

Electronic Supplementary Information

Sluggish Reactivity by a Nonheme Iron(IV)-Tosylimido Complex as Compared to its Oxo Analogue

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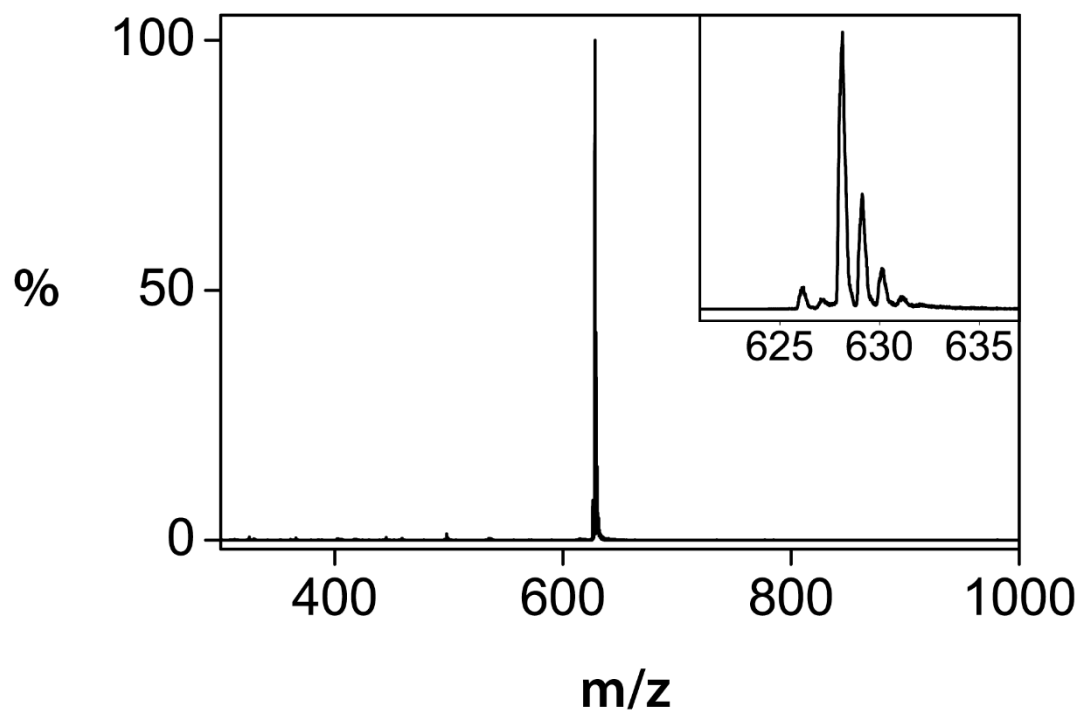


Fig. S1. ESI-MS spectrum of $[\text{Fe}^{\text{II}}(\text{Bntpen})(\text{OTf})]^+$ in CH_3CN at 298 K. Inset shows the isotopic distribution pattern for the peak at m/z 628.11 corresponding to $[\text{Fe}^{\text{II}}(\text{Bntpen})(\text{OTf})]^+$.

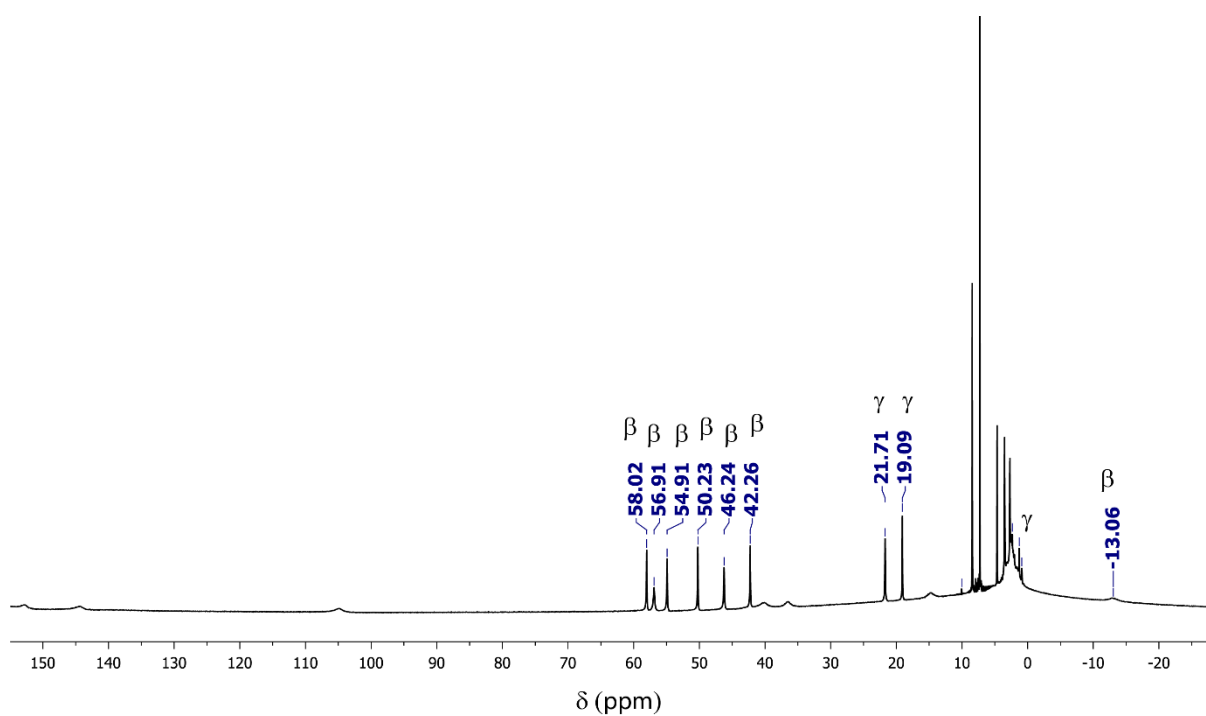


Fig. S2. ¹H-NMR (400 MHz) spectrum of the complex, [Fe^{II}(Bntpen)(OTf)]²⁺ in CDCl₃ at 295 K with a spectral width of ~200 ppm (scans: 128). The peaks have been assigned based of previously reported literature.¹

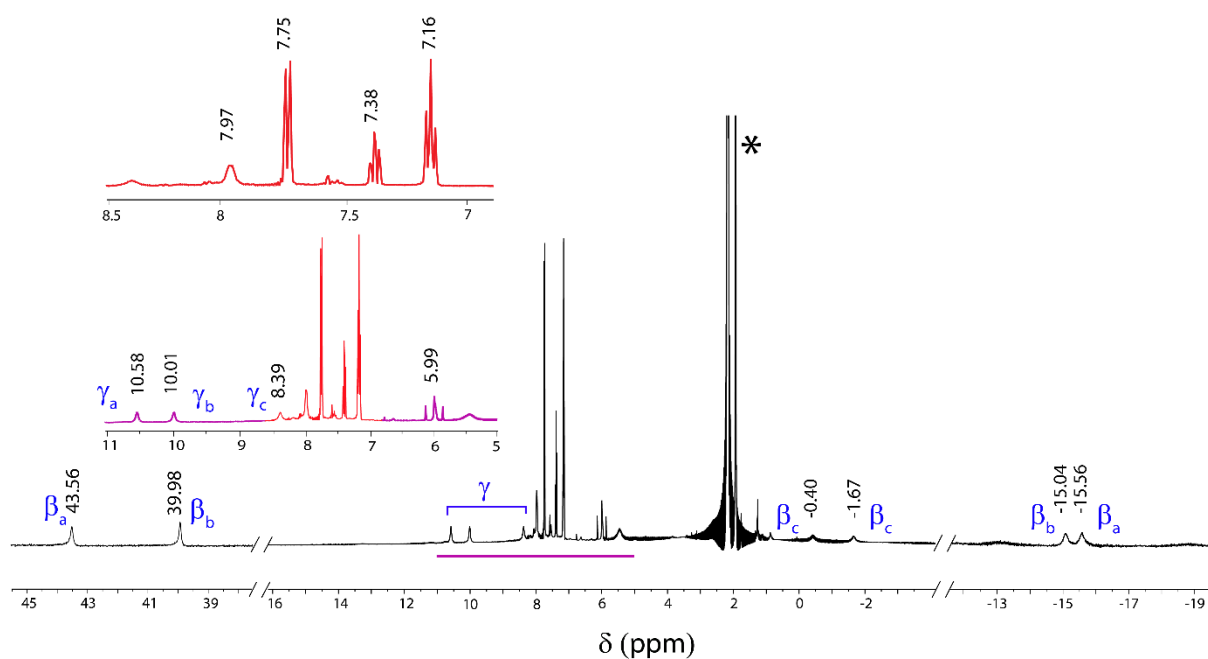


Fig. S3. $^1\text{H-NMR}$ (400 MHz) spectrum of the complex, $[\text{Fe}^{\text{IV}}(\text{Bntpen})(\text{O})]^{2+}$ (**3**) in CD_3CN at 295 K with a spectral width of ~ 200 ppm (scans: 256). The peaks have been assigned based on previously reported literature.² Residual solvent peaks are denoted by *.

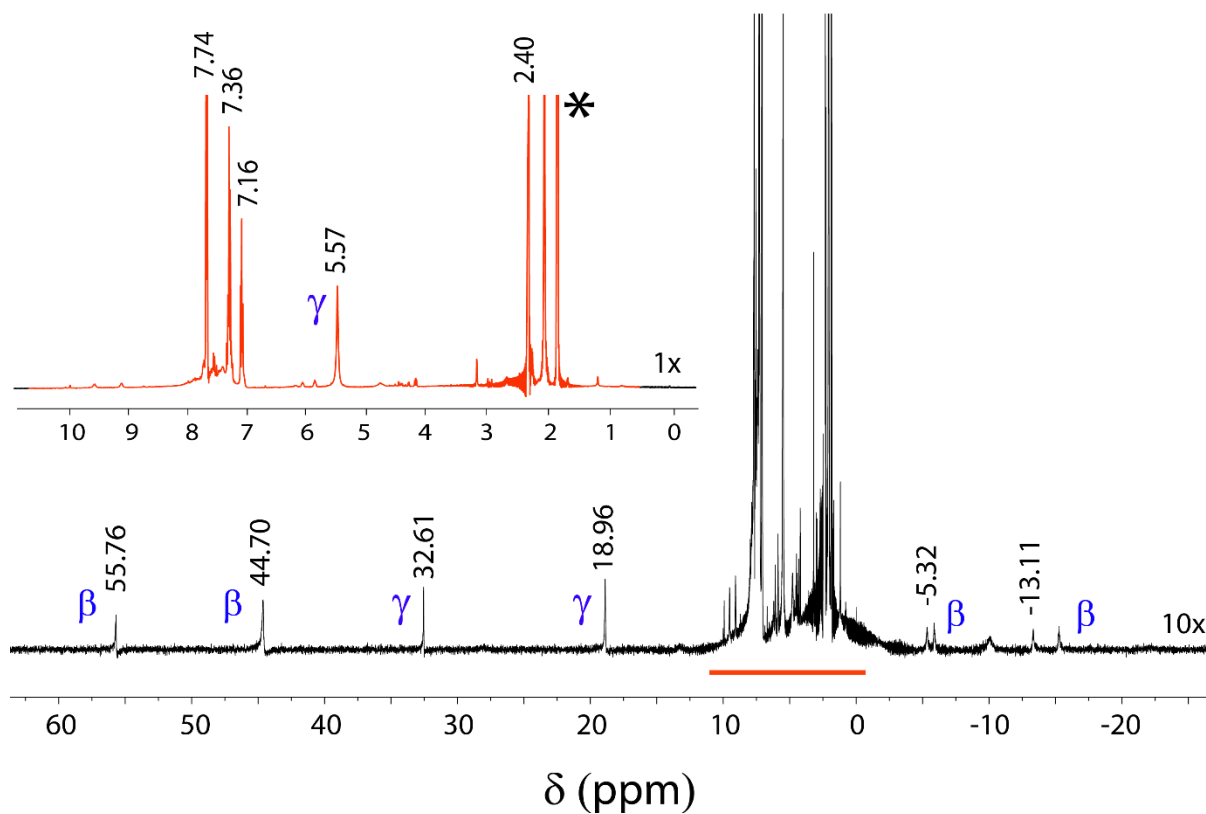


Fig. S4. ¹H-NMR (400 MHz) spectrum of the complex, $[\text{Fe}^{\text{IV}}(\text{Bntpen})(\text{NTs})]^{2+}$ (**4**) in CD_3CN at 295 K with a spectral width of ~ 200 ppm (scans: 256). The peaks have been assigned based on previously reported literature.^{2d,3} Peaks at δ 7.74 and δ 7.36 ppm correspond to tosyl resonances belonging to the tosylimide ligated to the iron centre as reported for similar $\text{Fe}(\text{IV})=\text{NTs}$ complex, **2**.³ The ¹H-NMR spectrum of the oxidant, PhINTs, is reported to signal at δ 2.30 ppm (CH_3) and δ 7.00-7.80 ppm (aromatic protons)⁴. Residual solvent peaks are denoted by *.

FTIR Spectroscopy:

FTIR spectra were recorded on a Perkin Elmer FTIR spectrometer at 298 K. The Fe(IV)=O stretching vibrations are usually around 830-850 cm^{-1} . However, the resonance RAMAN studies on **2** indicates signals at around 998 cm^{-1} corresponding to the Fe=N stretching vibration.^{2d} Similar Fe(IV)=NTs complexes like $[\text{Fe}^{\text{IV}}(\text{NTs})(\text{MePy}_2\text{tacn})](\text{OTf})_2$ and $[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Me}_2(\text{CHPy}_2)\text{tacn})](\text{OTf})_2$ with pentadentate ligand frameworks have shown stretching vibrations around 984 cm^{-1} .^{2d} The FTIR spectrum shown here for **4** shows transmittance at 997 cm^{-1} , for the Fe=N vibration.

519 cm^{-1} (strong, CF_3 asy. str.), 665 cm^{-1} (strong, S-N str.), 764 cm^{-1} (strong, CF_3 sym. str.), 997 cm^{-1} (shoulder, Fe=N str.), 1030 cm^{-1} (very strong, SO_2 str.), 1275 cm^{-1} (very strong, SO_3 asy. str.), 1330 cm^{-1} (strong, SO_2 asy. str.).

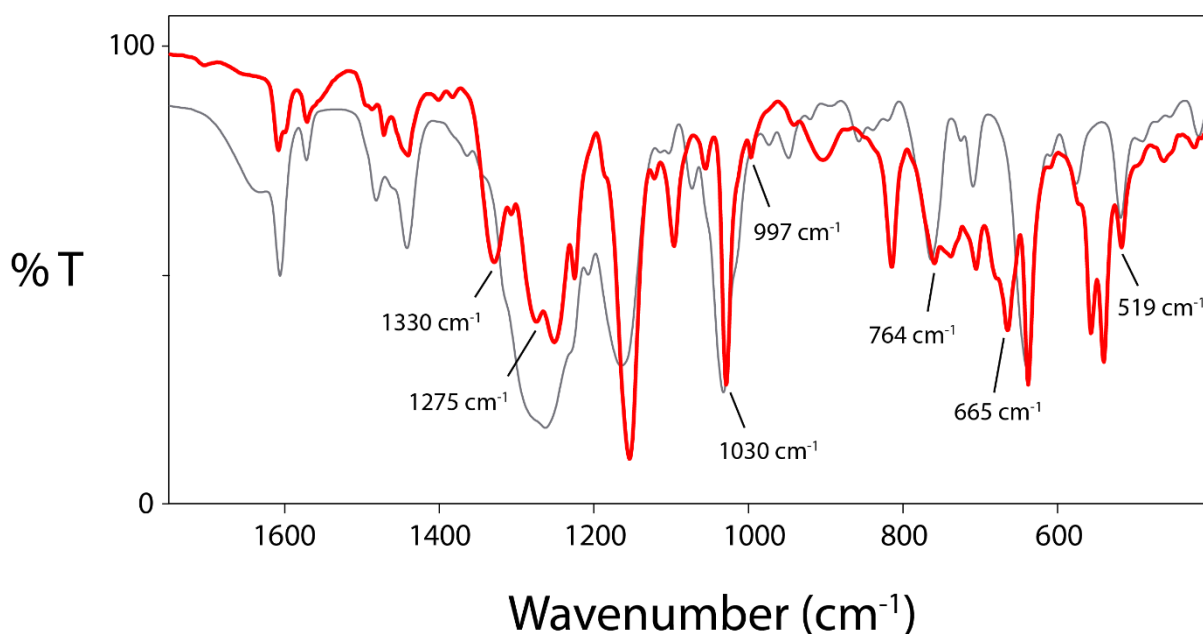


Fig. S5. FTIR spectra of complex $[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$, **4** (red line) in CH_3CN at 298 K. Black line shows the same for the Fe(II)-complex, $[\text{Fe}^{\text{II}}(\text{Bntpen})(\text{OTf})]^+$. The peak at 997 cm^{-1} is assigned to the Fe=N stretching frequency in **4**.

Table S1. Pseudo first-order and second-order rate constants determined for the reaction of **4** with *para*-X-thioanisole at 298 K.

X =	Concentration (mM)	$k_{\text{obs}} (\text{s}^{-1}) \times 10^{-3}$	$k_2 (\text{M}^{-1} \text{s}^{-1}) \times 10^{-2}$
-OMe	5	23.50	541.4
	10	52.16	
	15	76.57	
	20	113.63	
-Me	20	4.25	22.9
	30	7.04	
	40	9.25	
	50	11.63	
-H	50	2.28	5.4
	100	4.51	
	150	8.04	
	200	11.33	
-Cl	50	1.22	2.7
	100	2.42	
	150	3.68	
	200	5.83	

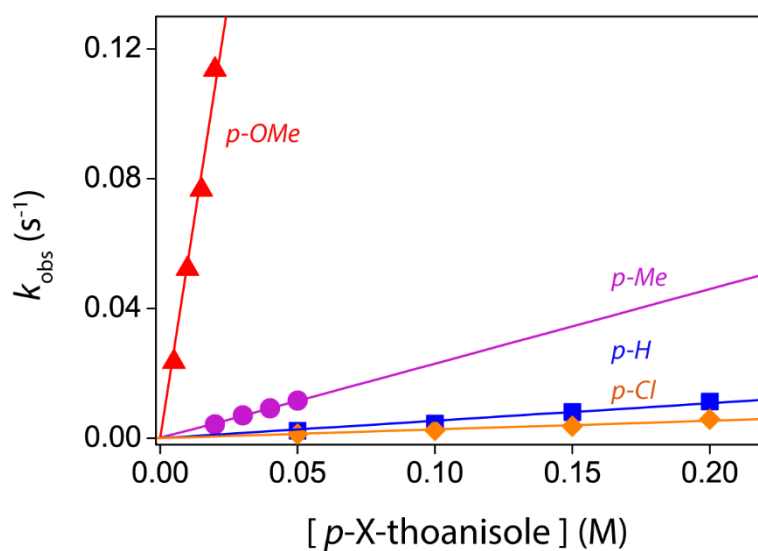


Fig. S6. Plot of k_{obs} against substrate concentration to determine second-order rate constants for the reactions of **4** (1mM) with *para*-X-thioanisole (X = -OMe ▲, -Me ●, -H ■, -Cl ◆) in CH_3CN at 298 K.

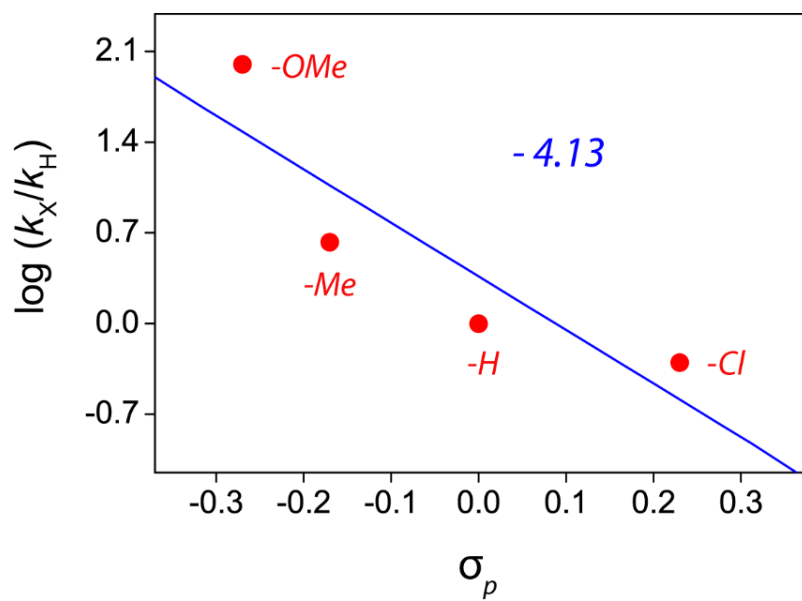


Fig. S7. Hammett plot obtained by plotting the $\log(k_X/k_H)$ values against σ_p values⁵ of *para*-X-thioanisole (X = OMe, Me, H and Cl) substrates for their reaction with **4** in CH_3CN at 298 K.

Table S2. Second-order rate constant (k_2) determined in the reaction of 3 (1 mM) and 4 (1 mM) with benzyl alcohol in CH₃CN at 298 K.

[Benzyl alcohol] (mM)	3	[Benzyl alcohol] (mM)	4
	$k_{\text{obs}} (\text{s}^{-1}) \times 10^{-3}$		$k_{\text{obs}} (\text{s}^{-1}) \times 10^{-3}$
20	21.98	200	0.73
40	44.97	300	1.06
60	70.57	400	1.67
80	92.55	-	-
$k_2 = 1.156 \text{ M}^{-1} \text{ s}^{-1}$		$k_2 = 0.004 \text{ M}^{-1} \text{ s}^{-1}$	

Table S3. Pseudo first-order rate constant (k_{obs}) for the reaction of 1 mM of [Fe^{IV}(NTs)(Bntpen)]²⁺ (4) with excess benzyl alcohol and benzyl alcohol-D₇ at 298 K.

