Supporting Information for

Octahedral Iron (IV) Tosylimido Complexes Exhibiting Single Electron Oxidation Reactivity

Gerard Sabenya,[a] Ilaria Gamba,[a] Laura Gómez,[a] Martin Clémancey,[b] Jonathan R Frisch,[c] Eric J. Klinker,[c] Geneviève Blondin,[b] Stéphane Torelli,[b] Lawrence Que, Jr,[c,*] Vlad Martin-Diaconescu, [a,d*] Jean-Marc Latour,[b,*] Julio Lloret-Fillol,[a,d,e*] Miquel Costas.[a,*]

a) Institut de Química Computacional i Catàlisi (IQCC) and Departament de Química, Universitat de Girona. Campus Montilivi, E17071 Girona, Catalonia (Spain) miquel.costas@udg.edu
b) Univ. Grenoble-Alpes, CNRS, CEA, IRIG, DIESE, CBM, Grenoble 38000, France
c) Department of Chemistry, University of Minnesota, Pleasant Str 207, Minneapolis, Minnesota
d) Institute of Chemical Research of Catalonia (ICIQ), The Barcelona Institute of Science and Technology, Avinguda Països Catalans 16, 43007 Tarragona, Spain. jlloret@iciq.es.
e) Catalan Institution for Research and Advanced Studies (ICREA), Passeig Lluïs Companys, 23, 08010, Barcelona (Spain).

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1. Experimental Section

Materials. Reagents were purchased from commercial sources and used as received, without any further purification. Compounds methyl *p* – tolyl sulfide, 4 – chlorothioanisole and formaldehyde were purchased from Fluorochem, Alfa Aesar and Scharlab respectively, while the rest of the compounds were purchased from Sigma – Aldrich. Solvents were purchased from SDS and Scharlab, purified and dried by passing through an activated alumina purification system (MBraun SPS – 800) and stored in an anaerobic glovebox under N_2.

Physical Methods. UV – VIS – NIR spectra were recorded on a Cary 50 diode array spectrophotometer (190 – 1100 nm range) in 1 cm quartz cells. A cryostat from Unisoku Scientific Instruments was used for the temperature control. Electrospray ionization mass spectrometry (ESI – MS) experiments were performed on a Bruker Daltonics Esquire 3000 Spectrometer or on a high – resolution mass spectrometer Bruker microTOF QII (Q – TOF) with a quadrupole analyser. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance 400 MHz spectrometer as solutions at 25°C and referenced to residual solvent peaks. The Mössbauer samples consisted of frozen 57Fe-enriched solutions contained in Delrin cups. Mössbauer spectra were recorded at 5 K on a low-field Mössbauer spectrometer equipped with a Janis CCR 5 K cryostat or at 4.2 K on a strong-field Mössbauer spectrometer equipped with an Oxford Instruments Spectromag 4000 cryostat containing an 8 T split-pair superconducting magnet. Both spectrometers were operated in a constant acceleration mode in transmission geometry. The isomer shifts were referenced against that of a room-temperature metallic iron foil. Analysis of the data was performed with the software WMOSS Mössbauer Spectral Analysis Software (http://www.wmoss.org), 2012-2013 (Web research, Edina).

X-band EPR spectra were recorded on a Bruker EMX spectrometer equipped with an Oxford ESR 910 cryostat for low temperature studies. The microwave frequency was calibrated with a frequency counter and the magnetic field with an NMR gaussmeter. The modulation amplitude employed was selected to optimize the signal-to-noise (S/N) ratio and resolution under conditions of nonsaturating microwave power.

XAS data collection and processing: Samples for X – ray absorption measurements were prepared as 4 mM solutions in acetone loaded in sample holders and stored at liquid nitrogen temperatures until run. XAS data on compounds **$1^{(IV)}$=NTs**, **$1^{(III)}$ – NHTs**, and **$2^{(III)}$ – NHTs** was collected at the ESRF synchrotron, Spline beamline, under anaerobic conditions at 90 K using a liquid nitrogen cryostat a 13 element detector and a Si(111) double crystal monochromator.. Compound **$2^{(IV)}$=NTs**, on the other hand was run at 25 K using a liquid helium cryostat from the SAMBA beamline at SOLEIL synchrotron, equipped with a Si (220) double crystal monochromator and a 35 – element Ge detector.

Data processing was carried out with the Athena software package.[1] A linear pre – edge together with a quadratic post – edge function were used for baseline subtraction and normalization of the edge jump to 1. Energy calibration was carried out using the first inflection point of Fe foil set as 7111.2 eV. The AUTOBK algorithm was used to extract EXAFS with E0 set as the first inflection point of the rising edge, together with an R_{bkg} of 1 and a spline with a k – range of 1 to 14.5 $Å^{-1}$. EXAFS analysis was carried out with Artemis, employing the Iffefit engine and FEFF6 code.[2, 3] The k^2 – weighted data was fit in R – space was fit in R – space between 1 and 3 Å, with a k – range of 2 – 12.5 Å, and a Hanning window with a dk of 2. Fits were carried out with a global S_0^2 of 0.9 as well as a global ΔE0. Scattering paths were fit in terms of ΔR_{eff} and σ^2, and the goodness of fit was the R_{fator} (%R) and reduced χ^2 (χ^2_v) were minimized as previously described.[4, 5]

2. Synthesis of complexes

Synthesis of $[Fe^{II}(CH_3CN)(MePy_2tacn)](X)_2$ (X = OTf or SbF_6, **$1^{(II)}$-OTf** or **$1^{(II)}$-SbF_6**) and $[Fe^{II}(CH_3CN)(Me_2(CHPy_2)tacn)](X)_2$ (X = OTf or SbF_6, **$2^{(II)}$-OTf** or **$2^{(II)}$-SbF_6**) were performed as previously described.[6, 7]

Preparation of $[Fe^{IV}(NTs)(MePy_2tacn)]^{2+}$ (**$1^{(IV)}$=NTs**) with PhINTs. In an anaerobic glovebox, **$1^{(II)}$** (1.8 mg, $2.5\cdot10^{-3}$ mmol) and PhINTs (1.12 mg, $3\cdot10^{-3}$ mmol) were mixed in CH_3CN (1 mL). The resulting solution was vigorously stirred 1 – 2 minutes. Removal of unreacted PhINTs was achieved by filtration, which afforded a golden solution of compound **$1^{(IV)}$=NTs**. The yield of the reaction was estimated according to the amount of Fe^{IV} determined by Mössbauer spectroscopy by preparation of ^{57}Fe enriched sample of compound **$1^{(IV)}$=NTs**. Yield: 87 %. ^{1}H – NMR (CD_3CN, 400 MHz, 300 K) δ, ppm: 41.04 (s, $PyH_{\beta a}$), 12.67 (s, $PyH_{\gamma a}$), -13.31 (s, $PyH_{\beta' a}$), 6.02 (s, 1H, $PyH_{\gamma b}$), -5.58 (s, 1H, $PyH_{\beta b}$) and

-6.93 (s, 1H, $PyH_{\beta'b}$). ESI-MS (m/z): $[M\text{-}2CF_3SO_3]^{2+}$ = 275.09 (100%), $[M\text{-}CF_3SO_3]^{+}$ = 699.13 (6%). UV-Vis (CH_3CN): λ_{max} = 455 nm, ε = 4500 $M^{-1}cm^{-1}$, λ = 750 nm, ε = 200 $M^{-1}cm^{-1}$.

Preparation of $[Fe^{IV}(NTs)(Me_2(CHPy_2)tacn)]^{2+}$ (**$2^{(IV)}$=NTs**) with PhINTs. In an anaerobic glovebox, **$2^{(II)}$** (1.8 mg, $2.5\cdot10^{-3}$ mmol) and PhINTs (1.12 mg, $3\cdot10^{-3}$ mmol) were mixed in CH_3CN (1 mL). The resulting solution was vigorously stirred until total formation of **$2^{(IV)}$=NTs**. Removal of unreacted PhINTs was achieved by filtration, which afforded a golden – orange solution of compound **$2^{(IV)}$=NTs**. The yield of the reaction was estimated according to the amount of Fe^{IV} determined by Mössbauer spectroscopy by preparation of a ^{57}Fe enriched sample of compound **$2^{(IV)}$=NTs**. Yield: 48 %. (The same procedure in acetone gave 81 % yield of **$2^{(IV)}$=NTs**). ^1H – NMR (CD_3CN, 400 MHz, 300 K) δ, ppm: 20.87 (s, PyHβ), 9.70 (s, PyHγ), -6.56 (s, PyHβ'). ESI – MS (m/z): $[M\text{-}2CF_3SO_3]^{2+}$ = 275.09 (100%), $[M\text{-}CF_3SO_3]^{+}$ = 699.13 (2%). UV-Vis (CH_3CN): λ_{max} = 456 nm, ε = 3600 $M^{-1}cm^{-1}$, λ = 740 nm, ε = 170 $M^{-1}cm^{-1}$. (Acetone): λ_{max} = 455 nm, ε = 4000 $M^{-1}cm^{-1}$, λ = 730 nm, ε = 230 $M^{-1}cm^{-1}$.

Preparation of $[Fe^{IV}(NTs)(N4Py)]^{2+}$ (**$3^{(IV)}$=NTs**) with PhINTs. **$3^{(IV)}$=NTs** was prepared as previously reported.[8]

Preparation of **$[Fe^{III}(NHTs)(MePy_2tacn)](X)_2$** (**$[1^{(III)}$ – NHTs]X**, X = OTf or SbF_6). **$[1^{(III)}$ – NHTs]X**, (X = OTf or SbF_6) was prepared in an anaerobic glovebox by reacting **$1^{(II)}$-X** (15 mg **$1^{(II)}$-OTf** or 18.6 mg of **$1^{(II)}$ – SbF_6**, $2.1\cdot10^{-2}$ mmol) with 1.2 eq of PhINTs (9.3 mg, $2.4\cdot10^{-2}$ mmol) in acetone (3 mL) at -40ºC. The resulting solution was vigorously stirred 1 – 2 minutes, covered with a layer of hexamethyldisiloxane or diethyl ether and stored at -40 ºC for several days. The resulting orange crystals were separated and characterised spectroscopically as described in the text.

Preparation of **$[Fe^{III}(NHTs)(Me_2(CHPy_2)tacn)]X_2$** (**$[2^{(III)}$ – NHTs]X**, X = OTf or $SbF_6$was done analogously to [**$1^{(III)}$ – NHTs]X**.

3. Reactivity studies

Kinetic Studies in the reaction with sulphides. The required amount of **$1^{(IV)}$=NTs** or **$2^{(IV)}$=NTs** (200 µL of a 2.5 mM solution of **$1^{(IV)}$=NTs** or **$2^{(IV)}$=NTs** in CH_3CN obtained by direct oxidation of **$1^{(II)}$** and **$2^{(II)}$** with PhINTs) was diluted in CH_3CN to obtain the desired final concentration of **$1^{(IV)}$=NTs** or **$2^{(IV)}$=NTs**.

Then, the desired quantity of thioanisole (^{X}PhSMe, dissolved in CH_3CN) was added. The progress of the reaction was monitored by UV – vis spectroscopy at 293 K.

Identification and quantification of sulfilimine. Reaction of **1$^{(IV)}$=NTs** or **2$^{(IV)}$=NTs** with sulfides (^{X}PhSMe) caused a decay of its characteristic absorption bands (λ_{max} = 455/456 and 750/740 nm). After full decay of this band, an internal standard was added to the solution (trimethoxybenzene) and the amount of formed sulfilimine was quantified by ^{1}H – NMR spectroscopy by comparison with independently prepared samples of the products. All quantifications had been done with 5 mg ($7\cdot10^{-3}$ mmol) of **1$^{(IV)}$=NTs** and **2$^{(IV)}$=NTs** and PhINTs (3.12 mg, $8.3\cdot10^{-3}$ mmol) in 2 ml of acetone. Blank experiments without iron complex revealed ≈ 0.1 eq of sulfilimine products.

HAT Kinetic Studies. The required amount of **1$^{(IV)}$=NTs** or **2$^{(IV)}$=NTs** (200 µL of a 2.5 mM solution of **1$^{(IV)}$=NTs** or **2$^{(IV)}$=NTs** in acetone obtained by direct oxidation of **1$^{(II)}$** and **2$^{(II)}$** with PhINTs) was diluted in acetone to obtain the desired final concentration of 0.25 mM. Then, the desired quantity of a selected substrate (xanthene, DHA, CHD and fluorene, dissolved in acetone) was added. The substrates were added in large excess (1 mM – 25 mM) compare to **1$^{(IV)}$=NTs** or **2$^{(IV)}$=NTs** (0.25 mM). The progress of the reaction was monitored by UV-Vis spectroscopy at 293 K. The decay kinetic of **1$^{(IV)}$=NTs** or **2$^{(IV)}$=NTs**, which is produced upon substrate addition, in acetone at 20 ºC and under N_2 atmosphere, lead to the formation of **1$^{(III)}$-NHTs** or **2$^{(III)}$-NHTs** species and substrate oxidation products.

The decay of **1$^{(IV)}$=NTs** or **2$^{(IV)}$=NTs** follow an exponential behaviour upon addition of different substrates and concentrations. Surprisingly, the observed rates (k_{obs}, s^{-1}), extrapolated from the exponential fits, do not vary linearly with the substrates concentrations and instead saturation profiles are observed (Figure 10 A and B of the main article). Saturation of the observed rates is generally observed when a fast pre-equilibrium reaction step precedes a slower irreversible step in the reaction mechanism. The values of k(s^{-1}) and Keq(M^{-1}) (extrapolated fitting the observed curves with the pre-equilibrium approximation, Equation 1 of the main article) are reported in Table 6 of the main article.

The extrapolated values of rates k (s^{-1}) (which in this model correspond to the rate of the slow and irreversible reaction step that follow the pre-equilibrium) shown a linear variation with the BDE of

the studied substrate and by plotting the logarithm of the rate corrected for the number of CH contained in each substrate (**Figure S11**).

4. Characterization and kinetic data

Spectroscopic and MS monitoring of the generation of $2^{(IV)}$=NTs

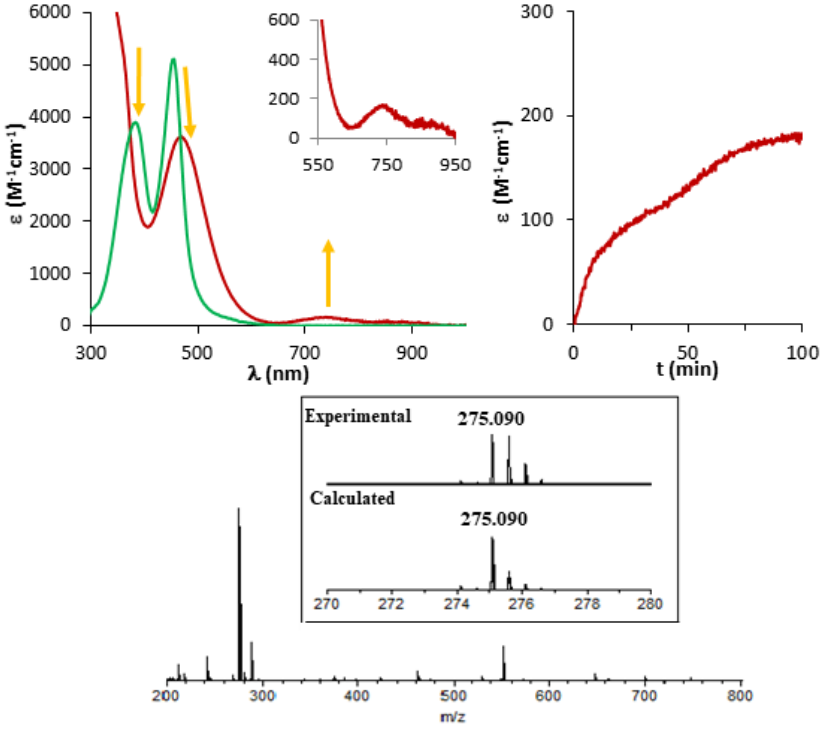


Figure S1. (Top) UV – vis spectra of oxidation of $\mathbf{2^{(II)}}$ to $\mathbf{2^{(IV)}}$**=NTs** in MeCN at 20ºC, HR – MS spectrum of $\mathbf{2^{(IV)}}$**=NTs** prepared in CH_3CN exhibiting a base peak at m/z 275.09; inset show amplification of major peak for $[Fe^{IV}(NTs)(Me_2(CHPy_2)tacn)]^{2+}$ species. Proper simulation of the peaks requires inclusion of ≈50 % of $[Fe^{III}(NHTs)(L)]^{2+}$ in the isotopic pattern corresponding to $[Fe^{IV}(NTs)(L)]^{2+}$.

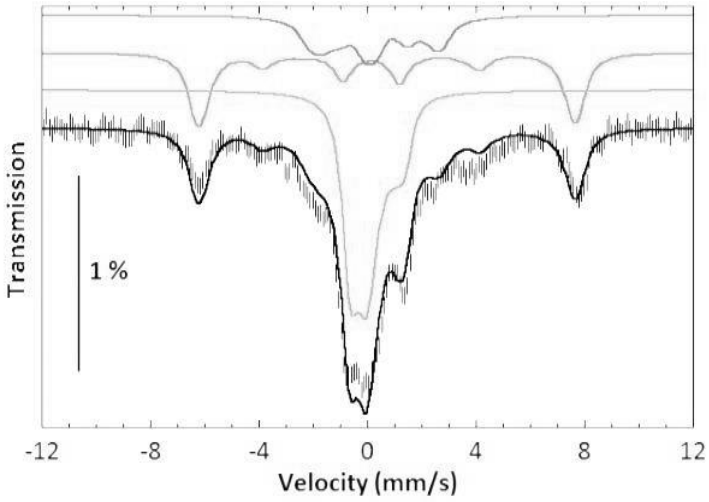


Figure S2. Mossbauer spectra of the reaction of **$2^{(II)}$OTf** with PhINTs in CH_3CN showing accumulation of 48% of **$2^{(IV)}$=NTS**.

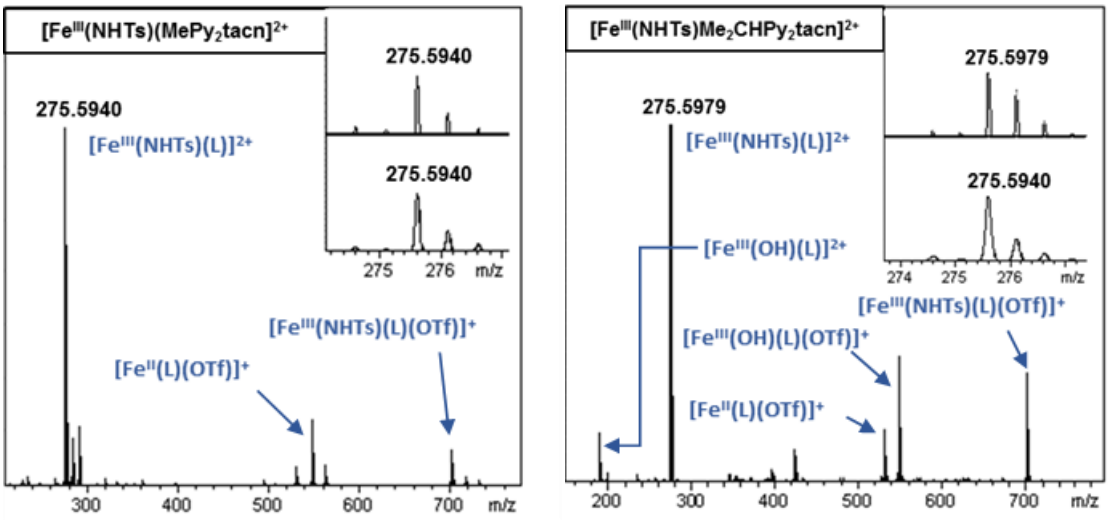


Figure S3. HR – MS of isolated [**$1^{(III)}$ – NHTs](OTf)$_2$** (left) and [**$2^{(III)}$ – NHTs](OTf)$_2$** (right) in CH_3CN.

