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Supporting Information

Modeling the *cis*-Oxo-Labile Binding Site Motif of Non-Heme Iron Oxygenases: Water Exchange and Oxidation Reactivity of a Non-Heme Iron(IV)-Oxo Compound Bearing a Tripodal Tetradentate Ligand

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1. Instrumentation

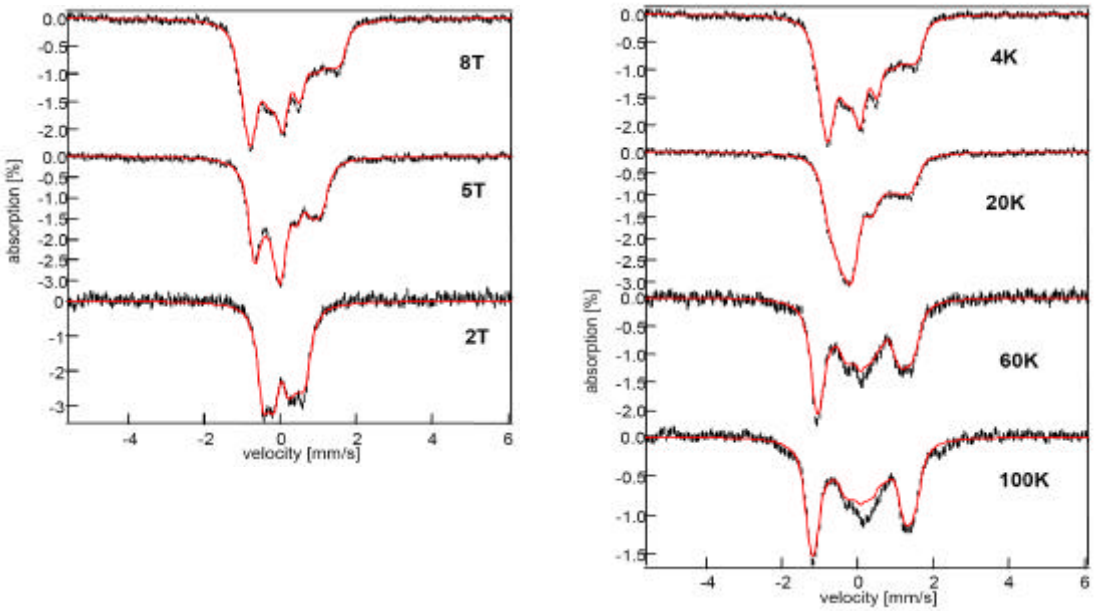
Product analyses were performed on a Shimadzu GC-2010 gas chromatograph (Cyclodex-B column, 30 m) and a flame ionization detector. GC-MS spectral analyses were performed on a ThermoQuest Trace GC 2000 Series chromatograph interfaced with a Finnigan ThermoQuest Trace MS mass spectrometer. The products were identified by comparison of their GC retention times and GC-MS with those of authentic compounds. NMR spectra were taken on Bruker DPX200 and DPX400 spectrometers. High-resolution electrospray mass spectrometry (ESI-MS) was performed on a Bruker (Billerica, MA) BioTOF II time-of-flight spectrometer. Exact-mass data were acquired using polypropylene glycol or polyethylene glycol as an internal standard. UV-vis spectroscopy was performed on a Cary 50 Scan (Varian) UV-vis spectrophotometer with 1 cm or 0.2 cm quartz cells. The low temperature control was performed with a cryostat from Unisoku Scientific Instruments (Japan). Mössbauer spectra were recorded with two spectrometers, using Janis Research Super-Varitemp dewars that allowed studies in applied magnetic fields up to 8.0 T in the temperature range from 1.5 to 200 K. Mössbauer spectral simulations were performed using the WMOSS software package (WEB Research, Edina, MN). Isomer shifts are quoted relative to Fe metal at 298 K. Resonance Raman spectra were collected on an Acton AM-506 spectrometer (1200 groove grating) using a Kaiser Optical holographic super-notch filters with a Princeton Instruments liquid-N_2-cooled (LN-1100PB) CCD detector with a 4 cm^{-1} spectral resolution.

2. Characterization of compound 2

Mössbauer spectroscopy

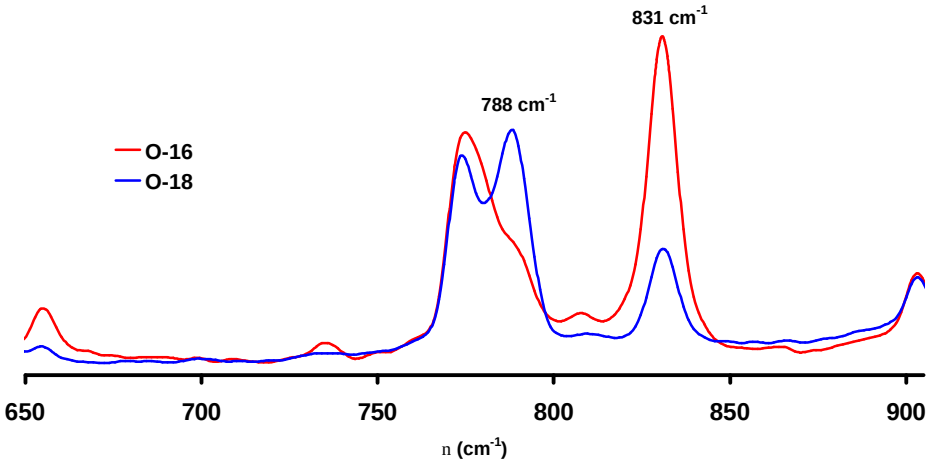
A ^{57}Fe sample of **2** for Mössbauer spectroscopy was prepared by reaction of [^{57}Fe(CF_3SO_3)$_2$(^{Me,H}Pytacn)] (**1**) with 2 equiv peracetic acid in acetonitrile at 15ºC. The ^{57}Fe enriched sample of **1** was synthesized following the reported experimental procedure[1] but using ^{57}Fe(CF_3SO_3)$_2$(CH_3CN)$_2$ as the iron source.

Figure S1. Left: Field dependence of the Mössbauer spectra of **2** at 4.2 K. Right: Temperature dependence of the Mössbauer spectra of **2** at 8 T. Black line: experimental data. Red line: simulated spectrum after subtraction of the intensity corresponding to the fast relaxing species **3** (which accounts for 15% of the sample).



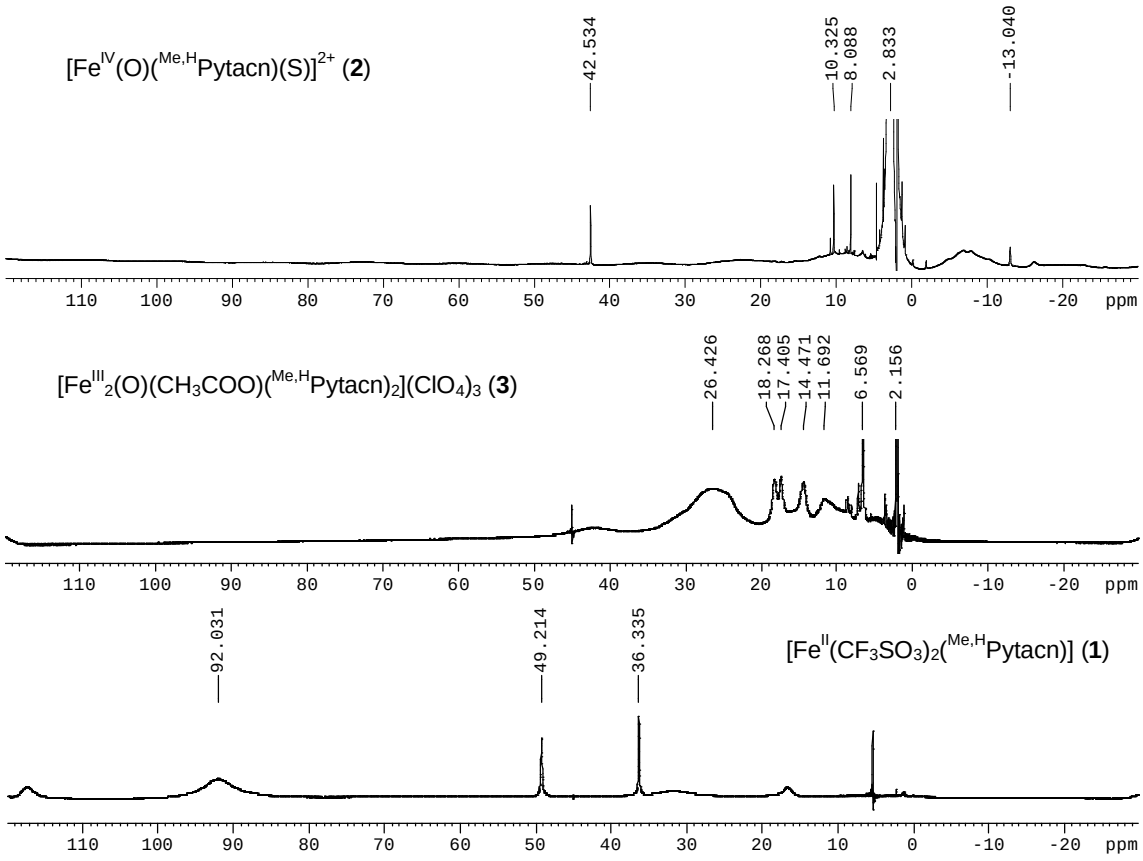
rRaman spectroscopy

Figure S2. Resonance Raman spectra of **2** before (red line) and after reaction with $H_2{}^{18}O$ (blue line) (λ_{exc} = 407.9 nm).



NMR spectroscopy

Figure S3. ^{1}H-NMR spectra of **1** (bottom), **2** (top) and **3** (middle) at 298K in CD_3CN. For compound **2** the spectrum shows a single set of sharp signals at 42, 10 and -13 ppm.