Complex	Substrate concentration [300 mM]		KIE
	Benzyl alcohol	Benzyl alcohol – D ₇	
4	1.064×10^{-3}	2.814×10^{-4}	4

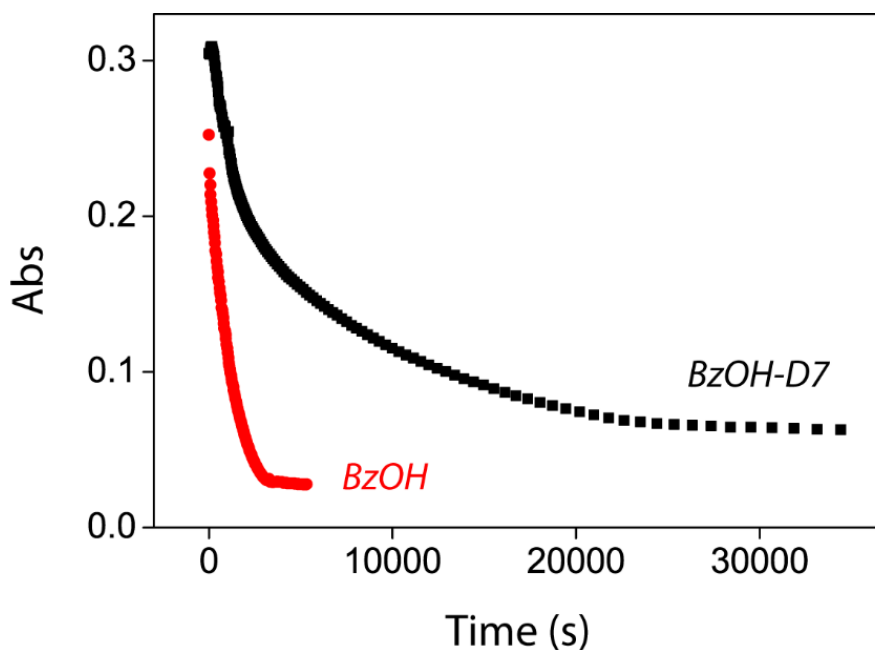


Fig. S8. Decay profile for the reaction of $[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ (1 mM) with 300 equivalents of benzyl alcohol (BzOH, ●) and benzyl alcohol- D_7 (BzOH- D_7 , ■) in CH_3CN at 298 K.

Table S4. Hammett parameters and second-order rate constants (k_2) determined for the reaction of **3** (1 mM) with various *para*-substituted benzyl alcohols in CH_3CN at 298 K.^a

<i>p</i> -X-benzyl alcohol	σ_p^b	σ_p^{+b}	k_2 ($\text{M}^{-1} \text{s}^{-1}$)	k_x/k_H^c	$\log(k_x/k_H)$
-OMe	-0.27	-0.78	0.865	1.469	0.167
-Me	-0.17	-0.31	0.623	1.058	0.024
-H	0.00	0.00	0.589	1.000	0.000
-Cl	0.23	0.11	0.371	0.628	-0.202

^a All the reactions were followed by monitoring the UV/Vis spectral changes of the reaction solution.

^b Data taken from ref. 5.

^c Relative rate constant obtained by dividing the k_2 of *p*-X-benzyl alcohol by k_2 of *p*-H-benzyl alcohol.

Computational data:

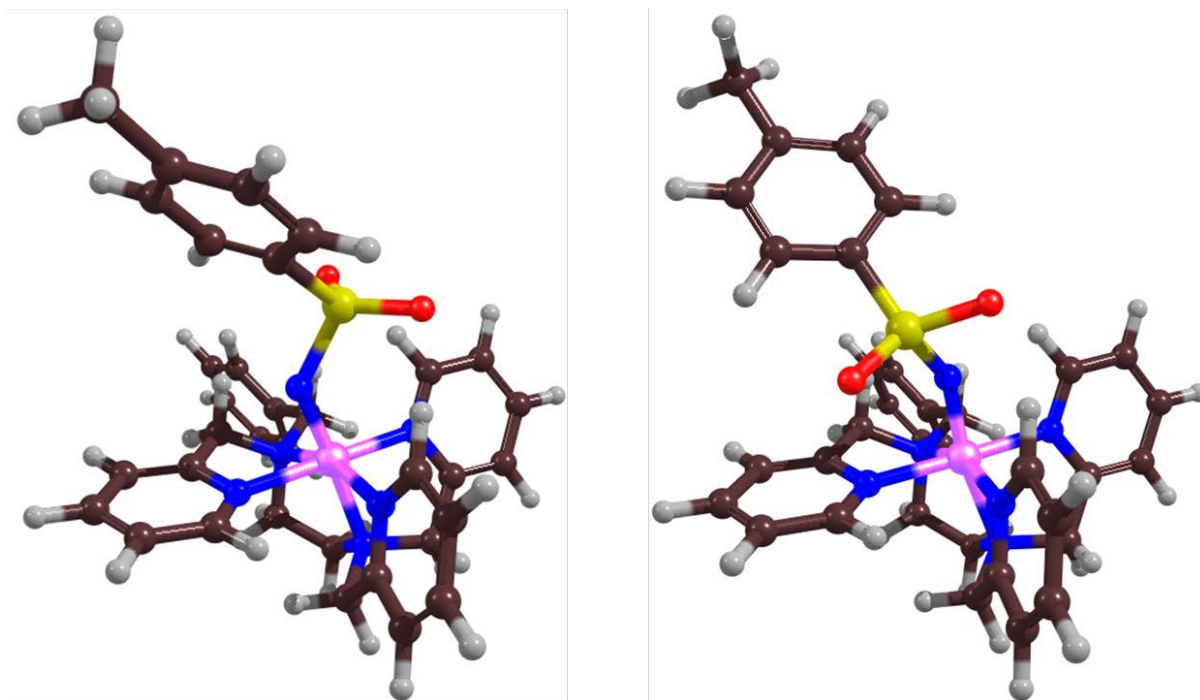


Fig. S9. UB3LYP/BS1 optimized structures of $^1[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ conformers, **14a** (left) vs **14b** (right, ground state).

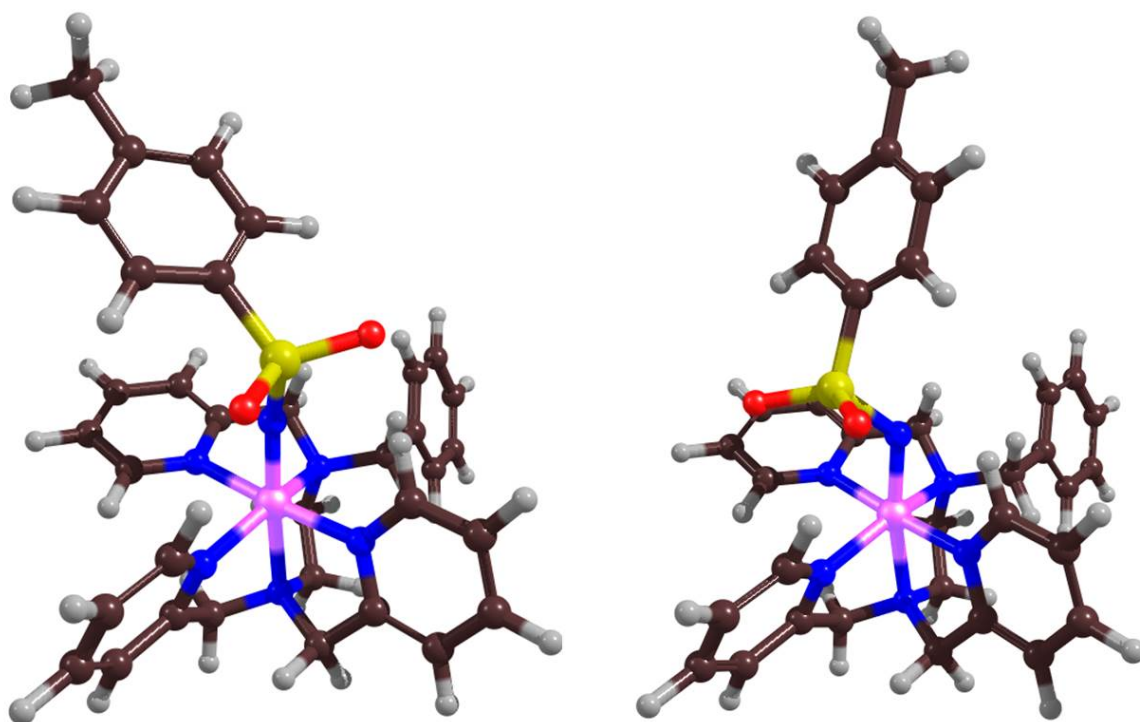


Fig. S10. UB3LYP/BS1 optimized structures of $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ conformers, **34a** (left) vs **34b** (right, ground state).

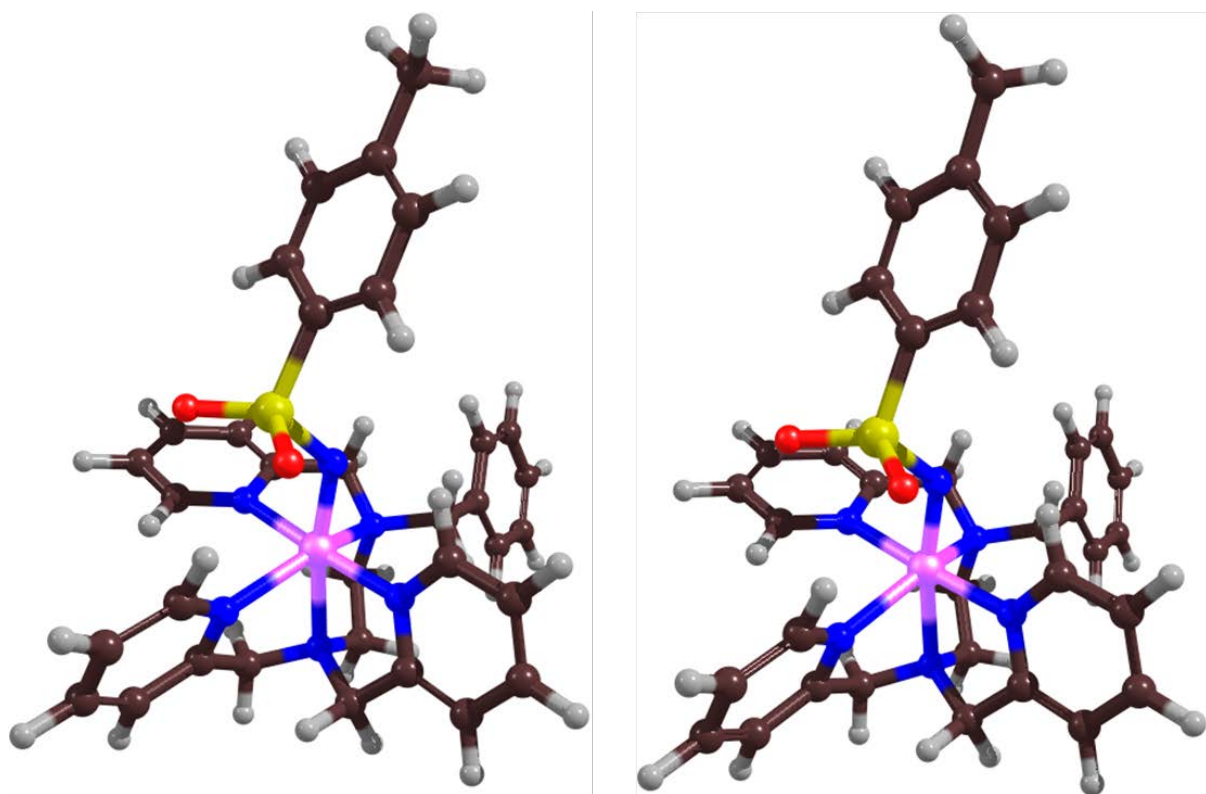


Fig. S11. UB3LYP/BS1 optimized structures of $^5[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{+2}$ conformers, **54a** (left) vs **54b** (right). In this multiplicity, the first conformer fell to the alternate configuration during the geometry optimization, maintaining only a rotation on the terminal methyl group.

Table S5: Absolute energies, zero-point energies and free energies (in au) of $^{1,3,5}\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ conformers (UB3LYP/BS2//UB3LYP/BS1):

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^1\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4a	-2316.747088	-2316.087420	-2316.158078	-2317.760018	-2317.954766	-2317.295099
$^1\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4b	-2316.756303	-2316.097270	-2316.169344	-2317.768880	-2317.963659	-2317.304626
$^3\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4a	-2316.760333	-2316.101261	-2316.173477	-2317.781553	-2317.978599	-2317.319527
$^3\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4b	-2316.767133	-2316.108765	-2316.181305	-2317.788015	-2317.983413	-2317.325044
$^5\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4a	-2316.758460	-2316.102277	-2316.175878	-2317.786669	-2317.979395	-2317.323211
$^5\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4b	-2316.758586	-2316.102211	-2316.177522	-2317.786538	-2317.979154	-2317.322779

Table S6: Relative energies (in kcal mol $^{-1}$) of $^{1,3,5}\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ conformers as calculated at UB3LYP/BS2//UB3LYP/BS1 in Gaussian:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^1\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4a	12.58	13.39	14.58	17.57	17.98	18.79
$^1\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4b	6.80	7.21	7.51	12.01	12.40	12.81
$^3\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4a	4.27	4.71	4.91	4.05	3.02	3.46
$^3\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4b	0.00	0.00	0.00	0.00	0.00	0.00
$^5\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4a	5.44	4.07	3.41	0.84	2.52	1.15
$^5\text{[Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4b	5.36	4.11	2.37	0.93	2.67	1.42

Table S7: Absolute energies, zero-point energies and free energies (in au) of the reaction of $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ with CHD and DMS as calculated at UB3LYP/BS2//UB3LYP/BS1 in Gaussian:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$ Conformer 4b	-2316.767133	-2316.108765	-2316.181305	-2317.788015	-2317.983413	-2317.325044
Isolated CHD	-233.3654783	-233.2417720	-233.2700250	-233.4714593	-233.4737984	-233.3500922
Isolated DMS	-477.9683283	-477.8917730	-477.9191340	-478.0558687	-478.0597978	-477.9832425
$^3\text{CHD_RC}$	-2550.136246	-2549.353602	-2549.439580	-2551.260678	-2551.454512	-2550.671868
$^3\text{CHD_TS1}$	-2550.121438	-2549.342958	-2549.422249	-2551.237799	-2551.426569	-2550.648089
$^3\text{CHD_IR1}$	-2550.163508	-2549.381481	-2549.465509	-2551.290150	-2551.484257	-2550.702230
$^3\text{CHD_Prd}$	-2550.246871	-2549.463347	-2549.548443	-2551.370938	-2551.556669	-2550.773145
$^3\text{DMS_RC}$	-2794.745784	-2794.009761	-2794.094298	-2795.852637	-2796.042962	-2795.306940
$^3\text{DMS_TS}$	-2794.713449	-2793.978496	-2794.059186	-2795.816205	-2796.002396	-2795.267443
$^3\text{DMS_Prd}$	-2794.765829	-2794.030557	-2794.114240	-2795.882169	-2796.057584	-2795.322312
$^3\text{DMS_Prd Alternative}$	-2794.741713	-2794.006349	-2794.092307	-2795.860315	-2796.048643	-2795.313280
$^3\text{CHD_TS1_Deuterium1}$	-2550.121438	-2549.344828	-2549.424178	-2551.237799	-2551.426569	-2550.649959
$^3\text{CHD_TS1_Deuterium2}$	-2550.121438	-2549.346334	-2549.425700	-2551.237799	-2551.426569	-2550.651465
$^5\text{DMS_RC}$	-2794.737517	-2794.003688	-2794.092102	-2795.851566	-2796.038992	-2795.305163
$^5\text{DMS_TS1}$	-2794.744280	-2794.010841	-2794.094415	-2795.854501	-2796.034029	-2795.300590
$^5\text{DMS_Prd}$	-2794.787983	-2794.054197	-2794.140388	-2795.907855	-2796.082901	-2795.349115
Isolated CHD Deuterium 1	-233.3654783	-233.2450530	-233.2734320	-233.4714593	-233.4737984	-233.353373
Isolated CHD Deuterium 2	-233.3654783	-233.2451330	-233.2735070	-233.4714593	-233.4737984	-233.353453

Table S8: Relative energies (in kcal mol⁻¹) of the reaction of $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ with CHD and DMS as calculated at UB3LYP/BS2//UB3LYP/BS1 in Gaussian:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	SCF	E+ZPC	G	SCF	SCF	E+ZPC
$^3\text{CHD_RC}$	-2.3	-1.9	7.4	-0.8	1.7	2.1
$^3\text{CHD_TS1}$	7.0	4.8	18.2	13.6	19.2	17.0
$^3\text{CHD_IR1}$	-19.4	-19.4	-8.9	-19.2	-17.0	-17.0
$^3\text{CHD_Prd}$	-71.7	-70.8	-60.9	-69.9	-62.4	-61.5
$^3\text{DMS_RC}$	-6.5	-5.8	3.9	-5.5	0.2	0.8
$^3\text{DMS_TS}$	13.8	13.8	25.9	17.4	25.6	25.6
$^3\text{DMS_Prd}$	-19.1	-18.8	-8.7	-24.0	-9.0	-8.8
$^3\text{DMS_Prd Alternative}$	-3.9	-3.6	5.1	-10.3	-3.4	-3.1
$^5\text{DMS_RC}$	-1.3	-2.0	5.2	-4.8	2.6	2.0
$^5\text{DMS_TS1}$	-5.5	-6.5	3.8	-6.7	5.8	4.8
$^5\text{DMS_Prd}$	-33.0	-33.7	-25.1	-40.1	-24.9	-25.6

Table S9: Kinetic Isotope Effects of CHD Reactions with $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ (UB3LYP/BS1) for the transition state for $\text{Fe}(\text{NTS})-\text{H}^1-\text{CH}^2\text{R}$:

Kinetic Isotope Effects	i Frequency	KIE Eyring	KIE Wigner
$^3\text{CHD_TS1_H}^1\text{H}^2$	842.3		
$^3\text{CHD_TS1_D}^1\text{H}^2$	663.0	4.79	5.66
$^3\text{CHD_TS1_H}^1\text{D}^2$	824.2	1.03	1.05

Table S10: Spin densities of key fragments of intermediates and transition states along the reaction of $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ at the UB3LYP/BS1//BS2//BS2+Solvent levels of theory:

$^3\text{CHD_RC}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	0.98	0.90	0.97
	(NTs)(Bntpen)	1.02	1.10	1.03
	Substrate	0.00	0.00	0.00
	Total	2.00	2.00	2.00
$^3\text{CHD_TS1}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	0.65	0.63	0.74
	(NTs)(Bntpen)	0.72	0.78	0.64
	Substrate	0.63	0.59	0.62
	Total	2.00	2.00	2.00
$^3\text{CHD_IR1}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	0.86	0.86	0.92
	(NTs)(Bntpen)	0.16	0.14	0.08
	Substrate	0.98	1.00	1.00
	Total	2.00	2.00	2.00
$^3\text{CHD_Prd}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	2.00	1.95	1.95
	(NTs)(Bntpen)	0.00	0.05	0.05
	Substrate	0.00	0.00	0.00
	Total	2.00	2.00	2.00
$^3\text{DMS_RC}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	0.97	0.85	0.94
	(NTs)(Bntpen)	1.03	1.15	1.06
	Substrate	0.00	0.00	0.00
	Total	2.00	2.00	2.00
$^3\text{DMS_TS}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	1.75	1.77	1.71
	(NTs)(Bntpen)	0.19	0.13	0.11
	Substrate	0.06	0.09	0.18
	Total	2.00	2.00	2.00
$^3\text{DMS_Prd}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	1.98	1.97	1.97
	(NTs)(Bntpen)	0.02	0.03	0.03
	Substrate	0.00	0.00	0.00
	Total	2.00	2.00	2.00
$^3\text{DMS_Prd_Alternative}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	2.02	2.01	1.99
	(NTs)(Bntpen)	-0.02	-0.01	0.01
	Substrate	0.00	0.00	0.00
	Total	2.00	2.00	2.00

Table S11: Scan Data for the pathway around CHD-TS2 calculated at UB3LYP/BS1 for $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$

NH Distance	Abs Energy a.u.	NH Distance	Abs Energy a.u.
2.2768	-2550.163357	1.5868	-2550.176742
2.2468	-2550.163571	1.5568	-2550.187398
2.2168	-2550.163798	1.5268	-2550.189256
2.1868	-2550.164042	1.4968	-2550.191536
2.1568	-2550.164305	1.4668	-2550.194308
2.1268	-2550.164583	1.4368	-2550.197595
2.0968	-2550.164880	1.4068	-2550.201368
2.0668	-2550.165196	1.3768	-2550.205520
2.0368	-2550.165534	1.3468	-2550.209956
2.0068	-2550.165895	1.3168	-2550.215145
1.9768	-2550.166279	1.2868	-2550.219789
1.9468	-2550.166688	1.2568	-2550.224391
1.9168	-2550.167124	1.2268	-2550.228862
1.8868	-2550.167593	1.1968	-2550.233110
1.8568	-2550.168100	1.1668	-2550.237028
1.8268	-2550.168656	1.1368	-2550.240499
1.7968	-2550.169269	1.1068	-2550.243379
1.7668	-2550.169951	1.0768	-2550.245508
1.7368	-2550.170715	1.0468	-2550.246696
1.7068	-2550.171583	1.0168	-2550.246719
1.6768	-2550.172579	0.9868	-2550.245312
1.6468	-2550.173745	0.9568	-2550.242157
1.6168	-2550.175115	0.9268	-2550.236878

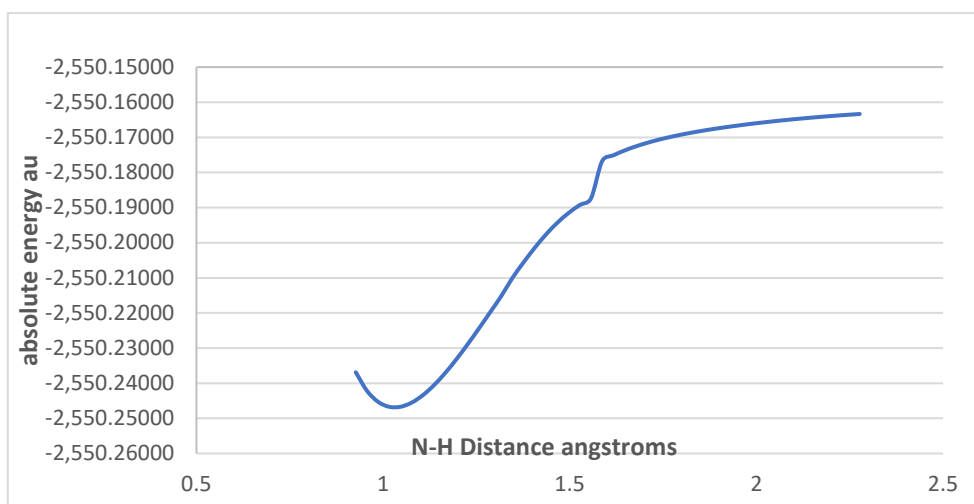


Fig. S12. Plot of the scan data for CHD_TS2, calculated at UB3LYP/BS1 for $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ starting at the radical intermediate on the right-hand-side. As can be seen the second H-atom abstraction is virtually barrierless and collapses to product rapidly.