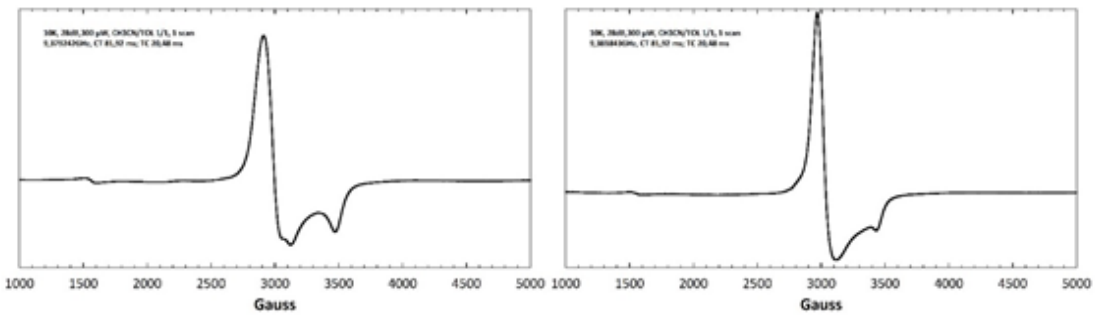


Figure S4. EPR spectra of isolated [**1$^{(III)}$ – NHTs](OTf)$_2$** (left) and [**2$^{(III)}$ – NHTs](OTf)$_2$** (right) at 4.2K.

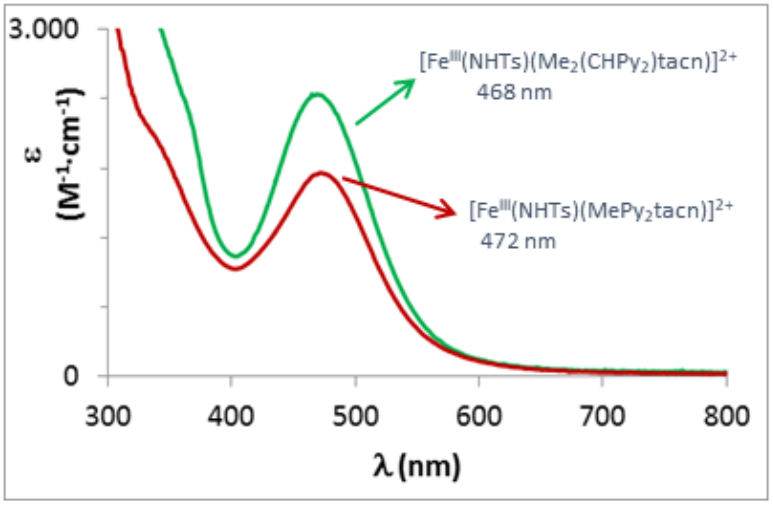


Figure S5. UV – vis spectra of isolated **1$^{(III)}$ – NHTs** and **2$^{(III)}$ – NHTs** in MeCN at 20 ºC.

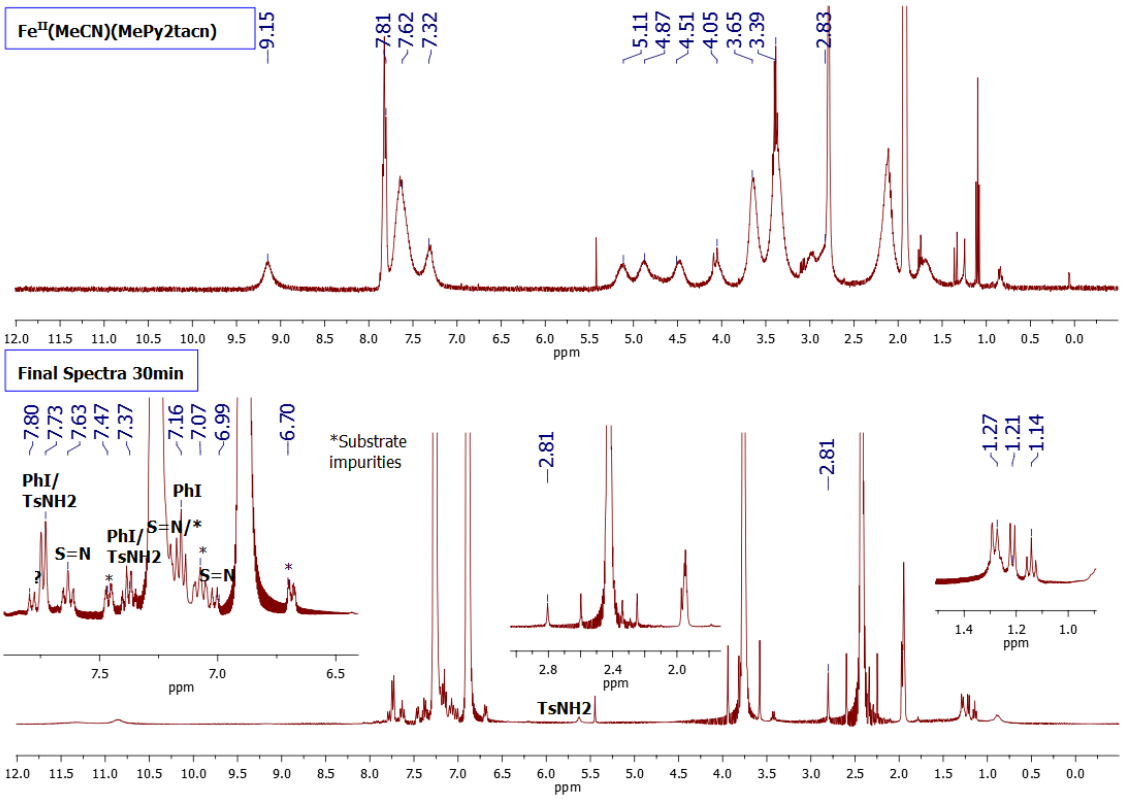


Figure S6. ^{1}H – NMR spectra of: (Top) [Fe^{II}(MeCN)(MePy$_2$tacn)](OTf)$_2$, **1$^{(II)}$OTf**, in CD_3CN; (below) reaction of **1$^{(IV)}$=NTs** with ^{MeO}PhSMe in CD_3CN after 30 minutes time.

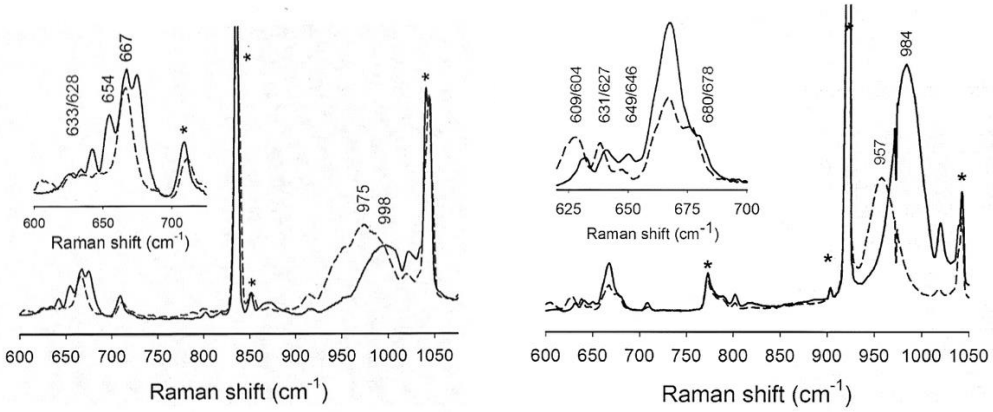
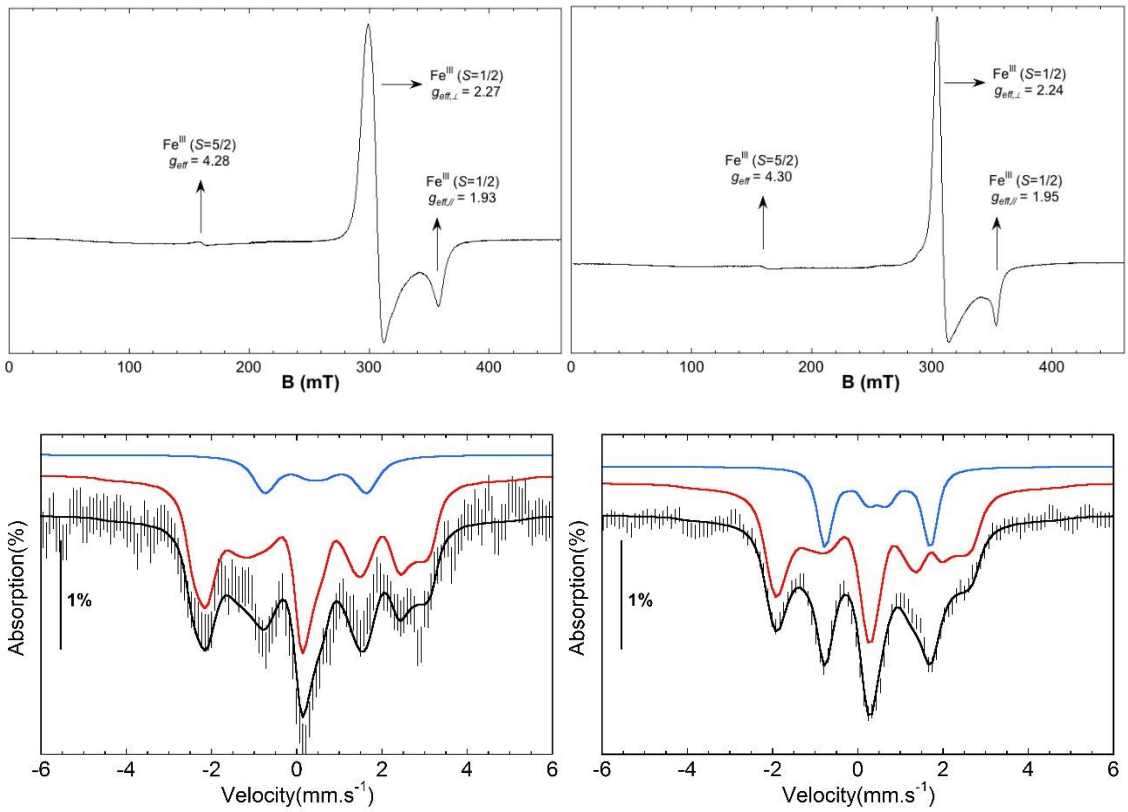


Figure S6A. Resonance Raman spectra of [Fe^{IV}(NTs)(N4Py)]$^{2+}$ (**3**) (left panel showing ^{14}NTs (solid line) and ^{15}NTs (dashed line) isotopomers) and [Fe^{IV}(NTs)(BnTPEN)]$^{2+}$ (**4**) (right panel showing ^{14}NTs (solid line) and ^{15}NTs (dashed line) isotopomers).[9]



Complex $1^{(IV)}$NTs	S	$g_x/g_y/g_z$	δ (mm.s^{-1})	ΔE_Q (mm.s^{-1})	Γ (mm.s^{-1})	H	$A_x/g_n\mu_n$ (T)	$A_y/g_n\mu_n$ (T)	$A_z/g_n\mu_n$ (T)	%
Fe^{III}	1/2	2.26/2.26/1.93	0.25	-1.8	0.38	0.66	-46	2	4	**86**
Fe^{II}	0		0.45	0.45	0.6	1				**14**
Complex $2^{(IV)}$NTs										
Fe^{III}	1/2	2.24/2.24/1.95	0.25	-1.7	0.42	0.66	-40.5	-3.8	2.1	**73**
Fe^{II}	0		0.47	0.55	0.3	0				**23**

Figure S7 and **Table S1.** Spectroscopic properties (EPR, top and Mossbauer, bottom) of iron species resulting from reaction of **$1^{(IV)}$=NTs** (left panels) and **$2^{(IV)}$=NTs** (right panels) with *p* - ^{MeO}PhSMe. Black

hatched bars: experimental spectrum, blue line Fe^{II} contribution, red line Fe^{III} contribution. Table S1 collects the corresponding spectroscopic parameters.

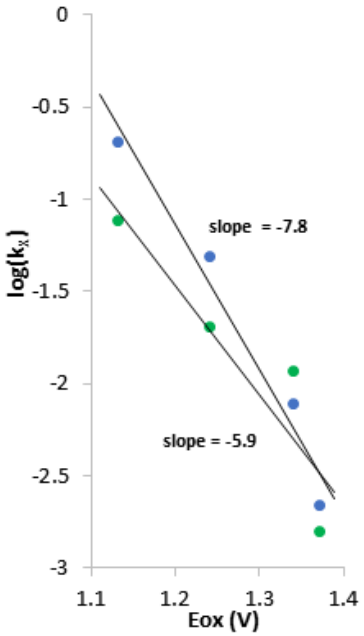


Figure S8. Plot Eox vs log(k_X) in the reactions of **$1^{(IV)}$=NTs** (green circles) and **$2^{(IV)}$=NTs** (blue circles) with *p* – ^{X}PhSMe substrates.

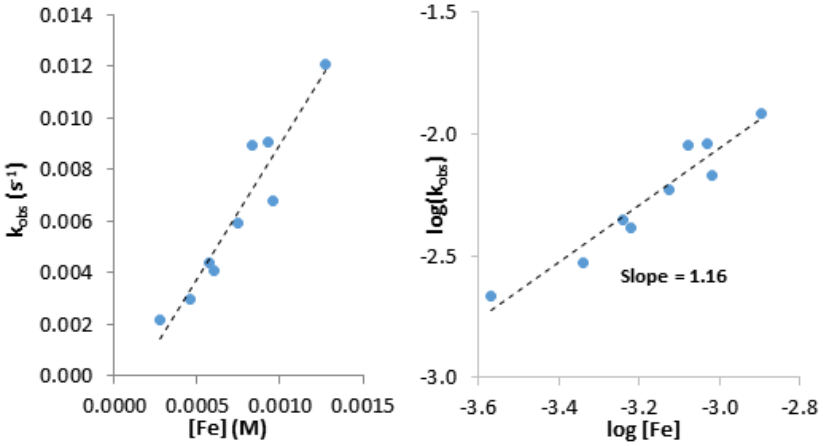


Figure S9. (Left) Rate dependence on [Fe] for the reaction of **$1^{(IV)}$=NTs** with ^{MeO}PhSMe. (Right) log(k_{obs}) vs log([**$1^{(IV)}$=NTs**]) in the reaction of **$1^{(IV)}$=NTs** with ^{MeO}PhSMe.

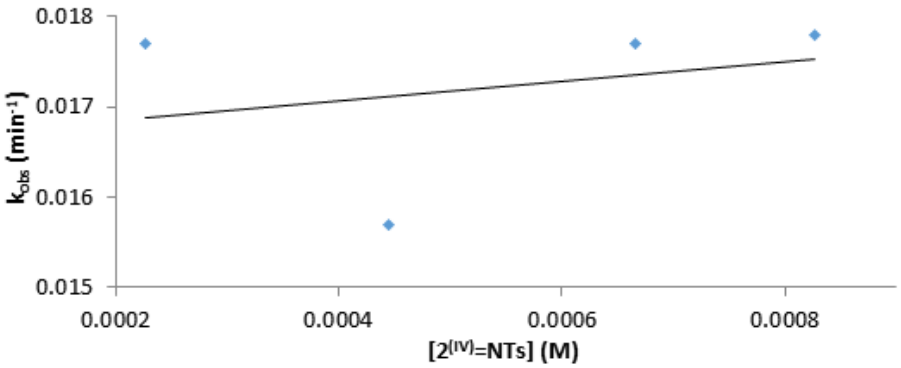


Figure S10. Dependence of k_{obs} on [Fe] in the reaction of **$2^{(IV)}$=NTs** with ^{Cl}PhSMe (0.09 M) in MeCN.

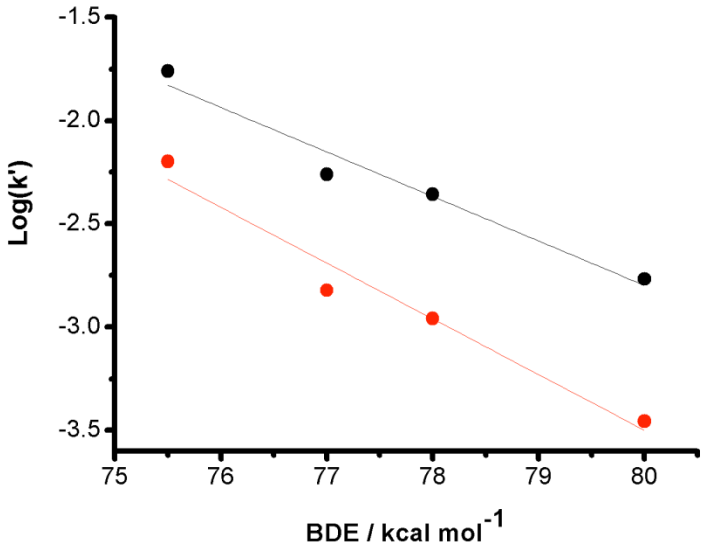


Figure S11. Plot of the logarithm of the extrapolated second order rate k (s^{-1}) values corrected by the number of CH (nH) contained in each substrate (Log(k / nH) = Log(k') for the reaction of different hydrocarbons substrates with **$1^{(IV)}$=NTs** (black dots) and **$2^{(IV)}$=NTs** (red dots), plotted versus the BDE of the studied substrates. The data exhibit linear regressions with slopes of -0.21 and -0.26 kcal*mol-1 for **$1^{(IV)}$=NTs** and **$2^{(IV)}$=NTs** complexes, respectively.

The procedure described before, and adopted to analyze the reaction kinetic in presence of different CH substrates and concentrations, was also applied to study DHA-d4. The profiles observed are shown in Figure **9 C** and **D** of the main manuscript and the corresponding k(s^{-1}) and Keq(M^{-1}) values reported in **Table S2.**

Table S2. k(s^{-1}) and Keq(M^{-1}) values for the reaction of **$1^{(IV)}$=NTs** and **$2^{(IV)}$=NTs** with DHA and DH4-d4.

	$1^{(IV)}$=NTs		**$2^{(IV)}$=NTs**	
Substrate	k, s^{-1}/ Keq,M^{-1}		k, s^{-1}/ Keq,M^{-1}	
DHA	2.2(∓0.2)E-02	315(∓81)	6.0(∓0.6)E-03	227(∓67)
DHA-d4	5.2(∓0.6)E-03	390(∓115)	8.3(∓0.4)E-04	314(∓74)

The reaction of **$1^{(IV)}$=NTs** with DHA was also studied in acetonitrile. The results obtained are represented in **Figure S12** and the k(s^{-1}) and Keq(M^{-1}) values reported in **Table S3**.

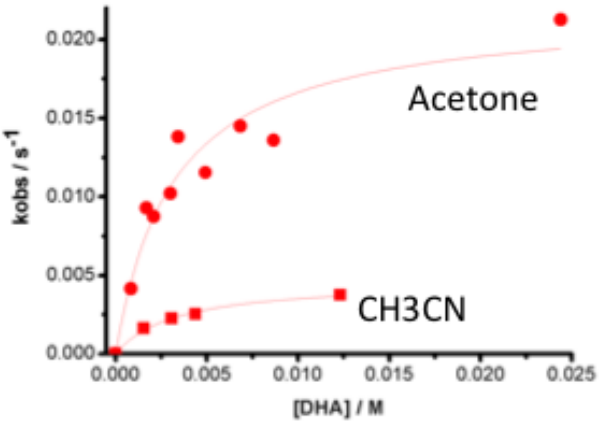


Figure S12. Plot of kobs vs substrate concentration for the reaction of **$1^{(IV)}$=NTs** complex with DHA in acetonitrile and acetone.

Table S3. k(s^{-1}) and Keq(M^{-1}) values for the reaction of **$1^{(IV)}$=NTs** with DHA in acetonitrile and acetone.