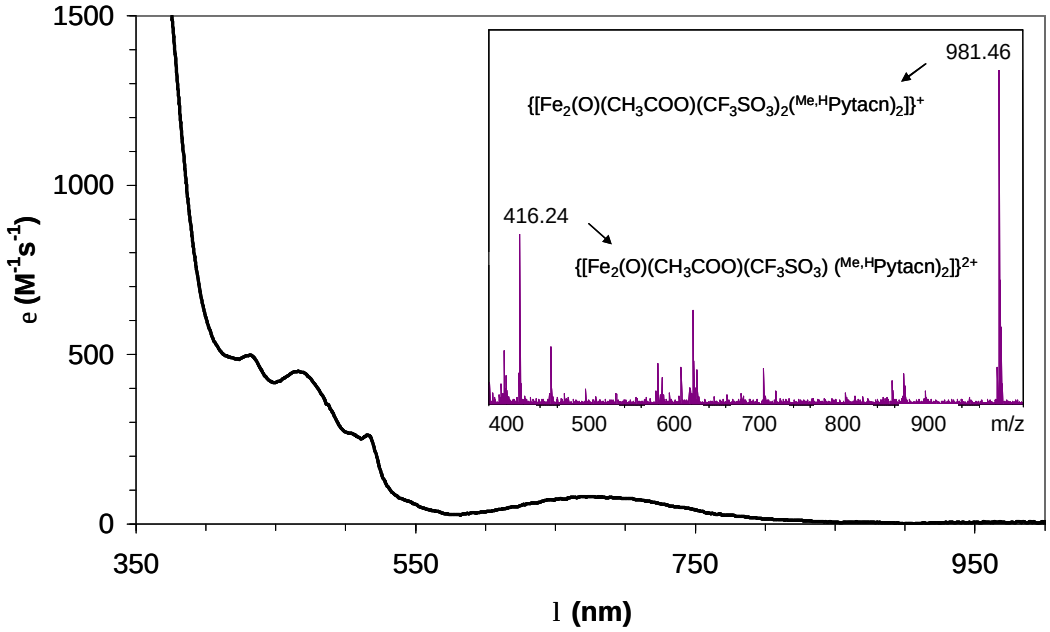


Experimental procedure for the preparation of the NMR sample of **2**: 5.4 mg of $[Fe(CF_3SO_3)_2(^{Me,H}Pytacn)]$ (**1**) (9 μmols) were dissolved in 1.2 mL CD_3CN and 20 μL D_2O. To the resulting solution 20 μL of a 0.95 M peracetic acid solution in CD_3CN (19 μmols) were added at once under stirring. The resulting solution was quickly transferred to a NMR tube and the ^{1}H-NMR spectrum was recorded.

3. Characterization of the decomposition species (3)

Thermal decay of **2** leads to a new species **3** that could be identified as $[Fe^{III}_2(\mu\text{-}O)(\mu\text{-}CH_3COO)(^{Me,H}Pytacn)_2]^{3+}$ (**3**) by means of UV-vis spectroscopy, ESI-MS and comparison with an independently prepared sample, characterized by X-ray crystallography.

Figure S4. UV-vis spectrum of the species derived from thermal decomposition of **2** recorded in CH_3CN at room temperature. Inset: ESI-MS spectrum.



Direct preparation of $[Fe^{III}_2(\mu\text{-}O)(\mu\text{-}CH_3COO)(^{Me,H}Pytacn)_2](ClO_4)_3\cdot CH_3CN$ (3·CH_3CN)

Synthesis of $[Fe^{III}_2(\mu\text{-}O)(\mu\text{-}CH_3COO)(^{Me,H}Pytacn)_2](ClO_4)_3\cdot CH_3CN$ (**3·CH_3CN**). 54.6 mg of compound **1** (90 μmols) were dissolved in CH_3CN (2 mL) under an inert atmosphere. 200 μL of an acetonitrile solution 0.30 M in CH_3COOH and Et_3N (60 μmols CH_3COOH and Et_3N) were added at once, which caused an immediate color change from dark pink to bright yellow. Immediately a balloon filled with O_2 was connected into the reaction vessel and the solution became red-brown in a few seconds. After stirring for 3 h, the solvent from the resulting solution was removed under reduced pressure affording a brown oil. The resulting product was dissolved in acetonitrile and 19 mg $NaClO_4\cdot H_2O$ (135 μmols) were added. The solution was stirred for about 2 hours, filtered through Celite© and diethyl ether was slowly diffused. 37 mg of brown crystals of **3·CH_3CN** suitable for X-ray diffraction were obtained (38 μmols, 84%). FT-IR (ATR) ν, cm^{-1}: 1611, 1523 (CH_3COO), 1447 ($C{=}C_{ar}$), 1073, 621 (ClO_4). ^{1}H-NMR ($CDCl_3$, 200 MHz, 300K) δ, ppm: 26.43, 18.27, 17.41, 14.47, 6.57. ESI-MS (m/z): 227.6 $[M\text{-}3ClO_4]^{3+}$, 880.9 $[M\text{-}ClO_4]^+$. UV-vis (CH_3CN) λ_{max}, nm (ε/Fe, $M^{-1}\cdot cm^{-1}$): 427 (660), 462 (690), 513 (500), 692 (58).

Crystal-structure determination. Crystals of $C_{32}H_{54}Cl_3Fe_2N_9O_{15}$ were grown from slow diffusion of diethyl ether into a CH_3CN solution of the compound, and used for low temperature (100(2)K) X-ray structure determination. The measurement was carried out on a BRUKER SMART APEX CCD diffractometer using graphite-monochromated Mo Kα radiation (λ =

0.71073 Å) from an X-Ray Tube. The measurements were made in the range 2.18 to 27.90° for ?. Full-sphere data collection was carried out with ? and f scans. A total of 61751 reflections were collected of which 10087 [R(int) = 0.0534] were unique. Programs used: data collection, Smart version 5.631 (Bruker AXS 1997-02); data reduction, Saint + version 6.36A (Bruker AXS 2001); absorption correction, SADABS version 2.10 (Bruker AXS 2001). Structure solution and refinement was done using SHELXTL Version 6.14 (Bruker AXS 2000-2003). The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2. The non-hydrogen atoms were refined anisotropically. The hydrogen-atoms were placed in geometrically optimized positions and forced to ride on the atom to which they are attached.

Table S1. Crystal data for **3·CH_3CN**.

Empirical formula	$C_{32}H_{54}Cl_3Fe_2N_9O_{15}$
Formula weight	1022.89
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 15.417(3) ? α = 90º b = 15.465(2) Å β = 90.807(3)° c = 17.759(3) Å γ = 90º
Volume	4233.8(12) $Å^3$
Density (calculated)	1.605 $g \cdot cm^{-3}$
Absorption coefficient	0.952 mm^{-1}
F(000)	2128
Cell formula units_Z	4
Crystal size	0.5 x 0.3 x 0.1 mm
? range for data collection	2.18 to 27.90°
Limiting indices	-20<=h<=20, -20<=k<=20, -23<=l<=23
Reflections collected	61751
Independent reflections	10087 [R(int) = 0.0534]
Completeness to ?	99.7% (? = 27.90º)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10087 / 7 / 584
Goodness-of-fit on F^2	1.115
Final R indices [I>2sigma(I)]	R1 = 0.0727**,** wR2 = 0.2234
R indices (all data)	R1 = 0.0819, wR2 = 0.2290
Largest diff. peak and hole	2.846 and -0.735 e. $Å^{-3}$

Table S2. Selected bond lengths (Å) and angles (º) for **3·CH_3CN**.

Fe1-N1	2.167(4)	O1-Fe1-O3	95.42(15)	O1-Fe2-O2	96.68(15)
Fe1-N2	2.225(4)	O1-Fe1-N4	99.75(16)	O2-Fe2-N6	85.54(15)
Fe1-N3	2.180(4)	N2-Fe1-N4	80.46(16)	N6-Fe2-N8	79.92(16)
Fe1-N4	2.197(4)	N2-Fe1-O3	85.06(15)	O1-Fe2-N8	98.33(16)
Fe1-O1	1.801(3)	N1-Fe1-O1	100.02(16)	N7-Fe2-N8	80.58(16)
Fe1-O3	2.062(4)	N1-Fe1-N2	73.99(16)	N6-Fe2-N7	77.70(15)
Fe2-N5	2.163(4)	N1-Fe1-N4	89.67(16)	O1-Fe2-N7	106.51(15)
Fe2-N6	2.247(4)	N1-Fe1-O3	93.34(15)	O2-Fe2-N7	89.95(15)
Fe2-N7	2.196(4)	N3-Fe1-O1	106.61(16)	O1-Fe2-N5	101.21(16)
Fe2-N8	2.184(4)	N3-Fe1-O3	89.53(15)	O2-Fe2-N5	90.70(16)
Fe2-O1	1.805(3)	N3-Fe1-N4	80.70(16)	N5-Fe2-N6	74.45(16)
Fe2-O2	2.017(3)	N2-Fe1-N3	79.36(16)	N5-Fe2-N8	91.72(16)

4. Oxygen-atom exchange with water

Figure S5. Plot of k_{obs} versus the concentration of $H_2{}^{18}O$ for the oxygen-atom exchange between **2** and $H_2{}^{18}O$ at 295K.

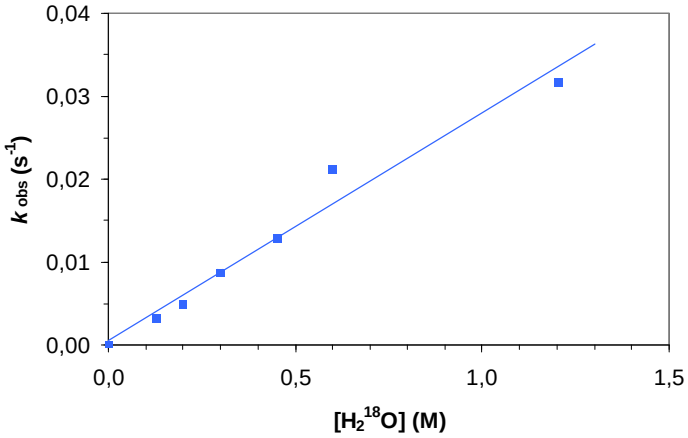


Table S3. Second order rate constants obtained in the oxygen-atom exchange of **2** (1 mM) with $H_2{}^{18}O$ (0.2 M) at different temperatures. Activation parameters obtained by fitting ln(k_{exc}/T) against 1/T: $\Delta H^{?}$ = 10.2±0.8 kcal·mol^{-1} and $\Delta S^{?}$ = -32±3 cal·K^{-1}·mol^{-1}

T (K)	k_{obs} (s^{-1})	k_{exc} ($M^{-1}s^{-1}$)
304.5	0.00850 ± 0.0002	0.043
295.0	0.0050 ± 0.0006	0.025
284.0	0.0021± 0.0001	0.0103
275.0	0.00135 ± 0.00004	0.0068

5. Sulfide oxidation: oxygen-atom transfer

Figure S6. UV-vis spectral changes of **2** upon addition of 5 equiv thioanisole. Experimental reaction conditions: to a solution of **2** (1 mM), 5 equiv of thioanisole (from a 70 mM acetonitrile solution) were added at once at 0 ºC and the kinetics were monitored at 750 nm (inset).