Table S12: Absolute energies, zero-point energies and free energies (in au) of $^{1,3,5}[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$ structures (UB3LYP/BS2//UB3LYP/BS1):

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^1[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$	-1517.92651	-1517.39483	-1517.45074	-1518.61811	-1518.82014	-1518.288458
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$	-1517.96994	-1517.43836	-1517.49499	-1518.66192	-1518.86381	-1518.332231
$^5[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$	-1517.95804	-1517.42866	-1517.48807	-1518.65803	-1518.85929	-1518.329914

Table S13: Relative (free) energies (in kcal mol⁻¹) of $^{1,3,5}[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$ structures as calculated at UB3LYP/BS2//UB3LYP/BS1 in Gaussian:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^1[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$	27.26	27.32	27.77	27.49	27.41	27.47
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$	0.00	0.00	0.00	0.00	0.00	0.00
$^5[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$	7.47	6.09	4.34	2.44	2.84	1.45

Table S14: Absolute energies, zero-point energies and free energies (in au) for the reaction of $^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$ with CHD and DMS as calculated at UB3LYP/BS2//UB3LYP/BS1:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$	-1517.969940	-1517.438360	-1517.494990	-1518.66192	-1518.86381	-1518.332231
$^3\text{CHD_RC}$	-1751.344524	-1750.688419	-1750.757365	-1752.13930	-1752.33665	-1751.680545
$^3\text{CHD_TS1}$	-1751.337924	-1750.687008	-1750.754127	-1752.12724	-1752.31879	-1751.667877
$^3\text{CHD_IR1}$	-1751.371465	-1750.717895	-1750.786324	-1752.16675	-1752.36175	-1751.708185
$^3\text{CHD_Prd}$	-1751.438452	-1750.784925	-1750.858622	-1752.23069	-1752.42205	-1751.768526
$^5\text{CHD_Prd}$	-2550.262082	-2549.482744	-2549.573178	-2551.384769	-2551.558106	-2550.778768
$^3\text{DMS_RC}$	-1995.948892	-1995.340033	-1995.409585	-1996.72676	-1996.92313	-1996.314270
$^3\text{DMS_TS}$	-1995.928610	-1995.322651	-1995.390831	-1996.71474	-1996.90530	-1996.299345
$^3\text{DMS_Prd}$	-1995.939938	-1995.33289	-1995.401201	-1996.73899	-1996.93043	-1996.323378
$^3\text{CHD_TS1_Deuterium1}$	-1751.337924	-1750.68914	-1750.756328	-1752.12724	-1752.31879	-1751.670009
$^3\text{CHD_TS1_Deuterium2}$	-1751.337924	-1750.690333	-1750.757531	-1752.12724	-1752.31879	-1751.671202
Isolated CHD Deuterium 1	-233.3654783	-233.2450530	-233.2734320	-233.4714593	-233.4737984	-233.353373
Isolated CHD Deuterium 2	-233.3654783	-233.2451330	-233.2735070	-233.4714593	-233.4737984	-233.353453
$^5\text{DMS_Prd}$	-1995.961117	-1995.320563	-1995.426797	-1996.7645093	-1996.9548948	-1996.31434

Table S15: Relative (free) energies (in kcal mol⁻¹) intermediates and transition states along the reaction of ³[Fe^{IV}(O)(Bntpen)]²⁺ with CHD and DMS as calculated at UB3LYP/BS2//UB3LYP/BS1:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
³ CHD_RC	-5.71	-5.20	4.80	-3.72	0.60	1.12
³ CHD_TS1	-1.57	-4.31	6.83	3.85	11.81	9.07
³ CHD_IR1	-22.62	-23.70	-13.37	-20.94	-15.15	-16.23
³ CHD_Prd	-64.65	-65.76	-58.74	-61.06	-52.99	-54.09
⁵ CHD_Prd	-81.2	-83.0	-76.5	-78.6	-63.3	-65.0
³ DMS_RC	-6.67	-6.21	2.85	-5.63	0.30	0.76
³ DMS_TS	6.06	4.69	14.62	1.91	11.49	10.12
³ DMS_Prd	-1.05	-1.73	8.11	-13.30	-4.28	-4.96
³ CHD_TS1_Deuterium1	-1.57	-3.59	7.59	3.85	11.81	9.79
³ CHD_TS1_Deuterium2	-1.57	-4.29	6.88	3.85	11.81	9.09
⁵ DMS_Prd	-14.34	6.01	-7.95	-29.32	-19.63	0.71

Table S16: Kinetic Isotope Effects for the CHD Reactions with ³[Fe^{IV}(O)(Bntpen)]²⁺ as calculated at UB3LYP/BS1 for Fe=O---H¹-CH²R:

Kinetic Isotope Effects	i Frequency	KIE Eyring	KIE Wigner
CHD_TS1_H ¹ H ²	-492.5543		
CHD_TS1_D ¹ H ²	-432.9967	3.59	3.75
CHD_TS1_H ¹ D ²	-472.2792	1.09	1.10

Table S17: Spin densities of key fragments of intermediates and transition states for the reaction of $^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$ as calculated at the UB3LYP/BS1//BS2//BS2+Solvent levels of theory:

$^3\text{CHD_RC}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	1.10	1.21	1.26
	O	0.96	0.91	0.87
	Bntpen	-0.07	-0.12	-0.13
	Substrate	0.00	0.00	0.00
	Total	2.00	2.00	2.00
$^3\text{CHD_TS1}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	0.84	0.82	0.91
	O	0.70	0.69	0.74
	Bntpen	-0.04	0.00	-0.02
	Substrate	0.50	0.48	0.37
	Total	2.00	2.00	2.00
$^3\text{CHD_IR1}$		BS1	BS2	BS2+Solvent
	Fe	0.92	0.91	0.93
	O	0.16	0.14	0.13
	Bntpen	-0.06	-0.04	-0.06
	Substrate	0.98	1.00	1.00
	Total	2.00	2.00	2.00
$^3\text{CHD_Prd}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	1.98	1.98	1.98
	O	0.02	0.02	0.02
	Bntpen	0.00	0.00	0.00
	Substrate	0.00	0.00	0.00
	Total	2.00	2.00	2.00
$^3\text{DMS_RC}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	1.10	1.10	1.20
	O	0.96	0.96	0.90
	Bntpen	-0.06	-0.06	-0.12
	Substrate	0.01	0.01	0.01
	Total	2.00	2.00	2.00
$^3\text{DMS_TS}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	2.32	2.42	2.42
	O	0.00	0.01	0.02
	Bntpen	0.03	0.02	0.01
	Substrate	-0.35	-0.45	-0.45
	Total	2.00	2.00	2.00
$^3\text{DMS_Prd}$	Fragment	BS1	BS2	BS2+Solvent
	Fe	1.96	1.96	1.96
	O	0.04	0.04	0.04
	Bntpen	0.00	-0.01	-0.01
	Substrate	0.00	0.00	0.00
	Total	2.00	2.00	2.00

Table S18: Absolute energies, zero-point energies and free energies (in au) of $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$ complexes and their reactivity with CHD and DMS as calculated at UB3LYP/BS2//UB3LYP/BS1:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$	-2159.57202	-2159.03031	-2159.09761	-2160.52518	-2160.72396	-2160.18224
$^3\text{CHD_TS1 } ^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$	-2392.93046	-2392.26860	-2392.34226	-2393.97862	-2394.16996	-2393.50810
$^3\text{DMS_TS1 } ^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$	-2637.51989	-2636.90181	-2636.97578	-2638.55474	-2638.74557	-2638.12748

Table S19: Relative (free) energies (in kcal mol⁻¹) of the transition states for the reaction of $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$ with CHD and DMS as calculated at UB3LYP/BS2//UB3LYP/BS1:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^3\text{CHD_TS1 } ^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$	4.4	2.2	15.9	11.3	17.4	15.2
$^3\text{DMS_TS1 } ^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$	12.8	12.7	25.7	16.5	24.0	23.8

Table S20: Absolute energies, zero-point energies and free energies (in au) of intermediates and transition states for the reaction of $^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$ with CHD and DMS as calculated at UB3LYP/BS2//UB3LYP/BS1:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$	-1360.774898	-1360.360408	-1360.411359	-1361.399098	-1361.604473	-1361.189983
$^3\text{CHD_TS1 } ^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$	-1594.141754	-1593.608439	-1593.670150	-1594.862335	-1595.055600	-1594.522285
$^3\text{DMS_TS1 } ^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$	-1838.726976	-1838.237678	-1838.299254	-1839.438430	-1839.629284	-1839.139986

Table S21: Relative (free) energies (in kcal mol⁻¹) for transition state for the reaction of $^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$ with CHD and DMS as calculated at UB3LYP/BS2//UB3LYP/BS1:

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^3\text{CHD_TS1 } ^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$	-0.86	-3.93	7.05	5.16	14.23	11.16
$^3\text{DMS_TS1 } ^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$	10.20	9.10	19.60	10.38	21.95	20.86

Table S22: Electron Affinities of Isolated compounds $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$, $^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$, $^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$ and $^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$ in kcal mol⁻¹

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$	193.3	193.8	193.8	193.5	118.2	118.8
$^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{N4Py})]^{2+}$	187.1	189.7	192.2	193.4	116.0	118.6
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$	174.1	176.0	176.4	176.3	93.3	95.2
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{N4Py})]^{2+}$	165.7	167.4	168.4	171.3	87.0	88.7

Table S23: BDE_{NH} and BDE_{OH} energies of Isolated compounds $^{2,4}[\text{Fe}^{\text{III}}(\text{NTs-H})(\text{Bntpen})]^{2+}$, $^{2,4}[\text{Fe}^{\text{III}}(\text{OH})(\text{Bntpen})]^{2+}$, $^{2,4}[\text{Fe}^{\text{III}}(\text{OH})(\text{N4Py})]^{2+}$ and $^{2,4}[\text{Fe}^{\text{III}}(\text{NTs-H})(\text{N4Py})]^{2+}$ in kcal mol⁻¹

System	BS1	BS1	BS1	BS2	BS2+Solvent	BS2+Solvent
	E	E+ZPE	G	E	E	E+ZPE
$^4[\text{Fe}^{\text{III}}(\text{NTs-H})(\text{Bntpen})]^{2+}$	86.3	80.0	75.2	91.3	92.0	85.6
$^2[\text{Fe}^{\text{III}}(\text{NTs-H})(\text{Bntpen})]^{2+}$	92.5	84.5	77.8	94.3	96.7	88.8
$^4[\text{Fe}^{\text{III}}(\text{O-H})(\text{Bntpen})]^{2+}$	85.2	79.7	74.7	88.7	87.6	82.0
$^2[\text{Fe}^{\text{III}}(\text{O-H})(\text{Bntpen})]^{2+}$	86.9	80.3	73.7	86.9	87.5	80.8
$^4[\text{Fe}^{\text{III}}(\text{NTs-H})(\text{N4Py})]^{2+}$	81.3	75.3	70.3	86.0	85.0	79.0
$^2[\text{Fe}^{\text{III}}(\text{NTs-H})(\text{N4Py})]^{2+}$	95.1	87.3	80.4	96.4	98.4	90.7
$^4[\text{Fe}^{\text{III}}(\text{O-H})(\text{N4Py})]^{2+}$	77.2	72.3	66.9	78.8	75.4	70.4
$^2[\text{Fe}^{\text{III}}(\text{O-H})(\text{N4Py})]^{2+}$	90.5	83.9	77.2	90.6	89.7	83.1

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Cartesian coordinates:

¹[Fe^{IV}(NTs)(Bntpen)]²⁺ Conformer 4a:

Fe	-0.751885000	0.270135000	-3.657851000
N	0.257452000	1.993968000	-4.013761000
N	-1.561533000	0.982020000	-1.926011000
N	-2.244501000	1.527444000	-4.449667000
N	-2.129900000	-1.254593000	-3.967217000
N	-0.049254000	-0.560563000	-5.478455000
C	1.365744000	2.448262000	-3.375944000
H	1.679199000	1.908173000	-2.488576000
C	2.045093000	3.584393000	-3.825621000
H	2.924704000	3.922047000	-3.291779000
C	1.571838000	4.270120000	-4.947197000
H	2.084498000	5.152171000	-5.313408000
C	0.400588000	3.822119000	-5.576053000
H	-0.016824000	4.360667000	-6.419337000
C	-0.242012000	2.686222000	-5.089129000
C	-1.561788000	2.168151000	-5.622283000
H	-2.165344000	2.984996000	-6.039181000
H	-1.425289000	1.416920000	-6.404202000
C	-2.582955000	2.593093000	-3.435674000
H	-3.610238000	2.943853000	-3.590678000
H	-1.930059000	3.455480000	-3.594120000
C	-2.389904000	2.061571000	-2.049739000
C	-3.011063000	2.648576000	-0.947547000
H	-3.667680000	3.499171000	-1.092030000
C	-2.780787000	2.129770000	0.330140000
H	-3.246678000	2.578876000	1.199483000
C	-1.956867000	1.009787000	0.454386000
H	-1.762816000	0.554876000	1.417514000
C	-1.374478000	0.454070000	-0.683948000
H	-0.780320000	-0.444336000	-0.601535000
C	-3.467689000	0.703832000	-4.759386000
H	-4.019374000	1.129091000	-5.607451000
H	-4.120546000	0.762979000	-3.884592000
C	-3.084056000	-0.737461000	-5.031676000
H	-3.971430000	-1.378410000	-5.065683000
H	-2.582761000	-0.820323000	-5.997260000
C	-1.343338000	-2.395841000	-4.558676000
H	-2.020484000	-3.157118000	-4.959340000
H	-0.760436000	-2.843347000	-3.748269000
C	-0.416836000	-1.867501000	-5.611709000
C	0.084213000	-2.666129000	-6.641942000
H	-0.246155000	-3.694392000	-6.732641000
C	1.013611000	-2.130076000	-7.537417000
H	1.417407000	-2.736557000	-8.339747000
C	1.415242000	-0.799357000	-7.376481000
H	2.140792000	-0.347457000	-8.041433000
C	0.867460000	-0.047086000	-6.340107000
H	1.167077000	0.978442000	-6.185981000
C	-2.858387000	-1.720785000	-2.691549000
H	-3.383471000	-0.846664000	-2.304593000
H	-2.061920000	-1.978912000	-1.989670000
C	-3.815309000	-2.878597000	-2.871548000
C	-5.177555000	-2.649445000	-3.145954000
H	-5.554746000	-1.631385000	-3.212205000
C	-6.067382000	-3.719078000	-3.289850000
H	-7.115592000	-3.527932000	-3.491853000
C	-5.607841000	-5.034258000	-3.151092000
H	-6.298207000	-5.864042000	-3.253888000
C	-4.260582000	-5.275246000	-2.854385000
H	-3.908480000	-6.291787000	-2.717372000
C	-3.371372000	-4.205313000	-2.712040000
H	-2.336622000	-4.402432000	-2.444557000
N	0.489512000	-0.793673000	-3.118786000

O	1.820429000	0.655135000	-0.833300000
S	1.552535000	-0.795373000	-1.560560000
O	0.572139000	-1.929469000	-0.833795000
C	3.175551000	-1.546418000	-2.033756000
C	3.193891000	-2.868582000	-2.477176000
C	4.323649000	-0.774464000	-1.861939000
H	4.260475000	0.234635000	-1.472389000
H	2.281935000	-3.447684000	-2.556208000
C	4.435123000	-3.432117000	-2.777617000
H	4.481669000	-4.462027000	-3.115373000
C	5.629048000	-2.696004000	-2.627608000
C	5.551475000	-1.365542000	-2.168866000
C	6.965495000	-3.334116000	-2.912261000
H	6.462535000	-0.792329000	-2.034329000
H	7.708988000	-2.593609000	-3.220445000
H	7.353794000	-3.829898000	-2.012506000
H	6.891879000	-4.095055000	-3.694651000

¹[Fe^{IV}(NTs)(Bntpen)]²⁺ Conformer 4b

Fe	-0.703051000	0.505373000	-3.505780000
N	-1.521298000	-0.951092000	-4.604040000
N	0.500308000	1.123766000	-5.042306000
N	-2.118501000	1.587094000	-4.693638000
N	-0.646430000	2.270884000	-2.390621000
N	-1.866583000	-0.039564000	-1.889559000
C	-0.938858000	-2.131780000	-4.932937000
H	0.091729000	-2.278150000	-4.627153000
C	-1.647900000	-3.120576000	-5.621440000
H	-1.154633000	-4.054692000	-5.858918000
C	-2.975244000	-2.887086000	-5.985517000
H	-3.543653000	-3.640996000	-6.517866000
C	-3.561160000	-1.650490000	-5.673833000
H	-4.578318000	-1.427046000	-5.975016000
C	-2.815981000	-0.697847000	-4.984828000
C	-3.318727000	0.689346000	-4.654279000
H	-4.089282000	1.010916000	-5.367210000
H	-3.751676000	0.734841000	-3.650632000
C	-1.602922000	1.696623000	-6.105539000
H	-2.020394000	2.584094000	-6.595292000
H	-1.952175000	0.829018000	-6.674023000
C	-0.102219000	1.707042000	-6.114919000
C	0.637665000	2.199255000	-7.192031000
H	0.129372000	2.670248000	-8.025778000
C	2.029199000	2.060335000	-7.187252000
H	2.620512000	2.431221000	-8.016399000
C	2.640107000	1.426363000	-6.100244000
H	3.712690000	1.281777000	-6.065679000
C	1.851907000	0.972938000	-5.044618000
H	2.270965000	0.469558000	-4.185304000
C	-2.312076000	2.962037000	-4.112018000
H	-3.337722000	3.315152000	-4.279269000
H	-1.645166000	3.637571000	-4.653569000
C	-1.973892000	2.967052000	-2.633997000
H	-1.925952000	3.990510000	-2.246875000
H	-2.737871000	2.433804000	-2.065766000
C	-0.605904000	1.811194000	-0.957595000
H	-0.797754000	2.647002000	-0.277099000
H	0.408112000	1.444168000	-0.763299000
C	-1.607587000	0.707472000	-0.773750000
C	-2.225048000	0.440312000	0.447048000
H	-2.009214000	1.064086000	1.306775000
C	-3.120562000	-0.631334000	0.542492000
H	-3.611434000	-0.854743000	1.482630000
C	-3.366120000	-1.407089000	-0.592414000
H	-4.035911000	-2.256921000	-0.558585000
C	-2.717583000	-1.092753000	-1.785635000

H	-2.859580000	-1.700630000	-2.663312000
C	0.556945000	3.174162000	-2.706929000
H	0.481871000	3.423455000	-3.766097000
H	1.432640000	2.534646000	-2.575327000
C	0.664465000	4.431354000	-1.871993000
C	0.115808000	5.644009000	-2.332170000
H	-0.373010000	5.684983000	-3.302882000
C	0.227281000	6.813447000	-1.572811000
H	-0.192569000	7.741959000	-1.943699000
C	0.897548000	6.787709000	-0.344028000
H	0.991071000	7.694827000	0.242523000
C	1.466763000	5.593499000	0.115628000
H	2.009199000	5.577547000	1.054591000
C	1.354419000	4.425067000	-0.644396000
H	1.829794000	3.512871000	-0.293108000
N	0.667538000	-0.142170000	-2.758439000
O	-0.439073000	-2.757150000	-1.593068000
S	0.897101000	-1.903202000	-1.999201000
O	1.738883000	-2.305779000	-3.377758000
C	2.045963000	-1.792528000	-0.548195000
C	3.371293000	-1.424502000	-0.777346000
C	1.543664000	-2.130591000	0.707715000
H	0.515989000	-2.453540000	0.826169000
H	3.730743000	-1.212226000	-1.777138000
C	4.229119000	-1.383961000	0.324177000
H	5.268833000	-1.112336000	0.175524000
C	3.775364000	-1.712348000	1.618317000
C	2.425739000	-2.082405000	1.789874000
C	4.725748000	-1.708838000	2.789533000
H	2.067266000	-2.353340000	2.777339000
H	5.531212000	-0.981330000	2.654192000
H	4.210526000	-1.482273000	3.727415000
H	5.194704000	-2.694942000	2.906516000

³[Fe^{IV}(NTs)(Bntpen)]²⁺ Conformer 4a

Fe	-0.750858000	0.448537000	-3.597837000
N	0.159833000	2.217135000	-3.978231000
N	-1.664346000	1.106338000	-1.905713000
N	-2.298240000	1.555888000	-4.453353000
N	-1.993764000	-1.201600000	-3.925753000
N	0.136709000	-0.364485000	-5.307697000
C	1.239807000	2.742224000	-3.346234000
H	1.619871000	2.204971000	-2.483149000
C	1.835643000	3.925988000	-3.794636000
H	2.695424000	4.317032000	-3.264873000
C	1.309754000	4.584192000	-4.908436000
H	1.756225000	5.503208000	-5.270452000
C	0.175623000	4.052804000	-5.541027000
H	-0.275833000	4.558521000	-6.387118000
C	-0.381305000	2.872197000	-5.057232000
C	-1.638162000	2.242213000	-5.613836000
H	-2.299237000	2.996962000	-6.058762000
H	-1.416620000	1.494196000	-6.380264000
C	-2.774921000	2.594412000	-3.464363000
H	-3.815750000	2.864121000	-3.677873000
H	-2.178132000	3.501538000	-3.593984000
C	-2.605483000	2.081944000	-2.067681000
C	-3.324630000	2.602249000	-0.991519000
H	-4.070999000	3.369593000	-1.163473000
C	-3.065635000	2.130111000	0.299193000
H	-3.607272000	2.527695000	1.149539000
C	-2.100965000	1.133322000	0.465167000
H	-1.864680000	0.732035000	1.442729000
C	-1.426672000	0.635952000	-0.649553000
H	-0.696839000	-0.152630000	-0.530499000
C	-3.435783000	0.628371000	-4.805938000