Substrate	k, s^{-1}/ Keq,M^{-1}	
DHA-acetone	2.2(∓0.2)E-02	315(∓81)
DHA-CH_3CN	4.7(∓0.3)E-03	301(∓44)

Table S4: Selected EXAFS fits for , **$1^{(III)}$ – NHTs**. Fits carried out in r-space (Δk = 2-12.0 Å^{-1}; Δr = 1-3 Å) with a Hanning window (dk 2), a *k*-weight = 3 and S_0 = 0.9. Bond distances and disorder parameters (Δr_{eff} and σ^2) were allowed to float having initial values of 0.0 Å and 0.003 Å^2 respectively, with a universal E_0 and ΔE_0 = 0 eV. (Fits highlighted in blue are the best models; σ^2 reported as x10^3 Å^2).

							Ni-N/O*			Ni-N/O*			Ni--C			Ni-C			Ni--C-N--Ni		
FIT	Δk	Δr	*Var.*	R_{FACTOR}	χ^2_v	ΔE_0	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2
1	2-12.0	1-2	3	0.072	255	1(3)	-	-	-	4	1.99(3)	3(2)									
2	2-12.0	1-2	3	0.045	158.5	0(3)	-	-	-	6	1.99(3)	8(2)									
3	2-12.0	1-2	3	0.051	177.2	0(3)	-	-	-	5	1.99(2)	5(2)									
4	2-12.0	1-2	3	0.041	144.1	-2(3)	1	1.84(2)	5(2)	5	1.99(2)	5(2)									
5	2-12.0	1-3	3	0.164	239.2	0(3)	1	1.85(3)	5(2)	5	2.00(3)	5(2)									
6	2-12.0	1-3	5	0.019	37.1	-2(1)	1	1.84(1)	4(1)	4	1.99(1)	4(1)	7	2.88(2)	4(1)	3	3.12(3)	4(1)	18	3.24(3)	4(1)
7	2-12.0	1-3	5	0.026	49.8	-1(1)	-	-	-	6	1.98(1)	9(1)	7	2.88(3)	9(1)	3	3.15(4)	9(1)	18	3.27(4)	9(1)
8	2-12.0	1-3	5	0.017	33.0	-1(1)	-	-	-	5	1.98(1)	6(1)	7	2.89(2)	6(1)	3	3.15(3)	6(1)	18	3.27(3)	6(1)
9	2-12.0	1-3	5	0.016	32.0	-2(1)	1	1.84(1)	6(1)	5	1.99(1)	6(1)	7	2.87(2)	6(1)	3	3.12(3)	6(1)	18	3.25(3)	6(1)

*Although EXAFS can not differentiate between O/N/C scattering paths, chemical intuition was used for description to facilitate comparison

Table S5: Selected EXAFS fits for , **$2^{(III)}$ – NHTs**. Fits carried out in r-space (Δk = 2-10.0 Å^{-1}; Δr = 1-3 Å) with a Hanning window (dk 2), a *k*-weight = 3 and S_0 = 0.9. Bond distances and disorder parameters (Δr_{eff} and σ^2) were allowed to float having initial values of 0.0 Å and 0.003 Å^2 respectively, with a universal E_0 and ΔE_0 = 0 eV. (Fits highlighted in blue are the best models; σ^2 reported as x10^3 Å^2).

							Ni-N/O*			Ni-N/O*			Ni--C			Ni--C			Ni-C			Ni--C-N--Ni		
FIT	Δk	Δr	*Var.*	R_{FACTOR}	χ^2_v	ΔE_0	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2
1	2-10	1-2	*3*	0.021	5.1	1(2)	-	-	-	6	2.01(2)	10(2)												
2	2-10	1-2	*3*	0.022	5.5	2(2)	-	-	-	5	2.01(2)	7(2)												
3	2-10	1-2	*3*	0.042	10.3	2(3)	-	-	-	4	2.01(3)	4(2)												
4	2-10	1-2	3	0.044	10.8	0(4)	1	1.84(3)	3(3)	4	2.01(3)	3(3)												
5	2-10	1-2	3	0.030	7.3	0(3)	1	1.84(3)	6(2)	5	2.01(3)	6(2)												
6	2-10	1-2	3	0.025	6.2	1(3)	0.5	1.83(3)	6(2)	5	2.01(3)	6(2)												
7	2-10	1-3	3	0.143	12.6	1(3)	1	1.85(4)	6(3)	5	2.02(4)	6(3)												
8	2-10	1-3	4	0.034	3.5	1(2)	-	-	-	6	2.00(2)	9(1)	4	2.87(5)	9(1)	3	3.02(5)	9(1)	3	3.12(5)	9(1)	18	3.27(5)	9(1)
9	2-10	1-3	4	0.019	2.0	0(1)	-	-	-	5	2.01(1)	7(1)	4	2.87(3)	7(1)	3	3.02(3)	7(1)	3	3.12(3)	7(1)	18	3.27(3)	7(1)
10	2-10	1-3	4	0.017	1.7	1(1)	-	-	-	4	2.00(1)	4(1)	4	2.87(2)	4(1)	3	3.02(2)	4(1)	3	3.12(2)	4(1)	18	3.27(2)	4(1)
11	2-10	1-3	4	0.028	2.9	0(1)	1	1.84(1)	3(1)	4	2.01(1)	3(1)	4	2.85(3)	3(1)	3	3.00(3)	3(1)	3	3.10(3)	3(1)	18	3.25(3)	3(1)
12	2-10	1-3	4	0.024	2.4	1(1)	0.5	1.83(1)	7(1)	5	2.01(1)	7(1)	4	2.86(3)	7(1)	3	3.01(3)	7(1)	3	3.11(3)	7(1)	18	3.26(3)	7(1)
11	2-10	1-3	4	0.032	3.9	0(1)	1	1.84(2)	7(3)	5	2.02(2)	7(3)	4	2.85(2)	7(3)	3	3.00(4)	7(3)	3	3.10(4)	7(3)	18	3.25(4)	7(3)

*Although EXAFS can not differentiate between O/N/C scattering paths, chemical intuition was used for description to facilitate comparison

Table S6: Selected EXAFS fits for , **$1^{(IV)}$ – NTs**. Fits carried out in r-space (Δk = 2-12.5 Å^{-1}; Δr = 1-3 Å) with a Hanning window (dk 2), a *k*-weight = 3 and S_0 = 0.9. Bond distances and disorder parameters (Δr_{eff} and σ^2) were allowed to float having initial values of 0.0 Å and 0.003 Å^2 respectively, with a universal E_0 and ΔE_0 = 0 eV. (Fits highlighted in blue are the best models; σ^2 reported as x10^3 Å^2).

							Ni-N/O*			Ni-N/O*			Ni--C			Ni-C			Ni--C-N--Ni		
FIT	Δk	Δr	*Var.*	R_{FACTOR}	χ^2_v	ΔE_0	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2
1	2-12.5	1-2	3	0.082	13.3		-	-	-	5	2.00(2)	3(2)									
2	2-12.5	1-2	3	0.010	16.7	1(3)	-	-	-	6	2.00(3)	6(2)									
3	2-12.5	1-2	3	0.059	9.5	-1(2)	1	1.71(2)	4(1)	6	1.98(2)	4(1)									
4	2-12.5	1-2	3	0.130	21.2	-1(4)	1	1.71(2)	1(2)	4	1.98(2)	1(2)									
5	2-12.5	1-2	3	0.070	11.9	-1(3)	1	1.71(2)	2(1)	5	1.98(2)	2(1)									
6	2-12.5	1-3	3	0.222	17.0	0(3)	1	1.72(2)	2(2)	5	1.99(2)	2(2)									
7	2-12.5	1-3	5	0.043	4.1	1(1)	1	1.71(1)	1(1)	4	1.98(1)	1(1)	7	2.84(2)	1(1)	4	3.06(3)	1(1)	10	3.23(3)	1(1)
8	2-12.5	1-3	5	0.059	5.6	2(1)	-	-	-	5	2.00(1)	3(1)	7	2.85(3)	3(1)	4	3.08(6)	3(1)	10	3.26(6)	3(1)
9	2-12.5	1-3	5	0.026	2.5	1(1)	1	1.71(1)	2(1)	5	1.99(1)	2(1)	7	2.84(1)	2(1)	4	3.07(3)	2(1)	10	3.25(3)	2(1)

*Although EXAFS can not differentiate between O/N/C scattering paths, chemical intuition was used for description to facilitate comparison

Table S7: Selected EXAFS fits for , **$2^{(IV)}$ – NTs**. Fits carried out in r-space (Δk = 2-12.5 $Å^{-1}$; Δr = 1-3 Å) with a Hanning window (dk 2), a *k*-weight = 3 and S_0 = 0.9. Bond distances and disorder parameters (Δr_{eff} and σ^2) were allowed to float having initial values of 0.0 Å and 0.003 $Å^2$ respectively, with a universal E_0 and ΔE_0 = 0 eV. (Fits highlighted in blue are the best models; σ^2 reported as x10^3 $Å^2$).

							Ni-N/O*			Ni-N/O*			Ni--C			Ni--C			Ni-C			Ni--C-N--Ni		
FIT	Δk	Δr	*Var.*	R_{FACTOR}	χ^2_ν	ΔE_0	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2	N	r(Å)	σ^2
1	2-12.5	1-2	3	0.112	33.8	-9(5)	-	-	-	6	1.99(2)	6(1)												
2	2-12.5	1-2	3	0.067	20.2	-8(4)	-	-	-	5	1.99(2)	4(1)												
3	2-12.5	1-2	3	0.0375	11.3	-8(3)	1	1.71(1)	3(1)	4	1.98(1)	3(1)												
4	2-12.5	1-2	3	0.016	4.9	-8(2)	1	1.71(1)	4.2(4)	5	1.99(1)	4.2(4)												
5	2-12.5	1-3	3	0.110	13.6	-8(3)	1	1.71(1)	4(1)	5	1.98(1)	4(1)												
6	2-12.5	1-3	4	0.042	5.8	-5(2)	1	1.71(1)	3.4(4)	4	1.99(1)	3.4(4)	5	2.84(2)	3.4(4)	3	2.97(2)	3.4(4)	2	3.09(2)	3.4(4)	14	3.23(2)	3.4(4)
7	2-12.5	1-3	4	0.087	11.8	-6(2)	-	-	-	5	2.00(1)	4(1)	5	2.84(3)	4(1)	3	2.97(3)	4(1)	2	3.09(3)	4(1)	14	3.23(3)	4(1)
8	2-12.5	1-3	4	0.024	3.3	-6(1)	1	1.72(1)	4.4(3)	5	1.99(1)	4.4(3)	5	2.84(1)	4.4(3)	3	2.97(1)	4.4(3)	2	3.09(1)	4.4(3)	14	3.22(1)	4.4(3)

*Although EXAFS can not differentiate between O/N/C scattering paths, chemical intuition was used for description to facilitate comparison

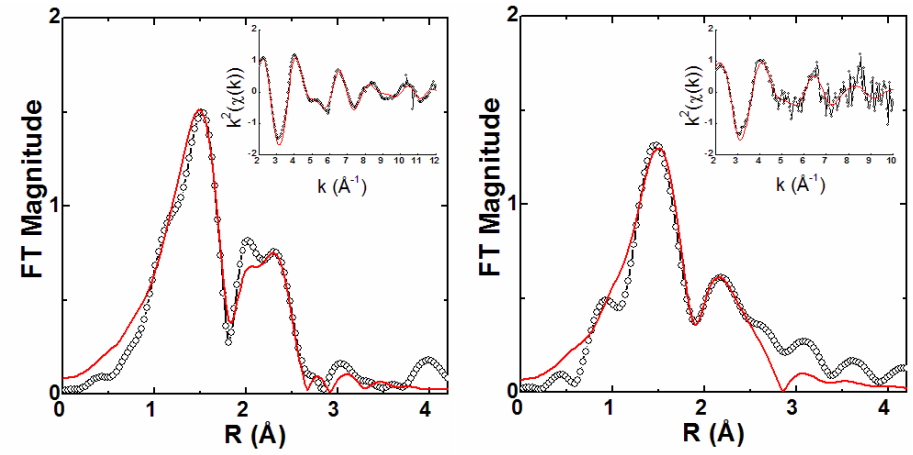


Figure S13: Non– phase shift corrected Fourier transforms for **$1^{(III)}$=NHTs** (left) and **$2^{(III)}$=NHTs** (right) with insets showing the k – space data and fits. Experimental data are shown in black and fits in red.

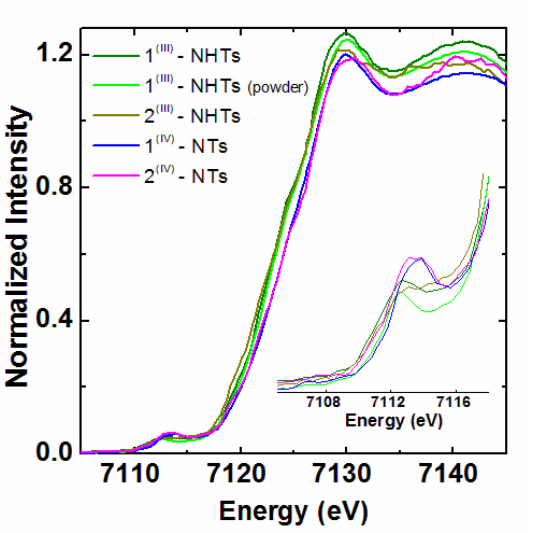


Figure S14: XANES spectra with inset showing 1s→ 3d features.

Table S8: Spectroscopic parameters from Fe-K edge X-ray absorption spectroscopy.

	1s→3d area (x10^2)	1s→3d (eV)	E_0' (eV)	Fe-N (Å)
$1^{(IV)}$=NTs	18.5	7113.2	7123.4	1.73
$2^{(IV)}$=NTs	18.0	7113.3	7123.3	1.72
$1^{(III)}$=NHTs	12.4	7112.5	7122.5	1.84
$2^{(III)}$=NHTs	10.5	7112.4	7122.3	1.84

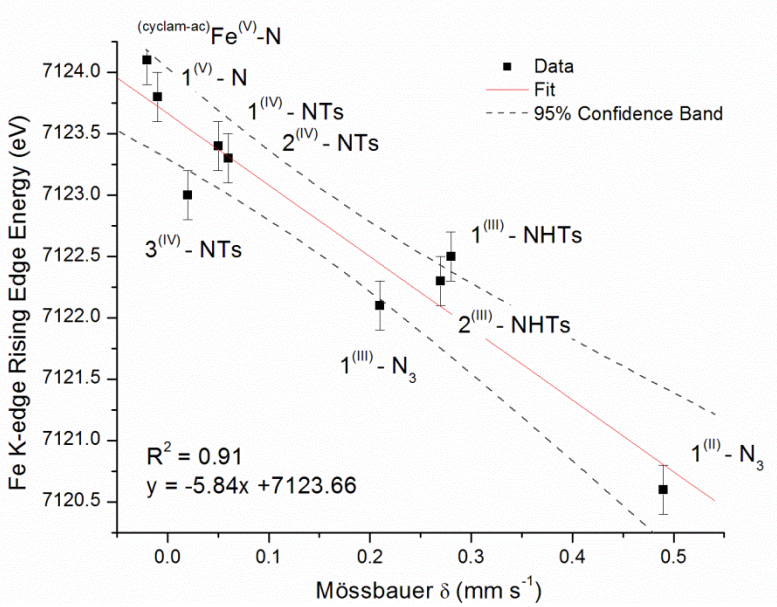


Figure S15: Correlation of Mössbauer and Fe K-edge rising edge energies for a series of related Fe-N^x complexes.(Data for complexes **$1^{(II)}$-N_3** and **$1^{(V)}$-N** was exctracted from Sabenya et al.[6, 10], and for complexes **$3^{(IV)}$-NTs** and **$^{(cyclam-ac)}Fe^{(V)}$-N** from Klinker et al,[8] and Aliaga-Alcalde et al.[11] respectively.

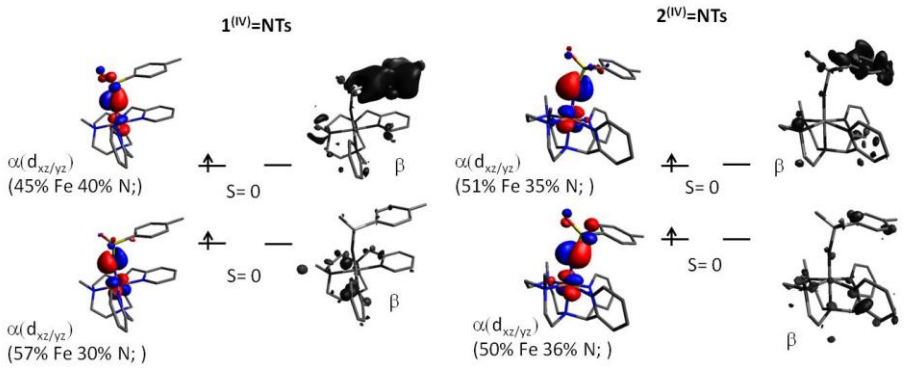


Figure S16: Schematic of Fe=NTs molecular orbitals showing the Fe d-manifold using unrestricted corresponding orbitals (0.05 isovalue) for **1$^{(IV)}$=NTs** (left) and **2$^{(IV)}$=NTs** (right).

5. Computational details

The geometries of the Fe(III) and Fe(IV) structures were optimized at the DFT level B3LYP and 6-311G** 6d basis set for all atoms using the Gaussian09 program.[12] The solvation effect of acetonitrile was introduced in geometry optimizations and energy through the IEFPCM-SMD polarizable continuum model.[13] Dispersion effects were also included using the Grimme D_3 correction.[14] Stationary points were characterized by analytical frequency calculations. Electronic energies have been corrected using a B3LYP and cc-pVTZ 6d basis set for all atoms.

$$\mathrm{G} = \mathrm{E}^{cc-pVTZ} + G_{correction}^{6-311g^{**}} \quad (1)$$

Calculation of bond dissociation energy, pka and redox values. Bond dissociation energy (enthalpy, 0 K gas-phase BDEs) is defined as the enthalpy change of the dissociation reaction of homolytic bonds at 298.15 K, 1 atm.[15]

$$\mathrm{R–X} \rightarrow \mathrm{R^{\bullet}} + \mathrm{X^{\bullet}} \quad (2)$$

$$\mathrm{BDE(R–X)} = \mathrm{H(R^{\bullet})} + \mathrm{H(X^{\bullet})} - \mathrm{H(R–X)} \quad (3)$$

where H(R$^{\bullet}$) and H(X$^{\bullet}$) and H(R—X) are enthalpies of the radicals and the molecule.

The standard dissociation free energy change between an acid (AH) and its conjugate base (A^-) in aqueous (ΔG*) may be expressed as: [8]

$$\Delta G^* = G(A^-_{aq}) + G(H^+_{aq}) - G(AH_{aq}) + \Delta G^{o/*} \quad (3)$$

$$G(H^+_{aq}) = G(H^+_{gas}) + \Delta G^{H+}_{solv} \qquad (4)$$

where $G(AH_{aq})$ and $G(A^-_{aq})$ are standard free energies of the acid and its conjugate base in aqueous media, respectively. The $G(H^+_{aq})$ is the free energy of the proton in acetonitrile, obtained from the experimental solvation free energy ($\Delta G^{H+}_{solv} = -260.2\ \text{kcal} \cdot \text{mol}^{-1}$) and its gas-phase free energy ($G(H^+_{gas}) = -6.3\ \text{kcal} \cdot \text{mol}^{-1}$). $\Delta G^{o/*}$ is the free energy change associated with the conversion from a standard state of 1 M in the aqueous phase and 1 atm in gas phase, to the desired concentration in both phases. ΔG^* values are derived with the following expression:

$$\Delta G^{o/*} = RT \ln(24.4 * c) \qquad (5)$$

where *R* is the universal gas constant (1.987 cal·mol^{-1}·K^{-1}), *T* is the temperature in Kelvin and *c* the concentration in mol·L^{-1}.

The standard one electron redox potentials relative to the SHE electrode were calculated by:

$$E^o = -\frac{\Delta G^0 - \Delta G_{SHE}}{F} \qquad (6)$$

where ΔG^0 is the standard free energy change associated with the reduction reaction, *F* is the Faraday constant (23.061 kcal·mol^{-1}V^{-1}) and ΔG_{SHE} is the free energy change associated with the proton reduction to H_2 (-4.24 eV). The ΔG_{SHE} value was derived using the Fermi-Dirac statistics for the treatment of electron thermodynamics.