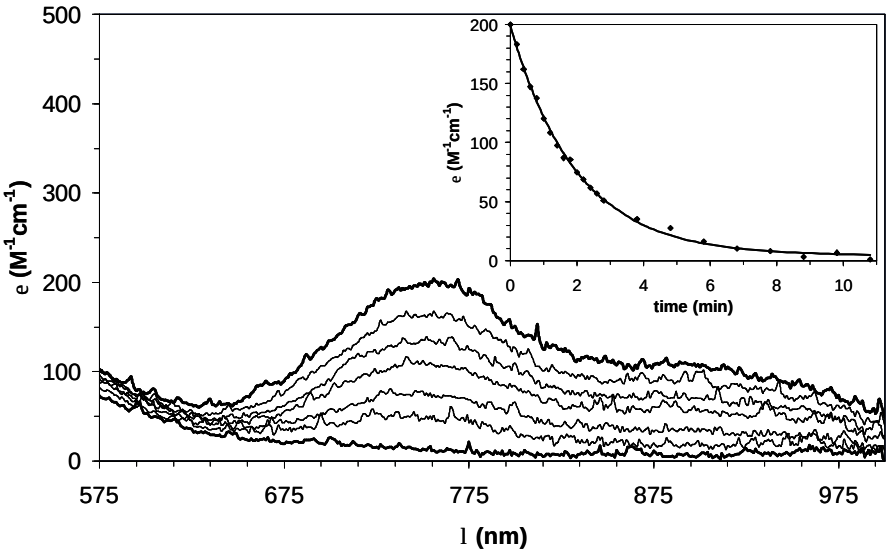
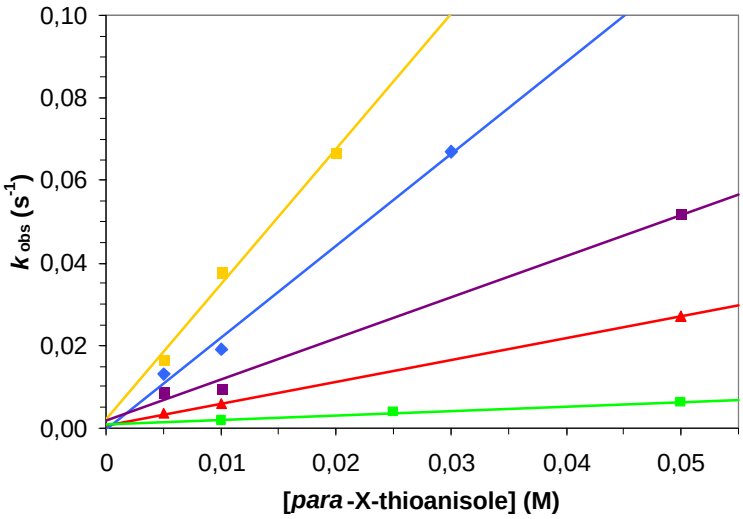
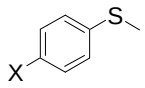


Figure S7. Plot of k_{obs} against substrate concentration for the reaction of **2** (1 mM) at 0 ºC with *p*-X-thioanisoles (the slope of each line corresponds to the second-order rate constant, k_2). X = CH_3O (yellow), CH_3 (blue), H (purple), Cl (red) and CN (green).





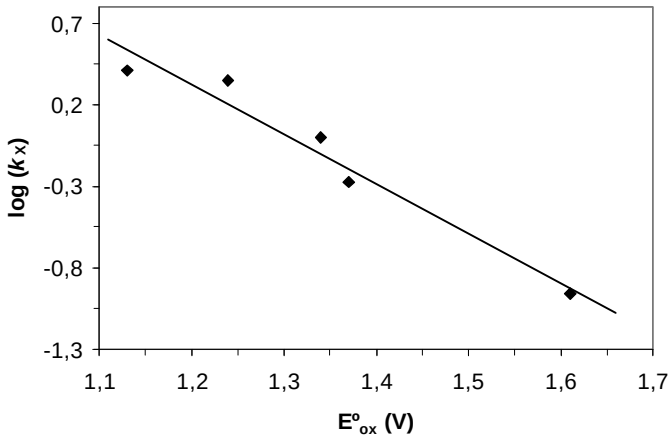
p-X-thioanisole
X = OCH_3, CH_3, H, Cl, CN

Table S4. Second-order rate constants (k_2) determined in the reaction of **2** with *p*-X thioanisoles.

X	E^o_{ox} vs. SCE (V)[a]	σ_p[b]	k_X ($M^{-1}s^{-1}$)[c]
OCH_3	1.13	-0.27	2.6 ± 0.3
CH_3	1.24	-0.17	2.2 ± 0.2
H	1.34	0.00	1.0 ± 0.1
Cl	1.37	0.23	0.53 ± 0.01
CN	1.61	0.66	0.11 ± 0.01

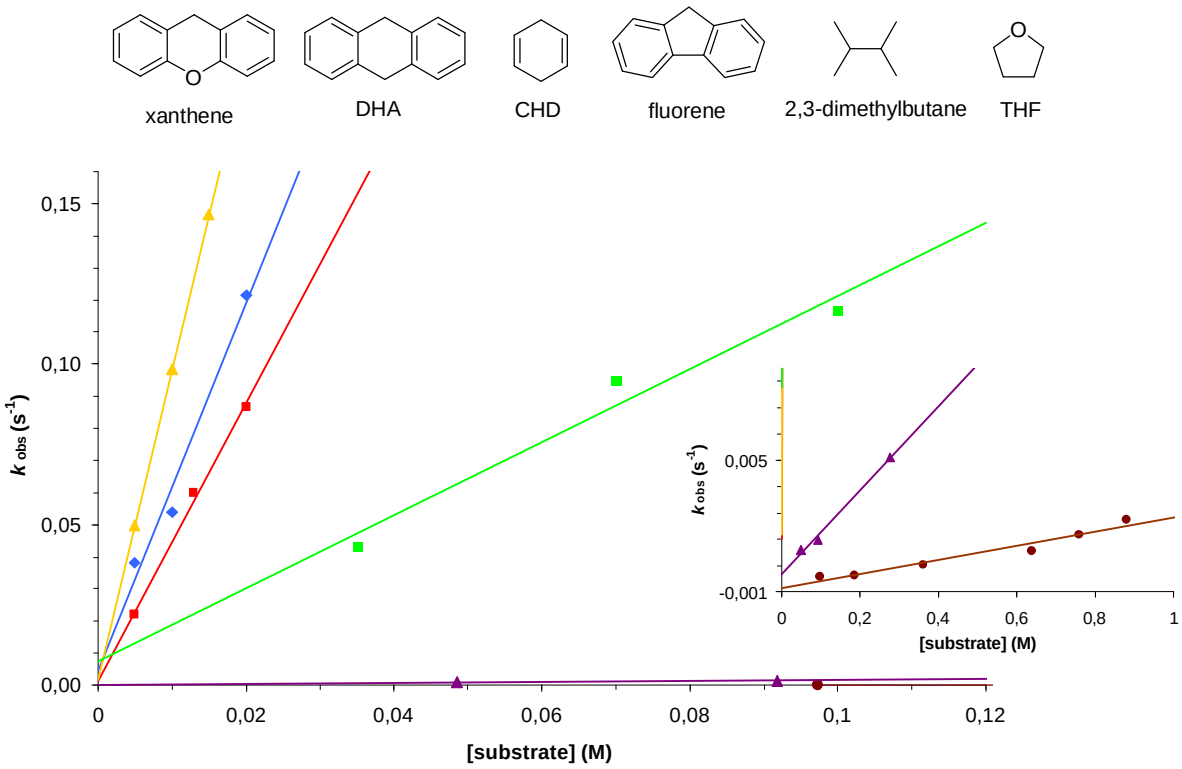
[a]One-electron oxidation potentials for *p*-X-thioanisoles. Data obtained from reference 2. [b]Hammett parameters. [c]Second-order rate constants in the reaction of **2** with *p*-X-thioanisoles.

Figure S8. Plot of log(k_X) against the one-electron oxidation potentials (E^o_{ox}) of *p*-X-thioanisoles. A linear correlation with a slope of -3.0 is obtained.



6. Oxidation of activated C-H bonds: hydrogen-atom abstraction

Figure S9. Plot of k_{obs} against substrate concentration for the reaction of **2** (1 mM) at -15 ºC with xanthene (yellow), DHA (blue), CHD (red), fluorene (green), 2,3-dimethylbutane (purple) and THF (brown) (the slope of each line corresponds to the second-order rate constant, k_2).



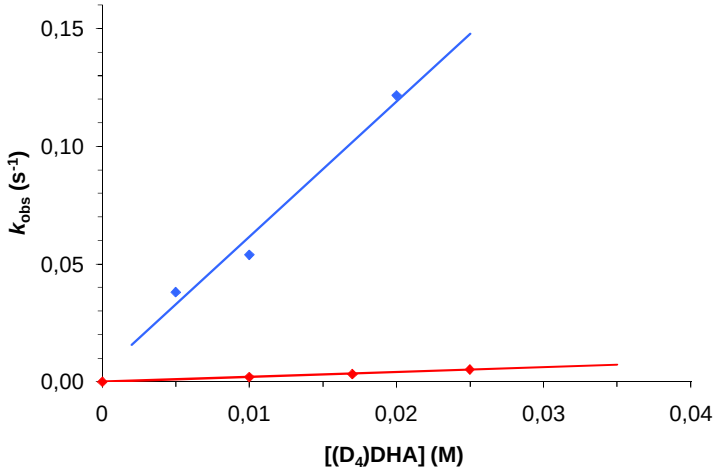
Determination of the kinetic isotope effect (KIE)

Dihydroanthracene (DHA). An exact amount of DHA or D_4-DHA (diluted in 200 μL acetonitrile) were added at once under stirring to a 2 mL of a 1 mM solution of **2** (2 μmols) in acetonitrile at -15ºC. Reactions were monitored by UV-vis spectroscopy by following the decay of the absorption band at λ = 750 nm which was fitted to a single exponential function. Plotting the obtained k_{obs} against substrate concentration gave a second-order rate constants (k_2) of 5.7±0.9 $M^{-1}s^{-1}$ and 0.21±0.2 $M^{-1}s^{-1}$ for DHA and D_4-DHA respectively. Dividing the obtained rate constants, a KIE value of 27 was obtained for the reaction of **2** with DHA at -15ºC.