H	-3.981090000	1.005391000	-5.680212000
H	-4.128584000	0.637871000	-3.960751000
C	-2.923326000	-0.777994000	-5.048087000
H	-3.755348000	-1.486204000	-5.126543000
H	-2.363324000	-0.825377000	-5.984022000
C	-1.080541000	-2.279096000	-4.441038000
H	-1.659442000	-3.105334000	-4.866763000
H	-0.517365000	-2.662787000	-3.584902000
C	-0.129634000	-1.695879000	-5.444343000
C	0.488532000	-2.469521000	-6.429126000
H	0.238478000	-3.520150000	-6.520879000
C	1.426519000	-1.878926000	-7.280175000
H	1.917771000	-2.464317000	-8.048667000
C	1.719032000	-0.520275000	-7.119839000
H	2.445135000	-0.023881000	-7.751683000
C	1.059695000	0.203022000	-6.128407000
H	1.273435000	1.249615000	-5.977446000
C	-2.755302000	-1.699448000	-2.685679000
H	-3.361368000	-0.861347000	-2.339869000
H	-1.983518000	-1.887977000	-1.935519000
C	-3.621234000	-2.922899000	-2.894765000
C	-4.984140000	-2.786754000	-3.222434000
H	-5.425907000	-1.796450000	-3.307866000
C	-5.793809000	-3.913965000	-3.397642000
H	-6.843783000	-3.793828000	-3.640918000
C	-5.252613000	-5.195065000	-3.238193000
H	-5.880902000	-6.069566000	-3.365369000
C	-3.904409000	-5.344547000	-2.889921000
H	-3.489987000	-6.335133000	-2.737803000
C	-3.095981000	-4.216760000	-2.715676000
H	-2.061285000	-4.344145000	-2.408670000
N	0.514934000	-0.470448000	-2.748176000
O	2.365180000	0.970204000	-1.134141000
S	1.784190000	-0.540873000	-1.387104000
O	0.976289000	-1.319256000	-0.190178000
C	3.139722000	-1.633363000	-2.031638000
C	3.023782000	-3.006562000	-1.825348000
C	4.244025000	-1.028853000	-2.628222000
H	4.312423000	0.048955000	-2.717142000
H	2.168931000	-3.424725000	-1.306643000
C	4.076381000	-3.813826000	-2.263968000
H	4.022892000	-4.885543000	-2.104306000
C	5.216011000	-3.259413000	-2.881634000
C	5.280507000	-1.861835000	-3.056605000
C	6.365824000	-4.139649000	-3.304384000
H	6.160682000	-1.420157000	-3.511780000
H	6.029463000	-5.147624000	-3.563479000
H	6.899782000	-3.722330000	-4.163033000
H	7.092810000	-4.239747000	-2.487487000

$^3[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4b

Fe	-0.759337000	0.587683000	-3.443060000
N	-1.528250000	-0.925041000	-4.564192000
N	0.506299000	1.088033000	-4.936696000
N	-2.111950000	1.610229000	-4.705901000
N	-0.765013000	2.366270000	-2.361803000
N	-1.948698000	0.051925000	-1.850810000
C	-0.935352000	-2.105488000	-4.872280000
H	0.098894000	-2.239997000	-4.575784000
C	-1.632021000	-3.106874000	-5.555917000
H	-1.130057000	-4.040052000	-5.778225000
C	-2.956763000	-2.886188000	-5.936490000
H	-3.515950000	-3.651455000	-6.462350000
C	-3.550477000	-1.645776000	-5.655353000
H	-4.563045000	-1.429657000	-5.976730000
C	-2.816422000	-0.680756000	-4.972300000

C	-3.320049000	0.714715000	-4.682077000
H	-4.064806000	1.030380000	-5.423878000
H	-3.780945000	0.784664000	-3.692264000
C	-1.540844000	1.670835000	-6.102582000
H	-1.910170000	2.562286000	-6.622098000
H	-1.901830000	0.805061000	-6.666081000
C	-0.040353000	1.631092000	-6.060070000
C	0.752744000	2.042192000	-7.132327000
H	0.291157000	2.482764000	-8.008764000
C	2.138750000	1.863557000	-7.066286000
H	2.770850000	2.170999000	-7.891261000
C	2.691488000	1.277323000	-5.923110000
H	3.757490000	1.107794000	-5.838723000
C	1.852322000	0.906509000	-4.874347000
H	2.231385000	0.450615000	-3.972038000
C	-2.338022000	3.003753000	-4.177494000
H	-3.353341000	3.346811000	-4.412884000
H	-1.642301000	3.663086000	-4.702296000
C	-2.079751000	3.047985000	-2.685142000
H	-2.058287000	4.080934000	-2.321228000
H	-2.867542000	2.521697000	-2.142723000
C	-0.782117000	1.957480000	-0.915345000
H	-1.027027000	2.811530000	-0.275971000
H	0.226594000	1.618384000	-0.661290000
C	-1.754242000	0.828057000	-0.742747000
C	-2.384533000	0.544949000	0.468031000
H	-2.222432000	1.191689000	1.322525000
C	-3.213680000	-0.578555000	0.563595000
H	-3.710383000	-0.816611000	1.497040000
C	-3.380862000	-1.390545000	-0.560789000
H	-3.993488000	-2.282394000	-0.524468000
C	-2.730387000	-1.053999000	-1.746687000
H	-2.810894000	-1.684843000	-2.615766000
C	0.454032000	3.254730000	-2.658455000
H	0.419110000	3.478986000	-3.725822000
H	1.318582000	2.611994000	-2.478050000
C	0.543144000	4.531368000	-1.850930000
C	0.000870000	5.732202000	-2.347811000
H	-0.468745000	5.751727000	-3.328685000
C	0.096058000	6.918107000	-1.611929000
H	-0.318382000	7.837468000	-2.010703000
C	0.743631000	6.920590000	-0.370846000
H	0.824860000	7.840556000	0.197237000
C	1.306264000	5.737943000	0.125165000
H	1.831021000	5.743344000	1.074232000
C	1.210159000	4.552962000	-0.611206000
H	1.679361000	3.649163000	-0.231321000
N	0.599476000	-0.079404000	-2.441446000
O	-0.295190000	-2.700218000	-1.733227000
S	1.051386000	-1.846329000	-2.112085000
O	1.879857000	-2.215968000	-3.492524000
C	2.210572000	-1.840457000	-0.664032000
C	3.563764000	-1.611855000	-0.902705000
C	1.681539000	-2.106215000	0.596697000
H	0.627531000	-2.323245000	0.724237000
H	3.937465000	-1.454794000	-1.907613000
C	4.426017000	-1.640356000	0.195940000
H	5.487167000	-1.477440000	0.039911000
C	3.946358000	-1.897085000	1.496596000
C	2.567775000	-2.127884000	1.676870000
C	4.897714000	-1.964670000	2.665535000
H	2.187482000	-2.343896000	2.669692000
H	5.747346000	-1.288386000	2.533226000
H	4.400450000	-1.712498000	3.606397000
H	5.303995000	-2.979156000	2.773134000

⁵[Fe^{IV}(NTs)(Bntpen)]²⁺ Conformer 4a

Fe	-0.620379000	0.502745000	-3.660612000
N	0.073504000	2.585816000	-4.010195000
N	-1.345253000	0.843115000	-1.758520000
N	-2.398685000	1.618365000	-4.134845000
N	-1.933841000	-1.210285000	-4.297106000
N	0.121702000	0.020151000	-5.634570000
C	1.197562000	3.193111000	-3.546629000
H	1.782322000	2.648973000	-2.813790000
C	1.569759000	4.466217000	-3.987788000
H	2.474508000	4.919807000	-3.602773000
C	0.763040000	5.131862000	-4.915001000
H	1.032631000	6.119003000	-5.272733000
C	-0.417441000	4.518722000	-5.360474000
H	-1.079682000	5.028006000	-6.051629000
C	-0.737310000	3.246589000	-4.890097000
C	-2.004296000	2.516610000	-5.273525000
H	-2.810102000	3.226636000	-5.502998000
H	-1.849970000	1.890947000	-6.157779000
C	-2.767963000	2.439973000	-2.921671000
H	-3.840241000	2.669027000	-2.936069000
H	-2.235331000	3.393844000	-2.975450000
C	-2.371527000	1.736398000	-1.654029000
C	-2.955995000	2.020952000	-0.419070000
H	-3.777206000	2.725830000	-0.357729000
C	-2.462896000	1.395482000	0.731955000
H	-2.901481000	1.609595000	1.699790000
C	-1.399029000	0.493065000	0.617023000
H	-0.988808000	-0.003460000	1.487210000
C	-0.864773000	0.235065000	-0.642663000
H	-0.046978000	-0.455026000	-0.792465000
C	-3.528314000	0.677419000	-4.481139000
H	-4.254581000	1.185811000	-5.128686000
H	-4.040552000	0.435638000	-3.546539000
C	-3.011517000	-0.590379000	-5.141042000
H	-3.833506000	-1.299553000	-5.297332000
H	-2.584216000	-0.366495000	-6.121792000
C	-1.037999000	-2.069315000	-5.129425000
H	-1.614107000	-2.819858000	-5.682467000
H	-0.370471000	-2.599060000	-4.441019000
C	-0.208330000	-1.230311000	-6.064311000
C	0.260221000	-1.724615000	-7.283087000
H	-0.035159000	-2.715242000	-7.609371000
C	1.114468000	-0.937520000	-8.062599000
H	1.491125000	-1.308662000	-9.008762000
C	1.481320000	0.327816000	-7.595944000
H	2.158885000	0.959804000	-8.156047000
C	0.972489000	0.774444000	-6.377648000
H	1.262875000	1.728523000	-5.969943000
C	-2.471266000	-1.984564000	-3.091401000
H	-3.041392000	-1.274730000	-2.487705000
H	-1.585273000	-2.270841000	-2.517824000
C	-3.322547000	-3.193042000	-3.419860000
C	-4.722324000	-3.076132000	-3.515831000
H	-5.201865000	-2.118864000	-3.323940000
C	-5.513947000	-4.189754000	-3.816400000
H	-6.591743000	-4.086816000	-3.878998000
C	-4.915658000	-5.439178000	-4.017372000
H	-5.528518000	-6.304685000	-4.243221000
C	-3.526307000	-5.573458000	-3.904460000
H	-3.062785000	-6.545236000	-4.034902000
C	-2.736117000	-4.459098000	-3.604821000
H	-1.662620000	-4.582305000	-3.488154000
N	0.686594000	-0.569753000	-3.053290000
O	3.060201000	0.404375000	-4.259517000
S	2.476941000	-0.067832000	-2.804854000
O	2.399381000	1.020919000	-1.573585000

C	3.336695000	-1.606394000	-2.229707000
C	3.424581000	-1.831960000	-0.856586000
C	3.896046000	-2.444742000	-3.190551000
H	3.843249000	-2.203189000	-4.245662000
H	3.016849000	-1.122213000	-0.146364000
C	4.106038000	-2.974765000	-0.435070000
H	4.207706000	-3.168101000	0.627707000
C	4.683419000	-3.867564000	-1.362934000
C	4.571626000	-3.581613000	-2.738055000
C	5.410976000	-5.098919000	-0.883633000
H	5.032875000	-4.245582000	-3.461024000
H	4.709177000	-5.830088000	-0.462224000
H	5.954287000	-5.588819000	-1.695271000
H	6.129541000	-4.852370000	-0.094439000

$^5[\text{Fe}^{\text{IV}}(\text{NTs})(\text{Bntpen})]^{2+}$ Conformer 4b

Fe	-0.650385000	0.535203000	-3.378511000
N	-1.623563000	-1.069003000	-4.570636000
N	0.712057000	1.049341000	-4.839739000
N	-1.952195000	1.560994000	-4.754786000
N	-0.842698000	2.485228000	-2.275279000
N	-2.015905000	0.058883000	-1.770169000
C	-1.178176000	-2.329328000	-4.814032000
H	-0.170267000	-2.563541000	-4.491760000
C	-1.982601000	-3.270674000	-5.462526000
H	-1.599728000	-4.268250000	-5.637894000
C	-3.266456000	-2.903925000	-5.876080000
H	-3.909040000	-3.617915000	-6.378476000
C	-3.707844000	-1.590193000	-5.658047000
H	-4.684930000	-1.269669000	-6.001842000
C	-2.864071000	-0.693954000	-5.004838000
C	-3.220855000	0.754425000	-4.761187000
H	-3.909782000	1.122907000	-5.532992000
H	-3.707436000	0.885298000	-3.789886000
C	-1.303605000	1.533235000	-6.118836000
H	-1.662794000	2.375330000	-6.722321000
H	-1.614469000	0.617532000	-6.630437000
C	0.195444000	1.537527000	-6.004764000
C	1.029248000	1.940755000	-7.048772000
H	0.601003000	2.335521000	-7.962983000
C	2.416122000	1.818587000	-6.903614000
H	3.077600000	2.121646000	-7.707057000
C	2.935778000	1.299783000	-5.711997000
H	4.002655000	1.183974000	-5.569152000
C	2.057803000	0.928130000	-4.697205000
H	2.401491000	0.524724000	-3.755637000
C	-2.158808000	2.990493000	-4.311290000
H	-3.114311000	3.368426000	-4.698044000
H	-1.365479000	3.586116000	-4.769898000
C	-2.102318000	3.114809000	-2.797932000
H	-2.157104000	4.169320000	-2.501249000
H	-2.951042000	2.602268000	-2.338147000
C	-1.007272000	2.082620000	-0.845605000
H	-1.331109000	2.930527000	-0.231335000
H	-0.022576000	1.764521000	-0.485924000
C	-1.968946000	0.930365000	-0.723237000
C	-2.731873000	0.722293000	0.427362000
H	-2.690806000	1.443612000	1.235479000
C	-3.532401000	-0.420979000	0.525113000
H	-4.127056000	-0.599859000	1.413504000
C	-3.544308000	-1.330494000	-0.536090000
H	-4.132072000	-2.238723000	-0.492549000
C	-2.772597000	-1.064055000	-1.665832000
H	-2.730237000	-1.760191000	-2.486971000
C	0.399584000	3.358143000	-2.464293000
H	0.499588000	3.533438000	-3.537920000

H	1.240030000	2.732172000	-2.151552000
C	0.391458000	4.674081000	-1.715675000
C	-0.083007000	5.846203000	-2.334549000
H	-0.420601000	5.816446000	-3.368131000
C	-0.089049000	7.065017000	-1.647787000
H	-0.449504000	7.961808000	-2.139714000
C	0.387329000	7.129329000	-0.333089000
H	0.389965000	8.074711000	0.197891000
C	0.880402000	5.974737000	0.287361000
H	1.272908000	6.026850000	1.297037000
C	0.885376000	4.756921000	-0.400182000
H	1.299616000	3.874469000	0.080388000
N	0.631657000	-0.096853000	-2.291106000
O	-0.280371000	-2.692638000	-1.580316000
S	1.070221000	-1.911196000	-2.074946000
O	1.746791000	-2.307992000	-3.521387000
C	2.356822000	-1.945996000	-0.741262000
C	3.695748000	-1.885299000	-1.121333000
C	1.929659000	-2.069778000	0.579393000
H	0.877123000	-2.155571000	0.822549000
H	3.978829000	-1.832878000	-2.166084000
C	4.655421000	-1.944939000	-0.108058000
H	5.706907000	-1.913573000	-0.372796000
C	4.283189000	-2.064088000	1.246493000
C	2.911911000	-2.125212000	1.570452000
C	5.331856000	-2.164953000	2.325611000
H	2.612007000	-2.233023000	2.607438000
H	6.258522000	-1.661345000	2.036419000
H	4.984219000	-1.731968000	3.268117000
H	5.580329000	-3.216327000	2.523175000

BnTPEN: ³TS1_{NTs,CHD}

Fe	-0.150957000	0.939272000	-2.945593000
N	-0.834505000	-0.563488000	-4.155610000
N	1.065627000	1.508334000	-4.488362000
N	-1.572180000	1.943771000	-4.168233000
N	-0.238666000	2.726715000	-1.806857000
N	-1.363624000	0.354989000	-1.382216000
C	-0.177456000	-1.673068000	-4.573003000
H	0.864244000	-1.771729000	-4.297083000
C	-0.813540000	-2.657076000	-5.335813000
H	-0.255005000	-3.533282000	-5.639650000
C	-2.155415000	-2.495666000	-5.681834000
H	-2.672662000	-3.250541000	-6.262746000
C	-2.820063000	-1.322065000	-5.295921000
H	-3.847024000	-1.142056000	-5.593386000
C	-2.136529000	-0.370556000	-4.543406000
C	-2.720852000	0.976301000	-4.177486000
H	-3.492824000	1.277677000	-4.898020000
H	-3.173761000	0.974290000	-3.182271000
C	-1.026564000	2.113159000	-5.562221000
H	-1.436818000	3.018628000	-6.023664000
H	-1.362227000	1.270903000	-6.176006000
C	0.474385000	2.114276000	-5.556073000
C	1.216556000	2.571846000	-6.647558000
H	0.715129000	3.067727000	-7.471122000
C	2.595766000	2.347231000	-6.680242000
H	3.188048000	2.684725000	-7.522874000
C	3.186181000	1.646783000	-5.623504000
H	4.240747000	1.399832000	-5.636804000
C	2.398056000	1.245910000	-4.545912000
H	2.794636000	0.662460000	-3.731108000
C	-1.878316000	3.299200000	-3.588369000
H	-2.916914000	3.584745000	-3.800247000
H	-1.234901000	4.021063000	-4.096938000
C	-1.603457000	3.318595000	-2.101684000
H	-1.658153000	4.341142000	-1.713002000
H	-2.347436000	2.723209000	-1.571175000
C	-0.239673000	2.261578000	-0.379716000
H	-0.520257000	3.075627000	0.298416000
H	0.778165000	1.942323000	-0.138485000
C	-1.183163000	1.098652000	-0.250209000
C	-1.822168000	0.777724000	0.947219000
H	-1.674332000	1.403076000	1.820304000
C	-2.654917000	-0.346808000	1.001428000
H	-3.163223000	-0.610390000	1.921846000
C	-2.818199000	-1.119021000	-0.150687000
H	-3.439550000	-2.005581000	-0.150775000
C	-2.154594000	-0.746658000	-1.320092000
H	-2.228728000	-1.347165000	-2.210618000
C	0.892306000	3.716322000	-2.086028000
H	0.933404000	3.837222000	-3.170054000
H	1.807827000	3.205644000	-1.781341000
C	0.770308000	5.073702000	-1.421728000
C	0.317039000	6.181541000	-2.162607000
H	0.071310000	6.062954000	-3.215428000
C	0.205557000	7.444846000	-1.571685000
H	-0.138225000	8.289060000	-2.159333000
C	0.549080000	7.619772000	-0.226226000
H	0.466356000	8.598335000	0.233483000
C	1.015362000	6.530299000	0.519743000
H	1.298894000	6.667187000	1.557894000
C	1.129741000	5.268808000	-0.074276000
H	1.527550000	4.441528000	0.505296000
N	1.263547000	0.231310000	-1.982667000
O	0.058927000	-2.361622000	-1.762139000
S	1.513931000	-1.595485000	-1.759049000

O	2.606004000	-1.964243000	-2.945631000
C	2.318332000	-2.019913000	-0.128353000
C	3.622016000	-2.507262000	-0.158946000
C	1.561203000	-1.944178000	1.038564000
H	0.528021000	-1.617215000	1.017670000
H	4.148885000	-2.600419000	-1.101886000
C	4.200549000	-2.905608000	1.051174000
H	5.211543000	-3.299862000	1.050498000
C	3.485999000	-2.829288000	2.262560000
C	2.163346000	-2.342306000	2.236042000
C	4.106683000	-3.303903000	3.554130000
H	1.593816000	-2.297730000	3.158719000
H	5.189776000	-3.150046000	3.561874000
H	3.680569000	-2.790409000	4.420975000
H	3.931350000	-4.378743000	3.693757000
H	4.686743000	0.442033000	0.756953000
H	2.957318000	0.499059000	0.804490000
C	3.822909000	1.026857000	0.385394000
C	3.928552000	2.405599000	0.963910000
H	3.736838000	2.520513000	2.027369000
H	4.471633000	4.447125000	0.674746000
C	4.338864000	3.472068000	0.218856000
C	4.641964000	3.309958000	-1.179659000
H	5.076161000	4.143372000	-1.722132000
H	2.630313000	0.803132000	-1.548795000
H	4.681431000	2.017708000	-2.870859000
C	4.417102000	2.110213000	-1.821987000
C	3.826032000	0.964668000	-1.149347000
H	4.202823000	0.010804000	-1.535823000

BnTPEN: ³IR1_{NTs,CHD}

Fe	-0.299480000	0.861596000	-3.036923000
N	-0.998864000	-0.615316000	-4.243697000
N	1.020347000	1.464830000	-4.488439000
N	-1.619641000	1.901191000	-4.277962000
N	-0.312536000	2.608761000	-1.873627000
N	-1.585729000	0.296464000	-1.530524000
C	-0.373598000	-1.762961000	-4.601898000
H	0.650860000	-1.901777000	-4.277852000
C	-1.026306000	-2.739487000	-5.361264000
H	-0.497219000	-3.648542000	-5.617625000
C	-2.344676000	-2.527664000	-5.765935000
H	-2.871803000	-3.274567000	-6.348258000
C	-2.974037000	-1.317544000	-5.433806000
H	-3.981929000	-1.104858000	-5.771992000
C	-2.279637000	-0.378000000	-4.678029000
C	-2.818002000	0.994490000	-4.338503000
H	-3.537396000	1.337030000	-5.093205000
H	-3.314752000	1.015535000	-3.364851000
C	-1.025550000	2.043717000	-5.657440000
H	-1.426822000	2.937766000	-6.147759000
H	-1.333362000	1.185532000	-6.262460000
C	0.471148000	2.063011000	-5.585148000
C	1.255264000	2.553639000	-6.630684000
H	0.782049000	3.037257000	-7.477747000
C	2.642443000	2.388843000	-6.583168000
H	3.268551000	2.755212000	-7.388305000
C	3.199823000	1.723437000	-5.487576000
H	4.265457000	1.542097000	-5.424214000
C	2.367365000	1.279002000	-4.462077000
H	2.772482000	0.744121000	-3.619905000
C	-1.867319000	3.275796000	-3.703673000
H	-2.882101000	3.614281000	-3.947289000
H	-1.169292000	3.957725000	-4.195683000
C	-1.634491000	3.282190000	-2.208492000
H	-1.634029000	4.306650000	-1.822145000