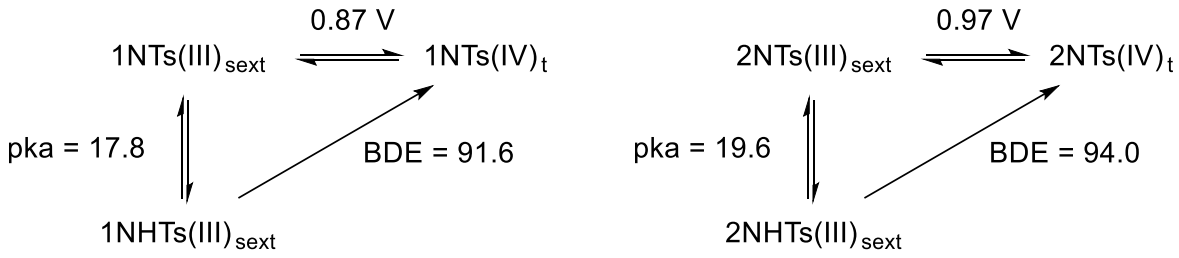
Property calculations and electronic structure: The electronic structure and Mössbauer parameters were were explored with the ORCA software package.[16] Single point calculations on the above

optimized geometries were carried out using the B3LYP functional with a def2 – TZVP as well as a def2 – TZVP/J auxiliary basis set on all atoms.[17, 18] The calculations employed a dense integration grid (ORCA Grid 5 = Lebedev 434 points) along with the Grimme and coworkers DFT – D3BJ dispersion correction.[14, 19]. In addition solvent effects were included using a conductor like screening model (COSMO) using acetonitrile as solvent.[20] Mössbauer parameters were also calculated, but in order to allow comparison with previously calibrated approaches the B3LYP functional was employed together with expanded CP(PPP) basis set[21] on the iron, TZVP basis set on the remaining atoms and a COSMO model simulating an aqueous solution environment.[22] As such, the calculated isotropic shift was adjusted to a linear calibration line of the form A(p-C) + B where A is -0.366, B is 2.852 and C is 11810 and p is the electron density at the nucleus. [21,22] Quadrupole splittings were taken from theoretical calculations as is. Similarly calculated vibrational frequencies were reported without further scaling.

Table S9. Energies calculated for the different species of Fe^{III}-NTs and Fe^{IV} =NTs.

Entry	Name	E[a]	H[b]	G[c]
1	**1NTs(III)d**	-3152.763272	-3152.144742	-3152.237112
2	**1NTs(III)q**	-3152.763679	-3152.145179	-3152.240579
3	**1NTs(III)sext**	-3152.774364	-3152.157374	-3152.255594
4	**1NHTs(III)d**	-3153.250327	-3152.617377	-3152.710737
5	**1NHTs(III)q**	-3153.239081	-3152.606241	-3152.701961
6	**1NHTs(III)sext**	-3153.25003	-3152.61953	-3152.71604
7	**1NTs(IV)t**	-3152.594317	-3151.974231	-3152.067744
8	**1NTs(IV)q**	-3152.58198	-3151.963276	-3152.059548
9	**2NTs(III)d**	-3152.743342	-3152.124508	-3152.215807
10	**2NTs(III)q**	-3152.749719	-3152.132559	-3152.227756
11	**2NTs(III)sext**	-3152.762106	-3152.145213	-3152.242067
12	**2NHTs(III)d**	-3153.236299	-3152.603283	-3152.694389
13	**2NHTs(III)q**	-3153.22501	-3152.593712	-3152.689552
14	**2NHTs(III)sext**	-3153.237014	-3152.607055	-3152.706353
15	**2NTs(IV)t**	-3152.578261	-3151.957805	-3152.050469
16	**2NTs(IV)q**	-3152.563488	-3151.945098	-3152.040315

[a] Electronic energies calculated at B3LYP/6-311+g**//B3LYP/cc-pVTZ level including solvent effects (SMD) and Grimme-D_3 dispersion correction. [b] Enthalpy energies (H) calculated as $\mathrm{H} = \mathrm{E}^{cc-pVTZ} + H_{correction}^{6-311g**}$. [c] Gibbs energies (G) obtained as $\mathrm{G} = \mathrm{E}^{cc-pVTZ} + G_{correction}^{6-311g**}$. All energies are given in hartrees.

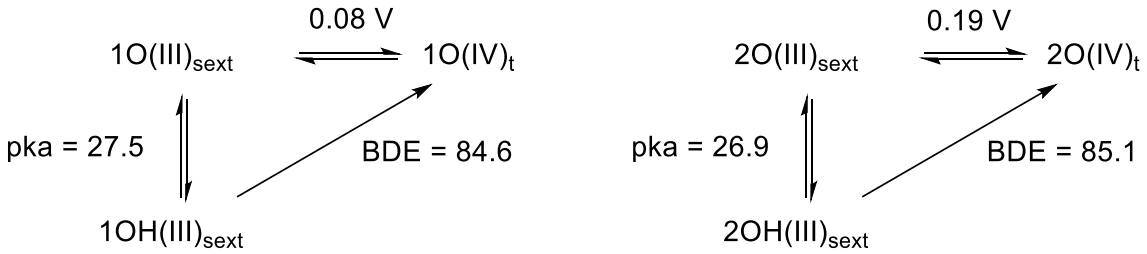


Scheme S1. Calculated $E_{1/2}$ ($Fe^{III/IV}$), pka of Fe^{III} protonation and BDE values for the protonation of **1** and **2** complexes. Theoretical values are calculated at B3LYP/6-311g**//B3LYP/cc-pVTZ level including solvent effects (SMD) and Grimme-D_3 dispersion correction. All redox potentials are given in V *vs* SHE. BDE in kcal mol^{-1}.

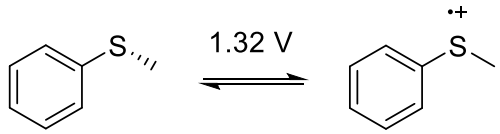
Table S9. Energies calculated for the different species of Fe^{III}-O and Fe^{IV} = O.

Entry	Name	E[a]	H[b]	G[c]
1	**1O(III)d**	-2353.42267	-2352.94451	-2353.01383
2	**1O(III)q**	-2353.44761	-2352.97006	-2353.04313
3	**1O(III)sext**	-2353.44745	-2352.97063	-2353.04561
4	**1OH(III)d**	-2353.94547	-2353.45318	-2353.52335
5	**1OH(III)q**	-2353.93040	-2353.43972	-2353.51292
6	**1OH(III)sext**	-2353.94242	-2353.45242	-2353.52692
7	**1O(IV)t**	-2353.29939	-2352.81820	-2352.88671
8	**2O(III)d**	-2353.40471	-2352.92689	-2352.99627
9	**2O(III)q**	-2353.43432	-2352.95758	-2353.03178
10	**2O(III)sext**	-2353.43510	-2352.95865	-2353.03420
11	**2OH(III)d**	-2353.93096	-2353.43871	-2353.50779
12	**2OH(III)q**	-2353.91351	-2353.42333	-2353.49734
13	**2OH(III)sext**	-2353.92688	-2353.43779	-2353.51434
14	**2O(IV)t**	-2353.28366	-2352.80274	-2352.87132

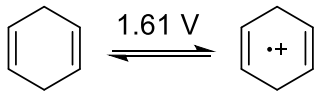
[a] Electronic energies calculated at B3LYP/6-311+g**//B3LYP/cc-pVTZ level including solvent effects (SMD) and Grimme-D_3 dispersion correction. [b] Enthalpy energies (H) calculated as $\mathrm{H} = \mathrm{E}^{cc-pVTZ} + H^{6-311g^{**}}_{correction}$. [c] Gibbs energies (G) obtained as $\mathrm{G} = \mathrm{E}^{cc-pVTZ} + G^{6-311g^{**}}_{correction}$. All energies are given in hartrees.



Scheme S2. Calculated $E_{1/2}$ ($Fe^{III/IV}$), pka of Fe^{III} protonation and BDE values for the protonation of **1** and **2** *oxo*- analogues. Theoretical values are calculated at B3LYP/6-311g**//B3LYP/cc-pVTZ level including solvent effects (SMD) and Grimme-D_3 dispersion correction. All redox potentials are given in V *vs* SHE. BDE in kcal mol^{-1}.



Scheme S3. Calculated $E_{1/2}$ ($PhSMe^{0/+}$). Theoretical values are calculated at B3LYP/6-311g**//B3LYP/cc-pVTZ level including solvent effects (SMD) and Grimme-D_3 dispersion correction. All redox potentials are given in V *vs* SHE. BDE in kcal mol^{-1}.



Scheme S4. Calculated $E_{1/2}$ ($CHD^{+/0}$). Theoretical values are calculated at B3LYP/cc-pVTZ level including solvent effects (SMD) and Grimme-D_3 dispersion correction. All redox potentials are given in V *vs* SHE.

6. Cartesian Coordinates

1NTs(III)d
E = -3152.763272
G = -3152.237112
1,2

N	+2.06052	+1.49886	-0.01615
N	+2.51817	-0.74542	-1.37913
N	+2.28931	-1.16756	+1.36932
N	+0.31646	-2.08254	-0.38060
N	-0.27265	+0.29365	-1.43323
C	+2.02652	+2.45513	+0.92715
H	+1.34391	+2.29233	+1.74469
C	+2.83023	+3.58388	+0.86840
H	+2.76548	+4.32536	+1.65424
C	+3.70922	+3.73114	-0.20003
H	+4.35334	+4.59947	-0.27090
C	+3.76124	+2.73461	-1.16909
H	+4.44380	+2.79685	-2.00710
C	+2.92534	+1.63265	-1.04872
C	+2.89354	+0.51825	-2.05732
H	+3.84850	+0.42841	-2.58066
H	+2.12972	+0.74412	-2.80311
C	+3.68922	-1.35962	-0.66392
H	+4.62178	-1.01085	-1.11083
H	+3.65284	-2.43648	-0.80953
C	+3.66669	-1.02496	+0.81972
H	+4.36767	-1.67089	+1.35920
H	+3.96903	+0.00781	+0.98355
C	+2.25477	-0.58186	+2.73038
H	+2.96615	-1.10273	+3.38019
H	+1.24458	-0.66407	+3.12048
H	+2.52019	+0.47197	+2.67927
C	+1.87057	-2.61654	+1.44028
H	+1.92574	-2.96541	+2.47276
H	+2.57746	-3.21681	+0.87097
C	+0.45331	-2.80257	+0.91518
H	+0.22023	-3.86608	+0.80241
H	-0.25657	-2.34226	+1.59857
C	+1.10031	-2.74598	-1.48726
H	+0.42009	-3.29871	-2.13669
H	+1.77389	-3.47457	-1.04382
C	+1.87928	-1.72033	-2.30459
H	+2.62607	-2.21963	-2.92929
H	+1.20955	-1.16767	-2.95877
C	-1.09437	-1.87944	-0.78952
H	-1.66898	-1.65433	+0.10907
H	-1.51185	-2.77168	-1.26146
C	-1.17346	-0.68208	-1.69409
C	-2.13220	-0.54644	-2.68857
H	-2.82487	-1.35732	-2.87440
C	-2.18873	+0.63821	-3.41444
H	-2.92917	+0.76809	-4.19465
C	-1.28895	+1.65625	-3.11335
H	-1.30726	+2.60137	-3.64026
C	-0.34944	+1.44757	-2.11452
H	+0.35748	+2.21475	-1.84016
Fe	+1.03531	-0.22794	-0.00234
N	-0.18980	+0.12450	+1.33022
S	-1.19464	+1.33541	+1.46148
O	-1.32480	+1.74023	+2.89580
O	-0.98862	+2.49924	+0.54294
C	-2.82391	+0.66933	+1.02051
C	-3.53180	+1.19250	-0.05520
C	-3.35335	-0.39574	+1.75540
C	-4.76898	+0.64691	-0.40173
H	-3.11049	+2.01486	-0.61890
C	-4.58368	-0.93408	+1.39979
H	-2.80268	-0.80237	+2.59534
C	-5.31151	-0.42461	+0.31221
H	-5.31438	+1.05866	-1.24480
H	-4.99100	-1.76158	+1.97219
C	-6.63214	-1.03816	-0.07832
H	-7.18614	-0.39254	-0.76304
H	-6.48087	-2.00160	-0.57757
H	-7.25708	-1.22612	+0.79925

1NTs(III)q
E = -3152.763679
G = -3152.240579
1,4

N	+2.15703	+0.61938	-1.56525
N	+2.47685	-1.44652	+0.19006
N	+2.26896	+0.94219	+1.72654
N	+0.30573	-1.15243	+1.96087
N	-0.44884	-1.15407	-0.67599
C	+2.20016	+1.81482	-2.16774
H	+1.48336	+2.54233	-1.81485
C	+3.10644	+2.10000	-3.18100
H	+3.11098	+3.07913	-3.64275
C	+4.00103	+1.10807	-3.57440
H	+4.72723	+1.29941	-4.35568
C	+3.95946	-0.13298	-2.94386
H	+4.64498	-0.92602	-3.21550
C	+3.01872	-0.34290	-1.94283
C	+2.85227	-1.65948	-1.23066

H +3.75510 -2.27076 -1.31145
H +2.03773 -2.20367 -1.71346
C +3.65938 -0.98760 +1.00117
H +4.58411 -1.22984 +0.47349
H +3.67579 -1.55004 +1.93179
C +3.61959 +0.50783 +1.28876
H +4.37384 +0.75350 +2.04632
H +3.85512 +1.07206 +0.38772
C +2.20151 +2.41810 +1.74388
H +2.95427 +2.82905 +2.42681
H +1.20581 +2.72392 +2.05620
H +2.37103 +2.79655 +0.73675
C +1.89520 +0.38751 +3.06844
H +1.95690 +1.17524 +3.82239
H +2.62212 -0.37075 +3.35312
C +0.48202 -0.19611 +3.07577
H +0.28494 -0.66270 +4.04854
H -0.23996 +0.60625 +2.92201
C +1.13766 -2.38068 +2.07414
H +0.51245 -3.23954 +2.33301
H +1.84529 -2.25496 +2.89065
C +1.87297 -2.68223 +0.76451
H +2.64127 -3.44427 +0.93209
H +1.17274 -3.07037 +0.02787
C -1.09918 -1.45367 +1.64329
H -1.68632 -0.55035 +1.81502
H -1.50442 -2.24769 +2.27813
C -1.25044 -1.81640 +0.18389
C -2.17617 -2.74709 -0.26871
H -2.79864 -3.27046 +0.44590
C -2.28555 -2.98433 -1.63536
H -3.00248 -3.70626 -2.00818
C -1.46778 -2.28108 -2.51520
H -1.52482 -2.43194 -3.58534
C -0.56046 -1.37044 -1.99505
H +0.09169 -0.78459 -2.62694
Fe +0.92898 +0.11336 +0.18882
N -0.16919 +1.54522 +0.21612
S -1.28256 +1.99805 -0.82196
O -1.56826 +3.44105 -0.59117
O -1.00240 +1.64118 -2.24116
C -2.82228 +1.14141 -0.40232
C -3.51622 +0.42079 -1.36784
C -3.31881 +1.23250 +0.89978
C -4.70231 -0.22737 -1.02403
H -3.12091 +0.35817 -2.37303
C -4.49977 +0.57965 +1.23171
H -2.77851 +1.79639 +1.65116
C -5.20938 -0.16495 +0.27709
H -5.23435 -0.79775 -1.77836
H -4.87951 +0.64550 +2.24620
C -6.46427 -0.90587 +0.66241
H -7.08328 -1.12634 -0.21001
H -6.21568 -1.85962 +1.14145
H -7.06186 -0.33146 +1.37498

1NTs(III)sext

E = -3152.774364
G = -3152.255594
1,6
N -1.94700 +1.29518 +0.91871
N -2.52850 -1.38862 +0.84018
N -2.52337 -0.46261 -1.88972
N -0.44130 -2.18114 -0.93769
N +0.53841 -0.73784 +1.14126
C -1.81735 +2.61748 +0.70869
H -1.09957 +2.90544 -0.05080
C -2.54960 +3.54745 +1.43143
H -2.42228 +4.60448 +1.23610
C -3.44447 +3.08876 +2.39600
H -4.03958 +3.78914 +2.97030
C -3.56995 +1.72003 +2.61443
H -4.25519 +1.32889 +3.35608
C -2.79773 +0.84392 +1.85989
C -2.80219 -0.64939 +2.08773
H -3.74179 -0.96382 +2.55217
H -1.99872 -0.86851 +2.79533
C -3.75249 -1.54368 -0.00101
H -4.64880 -1.42380 +0.61288
H -3.77772 -2.56004 -0.38915
C -3.80665 -0.53748 -1.14777
H -4.63151 -0.79880 -1.82171
H -3.99914 +0.46230 -0.75692
C -2.53962 +0.69911 -2.80566
H -3.36644 +0.61917 -3.52145
H -1.59134 +0.74698 -3.33584
H -2.64857 +1.61371 -2.22210
C -2.20119 -1.72066 -2.63319
H -2.34570 -1.56644 -3.70475
H -2.89982 -2.50032 -2.33700
C -0.75730 -2.16493 -2.39038
H -0.58970 -3.14839 -2.84393
H -0.07664 -1.44802 -2.84925
C -1.20050 -3.22851 -0.18595
H -0.53269 -4.05030 +0.08385
H -1.95640 -3.64569 -0.84785
C -1.85715 -2.68687 +1.08935
H -2.56227 -3.43410 +1.47279
H -1.10139 -2.52107 +1.85349
C +1.01352 -2.25470 -0.67856
H +1.51100 -1.60285 -1.40003
H +1.39575 -3.27124 -0.80885
C +1.33395 -1.72899 +0.70013
C +2.40293 -2.19434 +1.45776
H +3.02263 -2.99675 +1.07779
C +2.65367 -1.61262 +2.69667

H +3.48182 -1.95778 +3.30411
C +1.82987 -0.58291 +3.14404
H +1.99366 -0.10153 +4.09952
C +0.78214 -0.17326 +2.33173
H +0.11073 +0.62333 +2.62802
Fe -0.96782 -0.12597 -0.34094
N +0.18537 +0.86727 -1.31948
S +1.28792 +1.91256 -1.66486
O +1.57609 +1.98879 -3.12412
O +1.03592 +3.23825 -1.02503
C +2.79036 +1.26485 -0.89412
C +3.13079 +1.65346 +0.39889
C +3.54980 +0.30343 -1.56234
C +4.23587 +1.07801 +1.02160
H +2.53792 +2.40326 +0.90790
C +4.64970 -0.26585 -0.92851
H +3.28428 +0.01204 -2.57137
C +5.00656 +0.10605 +0.37483
H +4.49620 +1.38177 +2.02994
H +5.23837 -1.01339 -1.45068
C +6.16179 -0.56043 +1.07572
H +6.52941 +0.04565 +1.90658
H +5.85266 -1.52920 +1.48446
H +6.99153 -0.74790 +0.38933