The deuterated substrate D_4-9,10-dihydroanthracene (D_4-DHA) was prepared following the procedure described in the literature with slight modifications thereof.[3] NaH 60% in mineral oil (0.33 g, 8.2 mmols) was added to a mixture of 9,10-dihydroanthracene (0.5 g, 2.7 mmol) in D_6-DMSO (3 mL) under an inert atmosphere. The resulting deep red mixture was stirred at room temperature for 8 h and the reaction was quenched by careful addition of D_2O (5 mL). The crude product was filtered and washed with copious amounts of H_2O (20 mL). The resulting pink

solid was treated with H_2O (5 mL) and extracted with CH_2Cl_2 (3 x 5 mL). The combined organic layers were dried over $MgSO_4$ and filtered. The solvent was removed under reduced pressure to yield 0.45 g of a pale pink solid corresponding to D_4-9,10-dihydroanthracene (2.4 mmols, 89%). ^{1}H-NMR spectroscopy confirmed 98% deuteration. ^{1}H-NMR ($CDCl_3$, 200 MHz, 300K) δ, ppm: 7.32 – 7.27 (m, 4H, Ar**H**), 7.21 – 7.16 (m, 4H, Ar**H**).

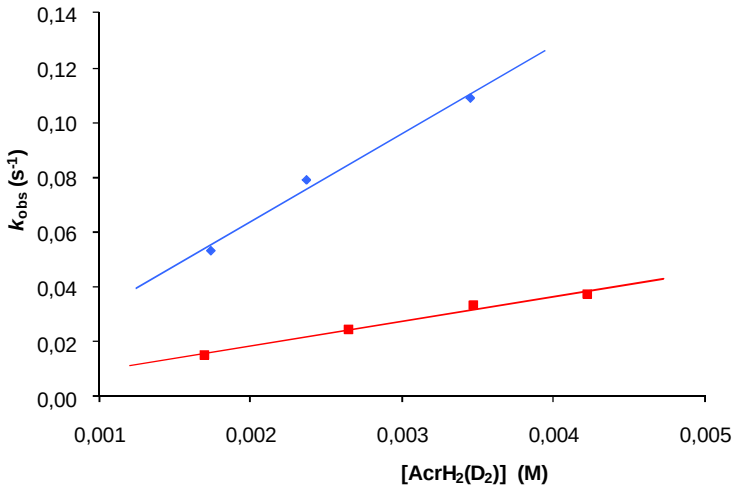
Figure S10. Plot of k_{obs} against substrate concentration for the reaction of **2** with DHA (blue line) and D_4-DHA (red line) at -15ºC (the slope of each line corresponds to the second-order rate constant, k_2).



9,10-dihydro-10-methylacridine ($AcrH_2$). An exact amount of $AcrH_2$ or $AcrD_2$ (diluted in acetonitrile) were added at once under stirring to a 1.2 mL of a 1 mM solution of **2** (1.2 μmols) in acetonitrile at -15 ºC. Reactions were monitored by UV-vis spectroscopy by following the decay of the absorption band at λ = 750 nm which was fitted to a single exponential function. Plotting the obtained k_{obs} against substrate concentration gave a second-order rate constants (k_2) for $AcrH_2$ and $AcrD_2$ respectively. Dividing the obtained rate constants, a KIE value of 3.5 was obtained for the reaction of **2** with $AcrH_2$ at -15 ºC.

The deuterated substrate [9,9'-D_2]-10-methylacridine ($AcrD_2$) was synthesized according to the procedure described in the literature.[4]

Figure S11. Plot of k_{obs} against substrate concentration for the reaction of **2** with $AcrH_2$ (blue line) and $AcrD_2$ (red line) at -15ºC (the slope of each line corresponds to the second-order rate constant, k_2).



7. DFT calculations

Figures S12-S20 show the optimized structures studied in this work calculated at the B3LYP.

Figure S12: Structure of **2a** calculated at the B3LYP level of theory in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms.

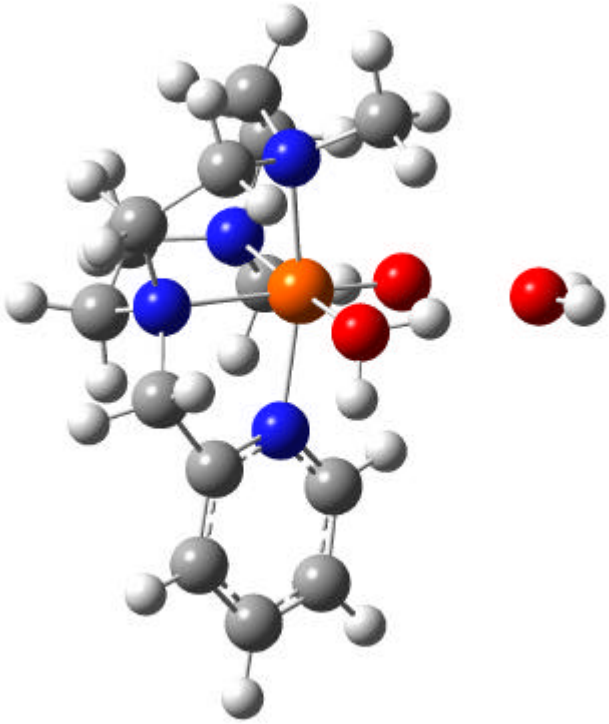


Figure S13: Structure of **2b** calculated at the B3LYP level of theory in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms.

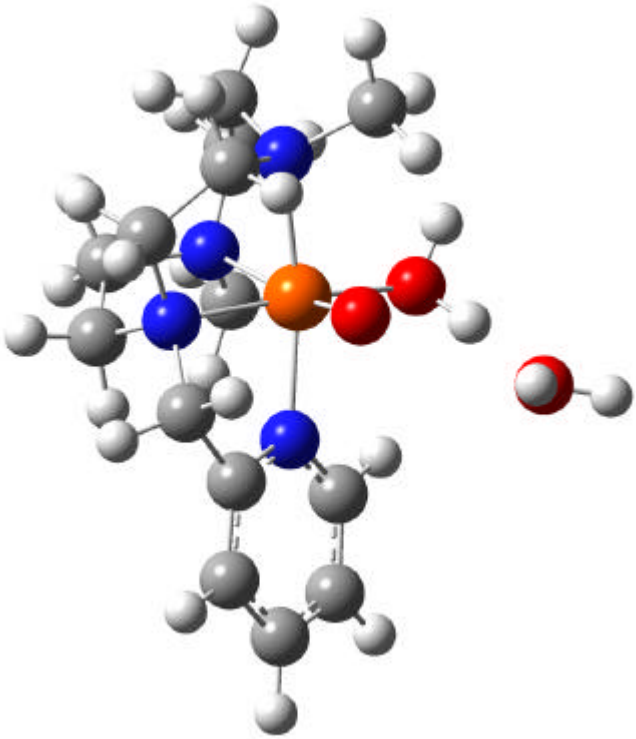


Figure S14: Structure of $[Fe^{IV}(O)(^{Me,H}Pytacn)(H_2O)]^{2+}$+$H_2O$+ CH_3CN calculated at the B3LYP level of theory in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms.

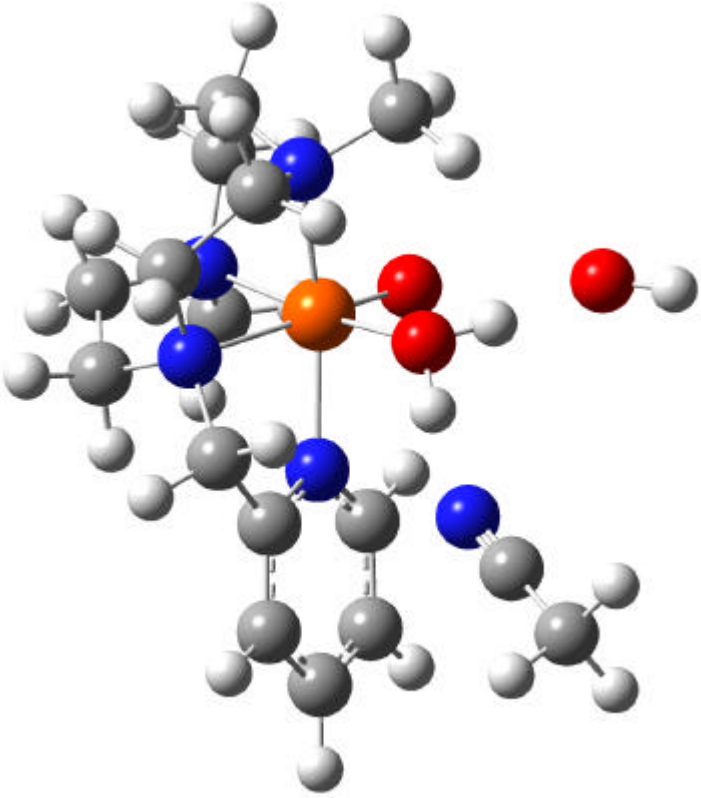


Figure S15: Structure of $[Fe^{IV}(O)(^{Me,H}Pytacn)(CH_3CN)]^{2+}+2H_2O$ calculated at the B3LYP level of theory in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms.

