.81566800 -1.81124900
C -2.49860500 -3.28617100 3.05302500
H -3.03184600 -3.98077100 3.69453400
N 1.42309600 -0.02800200 -1.38290600
N -1.13981300 -1.47755500 1.41611900
N 1.42309600 -0.02800200 1.38290600
C 1.66622800 1.20209400 1.87900900
H 1.01273100 1.99855000 1.54308700
C 2.70035700 1.44895900 2.77594100

H 2.85722600 2.45444900 3.15052700
C 3.52020300 0.38981200 3.16924100
H 4.34016100 0.55068100 3.86202300
C 3.26998500 -0.88264400 2.65487800
H 3.88615700 -1.72963300 2.93996900
C -0.06485300 4.18210500 0.00000000
C -0.79277700 4.49972100 1.27328400
C -0.79277700 4.49972100 -1.27328400
H -1.70463800 3.88807800 1.35116800
H -0.18080700 4.29325800 2.15965600
H -1.70463800 3.88807800 -1.35116800
H -0.18080700 4.29325800 -2.15965600
H 1.02278000 4.28331700 0.00000000
H -0.41874700 1.86995200 0.00000000
C -1.22946200 5.99699600 1.27192900
C -1.22946200 5.99699600 -1.27192900
C -2.01909100 6.33840800 0.00000000
H -0.33554200 6.63066400 1.33467100
H -1.82718100 6.19835900 2.16821200
H -2.27885500 7.40294400 0.00000000
H -2.96957300 5.78598500 0.00000000
H -0.33554200 6.63066400 -1.33467100
H -1.82718100 6.19835900 -2.16821200

S=2, ^{5}\{[Fe^{II}(N4Py^{Me2})($C_6H_{11}OH$)]$^{2+}$\}

E(gas) = -1676.226067 Eh
E(sol) = -1676.525457 Eh
H(corr) = 0.668746 Eh
G(corr) = 0.562814 Eh

Fe -0.14599100 -0.00587700 -0.04773100
N -1.49698600 -1.80230000 -0.63358700
N -2.01523400 0.32178600 1.11125600
O 1.69337200 -0.35662000 -1.11657300
C -3.01969300 -0.03320300 0.05924000
H -4.04750500 0.07228600 0.42908300
C 1.57704200 -1.38261500 2.30434800
H 2.35659600 -1.39262600 1.55037100
C -1.28776200 1.80976300 -2.62963500
C -2.82447400 0.87313700 -1.15085200
C -2.78575700 -1.47317900 -0.38555100
C -0.45318700 -1.30683800 4.12750500
H -1.28141200 -1.26056500 4.82798800
C -0.64653200 -0.94901900 2.79147100
C -1.21554700 -3.05079300 -1.06983300
C -2.23460600 -3.99286300 -1.27256900
H -1.97927400 -4.98767800 -1.62172800

C -0.71946900 2.41182000 1.67094500
C 1.84632000 -1.77336400 3.61259200
H 2.84393600 -2.09659200 3.88919900
C -3.55882900 -3.64769900 -1.02441300
H -4.35619800 -4.36864000 -1.17627900
C -2.03108700 -0.60164700 2.27596200
H -2.51002700 -1.53682400 1.96827100
H -2.64308300 -0.19131900 3.08763100
C -2.07844100 1.74942000 1.52660500
H -2.64301200 1.85235500 2.46057200
H -2.63413200 2.30781300 0.76656400
C -2.33095200 2.40932600 -3.35034500
H -2.09861500 3.02191800 -4.21506200
C -3.90442400 1.44114200 -1.81862600
H -4.91761200 1.28489700 -1.46253400
C 0.80876900 -1.73060500 4.54512400
H 0.97863200 -2.01734500 5.57810500
C 0.14327500 1.98953000 -3.05643100
H 0.80416700 2.08898900 -2.19375400
H 0.48002500 1.12698300 -3.64459300
H 0.25527700 2.87433100 -3.68629700
C 0.21858400 -3.40048800 -1.35550600
H 0.37059400 -4.48161300 -1.34127800
H 0.50759800 -3.04978500 -2.35560100
H 0.88514000 -2.94207000 -0.62343000
C -3.84338800 -2.35845900 -0.56665200
H -4.86181100 -2.05190900 -0.35104500
C -3.64876600 2.22582400 -2.94621900
H -4.46412700 2.69081500 -3.49161100
N 0.35944400 -0.98058900 1.89139500
N -1.54222400 1.04716700 -1.54182200
N 0.28851100 1.94637200 0.90407800
C 1.47426500 2.58587000 0.94426200
H 2.25726700 2.18201700 0.31078700
C 1.71066000 3.70161800 1.74114100
H 2.68333000 4.18139700 1.73122600
C 0.67365300 4.17185400 2.54917800
H 0.81961700 5.03050000 3.19694000
C -0.55689200 3.51609000 2.51098700
H -1.38430700 3.85650500 3.12597000
C 3.16938200 -0.28178700 -0.94200200
C 3.77474100 0.70236600 -1.94075200
C 3.78744100 -1.67501800 -1.05671700
H 3.53578000 0.36773200 -2.96149300
H 3.32568600 1.69392500 -1.81278200
H 3.54940800 -2.08911500 -2.04780900
H 3.34714700 -2.35051400 -0.31428200
H 3.28470100 0.09685400 0.07949300
H 1.52902800 -0.70262100 -2.00610700
C 5.30704800 0.77189500 -1.77877600
C 5.31876200 -1.60508100 -0.89108900
C 5.94555000 -0.62116900 -1.88918600