H	-2.427887000	2.736199000	-1.696341000
C	-0.391656000	2.120358000	-0.453371000
H	-0.653692000	2.941378000	0.222742000
H	0.599067000	1.749364000	-0.176056000
C	-1.391382000	1.003165000	-0.377127000
C	-2.063529000	0.680070000	0.801423000
H	-1.903041000	1.277190000	1.691815000
C	-2.941852000	-0.409862000	0.815363000
H	-3.473868000	-0.675590000	1.721553000
C	-3.115522000	-1.148086000	-0.357001000
H	-3.767573000	-2.011673000	-0.387151000
C	-2.417638000	-0.776242000	-1.505086000
H	-2.502276000	-1.355783000	-2.408345000
C	0.884924000	3.552620000	-2.068546000
H	0.950694000	3.745995000	-3.140416000
H	1.769322000	2.977701000	-1.779837000
C	0.814598000	4.858467000	-1.305333000
C	0.337484000	6.022743000	-1.937840000
H	0.042511000	5.988396000	-2.984418000
C	0.269361000	7.237340000	-1.247307000
H	-0.092452000	8.127245000	-1.750604000
C	0.683355000	7.305203000	0.088227000
H	0.635905000	8.246455000	0.624480000
C	1.179288000	6.159685000	0.722823000
H	1.524215000	6.216084000	1.749649000
C	1.249776000	4.945991000	0.030631000
H	1.684224000	4.078631000	0.518352000
N	1.045246000	0.044760000	-2.032646000
O	-0.205521000	-2.401961000	-1.623103000
S	1.285927000	-1.737382000	-1.732043000
O	2.285584000	-2.244518000	-2.940393000
C	2.201350000	-1.956178000	-0.123357000
C	3.485720000	-2.490530000	-0.189622000
C	1.543794000	-1.689418000	1.075521000
H	0.524208000	-1.321805000	1.090709000
H	3.935273000	-2.722167000	-1.148289000
C	4.148403000	-2.743114000	1.015809000
H	5.147058000	-3.166461000	0.990998000
C	3.535388000	-2.480410000	2.256378000
C	2.229846000	-1.947532000	2.265645000
C	4.244847000	-2.802546000	3.548865000
H	1.740190000	-1.753825000	3.214431000
H	5.328667000	-2.689426000	3.452785000
H	3.903908000	-2.163244000	4.368349000
H	4.052679000	-3.842308000	3.844831000
H	5.377117000	0.592525000	0.977179000
H	3.646919000	0.576957000	0.913390000
C	4.519947000	1.145536000	0.543154000
C	4.505739000	2.549825000	1.089492000
H	4.433981000	2.666471000	2.167160000
H	4.671872000	4.641324000	0.720464000
C	4.644438000	3.649034000	0.280425000
C	4.774922000	3.519260000	-1.131449000
H	4.921904000	4.398995000	-1.747572000
H	1.960493000	0.488200000	-1.878248000
H	4.897742000	2.140324000	-2.795227000
C	4.753876000	2.225629000	-1.720901000
C	4.604932000	1.087028000	-0.961821000
H	4.662559000	0.104470000	-1.424284000

BnTPEN: ³PrdNTs,CHD

Fe	-0.348817000	0.906536000	-2.639227000
N	-0.805736000	-0.642252000	-4.131172000
N	1.282686000	1.689861000	-3.631396000
N	-1.321971000	1.988088000	-4.422938000
N	-0.953939000	2.788373000	-1.629035000

N	-1.971334000	0.272287000	-1.552233000
C	-0.239402000	-1.870857000	-4.230878000
H	0.564591000	-2.092371000	-3.544741000
C	-0.696493000	-2.833069000	-5.132895000
H	-0.216600000	-3.802801000	-5.176367000
C	-1.778791000	-2.521950000	-5.961368000
H	-2.159283000	-3.248439000	-6.670124000
C	-2.359626000	-1.251385000	-5.869508000
H	-3.190287000	-0.974999000	-6.509308000
C	-1.854747000	-0.331383000	-4.948325000
C	-2.420857000	1.066203000	-4.806886000
H	-2.910233000	1.374171000	-5.743291000
H	-3.179276000	1.093019000	-4.016885000
C	-0.282451000	2.076989000	-5.483149000
H	-0.478619000	2.916821000	-6.164224000
H	-0.321640000	1.168515000	-6.092850000
C	1.093440000	2.198242000	-4.885740000
C	2.138705000	2.782710000	-5.608882000
H	1.943229000	3.179571000	-6.598729000
C	3.417287000	2.852090000	-5.053495000
H	4.236064000	3.298215000	-5.605915000
C	3.610634000	2.347818000	-3.763697000
H	4.573941000	2.396554000	-3.273100000
C	2.530068000	1.787072000	-3.089137000
H	2.661966000	1.426868000	-2.079905000
C	-1.755417000	3.334801000	-3.949101000
H	-2.622232000	3.697060000	-4.521179000
H	-0.934442000	4.030129000	-4.145138000
C	-2.090434000	3.326414000	-2.462526000
H	-2.351858000	4.339277000	-2.132885000
H	-2.960447000	2.691002000	-2.282181000
C	-1.486031000	2.306927000	-0.312238000
H	-2.043989000	3.094753000	0.207047000
H	-0.630076000	2.040882000	0.319527000
C	-2.339982000	1.090680000	-0.522244000
C	-3.420122000	0.793186000	0.307855000
H	-3.686787000	1.477243000	1.104923000
C	-4.134945000	-0.390596000	0.109717000
H	-4.972215000	-0.642462000	0.750135000
C	-3.743784000	-1.242777000	-0.925528000
H	-4.256347000	-2.179132000	-1.107191000
C	-2.666609000	-0.884012000	-1.732878000
H	-2.329473000	-1.536884000	-2.518998000
C	0.158588000	3.813404000	-1.430935000
H	0.567350000	4.026555000	-2.420577000
H	0.939884000	3.302268000	-0.859440000
C	-0.238984000	5.107539000	-0.747332000
C	-0.547885000	6.247711000	-1.512340000
H	-0.484264000	6.203813000	-2.597062000
C	-0.907731000	7.450577000	-0.894930000
H	-1.137181000	8.321497000	-1.499233000
C	-0.957926000	7.532538000	0.501321000
H	-1.231535000	8.465252000	0.981897000
C	-0.637743000	6.411025000	1.276291000
H	-0.658049000	6.476026000	2.358830000
C	-0.278056000	5.209683000	0.656450000
H	-0.010997000	4.354134000	1.271112000
N	1.069631000	-0.213641000	-1.207558000
O	-0.547173000	-0.856719000	0.966223000
S	0.376555000	-1.652209000	-0.112339000
O	-0.221227000	-2.668752000	-1.237376000
C	1.783918000	-2.485076000	0.781665000
C	2.486780000	-3.489368000	0.118505000
C	2.035375000	-2.102637000	2.098513000
H	1.427466000	-1.350773000	2.588170000
H	2.222630000	-3.793824000	-0.887664000
C	3.514852000	-4.125869000	0.818603000

H	4.074464000	-4.917541000	0.331991000
C	3.822050000	-3.774377000	2.149363000
C	3.068121000	-2.759023000	2.773425000
C	4.907034000	-4.498573000	2.905792000
H	3.280535000	-2.490672000	3.802814000
H	5.673909000	-4.893645000	2.233785000
H	5.392412000	-3.846237000	3.637446000
H	4.487230000	-5.349991000	3.457976000
H	4.116334000	-0.289484000	0.818222000
H	1.527998000	0.427601000	-0.543029000
C	4.131657000	0.778007000	0.620950000
C	3.152259000	1.612041000	1.184691000
H	2.384433000	1.192179000	1.829893000
H	2.480634000	3.652075000	1.449594000
C	3.211864000	3.000342000	0.981954000
C	4.248405000	3.553053000	0.218572000
H	4.309964000	4.628072000	0.085825000
H	1.790397000	-0.644946000	-1.799188000
H	6.052879000	3.153661000	-0.897398000
C	5.228384000	2.720116000	-0.340041000
C	5.169392000	1.333490000	-0.142280000
H	5.946959000	0.693861000	-0.547749000

BnTPEN: ³TS1_{NTs,DMS}

Fe	-0.687101000	0.663365000	-3.426635000
N	-1.379744000	-0.942350000	-4.544195000
N	0.424459000	1.222083000	-5.042439000
N	-2.281207000	1.562659000	-4.772267000
N	-1.015706000	2.556153000	-2.408011000
N	-1.788591000	0.071626000	-1.790614000
C	-0.672591000	-2.053434000	-4.873027000
H	0.368062000	-2.089725000	-4.581335000
C	-1.260281000	-3.112727000	-5.569579000
H	-0.665313000	-3.985371000	-5.807508000
C	-2.602922000	-3.025481000	-5.942381000
H	-3.083403000	-3.838176000	-6.474904000
C	-3.315275000	-1.854519000	-5.647881000
H	-4.344652000	-1.736012000	-5.966677000
C	-2.679990000	-0.824364000	-4.956653000
C	-3.336490000	0.509793000	-4.680113000
H	-4.156325000	0.688655000	-5.390392000
H	-3.759816000	0.542903000	-3.670859000
C	-1.715265000	1.671491000	-6.148669000
H	-2.147523000	2.526151000	-6.683702000
H	-1.995862000	0.778585000	-6.718588000
C	-0.210795000	1.749318000	-6.128370000
C	0.503261000	2.222210000	-7.232414000
H	-0.030503000	2.655971000	-8.070591000
C	1.895731000	2.103245000	-7.257448000
H	2.462844000	2.461500000	-8.108782000
C	2.535879000	1.487063000	-6.178049000
H	3.607242000	1.330377000	-6.176939000
C	1.773949000	1.061965000	-5.091909000
H	2.214240000	0.539712000	-4.259468000
C	-2.678082000	2.902264000	-4.241998000
H	-3.733833000	3.117280000	-4.460281000
H	-2.085050000	3.652310000	-4.771126000
C	-2.423391000	2.989806000	-2.749720000
H	-2.592913000	4.011726000	-2.390814000
H	-3.111076000	2.335198000	-2.210677000
C	-0.975340000	2.201102000	-0.951425000
H	-1.355477000	3.021946000	-0.332720000
H	0.069547000	2.020662000	-0.687038000
C	-1.762151000	0.939757000	-0.736164000
C	-2.409563000	0.652594000	0.465898000
H	-2.383675000	1.373186000	1.275304000

C	-3.091923000	-0.561176000	0.605800000
H	-3.603019000	-0.801091000	1.531113000
C	-3.103595000	-1.453868000	-0.468835000
H	-3.609407000	-2.408751000	-0.401338000
C	-2.439372000	-1.111905000	-1.646297000
H	-2.394115000	-1.796960000	-2.475274000
C	0.019779000	3.623667000	-2.764707000
H	-0.020107000	3.740928000	-3.849572000
H	0.990403000	3.186983000	-2.521452000
C	-0.151726000	4.966693000	-2.083642000
C	-0.855340000	6.007450000	-2.718500000
H	-1.265635000	5.855056000	-3.713933000
C	-1.006283000	7.252977000	-2.099547000
H	-1.544903000	8.046879000	-2.605304000
C	-0.448545000	7.478138000	-0.835683000
H	-0.559111000	8.444798000	-0.357068000
C	0.269260000	6.458011000	-0.199482000
H	0.721474000	6.636997000	0.770041000
C	0.418939000	5.214228000	-0.821170000
H	1.005556000	4.441164000	-0.331586000
N	0.875344000	0.183270000	-2.067974000
O	-0.031366000	-2.465080000	-2.032838000
S	1.377775000	-1.619805000	-2.091355000
O	2.346640000	-1.858569000	-3.412073000
C	2.359875000	-2.064036000	-0.572054000
C	3.615447000	-2.637296000	-0.759721000
C	1.763852000	-1.932986000	0.681123000
H	0.766401000	-1.522991000	0.790089000
H	4.014450000	-2.767216000	-1.758996000
C	4.316916000	-3.064649000	0.373050000
H	5.293614000	-3.520904000	0.249966000
C	3.768343000	-2.936259000	1.663810000
C	2.486467000	-2.363850000	1.797779000
C	4.517379000	-3.438938000	2.873632000
H	2.044238000	-2.271984000	2.784430000
H	5.600242000	-3.380005000	2.731004000
H	4.258239000	-2.873487000	3.773493000
H	4.272389000	-4.491349000	3.068578000
C	4.494012000	0.435580000	-2.318583000
S	2.896059000	1.341827000	-1.806739000
C	3.128492000	1.424818000	0.068541000
H	4.233734000	-0.249887000	-3.125639000
H	5.205450000	1.196298000	-2.641165000
H	4.869752000	-0.122580000	-1.462091000
H	4.048022000	1.979451000	0.261895000
H	2.273922000	1.965950000	0.472828000
H	3.175306000	0.417364000	0.478961000

BnTPEN: ³Prd_{NTs,DMS}

Fe	-0.838683000	0.598940000	-3.394890000
N	-1.505700000	-1.159454000	-4.255927000
N	0.315288000	1.064330000	-5.014092000
N	-2.426175000	1.307823000	-4.929282000
N	-1.158057000	2.585171000	-2.622849000
N	-1.871998000	0.170828000	-1.682952000
C	-0.803062000	-2.319211000	-4.267268000
H	0.176130000	-2.285275000	-3.806401000
C	-1.325738000	-3.485469000	-4.827618000
H	-0.739495000	-4.396084000	-4.826032000
C	-2.608215000	-3.451169000	-5.387269000
H	-3.039486000	-4.341365000	-5.830647000
C	-3.326059000	-2.248296000	-5.380665000
H	-4.315109000	-2.191540000	-5.821093000
C	-2.752205000	-1.110759000	-4.807976000
C	-3.445652000	0.239150000	-4.765714000
H	-4.229849000	0.286707000	-5.536316000

H	-3.932345000	0.381891000	-3.793977000
C	-1.787937000	1.279404000	-6.270677000
H	-2.205718000	2.054828000	-6.926952000
H	-2.018586000	0.320465000	-6.749638000
C	-0.286164000	1.413136000	-6.187794000
C	0.459694000	1.806517000	-7.302814000
H	-0.052039000	2.091645000	-8.215405000
C	1.855348000	1.816065000	-7.234951000
H	2.445744000	2.114457000	-8.093675000
C	2.469581000	1.426698000	-6.041221000
H	3.547684000	1.401781000	-5.942333000
C	1.675875000	1.063292000	-4.954611000
H	2.128351000	0.755792000	-4.023950000
C	-2.833244000	2.679899000	-4.510952000
H	-3.895474000	2.866599000	-4.727186000
H	-2.261063000	3.387043000	-5.118101000
C	-2.568809000	2.936780000	-3.027387000
H	-2.776346000	3.988078000	-2.791145000
H	-3.240925000	2.326706000	-2.419342000
C	-1.087842000	2.403424000	-1.134091000
H	-1.485428000	3.278713000	-0.606844000
H	-0.030949000	2.291934000	-0.860689000
C	-1.821723000	1.154705000	-0.739684000
C	-2.384976000	0.984529000	0.527956000
H	-2.340340000	1.794457000	1.246799000
C	-2.999943000	-0.227603000	0.851029000
H	-3.444805000	-0.375950000	1.828315000
C	-3.035541000	-1.241824000	-0.112205000
H	-3.500830000	-2.197552000	0.095649000
C	-2.465031000	-1.008828000	-1.361401000
H	-2.469240000	-1.772448000	-2.123537000
C	-0.132651000	3.608785000	-3.095433000
H	-0.187806000	3.626377000	-4.185424000
H	0.840327000	3.190247000	-2.823579000
C	-0.287321000	5.010576000	-2.538824000
C	-0.987383000	5.994588000	-3.260832000
H	-1.404211000	5.755411000	-4.236209000
C	-1.128648000	7.291187000	-2.753782000
H	-1.666489000	8.039915000	-3.325177000
C	-0.564886000	7.624209000	-1.516904000
H	-0.670120000	8.629655000	-1.124556000
C	0.148378000	6.659488000	-0.794607000
H	0.599422000	6.919283000	0.157227000
C	0.288533000	5.364494000	-1.303960000
H	0.856151000	4.626096000	-0.743172000
N	2.018627000	1.332493000	-0.190106000
O	0.795747000	-0.192035000	-2.126095000
S	2.294809000	-0.046333000	-1.398135000
O	3.580803000	0.187781000	-2.412430000
C	2.614137000	-1.638443000	-0.480941000
C	3.586775000	-2.495653000	-0.991510000
C	1.864276000	-1.923154000	0.658271000
H	1.125216000	-1.224880000	1.033667000
H	4.151650000	-2.225393000	-1.876188000
C	3.817950000	-3.695715000	-0.312280000
H	4.576730000	-4.376058000	-0.684833000
C	3.089759000	-4.033138000	0.845675000
C	2.116912000	-3.129394000	1.318482000
C	3.338052000	-5.341839000	1.555676000
H	1.556356000	-3.369993000	2.215799000
H	4.393456000	-5.627395000	1.513717000
H	3.039308000	-5.293785000	2.606479000
H	2.764353000	-6.153191000	1.088436000
C	4.390330000	2.980681000	-1.151191000
S	3.568306000	2.141258000	0.351735000
C	4.896494000	0.848081000	0.789272000
H	4.545248000	2.224204000	-1.919419000

H	3.696616000	3.757140000	-1.471339000
H	5.321408000	3.418641000	-0.787788000
H	5.744842000	1.409900000	1.182837000
H	4.465001000	0.208305000	1.557410000
H	5.159306000	0.292040000	-0.109787000

BnTPEN: ³Prd_AlternativeNTs,DMS

Fe	0.534029000	-0.976153000	-3.371403000
N	-0.951620000	-1.677396000	-4.529532000
N	1.057393000	0.440710000	-4.785625000
N	-1.000180000	0.508186000	-2.947351000
N	1.577619000	-0.196747000	-1.779876000
N	0.793417000	-2.715493000	-2.375880000
C	-0.830217000	-2.472543000	-5.623516000
H	0.175640000	-2.756247000	-5.908141000
C	-1.941739000	-2.910030000	-6.343273000
H	-1.807240000	-3.544245000	-7.210725000
C	-3.217395000	-2.513509000	-5.925829000
H	-4.099197000	-2.838519000	-6.465701000
C	-3.341244000	-1.678776000	-4.808109000
H	-4.316267000	-1.343149000	-4.473881000
C	-2.193675000	-1.272474000	-4.125117000
C	-2.217887000	-0.360446000	-2.915485000
H	-3.144588000	0.229090000	-2.889438000
H	-2.182369000	-0.953700000	-1.993427000
C	-1.042538000	1.503128000	-4.061863000
H	-1.246499000	2.508862000	-3.674146000
H	-1.882473000	1.252332000	-4.720469000
C	0.227172000	1.511006000	-4.894638000
C	0.510962000	2.557141000	-5.779083000
H	-0.156022000	3.409999000	-5.840755000
C	1.653783000	2.488682000	-6.581229000
H	1.884373000	3.289382000	-7.274409000
C	2.497542000	1.375571000	-6.473609000
H	3.392184000	1.288422000	-7.077521000
C	2.173466000	0.376216000	-5.559704000
H	2.807375000	-0.492066000	-5.424629000
C	-0.593512000	1.084979000	-1.618532000
H	-1.471312000	1.259077000	-0.982778000
H	-0.135517000	2.058540000	-1.802924000
C	0.399330000	0.173595000	-0.890213000
H	0.765743000	0.671350000	0.014573000
H	-0.083409000	-0.760305000	-0.584211000
C	2.368805000	-1.313395000	-1.143882000
H	2.556003000	-1.131918000	-0.081841000
H	3.356638000	-1.336458000	-1.615139000
C	1.695908000	-2.638829000	-1.351473000
C	2.015591000	-3.752997000	-0.568590000
H	2.754866000	-3.633047000	0.218242000
C	1.394004000	-4.972961000	-0.841476000
H	1.629615000	-5.850529000	-0.250371000
C	0.461368000	-5.050681000	-1.886179000
H	-0.041531000	-5.980659000	-2.121215000
C	0.184460000	-3.910032000	-2.629418000
H	-0.527414000	-3.928949000	-3.441319000
C	2.492152000	1.009720000	-2.040042000
H	1.949558000	1.682359000	-2.704817000
H	3.338765000	0.608936000	-2.605261000
C	2.951910000	1.775028000	-0.814460000
C	2.426803000	3.059190000	-0.571100000
H	1.712716000	3.492531000	-1.268437000
C	2.837832000	3.805351000	0.538101000
H	2.430303000	4.796707000	0.705255000
C	3.782117000	3.273339000	1.424088000
H	4.102424000	3.849807000	2.285325000
C	4.320354000	2.002419000	1.188425000

H	5.056900000	1.572420000	1.858557000
C	3.916581000	1.260460000	0.073249000
H	4.363163000	0.284018000	-0.079404000
N	6.286171000	-0.721309000	2.093330000
O	4.230205000	-2.175537000	0.896033000
S	5.637550000	-2.434354000	1.730614000
O	6.739627000	-3.444360000	1.020332000
C	5.220949000	-3.199162000	3.382018000
C	5.520678000	-4.545469000	3.569014000
C	4.594540000	-2.420368000	4.352631000
H	4.387677000	-1.371106000	4.177587000
H	6.014968000	-5.109375000	2.786223000
C	5.181237000	-5.130311000	4.793853000
H	5.409443000	-6.177717000	4.963134000
C	4.553120000	-4.384713000	5.808625000
C	4.265572000	-3.026287000	5.568194000
C	4.219553000	-5.017117000	7.139129000
H	3.783242000	-2.437253000	6.341803000
H	4.115154000	-6.102546000	7.053479000
H	5.011528000	-4.821886000	7.874179000
H	3.288870000	-4.616119000	7.552942000
C	8.747678000	-1.127128000	0.373148000
S	8.102878000	-0.649800000	2.102147000
C	8.844933000	-2.064708000	3.142261000
H	8.357662000	-2.116670000	0.136394000
H	8.367263000	-0.361169000	-0.301224000
H	9.837128000	-1.096158000	0.424882000
H	9.923241000	-1.900372000	3.156563000
H	8.422661000	-1.961425000	4.140783000
H	8.576013000	-3.012027000	2.676609000