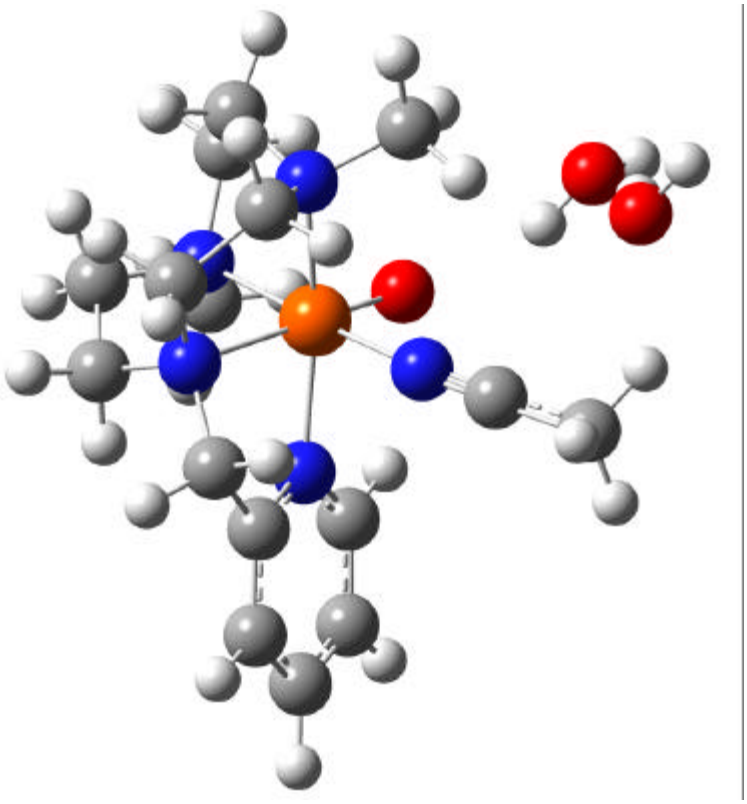


Figure S16: Structure of **I1** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

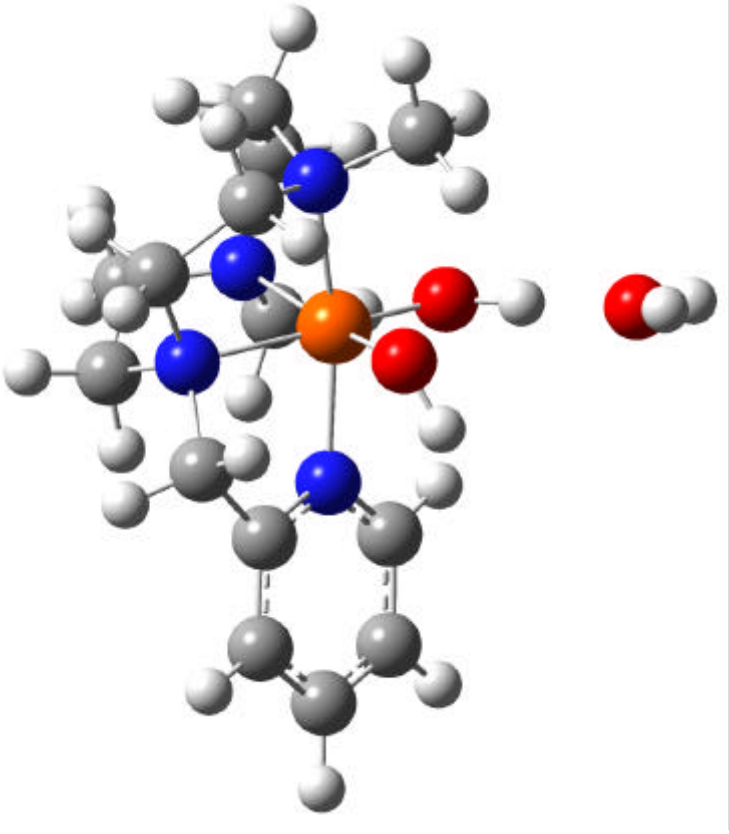


Figure S17: Structure of **I2** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

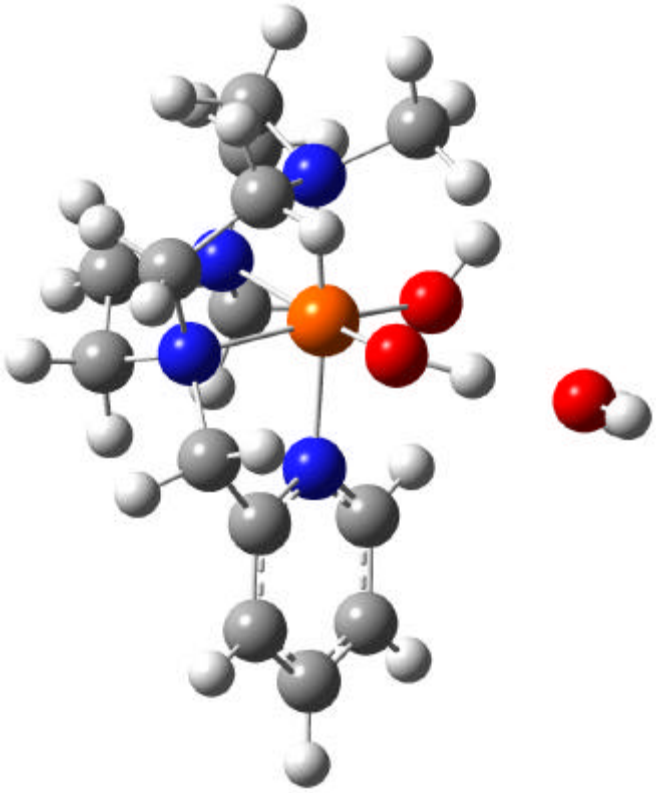


Figure S18: Structure of **TS1** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

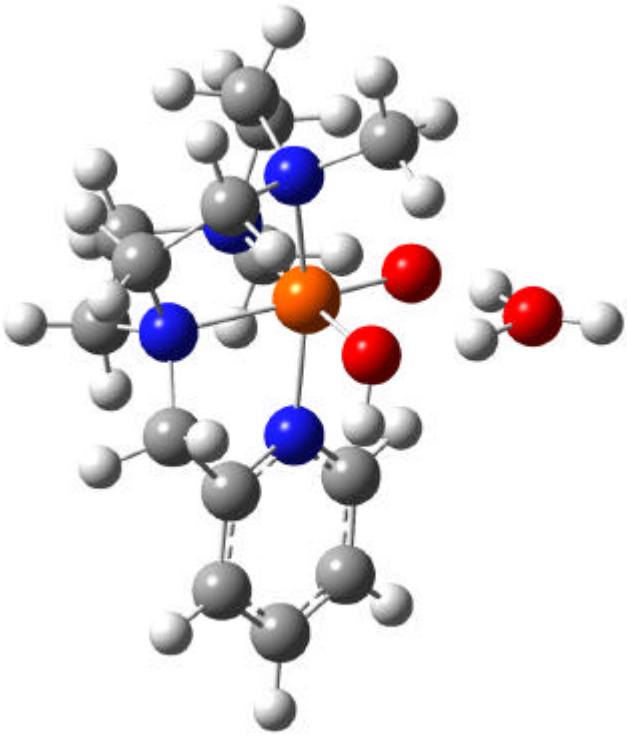


Figure S19: Structure of **TS2** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

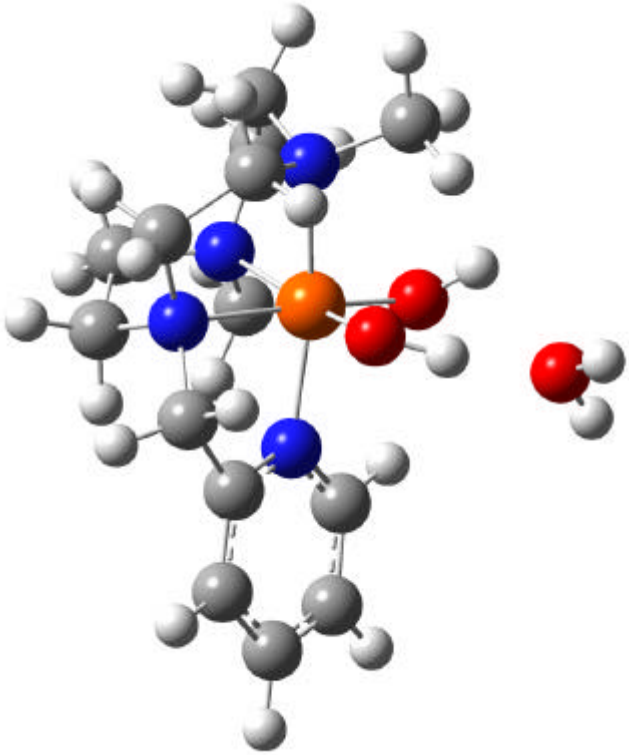


Figure S20: Structure of **TS3** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

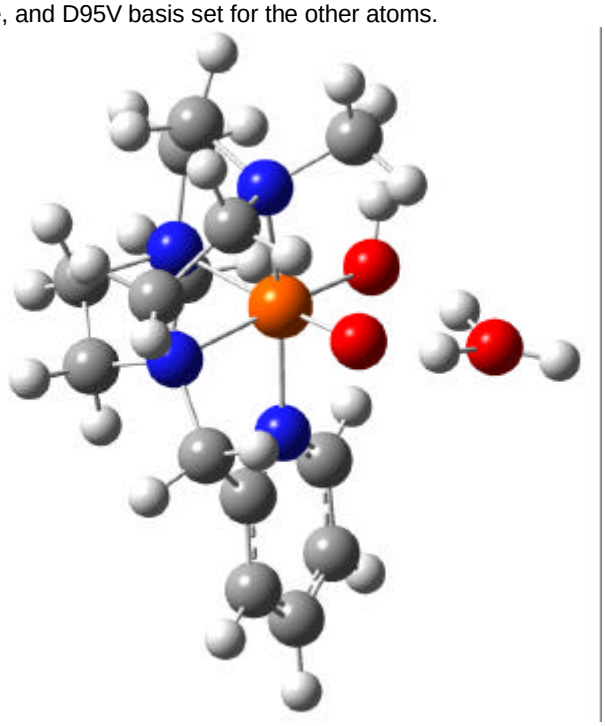


Table S5: Electronic energies, zero point energies, enthalpies and free energies (in kcal/mol) calculated for **2a**, **TS1**, **I1**, **TS2**, **I2**, **TS3** and **2b.**

	D**E**[a]	D**E+ZPVA**[b]	D**H(298ºK)**[c]	D**G(298ºK)**[c]
2a	0.48	1.56	1.33	2.20
TS1	11.19	9.83	8.79	11.53
I1	0.00	0.00	0.00	0.00
TS2	3.71	3.49	3.07	4.22
I2	4.37	4.21	4.21	4.19
TS3	13.34	11.42	10.47	12.97
2b	2.99	3.88	3.70	4.31

[a] The Electronic energies are computed at the B3LYP-D3 level in junction of the cc-pVTZ basis set for Fe, the atoms bond to Fe, and the H bond to oxygen atoms, and cc-pVDZ for the other atoms. The single point calculations include the Acetonitrile solvent effect computed through Gaussian09 PCM approach and the London dispersion effects calculated using the S. Grimme DFT-D3 method. The equilibrium geometries were calculated at the B3LYP level in junction of the LANL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

[b] The zero point energies include the B3LYP-D3/cc-pVTZ&cc-pVDZ//B3LYP/LANL2DZ &D95V electronic energies together with zero-point vibrational corrections at the B3LYP/LANL2DZ&D95V level.