H 5.55002200 1.21342000 -0.80205800
H 5.71809200 1.44859900 -2.53451700
H 7.02443700 -0.55021400 -1.71817600
H 5.81669600 -1.00124400 -2.91185400
H 5.55552300 -1.29040800 0.13490100
H 5.74252800 -2.60653000 -1.01569300

S=1, ^{3}{[Fe^{II}(N4Py^{Me2})($C_6H_{11}OH$)]$^{2+}$}

E(gas) = -1676.198219 Eh
E(sol) = -1676.498859 Eh
H(corr) = 0.670024 Eh
G(corr) = 0.568436 Eh

Fe -0.38246000 -0.00458000 0.01263900
N -1.40887600 1.50801400 -1.07066700
N -2.34033000 -0.08452900 1.03813300
O 1.97261400 0.05116000 -0.93116900
C -3.12295100 0.00622200 -0.22467800
H -4.20765200 -0.01616400 -0.05762900
C 1.24160200 1.80234200 1.82597000
H 2.04644700 1.53138900 1.15508700
C -0.94214400 -2.32180600 -2.08831600
C -2.72037900 -1.14993400 -1.13062100
C -2.74495000 1.29165600 -0.94862400
C -0.86551300 2.41117000 3.45311400
H -1.72429500 2.62873800 4.08075200
C -1.02040300 1.60329300 2.32504500
C -0.98332800 2.60868300 -1.73311100
C -1.90470200 3.50798000 -2.29441000
H -1.53348100 4.37991600 -2.82249600
C -1.03907600 -1.93026700 2.10482400
C 1.46562800 2.62401600 2.92437000
H 2.46208100 3.00471600 3.11971700
C -3.26887800 3.28153800 -2.17180000
H -3.98643100 3.97477900 -2.59939000
C -2.39839200 1.09281500 1.92875700
H -2.92636800 1.90435900 1.41756500
H -2.98107700 0.87208100 2.83073400
C -2.41154800 -1.37538200 1.75133200
H -3.01924800 -1.28807900 2.65971400
H -2.91843400 -2.10843200 1.11531400
C -1.85205500 -3.13356200 -2.78428100
H -1.46954700 -3.91549800 -3.43154500
C -3.66467900 -1.92375900 -1.79045500
H -4.72349300 -1.74221700 -1.63808300
C 0.39026300 2.93297300 3.75922300
H 0.52675800 3.56451200 4.63138000
C 0.53360700 -2.53136100 -2.27066500
H 0.90302400 -1.91963100 -3.10381700
H 0.74597700 -3.57270600 -2.52332200

H 1.09451300 -2.26052700 -1.37763900
C 0.49029200 2.84903100 -1.89356100
H 1.06802300 2.34879500 -1.11818500
H 0.71200900 3.91908700 -1.87201200
H 0.83001000 2.47294400 -2.86716400
C -3.70091900 2.14649600 -1.47828000
H -4.75730200 1.93518200 -1.34878500
C -3.21927100 -2.93842400 -2.64232500
H -3.92742700 -3.56576000 -3.17450100
N 0.02744500 1.29711000 1.52394800
N -1.37928400 -1.33225100 -1.27263800
N 0.01487600 -1.52781500 1.36011400
C 1.22731000 -2.06443600 1.60780800
H 2.03887800 -1.71056700 0.98394100
C 1.44183700 -3.01666400 2.59777100
H 2.43656500 -3.41900000 2.75497400
C 0.35844300 -3.42590500 3.37761800
H 0.48768900 -4.16004800 4.16660900
C -0.89553000 -2.87083700 3.12672000
H -1.75987800 -3.16504500 3.71426100
C 3.42283800 0.04859900 -0.66632400
C 4.09498300 -1.17753900 -1.28760200
C 4.07123500 1.34977800 -1.14261400
C 5.61189000 -1.18052900 -1.01083100
H 3.92584900 -1.15926000 -2.37491300
H 3.63379600 -2.09726200 -0.90767300
C 5.58758000 1.35057900 -0.86426800
H 3.90175200 1.45205200 -2.22521300
H 3.59170600 2.21098200 -0.66188000
C 6.27421500 0.12292600 -1.48083500
H 6.06796600 -2.04536600 -1.50344800
H 5.78357500 -1.31177600 0.06688200
H 6.02685200 2.27504400 -1.25290400
H 5.75759000 1.35946900 0.22162800
H 7.33760200 0.11780100 -1.22040600
H 6.22268900 0.18606500 -2.57656000
H 1.87001800 0.08214600 -1.89301800
H 3.48746200 -0.01478000 0.42682200

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