1NHTs(III)d
E = -3153.250327
G = -3152.710737
2,2
N +2.29567 +1.10321 +0.85393
N +2.52286 +0.25510 -1.64500
N +2.14438 -1.83096 +0.13234
N +0.16551 -1.14859 -1.67477
N -0.09522 +1.38575 -0.87746
C +2.30657 +1.23514 +2.19306
H +1.57128 +0.65910 +2.73545
C +3.20988 +2.05942 +2.84521
H +3.17753 +2.13521 +3.92409
C +4.14503 +2.76400 +2.09312
H +4.86859 +3.40967 +2.57581
C +4.14390 +2.62012 +0.70990
H +4.85939 +3.14059 +0.08638
C +3.20559 +1.78520 +0.12084
C +3.08002 +1.60724 -1.36189
H +4.03365 +1.75163 -1.87118
H +2.38347 +2.35354 -1.74707
C +3.60273 -0.80014 -1.57781
H +4.57747 -0.33483 -1.72352
H +3.45476 -1.49469 -2.40006
C +3.55836 -1.51828 -0.24469
H +4.14613 -2.43933 -0.28758
H +3.96724 -0.89269 +0.54627
C +2.14470 -2.28028 +1.55271
H +2.86485 -3.09545 +1.66982
H +1.15379 -2.62657 +1.82149
H +2.43166 -1.45285 +2.19666
C +1.57307 -2.92667 -0.74721
H +1.54818 -3.86231 -0.18868
H +2.24108 -3.07824 -1.59163
C +0.17055 -2.56999 -1.21599
H -0.14699 -3.23420 -2.02432
H -0.53034 -2.65662 -0.39195
C +0.90855 -1.00071 -2.98842
H +0.18927 -0.91697 -3.80298
H +1.48015 -1.90829 -3.15734
C +1.81592 +0.21651 -2.96271
H +2.53867 +0.17941 -3.78109
H +1.23874 +1.13273 -3.05773
C -1.19845 -0.56904 -1.78530
H -1.81093 -0.97412 -0.98160
H -1.66989 -0.84227 -2.73054
C -1.13284 +0.92235 -1.61123
C -2.11531 +1.77286 -2.09874
H -2.92586 +1.36479 -2.68866
C -2.04464 +3.12859 -1.80099
H -2.80375 +3.80919 -2.16705
C -0.99208 +3.59524 -1.01807
H -0.90413 +4.63995 -0.75075
C -0.03641 +2.69466 -0.57610
H +0.79216 +3.01706 +0.03766
Fe +1.10007 -0.11458 -0.23259
N -0.15765 -0.22688 +1.23051
S -1.27736 -1.13116 +2.00186
O -1.04706 -2.55921 +1.72008
O -1.32592 -0.70852 +3.41311
C -2.86442 -0.70098 +1.26681
C -3.22610 +0.64403 +1.16198
C -3.70298 -1.70656 +0.79685
C -4.43729 +0.97357 +0.57027
H -2.56783 +1.42907 +1.51567
C -4.91670 -1.35665 +0.20613
H -3.40529 -2.74428 +0.87646
C -5.30022 -0.01834 +0.07963
H -4.71463 +2.01777 +0.47463
H -5.56973 -2.13860 -0.16558
C -6.60332 +0.36576 -0.57055
H -7.23413 +0.92750 +0.12531
H -6.42950 +1.00977 -1.43826
H -7.15937 -0.51271 -0.90268
H -0.30953 +0.72198 +1.56991

1NHTs(III)q
E = -3153.239081
G = -3152.701961
2,4
N +2.39600 +1.18242 +0.72919

N +2.27916 -0.14354 -1.63381
N +1.98371 -2.02092 +0.44953
N -0.04739 -1.70684 -1.57803
N -0.50462 +0.90910 -0.95591
C +2.63044 +1.51944 +2.00657
H +1.97155 +1.07779 +2.74291
C +3.66352 +2.37426 +2.36402
H +3.82184 +2.62301 +3.40536
C +4.48378 +2.88577 +1.36136
H +5.30516 +3.54803 +1.60775
C +4.24608 +2.52671 +0.03734
H +4.87034 +2.89377 -0.76734
C +3.18716 +1.67286 -0.24205
C +2.80889 +1.25062 -1.63325
H +3.65212 +1.33308 -2.32186
H +2.01468 +1.90972 -1.98984
C +3.38895 -1.14628 -1.40896
H +4.35009 -0.67316 -1.61210
H +3.27068 -1.95122 -2.12901
C +3.37535 -1.69183 +0.00788
H +4.00216 -2.58651 +0.07028
H +3.76479 -0.95810 +0.70940
C +2.00625 -2.29811 +1.91070
H +2.73760 -3.08493 +2.11889
H +1.01751 -2.61194 +2.22824
H +2.27986 -1.38873 +2.44129
C +1.43496 -3.21824 -0.29681
H +1.42344 -4.07606 +0.37634
H +2.11789 -3.46297 -1.10706
C +0.02392 -2.98190 -0.82298
H -0.28131 -3.83384 -1.44052
H -0.66315 -2.89382 +0.01873
C +0.74144 -1.68316 -2.83755
H +0.07645 -1.73237 -3.70243
H +1.37722 -2.56426 -2.88068
C +1.57231 -0.40723 -2.92462
H +2.30106 -0.47832 -3.73678
H +0.92842 +0.44727 -3.12049
C -1.41899 -1.19848 -1.76564
H -2.03858 -1.56977 -0.94844
H -1.85997 -1.55293 -2.70070
C -1.45358 +0.30875 -1.70409
C -2.44265 +1.05625 -2.33236
H -3.18632 +0.54915 -2.93361
C -2.46115 +2.43547 -2.17020
H -3.22822 +3.03076 -2.65038
C -1.48696 +3.04147 -1.38011
H -1.46721 +4.11150 -1.22229
C -0.52400 +2.24422 -0.78733
H +0.25736 +2.65730 -0.16253
Fe +0.87249 -0.28480 -0.03058
N -0.05418 -0.02944 +1.65143
S -1.29788 -0.75019 +2.44970
O -1.16968 -2.20909 +2.30824
O -1.35228 -0.17718 +3.80428
C -2.80040 -0.26427 +1.58903
C -3.09541 +1.09281 +1.44405
C -3.64248 -1.24044 +1.06773
C -4.23915 +1.46384 +0.75172
H -2.43879 +1.85303 +1.85031
C -4.78812 -0.84918 +0.37573
H -3.40106 -2.28851 +1.18970
C -5.10022 +0.50208 +0.20122
H -4.46421 +2.51678 +0.62333
H -5.44250 -1.60855 -0.03805
C -6.30897 +0.93052 -0.58784
H -6.86345 +1.71529 -0.06613
H -6.00529 +1.34074 -1.55724
H -6.98450 +0.09346 -0.77394
H -0.15990 +0.97509 +1.80849

1NHTs(III)sext

E = -3153.25003
G = -3152.71604
2,6
N +2.36079 +0.98303 +1.07921
N +2.46554 +0.42684 -1.55271
N +2.17346 -2.05431 -0.12260
N +0.16585 -1.15264 -1.92718
N -0.41633 +1.22280 -0.76234
C +2.50733 +0.93278 +2.41735
H +1.84842 +0.25631 +2.94332
C +3.45543 +1.68989 +3.08524
H +3.53810 +1.61729 +4.16184
C +4.28915 +2.52307 +2.34346
H +5.04436 +3.12494 +2.83482
C +4.15303 +2.55925 +0.96007
H +4.79699 +3.17679 +0.34707
C +3.17886 +1.77376 +0.35682
C +2.94622 +1.75967 -1.12698
H +3.85037 +2.05125 -1.66805
H +2.16892 +2.49117 -1.35856
C +3.57720 -0.58545 -1.58308
H +4.54153 -0.07427 -1.59651
H +3.50414 -1.14055 -2.51576
C +3.54635 -1.54284 -0.39392
H +4.22506 -2.38052 -0.58424
H +3.88177 -1.03966 +0.51121
C +2.13123 -2.73056 +1.19967
H +2.82791 -3.57460 +1.21237
H +1.11699 -3.07742 +1.38720
H +2.40778 -2.01720 +1.97482
C +1.67539 -2.97382 -1.20081
H +1.68489 -4.00201 -0.83620
H +2.35939 -2.93314 -2.04541
C +0.25752 -2.60581 -1.61935

H -0.05502 -3.21079 -2.47662
H -0.42336 -2.79506 -0.78701
C +0.95582 -0.74431 -3.12759
H +0.28171 -0.56748 -3.96785
H +1.60409 -1.56850 -3.41376
C +1.77259 +0.51514 -2.86431
H +2.49437 +0.66305 -3.67435
H +1.12334 +1.38719 -2.83407
C -1.23574 -0.68160 -1.99752
H -1.81462 -1.23294 -1.25488
H -1.67314 -0.88164 -2.97873
C -1.32795 +0.78035 -1.64747
C -2.32306 +1.61619 -2.13854
H -3.03890 +1.23448 -2.85496
C -2.38205 +2.92962 -1.68542
H -3.15251 +3.59763 -2.05102
C -1.44591 +3.37422 -0.75405
H -1.46280 +4.38676 -0.37295
C -0.47571 +2.48770 -0.31458
H +0.27711 +2.77501 +0.40871
Fe +0.93135 -0.27657 -0.00206
N -0.14499 -0.37414 +1.66489
S -1.39076 -1.30112 +2.18162
O -1.21129 -2.65676 +1.63299
O -1.54068 -1.15410 +3.63938
C -2.85169 -0.59683 +1.40050
C -3.13475 +0.75807 +1.58781
C -3.66034 -1.39241 +0.59739
C -4.23553 +1.31243 +0.95115
H -2.49759 +1.37842 +2.20709
C -4.76168 -0.81778 -0.03749
H -3.42364 -2.43935 +0.45698
C -5.06361 +0.53704 +0.12426
H -4.45053 +2.36732 +1.08255
H -5.38811 -1.43472 -0.67239
C -6.23330 +1.17109 -0.58165
H -6.91687 +1.63586 +0.13509
H -5.89196 +1.96014 -1.25943
H -6.79357 +0.43924 -1.16621
H -0.18337 +0.50772 +2.17616

1NTs(IV)t
E = -3152.594317
G = -3152.067744
2,3
N -1.31773 +1.21928 -0.69761
N -2.00360 -0.73890 +0.94259
N -1.46363 -1.63510 -1.62611
N +0.23095 -2.25430 +0.48521
N +0.75504 +0.26193 +1.17272
C -1.07629 +2.02522 -1.74760
H -0.27410 +1.73129 -2.40631
C -1.80975 +3.18091 -1.96762
H -1.57900 +3.79951 -2.82502
C -2.83010 +3.51435 -1.08272
H -3.42558 +4.40623 -1.23635
C -3.07974 +2.68194 +0.00330
H -3.86533 +2.89990 +0.71522
C -2.30199 +1.54639 +0.17363
C -2.43797 +0.62498 +1.34815
H -3.45591 +0.61254 +1.73971
H -1.78077 +0.97310 +2.14695
C -3.11273 -1.45117 +0.19608
H -4.06968 -1.00233 +0.46096
H -3.14097 -2.48351 +0.53426
C -2.89661 -1.37579 -1.30299
H -3.53694 -2.10007 -1.81436
H -3.13624 -0.38493 -1.68363
C -1.22141 -1.28315 -3.05139
H -1.91065 -1.84865 -3.68472
H -0.19437 -1.52541 -3.31093
H -1.38454 -0.21829 -3.19714
C -1.09404 -3.08759 -1.40203
H -1.02680 -3.59620 -2.36365
H -1.89318 -3.57080 -0.84563
C +0.23342 -3.20457 -0.66916
H +0.39629 -4.22861 -0.32343
H +1.05261 -2.91305 -1.32255
C -0.70704 -2.71210 +1.58496
H -0.12541 -3.15486 +2.39275
H -1.34397 -3.49498 +1.18349
C -1.53493 -1.54890 +2.10751
H -2.38570 -1.91052 +2.68989
H -0.93785 -0.90206 +2.74491
C +1.58983 -1.99915 +1.03615
H +2.29408 -1.97956 +0.20462
H +1.89150 -2.79177 +1.72148
C +1.60643 -0.65078 +1.69760
C +2.46382 -0.32573 +2.73807
H +3.12345 -1.08330 +3.14044
C +2.45916 +0.97170 +3.23835
H +3.11921 +1.24609 +4.05205
C +1.60834 +1.91328 +2.66866
H +1.58788 +2.93951 +3.01046
C +0.77476 +1.52401 +1.63307
H +0.11113 +2.22880 +1.15482
Fe -0.37056 -0.50714 -0.29533
N +0.94540 -0.34411 -1.41011
S +2.22468 +0.22649 -2.19674
O +2.67557 -0.82623 -3.12361
O +1.90933 +1.54661 -2.77699
C +3.50068 +0.46968 -0.96770
C +3.57639 +1.68929 -0.29513
C +4.38822 -0.56805 -0.68329
C +4.55601 +1.86343 +0.67367
H +2.88509 +2.48776 -0.53143

C +5.35961 -0.37551 +0.29317
H +4.32590 -1.50469 -1.22290
C +5.45532 +0.83599 +0.98938
H +4.61889 +2.80896 +1.20057
H +6.05430 -1.17770 +0.51603
C +6.47395 +1.02388 +2.08129
H +6.88407 +2.03673 +2.07176
H +6.00830 +0.87132 +3.06148
H +7.29643 +0.31165 +1.99046

1NTs(IV)q
E = -3152.58198
G = -3152.059548
2,5
N +2.20890 +0.99733 -1.29404
N +2.51488 -1.44012 -0.23346
N +2.10708 +0.39914 +1.89786
N +0.20911 -1.63272 +1.33140
N -0.31641 -0.99304 -1.25108
C +2.18685 +2.32347 -1.51882
H +1.45482 +2.89238 -0.96574
C +3.06849 +2.92836 -2.39871
H +3.02040 +3.99786 -2.55492
C +4.00624 +2.13737 -3.05890
H +4.71207 +2.58362 -3.74899
C +4.03854 +0.76779 -2.81375
H +4.76187 +0.12320 -3.29597
C +3.12240 +0.22648 -1.92389
C +3.02773 -1.24085 -1.62164
H +3.98666 -1.74422 -1.75315
H +2.31819 -1.69228 -2.31790
C +3.61778 -1.22724 +0.78762
H +4.58339 -1.30098 +0.28779
H +3.56653 -2.04213 +1.50457
C +3.51092 +0.11779 +1.48874
H +4.17382 +0.13074 +2.36002
H +3.81663 +0.92369 +0.82289
C +1.96777 +1.82236 +2.29047
H +2.64770 +2.04969 +3.11752
H +0.93934 +2.00708 +2.59354
H +2.19995 +2.45780 +1.43744
C +1.62721 -0.49568 +3.00254
H +1.59114 +0.06685 +3.93657
H +2.34510 -1.29992 +3.14863
C +0.23932 -1.05255 +2.69922
H -0.03537 -1.80090 +3.44894
H -0.49547 -0.24804 +2.71887
C +1.06479 -2.85807 +1.19012
H +0.43416 -3.74847 +1.16325
H +1.69703 -2.94547 +2.06956
C +1.90600 -2.79964 -0.07973
H +2.69357 -3.55741 -0.05247
H +1.29179 -2.98555 -0.95705
C -1.16256 -1.87177 +0.83689
H -1.80117 -1.06153 +1.19445
H -1.56473 -2.81355 +1.21681
C -1.18491 -1.84269 -0.66930
C -2.07952 -2.58527 -1.42752
H -2.75745 -3.26876 -0.93285
C -2.09578 -2.41846 -2.80788
H -2.78828 -2.98595 -3.41765
C -1.21930 -1.50916 -3.39500
H -1.20619 -1.34216 -4.46390
C -0.34101 -0.81138 -2.58119
H +0.36305 -0.09591 -2.98250
Fe +1.00340 -0.01898 +0.07864
N -0.16877 +1.20354 +0.36572
S -1.31545 +2.09440 -0.38847
O -1.31568 +3.40483 +0.28133
O -1.13990 +2.06954 -1.84949
C -2.83125 +1.24715 +0.02186
C -3.48164 +0.48864 -0.94526
C -3.30248 +1.31233 +1.33614
C -4.62914 -0.21471 -0.58768
H -3.09309 +0.44115 -1.95433
C -4.44432 +0.60068 +1.67343
H -2.78434 +1.90771 +2.07775
C -5.12270 -0.17709 +0.72030
H -5.14023 -0.80902 -1.33658
H -4.81898 +0.64608 +2.69021
C -6.34074 -0.96823 +1.11608
H -6.88437 -1.33201 +0.24234
H -6.05227 -1.83631 +1.71848
H -7.02080 -0.36586 +1.72418

2NTs(III)d
E = -3152.743342
G = -3152.215807
1,2
N +1.71143 -1.02733 -2.17484
C +3.08646 -1.58132 -1.96367
C +3.16794 -2.25802 -0.61652
N +2.64999 -1.38726 +0.48098
C +3.58378 -0.29373 +0.91308
C +3.57888 +0.94649 +0.00589
N +2.26742 +1.14601 -0.70680
C +1.79398 +0.21349 -2.99211
C +2.46034 +1.34222 -2.19212
C +1.40196 +2.22619 -0.12307
C +0.08130 +2.14074 -0.86443
C +1.11346 +1.85488 +1.31032
N +0.75006 +0.56099 +1.44899
C +0.41385 +0.11126 +2.66813
C +0.43665 +0.93953 +3.78444
C +0.82266 +2.26772 +3.64166
C +1.16663 +2.73732 +2.37574

N -0.31967 +0.86558 -1.05130
C -1.45210 +0.62688 -1.72416
C -2.24791 +1.65877 -2.20384
C -1.85083 +2.97487 -1.98674
C -0.65780 +3.22322 -1.30990
Fe +0.99941 -0.43574 -0.29304
C +0.86558 -2.02224 -2.87077
C +2.42359 -2.28008 +1.64897
H +3.81366 -0.77785 -2.03554
H +3.32680 -2.29370 -2.75714
H +4.19533 -2.56818 -0.40033
H +2.53264 -3.14309 -0.61941
H +4.60288 -0.68465 +0.99133
H +3.26458 -0.00623 +1.91153
H +4.35559 +0.85889 -0.74673
H +3.81505 +1.82840 +0.60424
H +0.78103 +0.48729 -3.27414
H +2.35728 +0.02270 -3.91180
H +2.04438 +2.30126 -2.49828
H +3.52651 +1.38673 -2.39626
H +1.85558 +3.21439 -0.20666
H +0.09466 -0.92140 +2.72571
H +0.15144 +0.53654 +4.74771
H +0.85624 +2.92949 +4.49876
H +1.47377 +3.76187 +2.21085
H -1.70673 -0.41054 -1.86928
H -3.16111 +1.42484 -2.73390
H -2.45362 +3.79833 -2.35017
H -0.29702 +4.22933 -1.14017
H +0.82130 -2.93102 -2.27643
H -0.14418 -1.63023 -2.96780
H +1.27474 -2.23637 -3.86397
H +1.61041 -2.95957 +1.41108
H +3.34037 -2.83400 +1.87611
H +2.14916 -1.69508 +2.52104
N -0.07957 -1.90290 -0.07637
S -1.36543 -2.35502 +0.69330
O -1.14779 -2.47324 +2.17424
O -1.92134 -3.59634 +0.08072
C -2.73064 -1.15242 +0.54353
C -2.74130 +0.01176 +1.31232
C -3.73452 -1.36093 -0.40206
C -3.73359 +0.96685 +1.11690
H -1.98377 +0.17697 +2.06480
C -4.72688 -0.40073 -0.58837
H -3.72869 -2.26903 -0.99173
C -4.73871 +0.78243 +0.15875
H -3.72432 +1.87329 +1.71378
H -5.49830 -0.56909 -1.33303
C -5.81292 +1.82035 -0.04234
H -6.24735 +1.75500 -1.04255
H -6.62572 +1.68502 +0.68004
H -5.41846 +2.83001 +0.09812