¹[Fe^{IV}(O)(Bntpen)]²⁺

Fe	-0.702871000	0.523262000	-3.571773000
N	0.070550000	2.298672000	-3.983281000
N	-1.640984000	1.242211000	-1.940229000
N	-2.353296000	1.512311000	-4.524464000
N	-1.814493000	-1.154990000	-3.899914000
N	0.350264000	-0.292054000	-5.147292000
C	1.143300000	2.818696000	-3.334253000
H	1.536183000	2.241872000	-2.508034000
C	1.704251000	4.031713000	-3.735476000
H	2.560692000	4.426307000	-3.203067000
C	1.146626000	4.716718000	-4.821331000
H	1.565489000	5.661378000	-5.148429000
C	0.031073000	4.176105000	-5.477083000
H	-0.428260000	4.695568000	-6.310163000
C	-0.490517000	2.959254000	-5.040651000
C	-1.688716000	2.264409000	-5.642917000
H	-2.375765000	2.979722000	-6.112477000
H	-1.381318000	1.542988000	-6.407408000
C	-2.973993000	2.482639000	-3.547329000
H	-4.046900000	2.585232000	-3.744851000
H	-2.531237000	3.471259000	-3.709509000
C	-2.708761000	2.063167000	-2.127350000
C	-3.451110000	2.545975000	-1.047561000
H	-4.306453000	3.189063000	-1.221652000
C	-3.069360000	2.199639000	0.253302000
H	-3.631756000	2.566406000	1.104178000
C	-1.950777000	1.378544000	0.437424000
H	-1.618807000	1.097368000	1.429124000
C	-1.259678000	0.910680000	-0.678677000
H	-0.391914000	0.269046000	-0.608970000
C	-3.355389000	0.477733000	-4.969359000
H	-3.838062000	0.778099000	-5.907610000
H	-4.135902000	0.429736000	-4.206623000
C	-2.674496000	-0.869724000	-5.118524000

H	-3.408820000	-1.673057000	-5.239192000
H	-2.022025000	-0.878309000	-5.992898000
C	-0.799937000	-2.220608000	-4.250496000
H	-1.306426000	-3.094895000	-4.670529000
H	-0.306369000	-2.518419000	-3.320889000
C	0.211447000	-1.646601000	-5.195892000
C	0.991963000	-2.435579000	-6.041779000
H	0.847844000	-3.509524000	-6.063547000
C	1.960706000	-1.825800000	-6.844236000
H	2.584447000	-2.421106000	-7.500724000
C	2.110690000	-0.436121000	-6.783696000
H	2.851460000	0.074388000	-7.386443000
C	1.292555000	0.297820000	-5.927801000
H	1.395647000	1.369659000	-5.854797000
C	-2.650210000	-1.598283000	-2.676644000
H	-3.331165000	-0.776046000	-2.453361000
H	-1.932404000	-1.673039000	-1.857667000
C	-3.413334000	-2.890901000	-2.854524000
C	-4.741499000	-2.880557000	-3.323836000
H	-5.233241000	-1.936386000	-3.546856000
C	-5.457486000	-4.073413000	-3.465961000
H	-6.482332000	-4.050987000	-3.819581000
C	-4.857258000	-5.293369000	-3.130734000
H	-5.414178000	-6.218046000	-3.232562000
C	-3.545091000	-5.315549000	-2.641501000
H	-3.087930000	-6.256317000	-2.355541000
C	-2.828800000	-4.122812000	-2.501798000
H	-1.823334000	-4.150458000	-2.090262000
O	0.416814000	-0.216934000	-2.605446000

³[Fe^{IV}(O)(Bntpen)]²⁺

Fe	-0.709456000	0.548404000	-3.587938000
N	0.119379000	2.317801000	-3.966524000
N	-1.672788000	1.242320000	-1.964657000
N	-2.323434000	1.539969000	-4.539889000
N	-1.818755000	-1.165285000	-3.858556000
N	0.310706000	-0.284250000	-5.167512000
C	1.198612000	2.822914000	-3.323191000
H	1.592692000	2.228251000	-2.509648000
C	1.767342000	4.035740000	-3.717547000
H	2.630345000	4.420561000	-3.188652000
C	1.208305000	4.732016000	-4.795048000
H	1.631470000	5.676414000	-5.117459000
C	0.087514000	4.202219000	-5.452579000
H	-0.367990000	4.729616000	-6.282937000
C	-0.440382000	2.986238000	-5.021702000
C	-1.640215000	2.299251000	-5.643216000
H	-2.317410000	3.023849000	-6.112178000
H	-1.331587000	1.584069000	-6.412861000
C	-2.957392000	2.514078000	-3.573869000
H	-4.022229000	2.635353000	-3.801476000
H	-2.492161000	3.495647000	-3.713527000
C	-2.732921000	2.072230000	-2.156312000
C	-3.491885000	2.538939000	-1.081302000
H	-4.340094000	3.190184000	-1.259295000
C	-3.134996000	2.167114000	0.219445000
H	-3.710303000	2.521340000	1.066949000
C	-2.022232000	1.338953000	0.409057000
H	-1.707402000	1.040486000	1.401235000
C	-1.312823000	0.889291000	-0.702411000
H	-0.446070000	0.246998000	-0.619317000
C	-3.325970000	0.495667000	-4.974414000
H	-3.792234000	0.777728000	-5.926388000
H	-4.116705000	0.478575000	-4.220591000
C	-2.675016000	-0.875068000	-5.082221000
H	-3.435848000	-1.655881000	-5.188019000

H	-2.029461000	-0.922474000	-5.960164000
C	-0.793997000	-2.214889000	-4.206359000
H	-1.281932000	-3.114866000	-4.593440000
H	-0.272644000	-2.478912000	-3.280583000
C	0.184141000	-1.642846000	-5.189665000
C	0.951900000	-2.433866000	-6.045131000
H	0.820389000	-3.509597000	-6.045472000
C	1.890165000	-1.825637000	-6.884355000
H	2.501948000	-2.424118000	-7.549176000
C	2.026537000	-0.433611000	-6.848702000
H	2.744639000	0.075765000	-7.479149000
C	1.226009000	0.304977000	-5.980763000
H	1.322019000	1.378094000	-5.922413000
C	-2.656849000	-1.615953000	-2.648436000
H	-3.349495000	-0.800924000	-2.431720000
H	-1.947734000	-1.684315000	-1.820645000
C	-3.409659000	-2.915962000	-2.826225000
C	-4.736566000	-2.915978000	-3.298161000
H	-5.236262000	-1.975007000	-3.517444000
C	-5.441354000	-4.114938000	-3.447966000
H	-6.465472000	-4.100054000	-3.804210000
C	-4.830934000	-5.330749000	-3.117410000
H	-5.379017000	-6.260066000	-3.224857000
C	-3.519888000	-5.342858000	-2.625119000
H	-3.054559000	-6.280762000	-2.342763000
C	-2.815184000	-4.143909000	-2.477555000
H	-1.810469000	-4.163973000	-2.063400000
O	0.465009000	-0.076547000	-2.605587000

$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{Bntpen})]^{2+}$

Fe	-0.685048000	0.591604000	-3.425625000
N	0.200687000	2.414371000	-4.008264000
N	-1.731743000	1.298556000	-1.768310000
N	-2.297194000	1.571329000	-4.400140000
N	-1.811394000	-1.221260000	-3.869594000
N	0.393384000	-0.324655000	-5.179251000
C	1.322444000	2.957920000	-3.475503000
H	1.774329000	2.419616000	-2.651862000
C	1.859778000	4.142097000	-3.983007000
H	2.756131000	4.560551000	-3.542406000
C	1.222067000	4.769035000	-5.060631000
H	1.618443000	5.690950000	-5.470627000
C	0.059413000	4.201488000	-5.604186000
H	-0.452939000	4.676802000	-6.432911000
C	-0.431469000	3.015774000	-5.058274000
C	-1.659309000	2.286942000	-5.563057000
H	-2.370376000	2.977622000	-6.033260000
H	-1.379943000	1.534520000	-6.307659000
C	-2.914320000	2.579396000	-3.452730000
H	-3.959986000	2.759714000	-3.727304000
H	-2.382487000	3.529016000	-3.574626000
C	-2.778498000	2.132234000	-2.022269000
C	-3.592449000	2.597800000	-0.988844000
H	-4.428768000	3.252604000	-1.205336000
C	-3.303523000	2.217732000	0.328378000
H	-3.922530000	2.571824000	1.144767000
C	-2.206305000	1.383705000	0.580229000
H	-1.950725000	1.083230000	1.588647000
C	-1.438404000	0.935805000	-0.492503000
H	-0.579035000	0.289043000	-0.367918000
C	-3.323862000	0.530709000	-4.802700000
H	-3.864410000	0.863733000	-5.697675000
H	-4.051195000	0.472259000	-3.989297000
C	-2.682740000	-0.830242000	-5.040014000
H	-3.457331000	-1.589238000	-5.201763000
H	-2.053238000	-0.807091000	-5.931475000

C	-0.799496000	-2.249620000	-4.277468000
H	-1.295602000	-3.124630000	-4.711690000
H	-0.286097000	-2.575808000	-3.366215000
C	0.209283000	-1.670083000	-5.232877000
C	0.958577000	-2.477071000	-6.093647000
H	0.780447000	-3.545996000	-6.122543000
C	1.938506000	-1.892509000	-6.900547000
H	2.535850000	-2.502886000	-7.567791000
C	2.136041000	-0.508220000	-6.831436000
H	2.887269000	-0.017965000	-7.438185000
C	1.347883000	0.242206000	-5.962084000
H	1.479042000	1.310874000	-5.877146000
C	-2.616278000	-1.711909000	-2.654586000
H	-3.290208000	-0.899292000	-2.375506000
H	-1.882686000	-1.827770000	-1.852540000
C	-3.393941000	-2.992455000	-2.866548000
C	-4.729286000	-2.953847000	-3.311870000
H	-5.219475000	-1.997595000	-3.480664000
C	-5.453599000	-4.135725000	-3.499674000
H	-6.484022000	-4.091979000	-3.834812000
C	-4.853939000	-5.372788000	-3.234814000
H	-5.416937000	-6.289189000	-3.372100000
C	-3.533766000	-5.423911000	-2.770296000
H	-3.075991000	-6.379412000	-2.539222000
C	-2.809475000	-4.242013000	-2.585075000
H	-1.796705000	-4.293205000	-2.194072000
O	0.476497000	-0.064942000	-2.461018000

BnTPEN: ³RC_{O,CHD}

Fe	-0.395901000	0.479672000	-3.421301000
N	0.415933000	2.224134000	-3.939476000
N	-1.200236000	1.232890000	-1.741308000
N	-2.076140000	1.467652000	-4.255029000
N	-1.549284000	-1.221808000	-3.520901000
N	0.455598000	-0.426273000	-5.061539000
C	1.554570000	2.736419000	-3.415587000
H	2.012182000	2.166483000	-2.617835000
C	2.100354000	3.924283000	-3.906329000
H	3.011480000	4.315963000	-3.471581000
C	1.456398000	4.587218000	-4.956904000
H	1.860659000	5.511772000	-5.352737000
C	0.275048000	4.050474000	-5.490838000
H	-0.246682000	4.552844000	-6.297416000
C	-0.227435000	2.860818000	-4.965935000
C	-1.488590000	2.170333000	-5.446563000
H	-2.196006000	2.887394000	-5.881802000
H	-1.260565000	1.419707000	-6.210340000
C	-2.596273000	2.488506000	-3.270127000
H	-3.674746000	2.628655000	-3.404022000
H	-2.124214000	3.452632000	-3.486213000
C	-2.253519000	2.085062000	-1.864610000
C	-2.906169000	2.598259000	-0.742617000
H	-3.750561000	3.266954000	-0.865613000
C	-2.449570000	2.247039000	0.532755000
H	-2.941535000	2.637131000	1.416264000
C	-1.350067000	1.389228000	0.648088000
H	-0.963419000	1.097775000	1.616503000
C	-0.746327000	0.893247000	-0.506079000
H	0.096385000	0.213979000	-0.467246000
C	-3.131215000	0.427397000	-4.550317000
H	-3.682492000	0.682613000	-5.463799000
H	-3.846265000	0.453338000	-3.724660000
C	-2.514811000	-0.958511000	-4.666682000
H	-3.296159000	-1.725946000	-4.667332000
H	-1.957619000	-1.051433000	-5.599887000
C	-0.577013000	-2.301516000	-3.924381000

H	-1.114164000	-3.203887000	-4.234004000
H	0.023011000	-2.544617000	-3.039691000
C	0.308676000	-1.782407000	-5.018137000
C	0.975836000	-2.616813000	-5.916240000
H	0.828514000	-3.689208000	-5.863941000
C	1.832856000	-2.056220000	-6.867823000
H	2.364775000	-2.689024000	-7.568623000
C	1.992488000	-0.666400000	-6.898316000
H	2.650533000	-0.192862000	-7.616185000
C	1.293357000	0.116610000	-5.983100000
H	1.409655000	1.189391000	-5.974095000
C	-2.270995000	-1.616964000	-2.219946000
H	-2.868499000	-0.753309000	-1.925005000
H	-1.474876000	-1.748542000	-1.483149000
C	-3.140784000	-2.852031000	-2.310970000
C	-4.520776000	-2.734796000	-2.565988000
H	-4.970525000	-1.750940000	-2.681361000
C	-5.334546000	-3.870642000	-2.633062000
H	-6.397386000	-3.765188000	-2.820993000
C	-4.779031000	-5.140955000	-2.438934000
H	-5.409641000	-6.021858000	-2.483672000
C	-3.411737000	-5.270067000	-2.164855000
H	-2.984474000	-6.251203000	-1.988598000
C	-2.598567000	-4.133976000	-2.097328000
H	-1.547201000	-4.239795000	-1.846424000
O	0.871412000	-0.113460000	-2.539618000
H	2.645181000	-1.543547000	-1.208339000
C	2.901843000	-2.117942000	-0.300581000
H	3.969135000	-1.948582000	-0.121344000
C	2.645613000	-3.622726000	-0.548549000
C	2.079233000	-1.586076000	0.856269000
H	2.471856000	-0.749596000	1.429420000
C	0.879081000	-2.129840000	1.155015000
C	1.179832000	-3.983998000	-0.421568000
C	0.366262000	-3.281379000	0.398948000
H	-0.657866000	-3.601821000	0.573687000
H	0.286154000	-1.755807000	1.985911000
H	0.831481000	-4.895195000	-0.903904000
H	3.207070000	-4.222244000	0.187761000
H	3.040120000	-3.911521000	-1.529870000

BnTPEN: ³TS1_{o,CHD}

Fe	-0.811248000	0.211437000	-3.071321000
N	0.223102000	1.913127000	-3.222529000
N	-2.058977000	0.948012000	-1.668700000
N	-2.098477000	1.360481000	-4.311979000
N	-1.982896000	-1.397474000	-3.652829000
N	0.464005000	-0.692019000	-4.415689000
C	1.169243000	2.326520000	-2.346681000
H	1.325086000	1.692650000	-1.484199000
C	1.896965000	3.497201000	-2.571734000
H	2.646230000	3.810099000	-1.855375000
C	1.640573000	4.248902000	-3.723521000
H	2.190710000	5.162391000	-3.918019000
C	0.653414000	3.817257000	-4.621624000
H	0.426764000	4.390680000	-5.513248000
C	-0.044030000	2.641162000	-4.348973000
C	-1.140591000	2.069546000	-5.224386000
H	-1.639177000	2.857541000	-5.803714000
H	-0.737750000	1.338777000	-5.933511000
C	-2.839103000	2.367695000	-3.466383000
H	-3.811674000	2.600589000	-3.915030000
H	-2.266286000	3.301127000	-3.456772000
C	-2.977330000	1.873068000	-2.054073000
C	-3.922398000	2.378746000	-1.158913000

H	-4.652119000	3.107316000	-1.493750000
C	-3.904309000	1.941510000	0.170001000
H	-4.628589000	2.322003000	0.880978000
C	-2.935114000	1.012383000	0.566223000
H	-2.883462000	0.660084000	1.588961000
C	-2.027929000	0.532211000	-0.376648000
H	-1.248960000	-0.183172000	-0.147767000
C	-3.069091000	0.420228000	-4.984914000
H	-3.301935000	0.763886000	-6.000707000
H	-3.999471000	0.456800000	-4.413021000
C	-2.528150000	-1.001757000	-5.012980000
H	-3.311484000	-1.704684000	-5.317671000
H	-1.714314000	-1.083531000	-5.735317000
C	-1.001185000	-2.525233000	-3.812999000
H	-1.461729000	-3.375793000	-4.326258000
H	-0.715233000	-2.842022000	-2.805211000
C	0.209398000	-2.026168000	-4.546420000
C	1.041213000	-2.862758000	-5.293898000
H	0.799819000	-3.915083000	-5.389617000
C	2.175066000	-2.328169000	-5.913025000
H	2.832274000	-2.961125000	-6.497987000
C	2.441215000	-0.962057000	-5.768114000
H	3.307136000	-0.507305000	-6.233458000
C	1.569571000	-0.177415000	-5.014741000
H	1.755374000	0.876999000	-4.877685000
C	-3.090549000	-1.790514000	-2.665382000
H	-3.727813000	-0.912448000	-2.549586000
H	-2.577156000	-1.955380000	-1.715484000
C	-3.917647000	-2.997173000	-3.053490000
C	-5.115586000	-2.841804000	-3.776870000
H	-5.463790000	-1.846287000	-4.042778000
C	-5.890827000	-3.953088000	-4.124795000
H	-6.815309000	-3.817277000	-4.675233000
C	-5.482765000	-5.237007000	-3.744521000
H	-6.086737000	-6.098651000	-4.006188000
C	-4.305135000	-5.404185000	-3.005414000
H	-4.000577000	-6.395022000	-2.686540000
C	-3.530631000	-4.292224000	-2.659493000
H	-2.637037000	-4.431511000	-2.056635000
O	0.082238000	-0.558056000	-1.781970000
H	1.443509000	-1.096843000	-1.752179000
C	2.460939000	-1.695064000	-1.453517000
H	2.405774000	-2.579670000	-2.097854000
C	2.279711000	-2.041520000	0.032727000
C	3.605292000	-0.831212000	-1.758143000
H	3.982582000	-0.803850000	-2.776893000
C	4.165869000	-0.025256000	-0.800859000
C	2.783750000	-0.978735000	0.968839000
C	3.684322000	-0.043162000	0.565077000
H	4.088422000	0.673833000	1.272207000
H	4.997918000	0.625442000	-1.052127000
H	2.464239000	-1.023555000	2.006205000
H	2.829043000	-2.975994000	0.257353000
H	1.227693000	-2.273024000	0.242298000

BnTPEN: ³IR1_{o,CHD}

Fe	-0.859668000	0.137818000	-3.028546000
N	0.225377000	1.807838000	-3.075872000
N	-2.108385000	0.807626000	-1.611705000
N	-2.074074000	1.356847000	-4.218806000
N	-2.036841000	-1.421773000	-3.718681000
N	0.446916000	-0.729055000	-4.370215000
C	1.164152000	2.148833000	-2.161556000
H	1.297142000	1.472060000	-1.327914000
C	1.924885000	3.310564000	-2.315259000
H	2.670234000	3.561495000	-1.571374000

C	1.709734000	4.127217000	-3.429943000
H	2.286623000	5.034620000	-3.566828000
C	0.729980000	3.767925000	-4.368773000
H	0.535740000	4.391327000	-5.234051000
C	-0.000267000	2.598268000	-4.169884000
C	-1.091695000	2.092785000	-5.088179000
H	-1.573994000	2.914441000	-5.632223000
H	-0.694402000	1.389102000	-5.827071000
C	-2.809432000	2.343496000	-3.337613000
H	-3.760413000	2.627824000	-3.801651000
H	-2.207965000	3.255401000	-3.263413000
C	-2.997979000	1.774551000	-1.960401000
C	-3.949917000	2.247664000	-1.056274000
H	-4.656709000	3.011699000	-1.359553000
C	-3.966971000	1.730504000	0.244584000
H	-4.696913000	2.084449000	0.963448000
C	-3.026418000	0.758031000	0.603382000
H	-3.003388000	0.345264000	1.604281000
C	-2.109535000	0.312439000	-0.348129000
H	-1.348709000	-0.430710000	-0.149570000
C	-3.061223000	0.481250000	-4.959179000
H	-3.272997000	0.895556000	-5.952473000
H	-3.995898000	0.503541000	-4.393743000
C	-2.547427000	-0.945578000	-5.065628000
H	-3.337949000	-1.615643000	-5.421142000
H	-1.721120000	-1.002761000	-5.776445000
C	-1.074136000	-2.560549000	-3.914068000
H	-1.538230000	-3.370308000	-4.486076000
H	-0.826399000	-2.940322000	-2.917986000
C	0.166489000	-2.048690000	-4.585967000
C	0.999855000	-2.859789000	-5.358262000
H	0.739000000	-3.899300000	-5.519716000
C	2.162568000	-2.317484000	-5.914514000
H	2.822051000	-2.931588000	-6.516744000
C	2.455881000	-0.969412000	-5.681896000
H	3.347161000	-0.510753000	-6.091917000
C	1.582588000	-0.208188000	-4.907574000
H	1.792408000	0.829816000	-4.701004000
C	-3.171980000	-1.842902000	-2.771469000
H	-3.801481000	-0.962901000	-2.631412000
H	-2.680363000	-2.056519000	-1.819909000
C	-4.002736000	-3.020650000	-3.232054000
C	-5.176615000	-2.819310000	-3.983438000
H	-5.504515000	-1.809413000	-4.219391000
C	-5.956233000	-3.904953000	-4.396187000
H	-6.862431000	-3.734799000	-4.967061000
C	-5.577021000	-5.208355000	-4.053942000
H	-6.184967000	-6.050182000	-4.365993000
C	-4.424320000	-5.421474000	-3.287789000
H	-4.143321000	-6.428108000	-2.998316000
C	-3.644865000	-4.335310000	-2.877118000
H	-2.771639000	-4.510674000	-2.254180000
O	0.022446000	-0.750933000	-1.721299000
H	0.941507000	-1.073518000	-1.866053000
C	2.810386000	-2.048495000	-0.737434000
H	2.433318000	-3.060078000	-0.865789000
C	2.581909000	-1.385614000	0.597574000
C	3.561995000	-1.454874000	-1.725550000
H	3.758922000	-1.996599000	-2.647412000
C	4.136098000	-0.163822000	-1.549389000
C	3.189808000	-0.010335000	0.695037000
C	3.932652000	0.533022000	-0.324096000
H	4.404268000	1.502397000	-0.184823000
H	4.767613000	0.262175000	-2.321268000
H	3.070484000	0.524174000	1.633141000
H	2.993735000	-2.026913000	1.401436000
H	1.501509000	-1.347959000	0.829841000