[c] The zero point energies include the B3LYP-D3/cc-pVTZ&cc-pVDZ//B3LYP/LANL2DZ &D95V electronic energies together with thermal enthalpic corrections at the B3LYP/LANL2DZ&D95V level.

[d] The zero point energies include the B3LYP-D3/cc-pVTZ&cc-pVDZ//B3LYP/LANL2DZ &D95V electronic energies together with thermal free energy corrections at the B3LYP/LANL2DZ&D95V level.

Table S6: Electronic energies, zero point energies, enthalpies and free energies (in kcal/mol) calculated for $[Fe^{IV}(O)(^{Me,H}Pytacn)(H_2O)]^{2+}+H_2O+CH_3CN$ and $[Fe^{IV}(O)(^{Me,H}Pytacn)(CH_3CN)]^{2+}+2H_2O$**.**

	D**E**[a]	D**E+ZPVA**[b]	D**H(298ºK)**[c]	D**G(298ºK)**[c]
$[Fe^{IV}(O)(^{Me,H}Pytacn)(H_2O)]^{2+}+H_2O+CH_3CN$	0.00	0.00	0.00	0.00
$[Fe^{IV}(O)(^{Me,H}Pytacn)(CH_3CN)]^{2+}+2H_2O$	17.2	15.5	15.7	16.1

[a] The Electronic energies are computed at the B3LYP-D3 level in junction of the cc-pVTZ basis set for Fe, the atoms bond to Fe, and the H bond to oxygen atoms, and cc-pVDZ for the other atoms. The equilibrium geometries were calculated at the B3LYP level in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms..

[b] The zero point energies include the B3LYP/cc-pVTZ&cc-pVDZ//B3LYP/SDD&6-311G(d)&6-31G electronic energies together with zero-point vibrational corrections at the B3LYP/LANL2DZ&D95V level.

[c] The zero point energies include the B3LYP/cc-pVTZ&cc-pVDZ//B3LYP/SDD&6-311G(d)&6-31G electronic energies together with thermal enthalpic corrections at the B3LYP/LANL2DZ&D95V level.

[d] The zero point energies include the B3LYP/cc-pVTZ&cc-pVDZ//B3LYP/SDD&6-311G(d)&6-31G electronic energies together with thermal free energy corrections at the B3LYP/LANL2DZ&D95V level.

Table S7. Energies (in kcal/mol) for **2a**, **TS1**, **I1**, **TS2**, **2c**, **TS3**, and **2b** calculated at B3LYP/LANL2DZ &D95V level for S=0, 1, and 2.

	S=0	**S=1**	**S=2**
2a	10.38	0.00	12.90
TS1	36.05	8.64	26.23
I1	15.41	2.38	23.53
TS2	36.35	7.24	25.38
I2	17.20	7.04	27.65
TS3	39.58	10.27	29.95
2b	12.63	1.89	17.55

Tables S8-S16 show the optimized structures Cartesian xyz coordinates in Ångstroms for all structures studied in this work at the B3LYP level

Table S8: Optimized Cartesian xyz coordinates of **2a** calculated at the B3LYP level of theory in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms.

H	0.5409464504	1.8419410914	3.1055346569
H	2.8554752053	2.4170368879	1.3552921891
H	1.842799948	0.7367322331	2.7455774001
C	0.8465891149	1.0403300917	2.4308756833
H	3.2032867853	-0.0243015133	1.4750182817
H	0.0029727214	-0.6601273501	3.468965621
C	2.3517151007	1.7809432132	0.620318107
H	1.8333365394	-1.5613029625	2.3589143055
H	4.0325921715	0.5589844572	0.0529986214
C	0.1754590775	2.8587180749	0.9144874501
C	3.0450689002	0.4343948985	0.4999234878
N	0.9194585572	1.5686393576	1.0174602897
C	-0.1279959441	-0.1193212167	2.5262178898
H	2.3456939416	2.30100644	-0.3369156578
H	-1.1506345395	0.2545566791	2.5072218134
C	1.2641103818	-1.9122874686	1.4982194313
H	0.9799917066	-2.9436184022	1.7199581152
H	3.118896625	-2.2687667223	0.4323618863
N	0.0442734709	-1.0444139819	1.3609890711
N	2.2122667562	-0.4914766461	-0.350105906
C	2.1168776919	-1.8787716434	0.2258954024
H	-1.5869091146	-2.2423390937	2.0725466124
C	2.8204154609	-0.5620148162	-1.7146709508
C	-1.2292726118	-1.7834544231	1.1450033979
H	1.6693302134	-2.5011244196	-0.5466746786
Fe	0.2752344328	0.1704895046	-0.3476577817
H	-1.0454487239	-2.5935043948	0.4346137559
C	-2.2521072139	-0.8070104369	0.5930667586
N	-1.7371848796	0.2528217903	-0.0799308371
H	-4.014173159	-1.8131534243	1.2932146945
C	-3.6229297718	-0.9666099072	0.7419532776
C	-2.5627770871	1.160039692	-0.6322316394
H	-2.087835229	1.9643943442	-1.179043978
C	-4.4806960794	-0.0229026288	0.17722513
C	-3.9425411826	1.0555591473	-0.5192427201
H	-5.5536809241	-0.1296993992	0.2834439029
H	-4.5762588631	1.806444719	-0.9731743513
H	2.2094747701	-1.1699809726	-2.3744195095
H	3.8202658838	-0.9989112723	-1.644540128
H	2.8861953947	0.4433212689	-2.1256256882
H	-0.8531138607	2.713469033	1.2411466458
H	0.186907056	3.1954257546	-0.1192843191
H	0.6483772439	3.6093811615	1.5535214937
O	-0.1790340973	-1.3462500992	-1.6636115926
O	0.3866472017	1.2479510368	-1.5558477454
H	-1.1197089657	-1.5619457438	-1.6975780365
H	0.0423292044	-1.0742597391	-2.6080195744
H	0.3318665046	-1.1663951459	-4.9087666167
O	0.3916003855	-0.6477302044	-4.0978733778
H	0.3976074031	0.2828061724	-4.3501472737

Table S9: Optimized Cartesian xyz coordinates of **2b** calculated at the B3LYP level of theory in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms.

H	0.751176646	-2.7958561143	2.1592256479
H	2.9759587712	-0.8507352932	2.5371749826

H	2.0359591216	-2.5065978951	1.0158245999
C	1.0289446837	-2.1968716289	1.2891295142
H	3.3773926895	-1.2812068868	0.1526176565
H	0.2071315915	-3.4550524922	-0.275981273
C	2.4313034903	-0.2444149871	1.8043154392
H	2.0115600966	-2.45380049	-1.2788580738
H	4.1144061034	0.2495146141	0.5461773528
C	0.2606667319	-0.5064482361	2.8944750331
C	3.1534292472	-0.2620137874	0.4639672987
N	1.0309764075	-0.7356345753	1.6397535942
C	0.0558223945	-2.4608033499	0.1544082127
H	2.3823035565	0.7683768016	2.2097388957
H	-0.9674297062	-2.4151096469	0.5220756504
C	1.444736847	-1.6540904878	-1.7547341043
H	1.1681525527	-2.0135709106	-2.7475436102
H	3.3072229375	-0.6382079069	-2.1887518748
N	0.1989840696	-1.4205699448	-0.9290487352
N	2.3109061714	0.3970860501	-0.596202563
C	2.2877962143	-0.3825141905	-1.8820299557
H	-1.3522311266	-2.3802670468	-2.0546000399
C	2.8392549566	1.7644591173	-0.8775810182
C	-1.0763738494	-1.3766106313	-1.7183605316
H	1.8612971043	0.2775871813	-2.6340249998
Fe	0.3009135408	0.3811268266	-0.0915107623
H	-0.9150436143	-0.7409233593	-2.5902365257
C	-2.1417914374	-0.7714818154	-0.8321586863
N	-1.6761138922	0.0551039386	0.1353462877
H	-3.8481938105	-1.6935571151	-1.7484219291
C	-3.4975556327	-1.0218168273	-0.9745395967
C	-2.5368231508	0.6555583221	0.9731436356
H	-2.1089813416	1.3120101588	1.718756454
C	-4.3946133247	-0.3961061609	-0.1091779812
C	-3.9067269323	0.450122983	0.8815262976
H	-5.458958037	-0.5738026966	-0.2059566256
H	-4.57113591	0.9485064244	1.5752629209
H	2.1530517703	2.2873929103	-1.5392798838
H	3.8255829212	1.6957764669	-1.3449029151
H	2.9481643085	2.3192433242	0.0552122662
H	-0.7404712075	-0.9229487446	2.7905255511
H	0.1805634995	0.5622219724	3.0840573798
H	0.7555016616	-0.9889857196	3.7427342047
O	-0.0107846511	1.2016159435	-1.4615137403
O	0.233849075	2.0605211753	1.0405357974
H	-0.3452358186	2.7403370161	0.5657852526
H	1.0543417553	2.5181023547	1.2577402486
O	-1.303767667	3.6585789935	-0.2725609728
H	-1.5694150536	4.5712932835	-0.1094393827
H	-1.2554127476	3.5341981583	-1.2279381478

Table S10: Optimized Cartesian xyz coordinates of $[Fe^{IV}(O)(^{Me,H}Pytacn)(H_2O)]^{2+}$+$H_2O$+ CH_3CN calculated at the B3LYP level of theory in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms.