2NTs(III)q
E = -3152.749719
G = -3152.227756
1,4
N +2.20680 -1.40374 -1.82703
C +3.56480 -1.64524 -1.28205
C +3.48925 -1.94740 +0.20742
N +2.69824 -0.93989 +0.98198
C +3.40777 +0.36394 +1.21700
C +3.38997 +1.33259 +0.02635
N +2.18051 +1.16243 -0.85674
C +2.18841 -0.37400 -2.87625
C +2.57374 +0.99875 -2.30829
C +1.15998 +2.25927 -0.73415
C -0.07503 +1.76328 -1.46408
C +0.79572 +2.47818 +0.71981
N +0.53716 +1.35019 +1.39579
C +0.16282 +1.44269 +2.67838
C +0.03425 +2.66733 +3.32793
C +0.30887 +3.83529 +2.62245
C +0.69882 +3.74216 +1.28827
N -0.31793 +0.44601 -1.28929
C -1.36202 -0.12348 -1.90651
C -2.22751 +0.61212 -2.70363
C -1.99867 +1.97542 -2.86583
C -0.89931 +2.56109 -2.24104
Fe +1.02612 -0.48876 -0.11418
C +1.57942 -2.64851 -2.29824
C +2.39383 -1.52783 +2.31317
H +4.19167 -0.77723 -1.46744
H +4.04455 -2.48826 -1.79122
H +4.49432 -2.03124 +0.63271
H +2.97563 -2.89768 +0.34969
H +4.44317 +0.16340 +1.50918
H +2.90655 +0.82341 +2.06322
H +4.27384 +1.18524 -0.58602
H +3.43530 +2.35564 +0.40371
H +1.17568 -0.34307 -3.27530
H +2.86607 -0.62281 -3.70337
H +2.09884 +1.77603 -2.90596
H +3.64558 +1.15962 -2.38444
H +1.52864 +3.18615 -1.17687
H -0.05560 +0.50422 +3.17257
H -0.27487 +2.69652 +4.36523
H +0.22384 +4.80349 +3.10171
H +0.92553 +4.62220 +0.69969
H -1.48467 -1.18199 -1.73370
H -3.06408 +0.11922 -3.18019
H -2.65985 +2.57474 -3.48006
H -0.67278 +3.61291 -2.35871
H +1.58754 -3.38555 -1.49675
H +0.54111 -2.44728 -2.56190

H +2.10705 -3.05387 -3.17165
H +1.89776 -2.48278 +2.16956
H +3.32010 -1.66522 +2.88131
H +1.71758 -0.87250 +2.85233
N -0.00256 -1.85775 +0.36748
S -1.12208 -2.10722 +1.45250
O -0.84762 -1.49077 +2.78151
O -1.45336 -3.55514 +1.50617
C -2.61462 -1.28365 +0.84298
C -2.82561 +0.06653 +1.12212
C -3.49904 -1.97516 +0.01921
C -3.91748 +0.72184 +0.56521
H -2.14216 +0.59843 +1.76879
C -4.59155 -1.30784 -0.53236
H -3.33286 -3.02543 -0.18698
C -4.81340 +0.04979 -0.27789
H -4.07531 +1.77345 +0.78244
H -5.27805 -1.85061 -1.17371
C -5.96978 +0.78646 -0.90326
H -6.63772 +0.10638 -1.43551
H -6.55343 +1.32045 -0.14764
H -5.61002 +1.53363 -1.61877

2NTs(III)sext
E = -3152.762106
G = -3152.242067
1,6
N +2.15601 -1.47218 -1.67598
C +3.56522 -1.64253 -1.22307
C +3.63880 -1.81727 +0.28620
N +2.89180 -0.77267 +1.04201
C +3.55696 +0.55833 +1.09908
C +3.47048 +1.38983 -0.19309
N +2.20980 +1.19136 -0.97101
C +2.05869 -0.53113 -2.81619
C +2.47194 +0.89983 -2.41669
C +1.21516 +2.27913 -0.78637
C -0.06026 +1.87744 -1.51461
C +0.85483 +2.38392 +0.68559
N +0.57237 +1.20406 +1.26515
C +0.15760 +1.17565 +2.53833
C +0.02642 +2.33829 +3.29050
C +0.33731 +3.55911 +2.69966
C +0.75556 +3.58602 +1.36979
N -0.40579 +0.58866 -1.34674
C -1.52171 +0.12446 -1.92034
C -2.34737 +0.93793 -2.68680
C -1.99823 +2.27475 -2.85386
C -0.83252 +2.75616 -2.25895
Fe +0.96562 -0.55346 -0.03416
C +1.54639 -2.77397 -2.02164
C +2.69547 -1.26529 +2.42701
H +4.15006 -0.78480 -1.54039
H +4.00948 -2.51754 -1.70705
H +4.68615 -1.84254 +0.60853
H +3.18004 -2.77035 +0.55250
H +4.61310 +0.43698 +1.36720
H +3.07575 +1.10020 +1.90997
H +4.30522 +1.13966 -0.84101
H +3.59075 +2.44377 +0.07216
H +1.02239 -0.54521 -3.14886
H +2.68332 -0.87240 -3.65025
H +1.93111 +1.60401 -3.04923
H +3.52923 +1.06007 -2.61786
H +1.58004 +3.23978 -1.15882
H -0.08261 +0.19725 +2.93913
H -0.31262 +2.27918 +4.31682
H +0.25300 +4.48076 +3.26325
H +0.99878 +4.51527 +0.87055
H -1.74637 -0.91867 -1.74674
H -3.24447 +0.52807 -3.13119
H -2.62176 +2.93627 -3.44355
H -0.52227 +3.78719 -2.37159
H +1.62559 -3.44367 -1.16653
H +0.48990 -2.62591 -2.24393
H +2.04532 -3.22446 -2.88773
H +2.11269 -2.18369 +2.39789
H +3.66022 -1.45180 +2.91350
H +2.14660 -0.52576 +3.00535
N -0.12211 -1.80904 +0.68537
S -1.33056 -2.25066 +1.57577
O -1.21416 -1.75351 +2.97946
O -1.62302 -3.70452 +1.46794
C -2.76550 -1.39588 +0.87742
C -2.98721 -0.05475 +1.19535
C -3.57580 -2.03728 -0.05489
C -4.01029 +0.64158 +0.56445
H -2.36799 +0.43862 +1.93258
C -4.60133 -1.32771 -0.68031
H -3.40197 -3.07988 -0.29128
C -4.82706 +0.02154 -0.39205
H -4.17252 +1.68666 +0.80804
H -5.22593 -1.82935 -1.41192
C -5.91170 +0.80308 -1.08786
H -6.37581 +0.22156 -1.88700
H -6.69711 +1.09628 -0.38330
H -5.51127 +1.72373 -1.52280

2NHTs(III)d
E = -3153.236299
G = -3152.694389
2,2
N +2.13395 -0.65679 -1.81686
C +3.49895 -1.15656 -1.43734
C +3.39732 -1.99516 -0.18961
N +2.61335 -1.29649 +0.88016

C +3.37504 -0.22115 +1.61287
C +3.45027 +1.11403 +0.86485
N +2.26308 +1.33898 -0.04543
C +2.26229 +0.68146 -2.46753
C +2.69992 +1.73200 -1.44341
C +1.25169 +2.31721 +0.49439
C +0.09084 +2.26841 -0.47550
C +0.74404 +1.76681 +1.80019
N +0.45592 +0.44765 +1.73299
C -0.05283 -0.15377 +2.82001
C -0.29013 +0.54069 +3.99967
C +0.01624 +1.89462 +4.06743
C +0.54476 +2.52230 +2.94175
N -0.17603 +1.00867 -0.87852
C -1.14352 +0.79493 -1.77918
C -1.91243 +1.83715 -2.27812
C -1.66070 +3.13342 -1.83982
C -0.63211 +3.35789 -0.92602
Fe +1.08964 -0.31821 -0.05077
C +1.50848 -1.59585 -2.78475
C +2.25246 -2.34167 +1.88151
H +4.16340 -0.31187 -1.28680
H +3.91601 -1.74442 -2.25731
H +4.38819 -2.25986 +0.18821
H +2.85549 -2.91478 -0.41132
H +4.38477 -0.57792 +1.83099
H +2.86107 -0.08055 +2.55943
H +4.34574 +1.15261 +0.25479
H +3.51756 +1.92951 +1.58584
H +1.29737 +0.93189 -2.89792
H +2.98889 +0.62362 -3.28303
H +2.27432 +2.69923 -1.70396
H +3.77871 +1.85409 -1.44060
H +1.66740 +3.31867 +0.59828
H -0.29489 -1.20078 +2.72478
H -0.70915 +0.01292 +4.84640
H -0.15070 +2.45502 +4.97920
H +0.80308 +3.57305 +2.94134
H -1.28519 -0.22597 -2.09470
H -2.69297 +1.62516 -2.99566
H -2.24679 +3.96336 -2.21513
H -0.38162 +4.35195 -0.57991
H +1.54552 -2.61090 -2.39293
H +0.47302 -1.31128 -2.95140
H +2.05687 -1.56542 -3.72995
H +1.60574 -3.07919 +1.41607
H +3.16650 -2.82287 +2.24076
H +1.74077 -1.89626 +2.72739
N -0.00909 -1.85344 -0.23330
S -1.42394 -2.49004 +0.32122
O -1.41131 -2.64717 +1.78941
O -1.67983 -3.70658 -0.47195
C -2.71486 -1.30213 -0.04795
C -2.94807 -0.22978 +0.81213
C -3.47261 -1.47069 -1.20483
C -3.93000 +0.69738 +0.48687
H -2.37947 -0.11637 +1.72397
C -4.45897 -0.53753 -1.51011
H -3.29058 -2.31545 -1.85700
C -4.69448 +0.56463 -0.68007
H -4.10622 +1.53759 +1.14963
H -5.04918 -0.66483 -2.41081
C -5.72047 +1.60519 -1.04113
H -6.40792 +1.24228 -1.80747
H -6.30121 +1.90877 -0.16628
H -5.22806 +2.50326 -1.43030
H +0.44995 -2.63111 -0.70409

2NHTs(III)q

E = -3153.22501
G = -3152.689552
2,4
N +2.07507 -1.08412 -2.10878
C +3.44219 -1.48285 -1.67196
C +3.38227 -2.07449 -0.27774
N +2.67283 -1.18315 +0.70335
C +3.47234 +0.01804 +1.15770
C +3.47639 +1.19663 +0.17704
N +2.23206 +1.25358 -0.67532
C +2.09062 +0.12821 -2.94818
C +2.56673 +1.34794 -2.14859
C +1.26580 +2.34583 -0.30670
C -0.00267 +2.04398 -1.07977
C +0.94197 +2.27900 +1.16950
N +0.64980 +1.04530 +1.60500
C +0.29387 +0.87904 +2.88595
C +0.22038 +1.94725 +3.77433
C +0.53348 +3.22484 +3.32017
C +0.90318 +3.39794 +1.98821
N -0.29461 +0.72397 -1.15238
C -1.37049 +0.31354 -1.84050
C -2.22219 +1.21791 -2.45679
C -1.94420 +2.57758 -2.36500
C -0.81041 +2.99844 -1.67267
Fe +1.01780 -0.45557 -0.19448
C +1.39530 -2.18739 -2.81802
C +2.36548 -1.99814 +1.91451
H +4.10012 -0.61917 -1.69823
H +3.86542 -2.21990 -2.36040
H +4.38420 -2.29159 +0.10106
H +2.81060 -3.00117 -0.30141
H +4.49713 -0.30584 +1.35483
H +3.03025 +0.32691 +2.09923
H +4.33273 +1.13081 -0.48557
H +3.58002 +2.12499 +0.74036
H +1.07671 +0.28215 -3.31238

H +2.74291 -0.00440 -3.81885
H +2.11307 +2.24501 -2.56665
H +3.64188 +1.46974 -2.23703
H +1.66897 +3.32413 -0.56961
H +0.05121 -0.13049 +3.18841
H -0.07628 +1.77139 +4.80030
H +0.49255 +4.07473 +3.99081
H +1.15651 +4.37137 +1.58829
H -1.53535 -0.75145 -1.88474
H -3.08676 +0.85135 -2.99286
H -2.59442 +3.30390 -2.83703
H -0.54351 +4.04457 -1.60049
H +1.43108 -3.09205 -2.21157
H +0.35459 -1.91344 -2.99592
H +1.88321 -2.38909 -3.77818
H +1.81503 -2.88374 +1.61433
H +3.30323 -2.28106 +2.40077
H +1.75523 -1.41867 +2.59887
N -0.11086 -2.01285 -0.02505
S -1.28953 -2.41466 +1.04927
O -0.84153 -2.01301 +2.38972
O -1.66393 -3.81746 +0.81730
C -2.70258 -1.38989 +0.62971
C -2.80363 -0.10972 +1.17458
C -3.62247 -1.84272 -0.31254
C -3.83554 +0.72247 +0.76160
H -2.08717 +0.23091 +1.90865
C -4.65222 -0.99507 -0.71378
H -3.53738 -2.83938 -0.72756
C -4.76945 +0.29897 -0.19445
H -3.91267 +1.72007 +1.18044
H -5.37043 -1.34386 -1.44746
C -5.85566 +1.23260 -0.65885
H -6.54713 +0.73573 -1.34153
H -6.42662 +1.62266 +0.18878
H -5.42337 +2.09394 -1.17853
H -0.23152 -2.58193 -0.86130

2NHTs(III)sext
E = -3153.237014
G = -3152.706353
2,6
N +2.08536 -1.13369 -2.01376
C +3.49181 -1.45721 -1.62161
C +3.55079 -1.97851 -0.19832
N +2.85428 -1.09190 +0.78261
C +3.58214 +0.16376 +1.13289
C +3.50542 +1.27534 +0.07150
N +2.24181 +1.26958 -0.73966
C +2.02824 +0.03672 -2.92251
C +2.51611 +1.30842 -2.21721
C +1.27485 +2.33549 -0.35313
C -0.00925 +2.08896 -1.12804
C +0.93907 +2.18874 +1.11323
N +0.67631 +0.92415 +1.48945
C +0.29911 +0.68210 +2.75451
C +0.17950 +1.70164 +3.69092
C +0.46247 +3.00772 +3.30470
C +0.84858 +3.25798 +1.98960
N -0.37246 +0.79398 -1.18249
C -1.49117 +0.44295 -1.83201
C -2.30393 +1.38628 -2.44508
C -1.94105 +2.72791 -2.37695
C -0.77146 +3.08873 -1.70899
Fe +0.96513 -0.57119 -0.15356
C +1.44014 -2.30479 -2.65360
C +2.61881 -1.88340 +2.02052
H +4.11121 -0.57452 -1.74020
H +3.89506 -2.21443 -2.29864
H +4.59132 -2.12357 +0.10833
H +3.04126 -2.94119 -0.15058
H +4.63364 -0.06806 +1.32896
H +3.14471 +0.51665 +2.06264
H +4.34012 +1.17968 -0.61510
H +3.62387 +2.23811 +0.57285
H +0.99353 +0.14378 -3.24085
H +2.63779 -0.15168 -3.81281
H +2.02666 +2.17109 -2.66878
H +3.58360 +1.44801 -2.36745
H +1.66697 +3.33260 -0.56244
H +0.07915 -0.34830 +2.99738
H -0.13092 +1.46594 +4.70044
H +0.38403 +3.82229 +4.01471
H +1.07589 +4.25785 +1.64358
H -1.72088 -0.61252 -1.85271
H -3.20236 +1.06856 -2.95657
H -2.55638 +3.48702 -2.84470
H -0.44862 +4.11983 -1.64663
H +1.49898 -3.16195 -1.98380
H +0.39468 -2.07129 -2.85624
H +1.94315 -2.54798 -3.59472
H +1.97310 -2.72730 +1.78559
H +3.57075 -2.24468 +2.42307
H +2.13117 -1.26327 +2.76686
N -0.27819 -2.11517 -0.02228
S -1.44876 -2.51586 +1.05719
O -0.97551 -2.14745 +2.40024
O -1.87368 -3.90305 +0.81616
C -2.82532 -1.43719 +0.64865
C -2.89513 -0.16573 +1.21784
C -3.72909 -1.83217 -0.33468
C -3.87593 +0.71678 +0.78453
H -2.19570 +0.13103 +1.98690
C -4.70652 -0.93419 -0.75705
H -3.66724 -2.82238 -0.76892
C -4.78746 +0.35395 -0.21689

H -3.92845 +1.70830 +1.22124
H -5.40791 -1.23692 -1.52660
C -5.80596 +1.34719 -0.70879
H -6.48520 +0.90056 -1.43711
H -6.39997 +1.74437 +0.11953
H -5.30803 +2.19866 -1.18417
H -0.43839 -2.66206 -0.86670

2NTs(IV)t
E = -3152.578261
G = -3152.050469
2,3
N -1.83127 -1.46875 -0.21646
C -3.00946 -0.86783 +0.49615
C -3.28572 +0.51103 -0.04865
N -2.03935 +1.34205 -0.10876
C -1.59367 +1.91850 +1.20919
C -0.85247 +0.92315 +2.10168
N -0.11109 -0.11949 +1.29755
C -1.08430 -2.36062 +0.71727
C -0.39567 -1.52377 +1.79972
C +1.37077 +0.12198 +1.20383
C +1.89506 -0.93205 +0.24857
C +1.58324 +1.43798 +0.49855
N +0.79589 +1.56739 -0.59278
C +0.97422 +2.61518 -1.41007
C +1.92997 +3.58759 -1.14130
C +2.71234 +3.47729 +0.00244
C +2.54116 +2.37504 +0.83852
N +1.07524 -1.10829 -0.81015
C +1.41722 -1.96996 -1.77615
C +2.60562 -2.68639 -1.71882
C +3.45191 -2.50806 -0.62945
C +3.09031 -1.61434 +0.37842
Fe -0.55877 +0.07616 -0.68909
C -2.29180 -2.24924 -1.39489
C -2.34012 +2.49264 -1.00923
H -2.80253 -0.83270 +1.56079
H -3.88267 -1.50924 +0.36206
H -4.04322 +1.02406 +0.54913
H -3.64353 +0.43307 -1.07442
H -2.46106 +2.31894 +1.73962
H -0.93821 +2.75033 +0.96564
H -1.54997 +0.40637 +2.75185
H -0.15053 +1.45971 +2.74123
H -0.35960 -2.91730 +0.13067
H -1.77493 -3.07655 +1.17146
H +0.53411 -2.00203 +2.10153
H -1.01261 -1.44463 +2.68986
H +1.85343 +0.08396 +2.17968
H +0.34508 +2.66409 -2.28708
H +2.04644 +4.41647 -1.82702
H +3.45365 +4.23101 +0.23829
H +3.13948 +2.23331 +1.72875
H +0.72184 -2.07846 -2.59295
H +2.85427 -3.36544 -2.52343
H +4.38274 -3.05773 -0.56088
H +3.71473 -1.44745 +1.24620
H -2.88274 -1.60567 -2.04133
H -1.42890 -2.60826 -1.94980
H -2.89366 -3.09778 -1.05771
H -2.61370 +2.12163 -1.99131
H -3.16972 +3.06659 -0.58670
H -1.47348 +3.14005 -1.09393
N -0.91811 +0.12604 -2.37405
S -0.90220 +0.55167 -3.92712
O -0.68888 +2.00690 -4.06121
O -2.09792 -0.00983 -4.57506
C +0.53952 -0.28745 -4.56418
C +1.80257 +0.26039 -4.33544
C +0.38980 -1.53796 -5.16135
C +2.92627 -0.46416 -4.71156
H +1.90690 +1.23099 -3.86726
C +1.52753 -2.24745 -5.53149
H -0.59802 -1.95049 -5.32305
C +2.80882 -1.72930 -5.30445
H +3.91158 -0.04908 -4.53011
H +1.41870 -3.22314 -5.99200
C +4.03603 -2.50589 -5.69973
H +3.83663 -3.57919 -5.72472
H +4.37230 -2.20821 -6.69912
H +4.86095 -2.31873 -5.00840

2NTs(IV)q
E = -3152.563488
G = -3152.040315
2,5
N +1.73414 -1.05470 -2.28491
C +3.08187 -1.63633 -2.02748
C +3.11041 -2.33982 -0.68223
N +2.59576 -1.49432 +0.44465
C +3.53548 -0.41851 +0.91133
C +3.56847 +0.82064 +0.01337
N +2.25575 +1.08184 -0.69917
C +1.81928 +0.21654 -3.03962
C +2.47492 +1.30881 -2.18738
C +1.47172 +2.23227 -0.11770
C +0.13039 +2.22633 -0.82442
C +1.21301 +1.95759 +1.34509
N +0.80075 +0.69892 +1.58345
C +0.46613 +0.34974 +2.83326
C +0.54210 +1.24995 +3.89029
C +0.98261 +2.54575 +3.64392
C +1.32404 +2.91175 +2.34272
N -0.35031 +0.98242 -1.04240