BnTPEN: ³Prdo,CHD

Fe	-0.650850000	0.159663000	-3.103895000
N	0.205712000	2.116721000	-3.441485000
N	-1.817226000	0.707049000	-1.545305000
N	-2.293423000	1.375457000	-4.160311000
N	-1.912902000	-1.500620000	-3.780061000
N	0.520562000	-0.626842000	-4.589791000
C	1.253329000	2.649359000	-2.763285000
H	1.646740000	2.055146000	-1.948354000
C	1.803489000	3.886175000	-3.101885000
H	2.637000000	4.283035000	-2.535377000
C	1.255991000	4.597014000	-4.176569000
H	1.660602000	5.560831000	-4.463435000
C	0.167157000	4.053410000	-4.868623000
H	-0.287861000	4.590323000	-5.693431000
C	-0.340512000	2.810596000	-4.480382000
C	-1.527661000	2.160425000	-5.163496000
H	-2.149294000	2.924787000	-5.653256000
H	-1.185649000	1.470229000	-5.943757000
C	-2.900551000	2.247539000	-3.114824000
H	-3.943432000	2.492822000	-3.357452000
H	-2.357092000	3.198525000	-3.093671000
C	-2.813525000	1.615803000	-1.748014000
C	-3.691636000	1.973952000	-0.719665000
H	-4.479645000	2.692522000	-0.914969000
C	-3.547071000	1.402918000	0.546991000
H	-4.219635000	1.673564000	1.352594000
C	-2.526340000	0.467000000	0.751097000
H	-2.386929000	-0.010359000	1.713163000
C	-1.690689000	0.141256000	-0.313272000
H	-0.913322000	-0.601742000	-0.201450000
C	-3.267141000	0.395484000	-4.728352000
H	-3.720277000	0.776699000	-5.654694000
H	-4.079422000	0.281900000	-4.005199000
C	-2.617020000	-0.958994000	-5.000179000
H	-3.374916000	-1.673205000	-5.344753000
H	-1.873843000	-0.863537000	-5.796066000
C	-0.922726000	-2.549213000	-4.186942000
H	-1.392718000	-3.335650000	-4.789317000
H	-0.554592000	-3.023251000	-3.268658000
C	0.224586000	-1.918710000	-4.928550000
C	0.967222000	-2.614425000	-5.886030000
H	0.694720000	-3.632348000	-6.139826000
C	2.051961000	-1.988355000	-6.507179000
H	2.638000000	-2.514205000	-7.251990000
C	2.361312000	-0.670225000	-6.153469000
H	3.192065000	-0.147161000	-6.611020000
C	1.578745000	-0.022693000	-5.199712000
H	1.788033000	0.994426000	-4.905698000
C	-2.888850000	-2.055170000	-2.740910000
H	-3.517087000	-1.218475000	-2.429592000
H	-2.273641000	-2.338920000	-1.881498000
C	-3.745576000	-3.222065000	-3.187849000
C	-5.027646000	-3.003438000	-3.726686000
H	-5.419478000	-1.991815000	-3.802079000
C	-5.824961000	-4.077696000	-4.135818000
H	-6.813551000	-3.893826000	-4.542121000
C	-5.353454000	-5.389055000	-4.004128000
H	-5.973196000	-6.223078000	-4.314034000
C	-4.088349000	-5.622412000	-3.451106000
H	-3.730328000	-6.638363000	-3.324720000
C	-3.292642000	-4.546967000	-3.043010000
H	-2.326650000	-4.743541000	-2.584624000
O	0.925303000	-0.568658000	-1.826774000
H	1.713329000	-0.982336000	-2.225378000

C	2.148180000	-1.351294000	1.156151000
H	1.391349000	-1.668595000	1.866881000
C	2.496120000	0.007608000	1.059022000
C	2.823968000	-2.306320000	0.379754000
H	2.579498000	-3.358566000	0.481185000
C	3.842563000	-1.903283000	-0.496404000
C	3.523007000	0.407978000	0.187316000
C	4.192979000	-0.546712000	-0.591678000
H	5.009243000	-0.242608000	-1.238998000
H	4.389115000	-2.645450000	-1.069413000
H	3.824986000	1.449865000	0.148620000
H	2.009060000	0.739723000	1.695771000
H	1.111287000	-0.414202000	-0.874536000

BnTPEN: ³RC_{o,DMS}

Fe	-0.372151000	0.300644000	-3.083108000
N	0.612269000	2.005086000	-3.345974000
N	-1.533006000	1.081165000	-1.630503000
N	-1.768812000	1.365550000	-4.274861000
N	-1.533126000	-1.350713000	-3.507809000
N	0.823900000	-0.617988000	-4.475914000
C	1.625834000	2.443048000	-2.561675000
H	1.898006000	1.818035000	-1.720380000
C	2.313285000	3.618961000	-2.874223000
H	3.122096000	3.948370000	-2.234234000
C	1.948437000	4.343150000	-4.013129000
H	2.466112000	5.259751000	-4.271604000
C	0.901784000	3.874699000	-4.823151000
H	0.600445000	4.419939000	-5.710306000
C	0.249034000	2.695338000	-4.471623000
C	-0.879247000	2.066536000	-5.264363000
H	-1.432042000	2.819008000	-5.840705000
H	-0.495197000	1.321594000	-5.969021000
C	-2.484632000	2.390750000	-3.427947000
H	-3.494136000	2.566082000	-3.816058000
H	-1.947823000	3.342161000	-3.505476000
C	-2.501579000	1.965425000	-1.988239000
C	-3.384154000	2.496921000	-1.045514000
H	-4.155694000	3.191592000	-1.357532000
C	-3.248858000	2.132469000	0.298244000
H	-3.922485000	2.535787000	1.045407000
C	-2.227506000	1.246805000	0.662452000
H	-2.082599000	0.951758000	1.694220000
C	-1.387478000	0.735778000	-0.324193000
H	-0.580885000	0.049212000	-0.104915000
C	-2.752206000	0.374979000	-4.853873000
H	-3.043910000	0.668164000	-5.869913000
H	-3.652440000	0.417586000	-4.235770000
C	-2.177202000	-1.033512000	-4.848139000
H	-2.958768000	-1.770847000	-5.061049000
H	-1.409642000	-1.133932000	-5.616754000
C	-0.533945000	-2.463957000	-3.688860000
H	-1.010437000	-3.340173000	-4.139653000
H	-0.175897000	-2.742360000	-2.692722000
C	0.616032000	-1.966072000	-4.514036000
C	1.452745000	-2.813626000	-5.239638000
H	1.253115000	-3.878634000	-5.259733000
C	2.547024000	-2.275517000	-5.923737000
H	3.213467000	-2.918939000	-6.486088000
C	2.768686000	-0.896217000	-5.864583000
H	3.610415000	-0.441034000	-6.371114000
C	1.893559000	-0.098331000	-5.131702000
H	2.053760000	0.965308000	-5.052428000
C	-2.565065000	-1.725490000	-2.431206000
H	-3.227601000	-0.864751000	-2.326173000
H	-1.990033000	-1.820557000	-1.507347000

C	-3.364313000	-2.981280000	-2.701301000
C	-4.607854000	-2.912949000	-3.358803000
H	-5.011972000	-1.949046000	-3.660088000
C	-5.356529000	-4.071234000	-3.592716000
H	-6.316655000	-4.003491000	-4.092265000
C	-4.875339000	-5.313779000	-3.163249000
H	-5.458639000	-6.211153000	-3.336675000
C	-3.650434000	-5.393019000	-2.488845000
H	-3.288041000	-6.350762000	-2.131920000
C	-2.902361000	-4.234698000	-2.256298000
H	-1.970220000	-4.304637000	-1.701817000
O	0.585008000	-0.382909000	-1.920247000
S	3.911788000	-0.306680000	-1.441938000
C	5.757336000	-0.215800000	-1.038399000
H	6.206020000	-1.205120000	-1.138293000
H	5.899202000	0.169462000	-0.027601000
H	6.205356000	0.467142000	-1.761088000
C	3.358826000	-1.497320000	-0.081439000
H	3.557400000	-1.060016000	0.898484000
H	2.286701000	-1.646973000	-0.218022000
H	3.886887000	-2.446503000	-0.186414000

BnTPEN: ³TS1_{O,DMS}

Fe	-0.182583000	0.548185000	-2.932912000
N	0.516694000	2.664030000	-3.532275000
N	-1.496830000	1.178998000	-1.500590000
N	-1.784897000	1.448820000	-4.181053000
N	-1.352980000	-1.364698000	-3.590147000
N	1.037192000	-0.265411000	-4.361907000
C	1.435622000	3.438806000	-2.907682000
H	1.817173000	3.059739000	-1.967704000
C	1.861556000	4.657605000	-3.440061000
H	2.594361000	5.256422000	-2.912923000
C	1.316210000	5.088717000	-4.655839000
H	1.624901000	6.030959000	-5.093924000
C	0.350079000	4.298087000	-5.291563000
H	-0.105560000	4.621270000	-6.221055000
C	-0.030260000	3.089235000	-4.702420000
C	-1.086424000	2.176905000	-5.290470000
H	-1.802808000	2.755410000	-5.890590000
H	-0.633369000	1.429516000	-5.950822000
C	-2.530682000	2.424881000	-3.309633000
H	-3.545123000	2.586857000	-3.694750000
H	-2.017397000	3.389942000	-3.348552000
C	-2.551136000	1.951268000	-1.885736000
C	-3.543477000	2.331455000	-0.978704000
H	-4.375830000	2.939332000	-1.314490000
C	-3.444589000	1.929125000	0.356932000
H	-4.204658000	2.216656000	1.074118000
C	-2.348694000	1.152549000	0.749411000
H	-2.232810000	0.825888000	1.775420000
C	-1.397377000	0.793364000	-0.202851000
H	-0.525948000	0.198945000	0.032743000
C	-2.729801000	0.385819000	-4.679256000
H	-3.195756000	0.703978000	-5.621603000
H	-3.530030000	0.296098000	-3.940276000
C	-2.041316000	-0.960236000	-4.855302000
H	-2.776691000	-1.715084000	-5.163208000
H	-1.291479000	-0.900917000	-5.648922000
C	-0.234830000	-2.303381000	-3.865753000
H	-0.562536000	-3.188425000	-4.426796000
H	0.137648000	-2.659104000	-2.897400000
C	0.879619000	-1.601560000	-4.598757000
C	1.740480000	-2.292211000	-5.457097000
H	1.576952000	-3.348179000	-5.639145000
C	2.799052000	-1.617293000	-6.070492000

H	3.473643000	-2.142136000	-6.737074000
C	2.967329000	-0.252321000	-5.811244000
H	3.774247000	0.310204000	-6.264591000
C	2.072540000	0.387903000	-4.957557000
H	2.170273000	1.438054000	-4.730954000
C	-2.298994000	-1.905749000	-2.531683000
H	-3.015364000	-1.109821000	-2.314248000
H	-1.689482000	-2.043871000	-1.633122000
C	-3.028635000	-3.186141000	-2.887134000
C	-4.307057000	-3.143310000	-3.474374000
H	-4.792854000	-2.185444000	-3.645434000
C	-4.981591000	-4.322793000	-3.808402000
H	-5.969754000	-4.273815000	-4.252779000
C	-4.388521000	-5.564552000	-3.552699000
H	-4.913261000	-6.479521000	-3.804204000
C	-3.124959000	-5.622583000	-2.951923000
H	-2.673238000	-6.583509000	-2.730450000
C	-2.452600000	-4.442076000	-2.619648000
H	-1.486465000	-4.500790000	-2.124431000
O	0.879625000	0.073132000	-1.608583000
S	2.731316000	-0.880697000	-1.574679000
C	2.324636000	-1.899373000	-0.044645000
H	1.766873000	-1.268746000	0.647244000
H	3.258385000	-2.250835000	0.396945000
H	1.720742000	-2.743658000	-0.374395000
C	3.646400000	0.558744000	-0.777677000
H	4.518954000	0.170981000	-0.249576000
H	3.956988000	1.221950000	-1.584014000
H	2.954765000	1.059055000	-0.099426000

BnTPEN: ³DMS-Prdo,_{DMS}

Fe	-0.395228000	-0.141087000	-2.925671000
N	-2.474161000	-0.570260000	-2.492749000
N	-0.138797000	-1.811365000	-4.041555000
N	-1.574217000	0.386012000	-4.850528000
N	1.100098000	1.146227000	-3.967391000
N	-0.482138000	1.565543000	-1.801717000
C	-2.910105000	-1.434922000	-1.543661000
H	-2.141281000	-1.988880000	-1.019480000
C	-4.266693000	-1.608312000	-1.266433000
H	-4.581478000	-2.313381000	-0.506694000
C	-5.203282000	-0.864614000	-1.994842000
H	-6.264436000	-0.976797000	-1.804191000
C	-4.753562000	0.010549000	-2.991036000
H	-5.458642000	0.577356000	-3.588787000
C	-3.380901000	0.136666000	-3.223501000
C	-2.806132000	1.022588000	-4.312503000
H	-3.559724000	1.194406000	-5.095960000
H	-2.532427000	2.002833000	-3.905338000
C	-1.867520000	-0.910840000	-5.526359000
H	-1.973954000	-0.778484000	-6.611445000
H	-2.832408000	-1.283093000	-5.165342000
C	-0.816637000	-1.946046000	-5.217363000
C	-0.595120000	-3.035366000	-6.065265000
H	-1.141377000	-3.106995000	-6.999076000
C	0.321412000	-4.024263000	-5.697447000
H	0.501917000	-4.874738000	-6.344688000
C	0.997624000	-3.894114000	-4.479664000
H	1.711438000	-4.640395000	-4.153105000
C	0.747942000	-2.779498000	-3.682477000
H	1.234924000	-2.623728000	-2.729994000
C	-0.717421000	1.273785000	-5.691532000
H	-1.327403000	1.974635000	-6.279818000
H	-0.191874000	0.636905000	-6.408193000
C	0.290729000	2.053716000	-4.853570000
H	0.950915000	2.634374000	-5.510180000

H	-0.233296000	2.763771000	-4.208760000
C	1.693419000	1.928732000	-2.841549000
H	2.279969000	2.783625000	-3.200302000
H	2.387006000	1.261553000	-2.315530000
C	0.611465000	2.380202000	-1.897061000
C	0.725137000	3.547330000	-1.136858000
H	1.598462000	4.178823000	-1.253377000
C	-0.290787000	3.889679000	-0.239704000
H	-0.218678000	4.792585000	0.355560000
C	-1.404529000	3.049147000	-0.133287000
H	-2.216956000	3.278324000	0.545560000
C	-1.467997000	1.905156000	-0.926538000
H	-2.315387000	1.238321000	-0.875246000
C	2.171661000	0.373030000	-4.727541000
H	1.647545000	-0.242979000	-5.460725000
H	2.618466000	-0.307590000	-3.996109000
C	3.240546000	1.206923000	-5.405424000
C	3.097748000	1.598693000	-6.749768000
H	2.226965000	1.279310000	-7.317432000
C	4.082256000	2.366914000	-7.380562000
H	3.961173000	2.654555000	-8.419254000
C	5.230206000	2.748684000	-6.676537000
H	5.997546000	3.337762000	-7.166382000
C	5.394906000	2.349964000	-5.344448000
H	6.294373000	2.623611000	-4.803532000
C	4.408726000	1.582482000	-4.716173000
H	4.563734000	1.251864000	-3.692021000
O	0.634711000	-1.108721000	-1.405125000
S	1.187630000	-0.556514000	0.155803000
C	0.128258000	-1.566318000	1.353356000
H	0.556339000	-1.456114000	2.351157000
H	0.137348000	-2.604370000	1.019904000
H	-0.874753000	-1.143820000	1.316702000
C	2.816138000	-1.505882000	0.306862000
H	2.614954000	-2.558227000	0.106669000
H	3.491977000	-1.085784000	-0.436595000
H	3.202960000	-1.349144000	1.314978000

BnTPEN: ⁵DMS-PrdCHD_{o,DMS}

Fe	-0.508509000	0.754023000	-2.952334000
N	0.197464000	2.754066000	-3.575290000
N	-1.872713000	1.450369000	-1.371466000
N	-2.250287000	1.707918000	-4.120269000
N	-1.568531000	-1.128913000	-3.634779000
N	0.853990000	-0.138188000	-4.569082000
C	1.205566000	3.453407000	-2.996491000
H	1.644470000	3.012903000	-2.109497000
C	1.644911000	4.675977000	-3.503517000
H	2.448696000	5.212217000	-3.014100000
C	1.018426000	5.194518000	-4.644022000
H	1.333931000	6.144074000	-5.061071000
C	-0.035665000	4.482992000	-5.229026000
H	-0.552402000	4.874856000	-6.097850000
C	-0.429324000	3.262219000	-4.672521000
C	-1.572071000	2.436725000	-5.229472000
H	-2.270928000	3.080573000	-5.783871000
H	-1.186026000	1.692484000	-5.935295000
C	-2.970088000	2.647444000	-3.205549000
H	-4.002604000	2.810034000	-3.543946000
H	-2.467996000	3.620218000	-3.254191000
C	-2.950395000	2.179641000	-1.767633000
C	-3.952066000	2.548650000	-0.864068000
H	-4.807110000	3.121018000	-1.206292000
C	-3.832823000	2.179101000	0.479755000
H	-4.599018000	2.458400000	1.193954000
C	-2.711586000	1.446346000	0.886911000

H	-2.583830000	1.148382000	1.920407000
C	-1.754923000	1.096854000	-0.064812000
H	-0.868379000	0.527771000	0.180155000
C	-3.140515000	0.593615000	-4.576228000
H	-3.690134000	0.879032000	-5.485432000
H	-3.887438000	0.438009000	-3.793204000
C	-2.369780000	-0.699120000	-4.832772000
H	-3.069863000	-1.491374000	-5.128097000
H	-1.670287000	-0.560041000	-5.661723000
C	-0.507052000	-2.100213000	-4.044107000
H	-0.933379000	-2.949786000	-4.591731000
H	-0.070004000	-2.504597000	-3.122824000
C	0.577783000	-1.438509000	-4.860279000
C	1.294024000	-2.139010000	-5.837172000
H	1.039831000	-3.169470000	-6.058680000
C	2.330347000	-1.496352000	-6.521380000
H	2.895152000	-2.023012000	-7.282100000
C	2.619725000	-0.161253000	-6.214573000
H	3.412098000	0.371913000	-6.725886000
C	1.859581000	0.482823000	-5.239171000
H	2.041635000	1.517069000	-4.978233000
C	-2.428847000	-1.709325000	-2.514390000
H	-3.123145000	-0.921815000	-2.214893000
H	-1.743237000	-1.868794000	-1.676158000
C	-3.183146000	-2.982321000	-2.841850000
C	-4.497735000	-2.928318000	-3.342160000
H	-4.989668000	-1.967120000	-3.470224000
C	-5.197619000	-4.101257000	-3.645087000
H	-6.212523000	-4.043451000	-4.023146000
C	-4.594452000	-5.348184000	-3.443845000
H	-5.138406000	-6.258149000	-3.671617000
C	-3.294592000	-5.417932000	-2.928098000
H	-2.832995000	-6.382971000	-2.748895000
C	-2.596938000	-4.243734000	-2.627263000
H	-1.599659000	-4.311844000	-2.199696000
O	0.700188000	0.033437000	-1.428462000
S	2.177571000	-0.884330000	-1.415532000
C	2.000100000	-1.817946000	0.219616000
H	1.771284000	-1.093399000	1.001096000
H	2.938434000	-2.341371000	0.409582000
H	1.182339000	-2.524671000	0.086432000
C	3.468442000	0.398462000	-0.901923000
H	4.380524000	-0.135905000	-0.630741000
H	3.640377000	1.034578000	-1.768979000
H	3.064515000	0.965160000	-0.062575000

BnTPEN: ⁵CHD-PrdCHD_{O,CHD}

Fe	-0.882886000	0.349334000	-3.026568000
N	0.089267000	2.269548000	-3.486608000
N	-2.102207000	0.901089000	-1.277140000
N	-2.528963000	1.636268000	-3.938435000
N	-2.240701000	-1.304274000	-3.790161000
N	0.272928000	-0.601160000	-4.750406000
C	1.244028000	2.730574000	-2.941914000
H	1.697468000	2.104159000	-2.183603000
C	1.816860000	3.938675000	-3.338689000
H	2.737682000	4.280139000	-2.882062000
C	1.175553000	4.695229000	-4.327390000
H	1.593799000	5.640289000	-4.654539000
C	-0.021097000	4.224198000	-4.881210000
H	-0.543800000	4.798845000	-5.637480000
C	-0.543724000	3.004183000	-4.443589000
C	-1.827564000	2.418368000	-4.996389000
H	-2.466150000	3.216006000	-5.403302000
H	-1.596753000	1.733834000	-5.820905000