H	0.8406493398	2.075375577	3.0506199065
H	3.0435747243	2.4017504594	1.1147993506
H	2.0372990426	0.8607632388	2.6786866806
C	1.043914484	1.2144329132	2.411039776
H	3.2735191095	-0.0423328913	1.3865435011
H	0.1585841926	-0.3517271249	3.6139187938
C	2.4562761724	1.7467379374	0.462919153
H	1.8451401722	-1.4501084723	2.4727848352
H	4.0288861872	0.397245868	-0.1245964594
C	0.3665270964	2.9641318347	0.8238399213
C	3.0696427055	0.3574115298	0.3939245999
N	1.0467728586	1.6444619272	0.9658308233
C	0.0050104781	0.1349317257	2.6453277142
H	2.4100296165	2.1975855985	-0.5276272119
H	-0.9901645685	0.5768245537	2.6587739263

C	1.2096617997	-1.8109500867	1.6637638883
H	0.8724407228	-2.8067991874	1.960401178
H	2.9870467178	-2.3394024275	0.5398188408
N	0.0409473607	-0.874288393	1.5386245367
N	2.1357321292	-0.576800517	-0.3304127649
C	1.9973452913	-1.910241682	0.351790097
H	-1.6200428514	-1.8973285802	2.4285634561
C	2.6476559273	-0.785478415	-1.7198968612
C	-1.2938862243	-1.5285342264	1.4505749239
H	1.4781493572	-2.5563717645	-0.3526307361
Fe	0.2372541407	0.194604278	-0.2695736504
H	-1.2276485863	-2.3882138941	0.780727172
C	-2.274645593	-0.5156553928	0.8945963052
N	-1.7340286261	0.4374092171	0.0993674525
H	-4.0473355558	-1.3066676511	1.8066985449
C	-3.6375062933	-0.5455804303	1.1543359299
C	-2.5260433455	1.355982076	-0.4792862301
H	-2.0319801219	2.0693650447	-1.125861922
C	-4.460431088	0.4136867567	0.5678652155
C	-3.8967071939	1.3764564118	-0.2643150915
H	-5.5265722482	0.4095412988	0.7606008691
H	-4.5032230883	2.1350525133	-0.7416813386
H	1.9547384036	-1.3968170883	-2.2883901044
H	3.6220123978	-1.2802315265	-1.67722709
H	2.7473753693	0.1812316618	-2.2089231224
H	-0.6427279744	2.8995253156	1.228029983
H	0.3201795941	3.2285572608	-0.2297519659
H	0.9213992063	3.7292809229	1.3738824146
O	-0.3160561899	-1.3666377108	-1.4286625394
O	0.3445576482	1.1916045986	-1.5484469213
H	-1.1750331157	-1.8468846424	-1.3564991905
H	-0.2445804844	-1.0873784968	-2.3843333797
H	-0.2497498832	-0.8395981973	-4.7645226585
O	0.0183922813	-0.5235877119	-3.8949504113
H	0.0895093644	0.4367792025	-3.9404263471
N	-2.5771602314	-2.9947453364	-1.4770263068
C	-3.309905737	-3.7981200732	-1.8576233316
C	-4.232989658	-4.8109837809	-2.3394006783
H	-3.7201588307	-5.4796697332	-3.0340066988
H	-4.6156380596	-5.3975139401	-1.5015354992
H	-5.0709433727	-4.3375721278	-2.8552306877

Table S11: Optimized Cartesian xyz coordinates of $[Fe^{IV}(O)(^{Me,H}Pytacn)(CH_3CN)]^{2+}+2H_2O$ calculated at the B3LYP level of theory in junction of the SDD basis set and associated ECP for Fe, 6-311G(d) basis set for the atoms bond to Fe, and 6-31G basis set for the other atoms.

H	-2.1570337973	-3.365111857	0.7071030035
H	0.6541344208	-3.8142241232	1.4877733149
H	-0.829588173	-3.6022317318	-0.4009034445
C	-1.4066554972	-2.8380595189	0.1151307867
H	1.0970011042	-3.3728744698	-0.9007682842
H	-2.5419332296	-2.4752538102	-1.6909697952
C	0.8208837868	-2.7798709359	1.1699436316
H	-0.3714365894	-2.6034411103	-2.4583976873
H	2.583341501	-3.0929183265	-0.0255226588
C	-1.1225372759	-1.9164975392	2.3753742737
C	1.5626733287	-2.7300859282	-0.1544781314
N	-0.4904804286	-2.0641739912	1.031627114
C	-2.0825295296	-1.9089999125	-0.874603935
H	1.3860494198	-2.2686358782	1.9481437334
H	-2.876964285	-1.3536393443	-0.378725428
C	-0.1878992094	-1.5289690421	-2.4447692891
H	-0.4365351786	-1.1637020445	-3.4437461463
H	1.9289285261	-1.9254846916	-2.6940940158
N	-1.0987480951	-0.916220144	-1.4166698279
N	1.5906870873	-1.3136625493	-0.6707593584
C	1.2855427261	-1.2334800446	-2.1408344373
H	-2.6782163318	0.0101258031	-2.5321963627

C	2.9513802721	-0.7399335053	-0.4137057964
C	-1.8508821541	0.2876747561	-1.8710751435
H	1.5467694778	-0.2250051386	-2.4555908076
Fe	0.0708246917	-0.2564631024	0.2029108637
H	-1.1754052291	0.9320615543	-2.4367274288
C	-2.3528137428	1.0165822837	-0.6413073944
N	-1.6311818208	0.8144679337	0.4864762108
H	-4.0354649373	1.9865367636	-1.5539887426
C	-3.4618539333	1.8506883594	-0.6451760251
C	-1.9694971019	1.4498335287	1.6209281403
H	-1.3317886578	1.2694636203	2.4763901225
C	-3.8223975455	2.5040413897	0.532438154
C	-3.064357276	2.3008921438	1.6818931341
H	-4.684649832	3.15985414	0.5502705965
H	-3.3103978398	2.7921171053	2.6143703238
H	3.0050587901	0.3032660128	-0.7123642702
H	3.6902430005	-1.318553826	-0.9758846928
H	3.1723841933	-0.7950866848	0.649694517
H	-2.0970162892	-1.4413149826	2.2723911466
H	-0.482292946	-1.3036522353	3.0052347612
H	-1.2552293314	-2.9014352212	2.8313858687
O	0.8181896188	0.1676279945	1.588056496
N	0.6972534539	1.4321594436	-0.717163544
C	1.1001010421	2.4794832397	-0.9741872812
C	1.6387761942	3.7859304372	-1.2758194789
H	1.6625988145	3.9450962314	-2.3563511119
H	1.0276714137	4.5604786325	-0.8071484103
H	2.6588810104	3.7961752254	-0.8727621108
O	3.5105401309	1.0647807271	2.2666804268
H	3.8483362847	1.2600663797	3.147263706
H	2.5544499494	0.9445266122	2.3528557699
H	3.9882519573	2.0091021212	0.7624234073
O	4.0390328779	2.3419628921	-0.1545123535
H	4.9759938967	2.4633899079	-0.339719293

Table S12: Optimized Cartesian xyz coordinates of **I1** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

H	0.4414919007	-2.5097842738	2.6052134617
H	2.834918208	-0.6928593462	2.6469067908
H	1.7480452568	-2.5355576622	1.4364399198
C	0.7647610015	-2.1060588275	1.6395401463
H	3.1973072704	-1.5399638909	0.3498435559
H	-0.1533179791	-3.5525142141	0.2942544797
C	2.3373372951	-0.1689109378	1.8192106241
H	1.7563615357	-2.8203210047	-0.8596222484
H	4.0357941248	-0.0036961474	0.488113975
C	0.1200305465	-0.069243336	2.9134520721
C	3.0438860176	-0.4672491661	0.4937972017
N	0.8841132366	-0.5929690832	1.7250414552
C	-0.2370343332	-2.4888365335	0.552882582
H	2.3446598575	0.9023340033	2.0317579136
H	-1.2572152	-2.3121715525	0.9009641739
C	1.2159285219	-2.0910969345	-1.4696001389
H	0.9031324717	-2.6103379231	-2.382343767
H	3.1155678774	-1.2504913586	-2.1211977611
N	-0.008086185	-1.6353651627	-0.6828739158
N	2.2238130736	0.0759813497	-0.6703941093
C	2.1149962986	-0.8993291676	-1.8351708469
H	-1.6689861375	-2.6065177271	-1.6641458506
C	2.8295529504	1.3715495796	-1.164202437
C	-1.282329796	-1.5931444089	-1.4993662748
H	1.688904802	-0.3355205841	-2.6657345965
Fe	0.2886179591	0.3218980256	-0.0850791044
H	-1.0498847914	-1.1441037106	-2.4694295695
C	-2.276099019	-0.7333933283	-0.7408212788
N	-1.7061560843	0.2045268248	0.0841521161
H	-4.1069765333	-1.5961160878	-1.4935837713

C	-3.666975824	-0.8450651313	-0.844887391
C	-2.4830206254	1.0536580548	0.8085498546
H	-1.9650409606	1.7801489408	1.4226802614
C	-4.4825982736	0.0305323506	-0.0985599743
C	-3.8823480806	0.9891664028	0.7398797282
H	-5.5639059232	-0.0375438897	-0.1693717166
H	-4.4808662891	1.6768276232	1.3273915837
H	2.1581962761	1.8161960733	-1.8982099425
H	3.8044081611	1.1645755252	-1.6238986864
H	2.9614862394	2.0533745904	-0.3218185443
H	-0.910941381	-0.4305419545	2.8788835475
H	0.1285232739	1.0210885658	2.88827014
H	0.5848376233	-0.4188998764	3.844410581
O	0.0076731484	0.9879891051	-1.7658145007
O	0.4791708064	1.8529177357	0.7195150888
H	-0.8623463363	1.4199118562	-1.9105466836
H	0.4611639245	4.3844628033	-1.3290887199
H	0.3784845232	4.9336553714	0.1846112338
O	0.3963120097	4.1420588237	-0.3866710691
H	0.4545751864	2.7506026711	0.2053687748

Table S13: Optimized Cartesian xyz coordinates of **I2** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