C -1.52618 +0.81630 -1.66304
C -2.28790 +1.90363 -2.06709
C -1.81024 +3.18772 -1.82382
C -0.57501 +3.35555 -1.19764
Fe +0.92445 -0.47872 -0.32071
C +0.85286 -2.01755 -2.98255
C +2.32663 -2.40417 +1.59247
H +3.83007 -0.85088 -2.07173
H +3.33372 -2.35482 -2.81200
H +4.12617 -2.67011 -0.44782
H +2.46134 -3.21347 -0.72058
H +4.54355 -0.83415 +0.99584
H +3.20599 -0.14073 +1.90838
H +4.33592 +0.71683 -0.74503
H +3.83159 +1.69129 +0.61508
H +0.80446 +0.50069 -3.30876
H +2.38774 +0.07701 -3.96497
H +2.06598 +2.27733 -2.46845
H +3.54575 +1.35668 -2.36150
H +2.00120 +3.17417 -0.26202
H +0.12495 -0.66665 +2.97424
H +0.26095 +0.92937 +4.88500
H +1.06004 +3.26447 +4.45089
H +1.66739 +3.90959 +2.10300
H -1.83948 -0.20229 -1.83458
H -3.23704 +1.73696 -2.55793
H -2.38659 +4.05326 -2.12714
H -0.16123 +4.33727 -1.00845
H +0.81689 -2.94788 -2.41903
H -0.15372 -1.60495 -3.03559
H +1.22880 -2.21115 -3.99275
H +1.62124 -3.17075 +1.28496
H +3.26328 -2.87054 +1.91246
H +1.90594 -1.84242 +2.42016
N -0.22161 -1.74258 -0.10135
S -1.40346 -2.38000 +0.82844
O -1.01712 -2.35983 +2.25058
O -1.75657 -3.68103 +0.24296
C -2.77534 -1.25886 +0.59723
C -2.84073 -0.08887 +1.35610
C -3.70777 -1.52496 -0.40342
C -3.85223 +0.82451 +1.09603
H -2.11672 +0.10765 +2.13496
C -4.71680 -0.59794 -0.64629
H -3.63963 -2.43524 -0.98559
C -4.79868 +0.59124 +0.08726
H -3.90404 +1.73867 +1.67736
H -5.44301 -0.79687 -1.42632
C -5.87587 +1.60499 -0.18957
H -6.41456 +1.37509 -1.11033
H -6.60113 +1.62931 +0.63058
H -5.45228 +2.60947 -0.27537

Fe 0.02954 -0.32435 -0.42433
O 0.25555 -0.32524 -2.15477

1O(III)d

E = -2353.422671
G = -2353.013827
1,2

N	-1.50149	0.92723	-0.35584
N	-0.36997	-0.44654	1.65093
N	-1.13229	-2.05514	-0.50077
N	1.58345	-1.53798	-0.02996
N	1.41551	1.11522	-0.25478
C	-2.17706	1.36872	-1.42875
H	-1.79073	1.01204	-2.37503
C	-3.27338	2.21093	-1.31170
H	-3.79359	2.54425	-2.20071
C	-3.68438	2.60511	-0.03988
H	-4.54319	3.25384	0.08560
C	-2.97634	2.15439	1.07112
H	-3.26227	2.44135	2.07547
C	-1.88025	1.32217	0.87992
C	-0.98326	0.85389	2.00137
H	-1.52626	0.81390	2.95015
H	-0.18026	1.58644	2.11215
C	-1.29561	-1.58981	1.92443
H	-2.00542	-1.32264	2.71100
H	-0.70920	-2.42548	2.30156
C	-2.05120	-1.99856	0.66429
H	-2.55238	-2.96092	0.82358
H	-2.81657	-1.25950	0.43137
C	-1.90164	-2.13806	-1.75882
H	-2.43289	-3.09427	-1.83319
H	-1.20042	-1.99001	-2.57785
H	-2.62562	-1.32430	-1.78547
C	-0.18102	-3.21516	-0.39815
H	-0.49786	-4.01895	-1.06685
H	-0.21929	-3.61893	0.61206
C	1.23783	-2.79089	-0.75542
H	1.94931	-3.59423	-0.53358
H	1.27621	-2.53605	-1.81257
C	1.72982	-1.73096	1.45639
H	2.78626	-1.70760	1.73210
H	1.36097	-2.72198	1.71200
C	0.97234	-0.65889	2.24871
H	0.90608	-0.95572	3.30157
H	1.50578	0.28784	2.19829
C	2.75826	-0.85148	-0.61798
H	2.69203	-0.98235	-1.69913
H	3.70135	-1.27441	-0.26067
C	2.67161	0.62565	-0.34748
C	3.78945	1.44744	-0.26637
H	4.77888	1.01130	-0.32705
C	3.61202	2.81923	-0.11457
H	4.46795	3.48058	-0.05055
C	2.31648	3.32489	-0.05128
H	2.12734	4.38544	0.05574
C	1.24910	2.44010	-0.12278
H	0.22837	2.79349	-0.07453

1O(III)q

E = -2353.447608
G = -2353.04313
1,4

N	1.58965	-1.09101	-0.41202
N	0.42637	0.31861	1.58892
N	1.27707	2.14692	-0.43065
N	-1.53055	1.62275	0.02970
N	-1.68742	-1.11150	-0.25325
C	2.33795	-1.49614	-1.44925
H	2.00972	-1.12891	-2.41374
C	3.44635	-2.31488	-1.28449
H	4.02519	-2.61978	-2.14718
C	3.79648	-2.71724	0.00314
H	4.66372	-3.34572	0.16772
C	3.01977	-2.29533	1.07976
H	3.26199	-2.58295	2.09542
C	1.91547	-1.48772	0.83611
C	0.96254	-1.02826	1.91165
H	1.43500	-1.04972	2.89762
H	0.12010	-1.72339	1.92884
C	1.40905	1.40135	1.93204
H	2.11845	1.03175	2.67644
H	0.86448	2.21903	2.40085
C	2.17613	1.90534	0.71216
H	2.74058	2.80673	0.98996
H	2.89427	1.14986	0.39321
C	2.03162	2.30511	-1.68080
H	2.65528	3.20983	-1.66681
H	1.32696	2.34204	-2.50912
H	2.66826	1.43222	-1.82736
C	0.32686	3.27142	-0.21975
H	0.62710	4.13931	-0.81471
H	0.36614	3.58783	0.82146
C	-1.10753	2.89349	-0.60835
H	-1.78466	3.71765	-0.35119
H	-1.14996	2.72278	-1.68338
C	-1.63526	1.71057	1.51887
H	-2.68491	1.69370	1.82406
H	-1.23352	2.66983	1.83882
C	-0.89787	0.56371	2.22287
H	-0.78882	0.79245	3.28876
H	-1.47209	-0.35465	2.13389
C	-2.74027	1.05203	-0.58826
H	-2.64472	1.19166	-1.66716
H	-3.64956	1.56103	-0.25017
C	-2.84693	-0.43987	-0.34650
C	-4.07559	-1.09353	-0.29420
H	-4.99415	-0.52264	-0.35789
C	-4.09654	-2.47890	-0.16234
H	-5.04041	-3.00999	-0.12051
C	-2.89032	-3.17182	-0.08345
H	-2.86290	-4.24946	0.01797
C	-1.70789	-2.44368	-0.12913

H	-0.74043	-2.92907	-0.06350
Fe	0.04694	0.26336	-0.54221
O	-0.12770	0.29836	-2.17304

1O(III)sext

E = -2353.447448

G = -2353.045607

1,6

N	1.67746	-1.03062	-0.39514
N	0.41202	0.31401	1.65867
N	1.10329	2.23226	-0.37695
N	-1.65461	1.52830	0.07739
N	-1.59827	-1.17113	-0.35787
C	2.45323	-1.39929	-1.42634
H	2.11545	-1.05647	-2.39680
C	3.60321	-2.15438	-1.24980
H	4.20775	-2.43189	-2.10375
C	3.95471	-2.53206	0.04490
H	4.85129	-3.11459	0.22244
C	3.14780	-2.14744	1.11208
H	3.39743	-2.41983	2.13019
C	2.00493	-1.39575	0.85727
C	1.03453	-0.98758	1.94501
H	1.53381	-1.00426	2.92050
H	0.24474	-1.74340	1.97034
C	1.30108	1.45700	1.99402
H	2.05559	1.15060	2.72525
H	0.70588	2.23197	2.47508
C	2.01801	2.03061	0.76926
H	2.51668	2.96819	1.04907
H	2.78802	1.33410	0.43500
C	1.86670	2.49391	-1.61143
H	2.43561	3.43011	-1.53956
H	1.17311	2.52532	-2.44862
H	2.55542	1.66619	-1.78471
C	0.08487	3.29541	-0.13570
H	0.33476	4.19269	-0.70866
H	0.11134	3.58317	0.91371
C	-1.32308	2.84095	-0.53066
H	-2.05077	3.61146	-0.24676
H	-1.36242	2.69968	-1.61068
C	-1.74318	1.56657	1.56548
H	-2.78702	1.48363	1.88073
H	-1.39465	2.53890	1.90827
C	-0.93644	0.44973	2.24538
H	-0.89358	0.65373	3.32357
H	-1.44628	-0.50221	2.11152
C	-2.83632	0.89731	-0.54092
H	-2.77399	1.07502	-1.61715
H	-3.77215	1.32837	-0.16972
C	-2.81596	-0.60029	-0.33299
C	-3.97227	-1.35755	-0.17866
H	-4.93712	-0.86676	-0.14709
C	-3.86157	-2.74080	-0.06517
H	-4.74837	-3.35160	0.05721
C	-2.59865	-3.32716	-0.10648
H	-2.46947	-4.39863	-0.02205
C	-1.49104	-2.50150	-0.25133
H	-0.48348	-2.89961	-0.28132
Fe	0.01961	0.29378	-0.71307
O	-0.16751	0.40525	-2.42158

1OH(III)d

E = -2353.945465

G = -2353.523349

2,2

N	-1.53265	0.89619	-0.34458
N	-0.35219	-0.43748	1.62486
N	-1.10314	-2.05200	-0.50843
N	1.58942	-1.51807	0.00459
N	1.40535	1.12141	-0.21836
C	-2.21042	1.33628	-1.41762
H	-1.85195	0.99224	-2.37733
C	-3.29907	2.18538	-1.29566
H	-3.82158	2.51540	-2.18385
C	-3.69712	2.59025	-0.02420
H	-4.55102	3.24465	0.10238
C	-2.98226	2.14826	1.08475
H	-3.25370	2.44755	2.08896
C	-1.89413	1.30927	0.89177
C	-0.98051	0.86011	1.99862
H	-1.50446	0.78636	2.95274
H	-0.18893	1.60373	2.11167
C	-1.29055	-1.58323	1.90916
H	-1.99703	-1.29580	2.68822
H	-0.70635	-2.41329	2.29895
C	-2.03840	-1.99573	0.65271
H	-2.51871	-2.96744	0.80255
H	-2.81334	-1.27229	0.40693
C	-1.89752	-2.20085	-1.75225
H	-2.55108	-3.07465	-1.67621
H	-1.23187	-2.34435	-2.60224
H	-2.50854	-1.31391	-1.90744
C	-0.14595	-3.21933	-0.38068
H	-0.45483	-4.02091	-1.05224
H	-0.20551	-3.61605	0.62954
C	1.27558	-2.79160	-0.71265
H	1.98910	-3.57449	-0.44230
H	1.36392	-2.57952	-1.77606
C	1.73802	-1.71623	1.49894
H	2.79484	-1.68834	1.76510
H	1.37200	-2.70843	1.75005
C	0.97702	-0.64265	2.27013
H	0.86399	-0.93077	3.31856
H	1.50961	0.30396	2.23008
C	2.77646	-0.82819	-0.57082
H	2.75683	-0.98522	-1.64942
H	3.70340	-1.24152	-0.17006
C	2.66606	0.64979	-0.32625
C	3.76826	1.49351	-0.28217
H	4.76403	1.07506	-0.35426
C	3.56468	2.86289	-0.15069

H	4.40857	3.54128	-0.11361
C	2.26217	3.34741	-0.07220
H	2.05535	4.40562	0.01979
C	1.20982	2.44530	-0.11010
H	0.18499	2.78316	-0.05251
Fe	0.02944	-0.33403	-0.38280
O	0.37917	-0.23529	-2.16282
H	-0.26683	-0.67904	-2.72410

1OH(III)q

E = -2353.930404

G = -2353.512924

2,4

N	-1.74054	0.88553	-0.36174
N	-0.36404	-0.38491	1.56481
N	-0.86476	-2.21928	-0.52319
N	1.79821	-1.43445	0.12759
N	1.44100	1.22635	-0.27726
C	-2.53091	1.21056	-1.39556
H	-2.17630	0.90634	-2.37208
C	-3.72485	1.89255	-1.21321
H	-4.34213	2.13899	-2.06722
C	-4.10240	2.24160	0.08188
H	-5.03284	2.76823	0.25801
C	-3.27700	1.90539	1.15247
H	-3.54212	2.15985	2.17075
C	-2.09395	1.22801	0.89236
C	-1.07702	0.87105	1.94315
H	-1.52855	0.77720	2.93219
H	-0.34084	1.67614	1.98655
C	-1.22523	-1.59502	1.85242
H	-2.00444	-1.32697	2.56624
H	-0.60335	-2.34788	2.32985
C	-1.86109	-2.14937	0.58753
H	-2.27635	-3.14264	0.78555
H	-2.67341	-1.50886	0.24827
C	-1.57163	-2.51157	-1.79566
H	-2.16917	-3.42186	-1.69027
H	-0.84461	-2.66944	-2.59212
H	-2.22734	-1.67986	-2.05177
C	0.18676	-3.26739	-0.26662
H	-0.00639	-4.13529	-0.89834
H	0.10395	-3.60400	0.76393
C	1.58643	-2.73546	-0.55507
H	2.33417	-3.47458	-0.24976
H	1.69464	-2.55525	-1.62439
C	1.84292	-1.53822	1.61849
H	2.86729	-1.41199	1.97502
H	1.53028	-2.53904	1.90800
C	0.95329	-0.47997	2.27273
H	0.79562	-0.71523	3.32884
H	1.42380	0.49805	2.20942
C	2.93752	-0.67456	-0.42620
H	2.99713	-0.88920	-1.49543
H	3.88180	-0.97814	0.03341
C	2.72087	0.81198	-0.27931
C	3.77460	1.71710	-0.21453
H	4.79356	1.35117	-0.19942
C	3.49396	3.07854	-0.17673
H	4.29943	3.80163	-0.12710
C	2.16661	3.49943	-0.20540
H	1.90403	4.54904	-0.18479
C	1.16722	2.53997	-0.25500
H	0.12080	2.81373	-0.27611
Fe	0.02145	-0.29899	-0.47477
O	0.31167	-0.15259	-2.24417
H	-0.11546	-0.82608	-2.78794

1OH(III)sext

E = -2353.942421

G = -2353.526917

2,6

N	-1.67532	0.98432	-0.36848
N	-0.41222	-0.34647	1.63905
N	-1.01456	-2.24291	-0.41468
N	1.68402	-1.48549	0.09251
N	1.54076	1.18411	-0.31349
C	-2.43159	1.35374	-1.41824
H	-2.07931	1.02517	-2.38717
C	-3.58560	2.10221	-1.25737
H	-4.17350	2.38032	-2.12218
C	-3.96433	2.47354	0.03166
H	-4.86687	3.05110	0.19252
C	-3.17807	2.09091	1.11448
H	-3.44682	2.35915	2.12829
C	-2.02953	1.34617	0.88107
C	-1.07284	0.93731	1.97284
H	-1.58049	0.89116	2.93918
H	-0.30318	1.71023	2.04067
C	-1.28706	-1.51960	1.95833
H	-2.05178	-1.22918	2.68124
H	-0.67821	-2.28364	2.43666
C	-1.96917	-2.08454	0.71670
H	-2.43477	-3.04608	0.95865
H	-2.75427	-1.41023	0.37460
C	-1.76535	-2.52189	-1.66164
H	-2.41414	-3.39379	-1.52903
H	-1.06380	-2.72315	-2.46906
H	-2.37178	-1.65356	-1.91935
C	0.01352	-3.30412	-0.16113
H	-0.21951	-4.19307	-0.75013
H	-0.03206	-3.60082	0.88402
C	1.41096	-2.81311	-0.52907
H	2.16213	-3.54849	-0.22437
H	1.47681	-2.67655	-1.60846
C	1.76676	-1.54921	1.58995
H	2.80637	-1.44398	1.90523
H	1.44124	-2.53640	1.90859
C	0.92987	-0.46249	2.26995
H	0.84376	-0.68583	3.33836
H	1.42047	0.50289	2.16856
C	2.87083	-0.82308	-0.50118

H	2.86290	-1.02350	-1.57510
H	3.79893	-1.22259	-0.08532
C	2.78633	0.67132	-0.31241
C	3.90376	1.48845	-0.19829
H	4.89246	1.04783	-0.18625
C	3.72290	2.86479	-0.09983
H	4.57965	3.52153	-0.00739
C	2.43190	3.38842	-0.11778
H	2.25149	4.45292	-0.04555
C	1.36324	2.51211	-0.22608
H	0.33795	2.85922	-0.23849
Fe	-0.00762	-0.27948	-0.58729
O	0.19514	-0.31997	-2.39664
H	-0.12446	-0.86478	-3.12230

1O(IV)t

E = -2353.299394

G = -2352.886708

2,3

N	-1.53296	0.88312	-0.35783
N	-0.33844	-0.43684	1.62781
N	-1.07716	-2.06518	-0.49232
N	1.60517	-1.50215	-0.03821
N	1.38871	1.13716	-0.24901
C	-2.22283	1.30597	-1.43067
H	-1.86817	0.94645	-2.38678
C	-3.31823	2.14548	-1.30708
H	-3.85073	2.46369	-2.19362
C	-3.71148	2.55431	-0.03518
H	-4.57095	3.20108	0.09316
C	-2.98789	2.12358	1.07221
H	-3.25914	2.42286	2.07646
C	-1.89230	1.29362	0.87966
C	-0.97965	0.85300	1.99253
H	-1.51248	0.78228	2.94226
H	-0.19695	1.60556	2.10955
C	-1.25059	-1.59679	1.92496
H	-1.95359	-1.32285	2.71227
H	-0.64780	-2.41684	2.30735
C	-2.00496	-2.02086	0.67627
H	-2.46967	-2.99977	0.82520
H	-2.79104	-1.30772	0.43617
C	-1.86860	-2.19573	-1.74277
H	-2.46022	-3.11470	-1.70694
H	-1.18937	-2.21717	-2.59101
H	-2.53481	-1.34185	-1.84021
C	-0.10850	-3.22540	-0.38302
H	-0.42643	-4.02579	-1.05133
H	-0.14987	-3.62192	0.62801
C	1.30346	-2.78840	-0.73844
H	2.02927	-3.55732	-0.46172
H	1.38011	-2.59108	-1.80561
C	1.76879	-1.68676	1.45940
H	2.82868	-1.64804	1.71144
H	1.41597	-2.68192	1.71672
C	1.00622	-0.62243	2.24376
H	0.92244	-0.91724	3.29328
H	1.52555	0.33150	2.19924
C	2.77820	-0.79662	-0.62405
H	2.74837	-0.94541	-1.70482
H	3.71449	-1.20454	-0.24073
C	2.65515	0.67607	-0.35819
C	3.74677	1.53083	-0.29794
H	4.74699	1.12376	-0.37167
C	3.52736	2.89610	-0.14858
H	4.36397	3.58256	-0.09937
C	2.22001	3.36704	-0.06912
H	2.00233	4.42171	0.03589
C	1.17581	2.45718	-0.12339
H	0.14783	2.78418	-0.06873
Fe	0.03435	-0.34162	-0.43993
O	0.22807	-0.32545	-2.06270