C	-3.053606000	2.523290000	-2.855662000
H	-4.059157000	2.891377000	-3.101452000
H	-2.402928000	3.402970000	-2.794443000
C	-3.059154000	1.842704000	-1.504178000
C	-3.969372000	2.210343000	-0.506976000
H	-4.728521000	2.955758000	-0.715792000
C	-3.886735000	1.612316000	0.754169000
H	-4.583080000	1.887966000	1.537808000
C	-2.896530000	0.649635000	0.987283000
H	-2.804829000	0.162090000	1.950032000
C	-2.029920000	0.317822000	-0.051406000
H	-1.262908000	-0.435363000	0.079943000
C	-3.583598000	0.710979000	-4.467371000
H	-4.120236000	1.171290000	-5.309315000
H	-4.315549000	0.562908000	-3.669022000
C	-3.001931000	-0.632309000	-4.903868000
H	-3.808332000	-1.284977000	-5.261645000
H	-2.306497000	-0.488257000	-5.735169000
C	-1.351921000	-2.378168000	-4.342391000
H	-1.926058000	-3.092778000	-4.944096000
H	-0.951200000	-2.935057000	-3.485952000
C	-0.209043000	-1.810447000	-5.147309000
C	0.358334000	-2.510375000	-6.217391000
H	-0.057638000	-3.464801000	-6.519790000
C	1.460254000	-1.966940000	-6.885408000
H	1.914238000	-2.496251000	-7.715280000
C	1.961795000	-0.727498000	-6.469987000
H	2.812200000	-0.273272000	-6.963767000
C	1.340719000	-0.074117000	-5.406462000
H	1.688655000	0.890164000	-5.060382000
C	-3.163390000	-1.888525000	-2.716187000
H	-3.733103000	-1.053562000	-2.304424000
H	-2.499769000	-2.251894000	-1.924956000
C	-4.099891000	-2.990695000	-3.168606000
C	-5.396572000	-2.686413000	-3.624738000
H	-5.742155000	-1.655374000	-3.630195000
C	-6.266115000	-3.700781000	-4.039528000
H	-7.264428000	-3.451226000	-4.382097000
C	-5.853703000	-5.037657000	-3.994904000
H	-6.529347000	-5.825462000	-4.308926000
C	-4.574459000	-5.356717000	-3.523508000
H	-4.260585000	-6.393201000	-3.464567000
C	-3.706083000	-4.340847000	-3.110957000
H	-2.727030000	-4.604221000	-2.718706000
O	0.705247000	-0.457175000	-1.851962000
H	1.435549000	-0.949083000	-2.270918000
C	2.287047000	-2.420566000	0.382259000
H	1.831807000	-3.390704000	0.552639000
C	1.862663000	-1.305950000	1.124233000
C	3.327536000	-2.287171000	-0.548843000
H	3.678863000	-3.155664000	-1.096635000
C	3.950795000	-1.042251000	-0.733330000
C	2.485417000	-0.058761000	0.938414000
C	3.532417000	0.070400000	0.011137000
H	4.043000000	1.021593000	-0.100502000
H	4.782779000	-0.950576000	-1.424135000
H	2.190086000	0.791206000	1.545691000
H	1.090975000	-1.419790000	1.879557000
H	0.896712000	-0.373582000	-0.892336000

BnTPEN: ⁵DMS-RC_{N_TS,DMS}

Fe	-0.902242000	0.332582000	-3.420711000
N	-1.867230000	-1.256845000	-4.669777000
N	0.544069000	0.826433000	-4.783575000
N	-2.105412000	1.379442000	-4.863238000

N	-1.088244000	2.303442000	-2.339830000
N	-2.357631000	-0.083432000	-1.887172000
C	-1.449731000	-2.529178000	-4.899185000
H	-0.463351000	-2.793484000	-4.537392000
C	-2.252825000	-3.445280000	-5.584615000
H	-1.891424000	-4.452987000	-5.747108000
C	-3.506554000	-3.040833000	-6.051136000
H	-4.147907000	-3.734750000	-6.582400000
C	-3.917016000	-1.714683000	-5.849241000
H	-4.867740000	-1.363809000	-6.234869000
C	-3.075219000	-0.845199000	-5.158480000
C	-3.396531000	0.613881000	-4.933324000
H	-4.033491000	1.002679000	-5.739181000
H	-3.926916000	0.763134000	-3.987785000
C	-1.381884000	1.321184000	-6.189165000
H	-1.691772000	2.160894000	-6.822621000
H	-1.679116000	0.403390000	-6.704392000
C	0.107300000	1.306177000	-5.985374000
C	1.010489000	1.692314000	-6.975395000
H	0.646144000	2.076616000	-7.921247000
C	2.384976000	1.571115000	-6.733685000
H	3.099343000	1.862416000	-7.495157000
C	2.821721000	1.077030000	-5.500199000
H	3.874170000	0.980402000	-5.267399000
C	1.876146000	0.714413000	-4.543607000
H	2.163046000	0.346096000	-3.569952000
C	-2.294262000	2.817194000	-4.439616000
H	-3.218524000	3.217346000	-4.876594000
H	-1.462700000	3.387925000	-4.860062000
C	-2.310919000	2.949468000	-2.925791000
H	-2.364316000	4.006184000	-2.637486000
H	-3.189656000	2.452400000	-2.507601000
C	-1.326444000	1.908976000	-0.918304000
H	-1.652662000	2.766919000	-0.319146000
H	-0.367333000	1.563362000	-0.516945000
C	-2.327847000	0.787369000	-0.838591000
C	-3.150288000	0.607049000	0.275301000
H	-3.120805000	1.327469000	1.084674000
C	-3.995730000	-0.505928000	0.334583000
H	-4.637327000	-0.662258000	1.194111000
C	-3.991765000	-1.414914000	-0.727158000
H	-4.614007000	-2.300823000	-0.712329000
C	-3.158716000	-1.178113000	-1.819218000
H	-3.102591000	-1.876772000	-2.637290000
C	0.174470000	3.159011000	-2.471326000
H	0.334635000	3.317576000	-3.540323000
H	0.997224000	2.539920000	-2.102203000
C	0.131713000	4.487339000	-1.744845000
C	-0.306457000	5.652371000	-2.402844000
H	-0.589782000	5.608869000	-3.452221000
C	-0.347795000	6.880281000	-1.733493000
H	-0.681026000	7.770786000	-2.255321000
C	0.056208000	6.960744000	-0.395631000
H	0.029411000	7.912428000	0.123484000
C	0.514827000	5.813779000	0.264154000
H	0.851812000	5.878609000	1.293126000
C	0.556623000	4.587029000	-0.406530000
H	0.950688000	3.711291000	0.101295000
N	0.292286000	-0.363335000	-2.267782000
O	-0.752524000	-2.925150000	-1.677686000
S	0.656418000	-2.190238000	-2.076873000
O	1.401490000	-2.594499000	-3.486733000
C	1.860182000	-2.332663000	-0.673297000
C	3.218820000	-2.357283000	-0.977182000
C	1.351350000	-2.467179000	0.616844000
H	0.283255000	-2.485064000	0.798789000
H	3.563515000	-2.290874000	-2.002415000

C	4.112972000	-2.521172000	0.085145000
H	5.177095000	-2.566401000	-0.121385000
C	3.656466000	-2.657005000	1.411925000
C	2.268243000	-2.624983000	1.658161000
C	4.629902000	-2.875953000	2.543375000
H	1.902270000	-2.743137000	2.672611000
H	5.625123000	-2.493491000	2.300693000
H	4.291141000	-2.394120000	3.465594000
H	4.735400000	-3.947678000	2.758070000
C	4.914390000	3.826826000	-2.156675000
S	4.031563000	2.183815000	-1.840901000
C	5.146452000	1.492517000	-0.480659000
H	4.361900000	4.338256000	-2.945816000
H	4.904696000	4.430898000	-1.248414000
H	5.938492000	3.638886000	-2.482249000
H	5.137261000	2.161701000	0.381045000
H	4.736760000	0.520662000	-0.202510000
H	6.161891000	1.374011000	-0.861969000

BnTPEN: ⁵DMS-TS1_{NTS,DMS}

Fe	-0.165993000	0.604873000	-2.965558000
N	-1.220942000	-1.153583000	-4.196284000
N	1.409078000	1.108654000	-4.425171000
N	-1.282252000	1.442251000	-4.896179000
N	-0.689210000	2.850981000	-2.416622000
N	-1.801613000	0.484535000	-1.532429000
C	-0.894600000	-2.470489000	-4.124091000
H	-0.023368000	-2.701920000	-3.528173000
C	-1.655314000	-3.456523000	-4.755177000
H	-1.360967000	-4.495855000	-4.675974000
C	-2.790395000	-3.079633000	-5.481076000
H	-3.401338000	-3.824374000	-5.978339000
C	-3.118156000	-1.721930000	-5.570367000
H	-3.978992000	-1.394662000	-6.142747000
C	-2.311456000	-0.785337000	-4.919626000
C	-2.573612000	0.696042000	-4.984430000
H	-3.113510000	0.953177000	-5.907783000
H	-3.201440000	1.008230000	-4.143212000
C	-0.404424000	1.141844000	-6.068032000
H	-0.674167000	1.771746000	-6.927065000
H	-0.571310000	0.103578000	-6.369102000
C	1.050652000	1.317393000	-5.721781000
C	1.999261000	1.639548000	-6.697860000
H	1.682237000	1.811080000	-7.720317000
C	3.347082000	1.737422000	-6.342259000
H	4.094346000	1.984270000	-7.087738000
C	3.711091000	1.525308000	-5.007324000
H	4.743440000	1.605938000	-4.689653000
C	2.720199000	1.220872000	-4.077026000
H	2.928005000	1.081000000	-3.025174000
C	-1.506386000	2.916479000	-4.760228000
H	-2.326757000	3.242456000	-5.416311000
H	-0.602003000	3.423583000	-5.104457000
C	-1.805891000	3.285080000	-3.318677000
H	-1.968341000	4.366628000	-3.229915000
H	-2.721176000	2.792655000	-2.978999000
C	-1.175618000	2.785050000	-1.006207000
H	-1.690282000	3.710902000	-0.721810000
H	-0.293413000	2.679312000	-0.370075000
C	-2.061032000	1.588779000	-0.781018000
C	-3.045329000	1.574180000	0.210945000
H	-3.246125000	2.472895000	0.782876000
C	-3.751734000	0.393806000	0.460458000
H	-4.515503000	0.364480000	1.229134000

C	-3.452276000	-0.748964000	-0.289958000
H	-3.963013000	-1.686981000	-0.111813000
C	-2.473028000	-0.669054000	-1.276377000
H	-2.192818000	-1.526528000	-1.868799000
C	0.539153000	3.751925000	-2.537648000
H	0.888386000	3.666357000	-3.568137000
H	1.295803000	3.296533000	-1.897387000
C	0.326705000	5.209755000	-2.177431000
C	0.000132000	6.153734000	-3.169658000
H	-0.079073000	5.842080000	-4.208573000
C	-0.191069000	7.500791000	-2.843466000
H	-0.435627000	8.216579000	-3.620807000
C	-0.051125000	7.925748000	-1.517267000
H	-0.193598000	8.970275000	-1.263163000
C	0.293384000	7.001762000	-0.523287000
H	0.426240000	7.332394000	0.501276000
C	0.484078000	5.655603000	-0.851802000
H	0.785744000	4.954633000	-0.078691000
N	1.334106000	0.976364000	-1.344729000
O	0.600290000	-1.047943000	0.642310000
S	1.358368000	-0.731385000	-0.774930000
O	0.537018000	-1.202390000	-2.207705000
C	2.944447000	-1.715800000	-0.785941000
C	3.657024000	-1.857003000	-1.974761000
C	3.342233000	-2.298041000	0.416748000
H	2.733960000	-2.193818000	1.307592000
H	3.303787000	-1.418323000	-2.899819000
C	4.831070000	-2.614533000	-1.944311000
H	5.400354000	-2.747033000	-2.858450000
C	5.282563000	-3.219764000	-0.753919000
C	4.521302000	-3.049298000	0.419329000
C	6.535397000	-4.060338000	-0.741721000
H	4.846706000	-3.518007000	1.342101000
H	7.215523000	-3.784300000	-1.552249000
H	7.074162000	-3.964525000	0.205705000
H	6.289244000	-5.122973000	-0.867863000
C	4.181380000	1.555412000	0.713983000
S	2.402810000	2.182014000	0.545565000
C	1.663035000	1.596761000	2.196412000
H	4.685257000	1.790161000	-0.223050000
H	4.651327000	2.096506000	1.536883000
H	4.190170000	0.481350000	0.897630000
H	0.794409000	2.226981000	2.385213000
H	1.365327000	0.551213000	2.107887000
H	2.412484000	1.748847000	2.974498000

BnTPEN: ⁵DMS-Prd_{NTS,DMS}

Fe	-0.697405000	0.560146000	-3.410099000
N	-1.538381000	-1.282281000	-4.242808000
N	0.545570000	1.073909000	-5.174495000
N	-2.241446000	1.251912000	-4.938800000
N	-1.156217000	2.579822000	-2.520175000
N	-1.989814000	0.146495000	-1.544291000
C	-0.959430000	-2.507040000	-4.194028000
H	0.029853000	-2.546281000	-3.755312000
C	-1.610354000	-3.645468000	-4.671242000
H	-1.122230000	-4.611054000	-4.622967000
C	-2.894494000	-3.510218000	-5.213184000
H	-3.423470000	-4.375744000	-5.595730000
C	-3.486937000	-2.242396000	-5.268024000
H	-4.475088000	-2.111172000	-5.694509000
C	-2.784445000	-1.140528000	-4.772533000
C	-3.349175000	0.267454000	-4.777913000
H	-4.107370000	0.372041000	-5.568170000
H	-3.842842000	0.470637000	-3.821217000
C	-1.635137000	1.169153000	-6.300793000

H	-2.141150000	1.852081000	-6.997050000
H	-1.799732000	0.155100000	-6.682287000
C	-0.145914000	1.427645000	-6.294194000
C	0.503052000	1.920884000	-7.429820000
H	-0.075290000	2.207013000	-8.301363000
C	1.897559000	2.026479000	-7.432315000
H	2.416894000	2.402622000	-8.306448000
C	2.606709000	1.631714000	-6.293733000
H	3.688168000	1.681092000	-6.261001000
C	1.902656000	1.165571000	-5.182765000
H	2.424229000	0.847098000	-4.288178000
C	-2.603893000	2.660027000	-4.581219000
H	-3.617111000	2.904717000	-4.933071000
H	-1.914700000	3.313285000	-5.123123000
C	-2.508298000	2.929517000	-3.080037000
H	-2.740640000	3.984576000	-2.884499000
H	-3.248529000	2.330580000	-2.543370000
C	-1.229646000	2.409409000	-1.034476000
H	-1.665376000	3.295539000	-0.556132000
H	-0.199282000	2.303139000	-0.671154000
C	-2.000870000	1.171194000	-0.653335000
C	-2.646879000	1.060712000	0.583671000
H	-2.653965000	1.903150000	1.266251000
C	-3.278253000	-0.138941000	0.921822000
H	-3.786393000	-0.242576000	1.873864000
C	-3.248350000	-1.200969000	0.009849000
H	-3.724565000	-2.147495000	0.235232000
C	-2.597950000	-1.019311000	-1.209573000
H	-2.549005000	-1.813140000	-1.941790000
C	-0.071573000	3.583179000	-2.896408000
H	0.003122000	3.574159000	-3.986088000
H	0.857163000	3.163731000	-2.498037000
C	-0.271580000	5.001579000	-2.398529000
C	-0.884445000	5.968419000	-3.216785000
H	-1.198318000	5.704163000	-4.223773000
C	-1.069845000	7.278979000	-2.762679000
H	-1.539243000	8.013854000	-3.407739000
C	-0.638281000	7.643651000	-1.482234000
H	-0.777903000	8.659811000	-1.130230000
C	-0.011929000	6.696253000	-0.663040000
H	0.338470000	6.979959000	0.323713000
C	0.172522000	5.387114000	-1.119594000
H	0.676006000	4.664075000	-0.483032000
N	1.986929000	1.339807000	-0.396551000
O	0.767249000	-0.324957000	-2.183890000
S	2.297893000	-0.092814000	-1.534339000
O	3.545878000	0.137976000	-2.591151000
C	2.672730000	-1.654881000	-0.588013000
C	3.718917000	-2.452729000	-1.046336000
C	1.890710000	-1.975329000	0.519635000
H	1.086851000	-1.327237000	0.849094000
H	4.297624000	-2.159083000	-1.914449000
C	3.992985000	-3.630496000	-0.344089000
H	4.805420000	-4.267469000	-0.678032000
C	3.236394000	-4.002496000	0.784624000
C	2.188375000	-3.157671000	1.203635000
C	3.531103000	-5.288434000	1.517725000
H	1.601587000	-3.427289000	2.075548000
H	4.600199000	-5.520577000	1.507876000
H	3.200752000	-5.244130000	2.559225000
H	3.012045000	-6.132816000	1.045084000
C	4.515029000	2.839031000	-1.267571000
S	3.512206000	2.153983000	0.205145000
C	4.738217000	0.872196000	0.898849000
H	4.681741000	2.029340000	-1.976413000
H	3.907680000	3.636562000	-1.693454000
H	5.438750000	3.237904000	-0.845358000

H	5.547334000	1.445819000	1.353402000
H	4.195815000	0.303083000	1.652142000
H	5.099432000	0.237078000	0.091026000

BnTPEN: ⁵CHD-PrdCHD_{NTS,CHD}

Fe	-0.578243000	0.731903000	-3.019228000
N	-1.317346000	-1.169197000	-3.835713000
N	0.699557000	1.250755000	-4.733673000
N	-2.088580000	1.332096000	-4.610051000
N	-1.117180000	2.776780000	-2.206452000
N	-1.798094000	0.338372000	-1.150057000
C	-0.696577000	-2.372584000	-3.758455000
H	0.282151000	-2.369543000	-3.295052000
C	-1.293092000	-3.538431000	-4.240517000
H	-0.772534000	-4.485413000	-4.167850000
C	-2.564884000	-3.455252000	-4.820339000
H	-3.052019000	-4.343180000	-5.207105000
C	-3.198429000	-2.209495000	-4.909654000
H	-4.176443000	-2.117724000	-5.368582000
C	-2.550365000	-1.077913000	-4.406880000
C	-3.163494000	0.309409000	-4.457832000
H	-3.901291000	0.369785000	-5.271535000
H	-3.693900000	0.516802000	-3.521330000
C	-1.431581000	1.240317000	-5.948270000
H	-1.936310000	1.887909000	-6.678047000
H	-1.543424000	0.212249000	-6.310959000
C	0.045313000	1.556658000	-5.888855000
C	0.725930000	2.055978000	-7.002723000
H	0.178567000	2.303503000	-7.905438000
C	2.113771000	2.220057000	-6.941305000
H	2.657757000	2.604377000	-7.796672000
C	2.785047000	1.874442000	-5.764200000
H	3.860511000	1.972917000	-5.683293000
C	2.050083000	1.396363000	-4.678883000
H	2.534851000	1.108567000	-3.755248000
C	-2.519175000	2.733687000	-4.301167000
H	-3.532816000	2.923717000	-4.683644000
H	-1.845349000	3.401558000	-4.844334000
C	-2.471535000	3.044870000	-2.806693000
H	-2.758882000	4.091687000	-2.643681000
H	-3.194496000	2.423982000	-2.270282000
C	-1.224797000	2.668275000	-0.717416000
H	-1.726913000	3.544600000	-0.289505000
H	-0.201366000	2.627060000	-0.324057000
C	-1.925321000	1.398725000	-0.309553000
C	-2.616073000	1.291903000	0.903242000
H	-2.716012000	2.160400000	1.544393000
C	-3.169670000	0.063173000	1.270742000
H	-3.711498000	-0.037571000	2.204356000
C	-3.017914000	-1.033483000	0.412679000
H	-3.430491000	-2.003139000	0.663514000
C	-2.330003000	-0.856965000	-0.785888000
H	-2.188588000	-1.675081000	-1.478042000
C	-0.070645000	3.817257000	-2.597485000
H	0.043302000	3.759233000	-3.682190000
H	0.864312000	3.470484000	-2.147828000
C	-0.366174000	5.244352000	-2.178181000
C	-1.014543000	6.131356000	-3.057503000
H	-1.283906000	5.801073000	-4.057988000
C	-1.290929000	7.448236000	-2.673646000
H	-1.786227000	8.121212000	-3.365229000
C	-0.915329000	7.899599000	-1.403271000
H	-1.124461000	8.921141000	-1.105373000
C	-0.252734000	7.033540000	-0.524777000
H	0.057558000	7.386750000	0.452888000
C	0.022533000	5.717759000	-0.911025000

H	0.560203000	5.060930000	-0.232604000
N	1.721650000	1.432781000	0.033661000
O	1.033954000	-0.291515000	-1.959062000
S	2.222543000	0.116997000	-0.881903000
O	3.641141000	0.386384000	-2.024100000
C	2.814693000	-1.387445000	0.050466000
C	3.660238000	-2.296501000	-0.585155000
C	2.333497000	-1.557795000	1.346767000
H	1.667349000	-0.833231000	1.801386000
H	4.016574000	-2.119938000	-1.592201000
C	4.052102000	-3.424760000	0.137886000
H	4.717431000	-4.144174000	-0.328213000
C	3.606359000	-3.643322000	1.459101000
C	2.745609000	-2.696437000	2.046389000
C	4.052459000	-4.866299000	2.221212000
H	2.392791000	-2.850037000	3.060431000
H	5.141565000	-4.873828000	2.349780000
H	3.598160000	-4.912315000	3.213731000
H	3.787362000	-5.784797000	1.684653000
H	6.453535000	2.701782000	-1.759738000
H	4.374311000	0.847375000	-1.525862000
C	5.987826000	2.525190000	-0.795232000
C	6.153421000	1.285533000	-0.152177000
H	6.757484000	0.510335000	-0.614238000
H	5.749837000	0.130545000	1.630121000
C	5.593859000	1.075046000	1.119323000
C	4.875031000	2.103065000	1.746189000
H	4.484032000	1.957693000	2.748765000
H	2.473948000	1.655574000	0.717043000
H	4.181535000	4.145430000	1.601347000
C	4.711034000	3.340585000	1.101715000
C	5.263900000	3.550296000	-0.168078000
H	5.157352000	4.513953000	-0.654641000