H	-0.9245950194	-3.4541224168	-0.8818138712
H	-3.0199763085	-1.6969662355	-2.0571881898
H	-2.1733765661	-2.6537579156	0.055807681
C	-1.1507760809	-2.5465101412	-0.3115537623
H	-3.4454248949	-1.0823796439	0.3062939895
H	-0.3784446178	-3.1104626118	1.6459367755
C	-2.4485100263	-0.8642830335	-1.624597363
H	-2.0923932115	-1.6348954712	2.1691353747
H	-4.0939226229	0.2013498359	-0.6989833076
C	-0.2543063728	-1.6467435322	-2.453910908
C	-3.1655452099	-0.2959205972	-0.3991884991
N	-1.0647401699	-1.3306052221	-1.2200577955
C	-0.1653428839	-2.392342816	0.8436574172
H	-2.3236384412	-0.1038725803	-2.4000089251
H	0.8532386056	-2.578010101	0.4960357118
C	-1.4592891263	-0.7460444859	2.2470810778
H	-1.1722112588	-0.6543654668	3.3004092226
H	-3.2629362708	0.4727753455	2.2025008766
N	-0.223146878	-0.9741507598	1.3876600204
N	-2.2525238841	0.6987731744	0.3079014367
C	-2.233069315	0.5196696814	1.8235076423
H	1.3697385207	-1.4502704532	2.7715607109
C	-2.6982178805	2.1079220175	-0.0105638515
C	1.1007678547	-0.6612239545	2.0586169581
H	-1.751267894	1.4094584685	2.2290088633
Fe	-0.2784243057	0.3482971959	-0.1694358614
H	0.9949929005	0.287082965	2.5934422436
C	2.1437738063	-0.5140946431	0.9633842124
N	1.654176674	-0.1129836803	-0.2540674361
H	3.8975895167	-1.0475014795	2.1048855094
C	3.5150715827	-0.7228264695	1.1422763768
C	2.4835813226	0.1235520901	-1.3015074238
H	2.0178044028	0.4859646937	-2.2102535455
C	4.3892174289	-0.4970266029	0.0579758588
C	3.8676398764	-0.0684655033	-1.1775002699
H	5.4573616818	-0.6506030202	0.1787320073
H	4.5147272497	0.1191681592	-2.0273799811
H	-1.9587671629	2.8194674468	0.3587874069
H	-3.6654343578	2.306648183	0.468251767
H	-2.8256658848	2.2255921387	-1.0909074215
H	0.7044568238	-2.0838083754	-2.1655442233
H	-0.0839364388	-0.7232152944	-3.0088424207
H	-0.7958965339	-2.3656839434	-3.0821330803
O	0.1368615576	1.6851234804	0.8828676844

O	-0.1695772777	1.2716673554	-1.7361372983
H	1.436235862	3.9244427245	-1.00023989
H	-0.8470574515	1.9542055793	-1.9316396274
O	1.1075890513	3.8134550748	-0.0890572558
H	1.3015507876	4.593466145	0.4646425576
H	0.5609638314	2.5313923028	0.4573327685

Table S14: Optimized Cartesian xyz coordinates of **TS1** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

H	0.498471	-3.043313	1.929276
H	2.839583	-1.259169	2.462486
H	1.806006	-2.747704	0.797340
C	0.813413	-2.405067	1.096822
H	3.228385	-1.497038	0.024816
H	-0.075517	-3.481531	-0.572715
C	2.344628	-0.550597	1.784668
H	1.814926	-2.446299	-1.495471
H	4.049206	-0.038545	0.554533
C	0.118175	-0.774299	2.841108
C	3.062762	-0.497796	0.435414
N	0.900426	-0.958577	1.562864
C	-0.179806	-2.518888	-0.055179
H	2.331627	0.433153	2.259617
H	-1.202304	-2.454262	0.323049
C	1.264743	-1.592018	-1.899661
H	0.970248	-1.861182	-2.920309
H	3.149669	-0.579631	-2.295036
N	0.031079	-1.375952	-1.033475
N	2.236148	0.315444	-0.555405
C	2.143220	-0.331095	-1.931838
H	-1.622475	-2.124546	-2.203468
C	2.855292	1.687542	-0.705721
C	-1.249313	-1.170840	-1.808892
H	1.709306	0.421752	-2.591350
Fe	0.290102	0.367038	0.070209
H	-1.039721	-0.520487	-2.664702
C	-2.256453	-0.537223	-0.861256
N	-1.703740	0.165530	0.182158
H	-4.069381	-1.205090	-1.826964
C	-3.645127	-0.637445	-1.004378
C	-2.500804	0.792342	1.087715
H	-2.000226	1.349469	1.870616
C	-4.479807	0.006027	-0.066878
C	-3.898879	0.727971	0.992614
H	-5.559439	-0.057938	-0.162333
H	-4.510661	1.236002	1.730177
H	2.247415	2.292581	-1.376056
H	3.864054	1.586061	-1.125874
H	2.914972	2.168811	0.272135
H	-0.904468	-1.134274	2.705183
H	0.104766	0.284968	3.099302
H	0.588944	-1.346095	3.651043
O	-0.044722	1.564030	-1.419242
O	0.420281	1.635682	1.190911
H	-0.951286	1.520509	-1.788205
H	0.112415	2.957455	-0.929634
H	0.198359	4.566036	-0.105763
O	0.250558	3.597520	-0.108610
H	0.355891	2.842672	0.728178

Table S15: Optimized Cartesian xyz coordinates of **TS2** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

H	0.7268779851	-3.387737869	1.204607311
H	2.922171162	-1.6210738006	2.2265916726
H	2.0344650653	-2.7528787554	0.2221673192

C	1.0139510513	-2.5535845495	0.5551985945
H	3.3674672346	-1.2735932649	-0.1953360763
H	0.2561324278	-3.2612764158	-1.3605132005
C	2.3914442346	-0.8124982263	1.705717564
H	2.0224048507	-1.9135494084	-2.0093033348
H	4.0845016106	0.0688127913	0.6793806952
C	0.1665734268	-1.4063336114	2.6018719601
C	3.1314505629	-0.4090706749	0.4298809172
N	0.9863774194	-1.2536981397	1.3441209371
C	0.0570548435	-2.4638540871	-0.6330207413
H	2.2968499685	0.0343098954	2.3898684488
H	-0.9742011413	-2.5782759754	-0.2928846151
C	1.4259635496	-1.0117668387	-2.1759163219
H	1.145551003	-1.0092349181	-3.2350488107
H	3.2696040672	0.146769933	-2.2341643482
N	0.1809178745	-1.1054200631	-1.3050153082
N	2.2647053994	0.5577091242	-0.3684354966
C	2.2416712133	0.2570940569	-1.8630711376
H	-1.4202921955	-1.6231219993	-2.6641293035
C	2.7714149029	1.9668038654	-0.1583599621
C	-1.1249741485	-0.7922760572	-2.0116007656
H	1.7871273829	1.1252934362	-2.3409580131
Fe	0.2824054808	0.3402913328	0.1394106593
H	-0.9772808981	0.1074213974	-2.6159438428
C	-2.1679158887	-0.5186334505	-0.9415070438
N	-1.6681452498	-0.0501897966	0.2474325562
H	-3.9367201471	-1.0594485694	-2.0558855611
C	-3.5459585591	-0.6814579879	-1.1163411412
C	-2.4924856159	0.2966096536	1.2683022575
H	-2.0181087835	0.7037468197	2.1532536138
C	-4.4154198085	-0.3403384524	-0.0588719933
C	-3.8825680094	0.1541138152	1.1470831818
H	-5.4885199854	-0.4565949796	-0.1773380389
H	-4.5254979761	0.4294362983	1.9760143184
H	2.0789887195	2.6775094784	-0.6107095959
H	3.757953183	2.0750640326	-0.6266586986
H	2.8727731723	2.1685594855	0.9110103732
H	-0.8127983427	-1.8235046241	2.3572778646
H	0.0464639091	-0.4255727311	3.06469156
H	0.6754316378	-2.0847174017	3.2988420946
O	-0.0927896205	1.6206631719	-1.0212848393
O	0.2505215825	1.4097106054	1.6036020076
H	-1.3645527468	4.1451282993	0.6173849874
H	0.6748531146	2.2934485512	1.5382234972
O	-0.7001263919	3.9501857583	-0.0711747867
H	-0.5279038625	4.7426574397	-0.6168184609
H	-0.4104209032	2.5176510233	-0.6441494501

Table S16: Optimized Cartesian xyz coordinates of **TS3** calculated at the B3LYP level of theory in junction of the LanL2DZ basis set and associated ECP for Fe, and D95V basis set for the other atoms.

H	0.764033	-2.988855	1.905681
H	2.955169	-1.073585	2.470295
H	2.053632	-2.584721	0.788441
C	1.035602	-2.319555	1.081985
H	3.403715	-1.219827	0.052130
H	0.249594	-3.443143	-0.610344
C	2.418625	-0.381023	1.806863
H	2.033534	-2.279109	-1.529439
H	4.098759	0.289907	0.611736
C	0.192130	-0.759132	2.824436
C	3.151960	-0.242237	0.470937
N	1.007460	-0.873451	1.557882
C	0.063084	-2.500452	-0.080061
H	2.355897	0.578588	2.329212
H	-0.964095	-2.525642	0.288760
C	1.439460	-1.442949	-1.909365
H	1.163137	-1.691614	-2.939757

H	3.289035	-0.342966	-2.231878
N	0.184830	-1.333147	-1.048197
N	2.278746	0.512011	-0.522918
C	2.261024	-0.138206	-1.903682
H	-1.399034	-2.174604	-2.257415
C	2.771988	1.934646	-0.659322
C	-1.114168	-1.208220	-1.823577
H	1.818384	0.592106	-2.581877
Fe	0.288954	0.390783	-0.003635
H	-0.960527	-0.485113	-2.630204
C	-2.164690	-0.692135	-0.856563
N	-1.669360	0.044651	0.189365
H	-3.921924	-1.496726	-1.819418
C	-3.539644	-0.907443	-0.991760
C	-2.503643	0.595949	1.107172
H	-2.040889	1.188687	1.886644
C	-4.417260	-0.343515	-0.041981
C	-3.892050	0.414448	1.021245
H	-5.488634	-0.495138	-0.131969
H	-4.539537	0.861857	1.767417
H	2.064921	2.510549	-1.257162
H	3.754777	1.942224	-1.147387
H	2.875184	2.393573	0.328013
H	-0.786906	-1.219629	2.674512
H	0.056631	0.294378	3.072950
H	0.701326	-1.273552	3.649625
O	-0.066641	1.341309	-1.380171
O	0.186657	1.868269	1.208734
H	-0.548981	2.962642	0.513665
H	1.016529	2.186798	1.616632
O	-0.926070	3.310149	-0.398791
H	-1.294571	4.190980	-0.569310
H	-0.599774	2.472239	-1.104107

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