2O(III)d

E = -2353.404711

G = -2352.996265

1,2

N	-1.95248	-1.43284	-0.02927
C	-3.12166	-0.69574	0.54259
C	-3.25273	0.66153	-0.11269
N	-1.95850	1.39589	-0.13752
C	-1.55157	2.02489	1.15791
C	-0.90114	1.06411	2.17943
N	-0.21406	-0.10550	1.54420
C	-1.33638	-2.29103	1.01557
C	-0.67005	-1.42452	2.10001
C	1.27597	-0.01231	1.46964
C	1.74017	-1.16890	0.58965
C	1.63722	1.23388	0.68363
N	0.92545	1.33909	-0.45918
C	1.24785	2.28197	-1.35194
C	2.26306	3.19947	-1.10770
C	2.96303	3.12945	0.09471
C	2.65420	2.11866	1.00464
N	0.99015	-1.29536	-0.52620
C	1.33132	-2.19040	-1.45915
C	2.42769	-3.02908	-1.29323
C	3.18597	-2.92695	-0.12858
C	2.84289	-1.97252	0.82996
Fe	-0.52583	-0.01701	-0.53205
C	-2.36107	-2.24374	-1.19381
C	-2.07740	2.44523	-1.17773
H	-2.98407	-0.58810	1.61535
H	-4.03920	-1.27353	0.39740
H	-4.02748	1.25678	0.38408
H	-3.53944	0.52680	-1.15516
H	-2.40780	2.52191	1.62735
H	-0.82918	2.79455	0.89610
H	-1.65734	0.67926	2.85793
H	-0.19356	1.63307	2.78793
H	-0.60122	-2.92236	0.52251
H	-2.08907	-2.94513	1.47072
H	0.17267	-1.96717	2.53013

H	-1.36395	-1.23380	2.91508
H	1.75664	-0.02854	2.45030
H	0.66809	2.26836	-2.26460
H	2.49613	3.95177	-1.85031
H	3.74983	3.84076	0.31561
H	3.19330	2.00757	1.93672
H	0.69822	-2.19260	-2.33709
H	2.67850	-3.74653	-2.06430
H	4.03868	-3.57619	0.03075
H	3.41555	-1.84996	1.74048
H	-2.69659	-1.57119	-1.97990
H	-1.49416	-2.78551	-1.56733
H	-3.14786	-2.95604	-0.91836
H	-2.10686	1.93638	-2.14005
H	-2.97391	3.05489	-1.01675
H	-1.20558	3.09390	-1.15002
O	-0.76961	-0.00251	-2.25037

2O(III)q

E = -2353.434321

G = -2353.031779

1,4

N	2.43723	0.95490	0.19802
C	3.26686	-0.12711	0.77041
C	3.08675	-1.42531	-0.01027
N	1.66244	-1.80839	-0.21373
C	0.98570	-2.38375	0.98727
C	0.50764	-1.34963	2.02627
N	0.17577	-0.00820	1.43699
C	1.88211	1.85435	1.21735
C	0.90089	1.11166	2.13967
C	-1.28849	0.29157	1.35934
C	-1.43764	1.54398	0.50627
C	-2.01497	-0.82183	0.62294
N	-1.42099	-1.20118	-0.51924
C	-2.03209	-2.10100	-1.29613
C	-3.25343	-2.67376	-0.95437
C	-3.85502	-2.29782	0.24406
C	-3.22743	-1.34995	1.04995
N	-0.63638	1.55250	-0.57979
C	-0.72411	2.56142	-1.45625
C	-1.61036	3.61493	-1.27402
C	-2.42828	3.61895	-0.14584
C	-2.34364	2.56303	0.76006
Fe	0.60590	-0.06603	-0.68893
C	3.13920	1.69371	-0.85642
C	1.60416	-2.79374	-1.31704
H	2.99885	-0.27540	1.81364
H	4.32892	0.14589	0.75916
H	3.63131	-2.23789	0.48513
H	3.50674	-1.29571	-1.00760
H	1.64392	-3.10851	1.48028
H	0.12238	-2.92552	0.60956
H	1.27357	-1.20291	2.78224
H	-0.36395	-1.75764	2.54280
H	1.36173	2.65148	0.68738
H	2.66716	2.31939	1.83050
H	0.18089	1.82732	2.53784
H	1.42371	0.69405	2.99709
H	-1.72320	0.43805	2.35092
H	-1.52054	-2.36551	-2.21431
H	-3.71509	-3.39875	-1.61289
H	-4.80058	-2.73245	0.54629
H	-3.66544	-1.02277	1.98461
H	-0.05819	2.48876	-2.30662
H	-1.65193	4.41561	-2.00161
H	-3.12314	4.43204	0.02692
H	-2.96474	2.52608	1.64608
H	3.44366	0.99884	-1.63723
H	2.45141	2.41083	-1.30478
H	4.01932	2.22463	-0.46627
H	1.95931	-2.30831	-2.22316
H	2.21042	-3.67898	-1.08944
H	0.57210	-3.09784	-1.47552
O	0.94555	-0.00668	-2.29053

2O(III)sext

E = -2353.435101

G = -2353.0342

1,6

N	-2.07290	-1.52287	0.10664
C	-3.14226	-0.73155	0.77282
C	-3.32366	0.63199	0.11647
N	-2.06024	1.39795	-0.03941
C	-1.51920	2.00053	1.20525
C	-0.82233	1.01845	2.17363
N	-0.14456	-0.13157	1.51656
C	-1.30496	-2.33358	1.07421
C	-0.54163	-1.45093	2.08595
C	1.32065	0.01629	1.38217
C	1.85469	-1.13581	0.53507
C	1.64847	1.29000	0.61421
N	0.97441	1.43361	-0.53998
C	1.26211	2.45997	-1.34647
C	2.22183	3.41171	-1.01776
C	2.90056	3.28225	0.19057
C	2.61568	2.19843	1.02043
N	1.13824	-1.39678	-0.57254
C	1.55961	-2.33851	-1.42366
C	2.71582	-3.07577	-1.19498
C	3.45388	-2.81605	-0.04331
C	3.01940	-1.82736	0.83782
Fe	-0.63249	-0.08277	-0.84387
C	-2.62224	-2.36400	-0.97179
C	-2.28398	2.45723	-1.04875
H	-2.90146	-0.61766	1.82563
H	-4.09361	-1.27242	0.73037
H	-4.06004	1.21774	0.68128
H	-3.71435	0.48463	-0.89093
H	-2.31364	2.52244	1.75379
H	-0.79965	2.75137	0.88492
H	-1.55510	0.62143	2.87036

H	-0.10925	1.59278	2.77381
H	-0.60487	-2.93439	0.49547
H	-1.96392	-3.02151	1.61998
H	0.33688	-2.00084	2.42837
H	-1.15399	-1.28135	2.97044
H	1.82796	0.02895	2.35208
H	0.69730	2.50558	-2.26923
H	2.42536	4.23185	-1.69428
H	3.64716	4.01112	0.48303
H	3.13206	2.05616	1.96129
H	0.94256	-2.49057	-2.30076
H	3.02546	-3.83262	-1.90422
H	4.35800	-3.37501	0.16780
H	3.56919	-1.59489	1.74123
H	-3.13111	-1.72690	-1.69279
H	-1.80181	-2.86375	-1.48674
H	-3.31931	-3.11642	-0.58004
H	-2.49635	1.97949	-2.00339
H	-3.10790	3.12066	-0.75677
H	-1.37716	3.04890	-1.15802
O	-0.99162	-0.06435	-2.51652

2OH(III)d

E = -2353.93096

G = -2353.507789

2,2

N	1.96017	1.41448	-0.02698
C	3.12972	0.69642	0.58195
C	3.27085	-0.66423	-0.05472
N	1.95607	-1.37807	-0.11311
C	1.52714	-2.01807	1.18214
C	0.88824	-1.04975	2.18905
N	0.20159	0.11327	1.51696
C	1.32630	2.29731	0.99745
C	0.64887	1.44638	2.07911
C	-1.29731	0.00735	1.47749
C	-1.76873	1.16027	0.60499
C	-1.65440	-1.23728	0.69098
N	-0.93414	-1.33809	-0.44629
C	-1.24261	-2.27122	-1.35263
C	-2.26581	-3.18441	-1.12570
C	-2.97639	-3.12050	0.06940
C	-2.67557	-2.11985	0.99405
N	-1.00594	1.29626	-0.50002
C	-1.33410	2.19292	-1.43569
C	-2.44259	3.01749	-1.28262
C	-3.21735	2.90250	-0.13169
C	-2.88038	1.95134	0.83190
Fe	0.53764	0.01830	-0.48501
C	2.40338	2.23251	-1.18271
C	2.10115	-2.46495	-1.12052
H	2.97595	0.60969	1.65311
H	4.03981	1.28177	0.43577
H	4.00810	-1.27295	0.47543
H	3.60054	-0.55112	-1.08739
H	2.38306	-2.51769	1.64348
H	0.80327	-2.78201	0.91052
H	1.64027	-0.65115	2.86176
H	0.16907	-1.59648	2.80100
H	0.60552	2.92708	0.48321
H	2.08310	2.94688	1.44690
H	-0.20535	1.98302	2.48931
H	1.32795	1.25510	2.90474
H	-1.74306	0.01971	2.47165
H	-0.65556	-2.25794	-2.26054
H	-2.49408	-3.92868	-1.87714
H	-3.76851	-3.83012	0.27512
H	-3.22417	-2.01472	1.92075
H	-0.69152	2.22112	-2.30518
H	-2.68738	3.73375	-2.05586
H	-4.08070	3.54033	0.01403
H	-3.46384	1.82044	1.73379
H	2.94764	1.60494	-1.88610
H	1.53477	2.65682	-1.68032
H	3.06062	3.03632	-0.83871
H	2.32171	-2.03306	-2.09337
H	2.91631	-3.13134	-0.82348
H	1.18313	-3.04019	-1.18490
O	0.67100	0.01164	-2.28654
H	1.58001	0.00128	-2.61239

2OH(III)q

E = -2353.913505

G = -2353.497337

2,4

N	-2.36467	-1.00435	0.17899
C	-3.24084	0.04978	0.75688
C	-3.09228	1.35102	-0.01744
N	-1.66357	1.77348	-0.20388
C	-1.02112	2.35954	1.02808
C	-0.54040	1.32764	2.06049
N	-0.16904	-0.00441	1.44810
C	-1.81852	-1.91134	1.21076
C	-0.86915	-1.15609	2.14874
C	1.31229	-0.27207	1.38783
C	1.48211	-1.51500	0.52503
C	1.99703	0.85970	0.64624
N	1.35341	1.21959	-0.47667
C	1.91507	2.11620	-1.29475
C	3.13691	2.71215	-1.00063
C	3.78668	2.36358	0.17979
C	3.21120	1.41211	1.02152
N	0.68052	-1.51691	-0.56308
C	0.75917	-2.50301	-1.46363
C	1.65386	-3.55299	-1.29982
C	2.47683	-3.56571	-0.17699
C	2.39565	-2.52835	0.75315
Fe	-0.58661	0.06482	-0.56935
C	-3.04752	-1.76598	-0.88518
C	-1.63352	2.81331	-1.26787
H	-2.98877	0.19551	1.80337
H	-4.28747	-0.26634	0.72512

H	-3.64373	2.15417	0.47890
H	-3.50543	1.22125	-1.01762
H	-1.72289	3.05083	1.50272
H	-0.17103	2.93611	0.67351
H	-1.31419	1.14691	2.79875
H	0.31767	1.73758	2.59477
H	-1.28498	-2.70452	0.68917
H	-2.62207	-2.37331	1.79502
H	-0.12672	-1.84825	2.54300
H	-1.40381	-0.75054	3.00289
H	1.73228	-0.40691	2.38476
H	1.36949	2.35457	-2.19916
H	3.56249	3.43403	-1.68556
H	4.73402	2.81991	0.44058
H	3.69127	1.09972	1.93987
H	0.08729	-2.42032	-2.30832
H	1.69893	-4.34139	-2.03970
H	3.17898	-4.37624	-0.02357
H	3.02318	-2.50546	1.63438
H	-3.44673	-1.07675	-1.62756
H	-2.32453	-2.41954	-1.37197
H	-3.86578	-2.36353	-0.46779
H	-2.07263	2.42067	-2.18229
H	-2.20564	3.68916	-0.94742
H	-0.60660	3.10809	-1.46468
O	-0.87450	-0.06519	-2.34233
H	-1.59208	0.48197	-2.68674

2OH(III)sext

E = -2353.926876

G = -2353.514338

2,6

N	-2.06995	-1.45676	0.12419
C	-3.13982	-0.65187	0.78935
C	-3.29963	0.70240	0.11969
N	-2.00874	1.43680	-0.04721
C	-1.46145	2.05378	1.19818
C	-0.79070	1.06678	2.17200
N	-0.13942	-0.10751	1.50438
C	-1.33355	-2.29225	1.10606
C	-0.55679	-1.41843	2.10728
C	1.34243	0.00459	1.39591
C	1.83390	-1.16529	0.55309
C	1.69238	1.26101	0.61809
N	0.98441	1.41614	-0.51810
C	1.27978	2.42390	-1.35022
C	2.28316	3.34047	-1.06043
C	2.99405	3.20177	0.12769
C	2.69970	2.13903	0.98129
N	1.08648	-1.39328	-0.54349
C	1.44602	-2.34669	-1.41283
C	2.57524	-3.12860	-1.20615
C	3.34397	-2.90593	-0.06686
C	2.97092	-1.90530	0.83013
Fe	-0.59733	-0.05894	-0.72414
C	-2.63408	-2.29901	-0.95574
C	-2.22167	2.50020	-1.06421
H	-2.89960	-0.53854	1.84158
H	-4.08918	-1.19128	0.74081
H	-4.00907	1.31831	0.68136
H	-3.69770	0.55786	-0.88505
H	-2.25829	2.58579	1.72755
H	-0.73308	2.79221	0.87185
H	-1.52863	0.68479	2.86973
H	-0.05563	1.61678	2.76432
H	-0.65411	-2.92538	0.53900
H	-2.03066	-2.94241	1.64513
H	0.31666	-1.97127	2.45237
H	-1.16101	-1.21786	2.98875
H	1.82511	0.00801	2.37492
H	0.69060	2.48709	-2.25594
H	2.49359	4.14420	-1.75364
H	3.77417	3.90740	0.38662
H	3.23975	1.98807	1.90691
H	0.80566	-2.46614	-2.27748
H	2.84053	-3.89306	-1.92452
H	4.22758	-3.50329	0.12333
H	3.54642	-1.70085	1.72374
H	-3.19338	-1.66958	-1.64600
H	-1.82119	-2.78432	-1.49461
H	-3.30112	-3.06099	-0.53958
H	-2.47846	2.03355	-2.01315
H	-3.02471	3.17414	-0.74874
H	-1.30695	3.07387	-1.19020
O	-0.94126	-0.14578	-2.49043
H	-1.56929	-0.55935	-3.09016

2O(IV)t

E = -2353.283663

G = -2352.871322

2,3

N	-1.93558	-1.43623	-0.05047
C	-3.11485	-0.71620	0.54331
C	-3.25802	0.64235	-0.09599
N	-1.94998	1.37343	-0.13050
C	-1.54110	2.01232	1.17120
C	-0.90735	1.04562	2.18297
N	-0.21737	-0.11407	1.51673
C	-1.30901	-2.30933	0.98608
C	-0.65408	-1.44844	2.07470
C	1.27656	0.00057	1.46632
C	1.75664	-1.15067	0.59589
C	1.62621	1.24748	0.68098
N	0.91029	1.35132	-0.45960
C	1.21830	2.29047	-1.36074
C	2.23418	3.20843	-1.12388
C	2.93989	3.14220	0.07345
C	2.64059	2.13490	0.99094
N	1.00226	-1.30134	-0.51372
C	1.34618	-2.19925	-1.44356
C	2.46037	-3.01260	-1.27850
C	3.22591	-2.88433	-0.12327

C	2.87307	-1.93164	0.83260
Fe	-0.54511	-0.01974	-0.54563
C	-2.36553	-2.25527	-1.21171
C	-2.09274	2.45439	-1.14610
H	-2.97476	-0.62789	1.61608
H	-4.01925	-1.30662	0.38520
H	-4.00620	1.24423	0.42575
H	-3.56871	0.52860	-1.13363
H	-2.40840	2.50316	1.61987
H	-0.82145	2.78320	0.90922
H	-1.66407	0.64632	2.85024
H	-0.19550	1.59587	2.80074
H	-0.57785	-2.93770	0.48578
H	-2.07036	-2.96039	1.42497
H	0.19911	-1.97696	2.49810
H	-1.34631	-1.26463	2.89109
H	1.72992	-0.00839	2.45726
H	0.63586	2.28735	-2.27126
H	2.45927	3.95834	-1.87049
H	3.72696	3.85509	0.28662
H	3.18533	2.02757	1.91957
H	0.70996	-2.24809	-2.31660
H	2.71550	-3.73059	-2.04661
H	4.09428	-3.51297	0.03183
H	3.44870	-1.79062	1.73792
H	-2.82599	-1.60768	-1.95407
H	-1.49660	-2.73627	-1.65399
H	-3.07811	-3.01635	-0.88215
H	-2.24076	2.00075	-2.12294
H	-2.94954	3.08267	-0.88723
H	-1.20019	3.07158	-1.16419
O	-0.76083	-0.01053	-2.15949

PhSMe

E = -669.9041

G = -669.808869

0,1

C	1.93666	-1.20708	0.10829
C	0.56737	-1.20998	-0.15496
C	-0.12318	0.00000	-0.28398
C	0.56737	1.20998	-0.15496
C	1.93666	1.20708	0.10829
C	2.62289	0.00000	0.23992
H	2.46572	-2.14839	0.20795
H	0.03506	-2.14837	-0.25909
H	0.03506	2.14837	-0.25909
H	2.46572	2.14839	0.20795
H	3.68796	0.00000	0.44303
S	-1.89082	0.00000	-0.63609
C	-2.55943	0.00000	1.07523
H	-2.23923	0.89468	1.61029
H	-3.64790	0.00000	0.98927
H	-2.23923	-0.89468	1.61029

PhSMe+

E = -669.700293

G -669.604701

1,2

C	1.66746	-1.40142	-0.00011
C	0.31690	-1.13406	-0.00008
C	-0.11597	0.21847	-0.00002
C	0.83537	1.28345	0.00013
C	2.18045	0.98885	0.00020
C	2.60291	-0.34932	-0.00005
H	2.01199	-2.42780	-0.00007
H	-0.39537	-1.94715	-0.00007
H	0.49788	2.31365	0.00045
H	2.90951	1.78915	0.00048
H	3.66201	-0.57746	-0.00026
S	-1.76332	0.70856	-0.00029
C	-2.75249	-0.81066	0.00036
H	-2.54552	-1.39064	0.90065
H	-3.78983	-0.47674	0.00001
H	-2.54541	-1.39188	-0.89910

CHD^0

E = -233.521741

G = -233.428861

0,1

C	-1.49446	-0.00001	0.00004
C	-0.66497	1.25201	-0.00002
C	0.66497	1.25201	-0.00002
C	1.49446	0.00000	0.00004
C	0.66497	-1.25200	-0.00003
C	-0.66497	-1.25201	-0.00002
H	-2.16890	-0.00000	0.86598
H	-1.20364	2.19340	-0.00006
H	1.20363	2.19341	-0.00007
H	2.16904	0.00001	-0.86580
H	1.20363	-2.19341	-0.00007
H	-1.20362	-2.19341	-0.00006
H	2.16889	0.00000	0.86600
H	-2.16902	-0.00000	-0.86582

CHD^+

E = -233.302381

G = -233.213980

1,2

C	-1.44363	0.00001	0.00001
C	-0.67956	1.25348	-0.00001
C	0.67957	1.25347	-0.00002
C	1.44363	-0.00001	0.00001
C	0.67957	-1.25347	-0.00002
C	-0.67958	-1.25347	-0.00001
H	-2.16684	0.00001	0.84026
H	-1.23214	2.18294	-0.00002
H	1.23216	2.18293	-0.00004
H	2.16696	-0.00001	-0.84013
H	1.23213	-2.18294	-0.00003
H	-1.23215	-2.18293	-0.00003
H	2.16679	-0.00002	0.84031
H	-2.16691	-0.00000	-0.84017

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