Electronic Supplementary Material (ESI) for ChemComm.

Why Metal-Oxos React with Dihydroanthracene and Cyclohexadiene at Comparable Rates, Despite Having Different C–H Bond Strengths. A Computational Study

Johannes E. M. N. Klein,[a,*] Büsra Dereli,[b] Lawrence Que, Jr.,[a] and Christopher J. Cramer[b]

[a] *Department of Chemistry and Center for Metals in Biocatalysis, University of Minnesota, 207 Pleasant St. S.E., Minneapolis, Minnesota 55455, United States. E-mail: kleinj@umn.edu.*

[b] *Department of Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota, 207 Pleasant Street SE, Minneapolis, Minnesota 55455, United States.*

Table of Contents

1. Computational Details

1.1 BDE calculations

All density functional theory (DFT) calculations were carried out with the electronic structure code Turbomole v6.6.[1] The M06-2X functional[2] was chosen as benchmark calculations have shown it to be accurate for the computation of bond dissociation energies to within an average error of about 2 kcal mol^{-1}.[3] The def2-TZVPP basis set was employed for all atoms.[4] Computations were accelerated using the multipole accelerated resolution of the identity approximation (*MARI-J*)[5] together with the def2-TZVPP/J auxiliary basis set.[6] The grid *m5* was used throughout. Thermal corrections (298.15 K) were obtained from frequency calculations using analytical second derivatives and the harmonic frequencies were scaled by 0.983 as recommended by Truhlar and co-workers for the M06-2X/def2-TZVPP combination of functional and basis set.[7] Frequency calculations were carried out to characterize stationary points giving no imaginary frequency for ground states and a single imaginary frequency for transition states. Small frequencies were raised to 100 cm^{-1} in order to compensate for the breakdown of the harmonic oscillator model.[8] For the hydrogen atom we add 5/2*RT (1.48 kcal mol^{-1} at 298.15 K) to the electronic energy as contribution from enthalpy.

Wave function theory (WFT) calculations were carried out with the electronic structure code Molpro Version 2012.1.[9] We computed energies using the *jun-jun* dual method of Truhlar and co-workers,[10] which is based on (R)CCSD(T)-F12a[11] and (R)MP2-F12[12] calculations including explicit correlation in combination with the calendar basis sets jun-cc-*p*V(N+d)Z (N = D,T).[13] The cc-pVNZ/JKFIT (N = D,T)[14] (JKFIT and OPTRI) and the cc-pVNZ (N = D,T)/MP2FIT[15] auxiliary basis sets were employed. For open-shell molecules, a restricted open-shell Hartree-Fock formalism was used.

The transition state for inversion of the DHA molecules was computed at the M06-2X/def2-TZVPP level of theory (*vide infra*).

1.2 HAT calculations

Two individual sets of calculations were carried out: (i) using the B3LYP[16] functional and (ii) using the B3LYP functional in combination with Grimme's D3[17] dispersion correction using the original zero-damping function. The details described below apply to both sets of calculations.

Geometries were optimized using the def2-SVP[4] basis set for all atoms except Fe and Cu where the def2-TZVP[4] basis set was used. Single point energies were computed using the def2-TZVPP[4] basis set for all atoms at the located stationary points. Solvation effects of MeCN (ε =

35.88[18] and refraction index = 1.344[19]) and CH_2Cl_2 (ε = 8.51[20] and refraction index = 1.421[21]) were modeled using the conductor-like screening model (COSMO)[22] in all calculations. All reported energies include the outlying charge correction.[23] The inclusion of a solvation model aids in the reduction of self-interaction error (SIE) in the HAT calculations for the Fe^{IV}(O) complexes as noted by Siegbahn and co-workers.[24]

Frequency calculations were carried out to characterize stationary points giving no imaginary frequency for ground states and a single imaginary frequency for transition states. Small frequencies were raised to 100 cm^{-1} in order to compensate for the breakdown of the harmonic oscillator model.[8] Frequency calculations for thermal corrections were carried out using frozen charges (NumForce –cosmo option). Frequencies were used without scaling. Free energies are referenced to a 1 M standard solution state (298.15 K) and include the concentration-change term RTln(24.5) = 1.89 kcal mol^{-1}.[25]

For the complexes $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ and $[Fe^{IV}(O)TMG_3tren]^{2+}$, as well as the associated reaction paths, the *S* = 2 spin state, as determined experimentally, was considered. For the HAT reaction by the Cu^{III}(OH)(L) complex the reactions studied require transitioning from two closed shell fragments to two open shell fragments resembling a singlet diradical. We use a broken symmetry approach to describe the bond-breaking process. Spin-densities/populations are analyzed to ensure that the correct electronic structure was obtained. The effect of applying a spin purification procedure to remove triplet-state spin contamination was evaluated according to $E_{singlet} = \frac{2E_{\langle S_Z\rangle=0} - \langle S^2\rangle E_{\langle S_Z\rangle=1}}{2 - \langle S^2\rangle}$.[26] The $\Delta\Delta G^{\ddagger}$ values discussed in the manuscript are only affected by 0.1 kcal/mol. The spin purified values are provided in brackets in Figure S4 (c) and (d) for completeness and are not further discussed.

The start and end points corresponding to the transition states are obtained from dynamic reaction coordinate calculations (DRC –t 150 -f).[27] Start geometries for the $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ complex were constructed from the crystal structure of the $[Fe^{II}TMG_2dienCl_2]$ complex (CCDC# 845701)[28] and for the $[Fe^{IV}(O)TMG_3tren]^{2+}$ complex from the corresponding crystal structure (CCDC# 818436).[29] For the Cu^{III}(OH)(L) based reaction paths start geometries were based on a previously reported transition state structure for DHA oxidation.[30]

Structural depictions and spin density plots were generated using IboView.[31]

2. Free Energy Profiles for all HAT Pathways

2.1 $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (σ) pathways

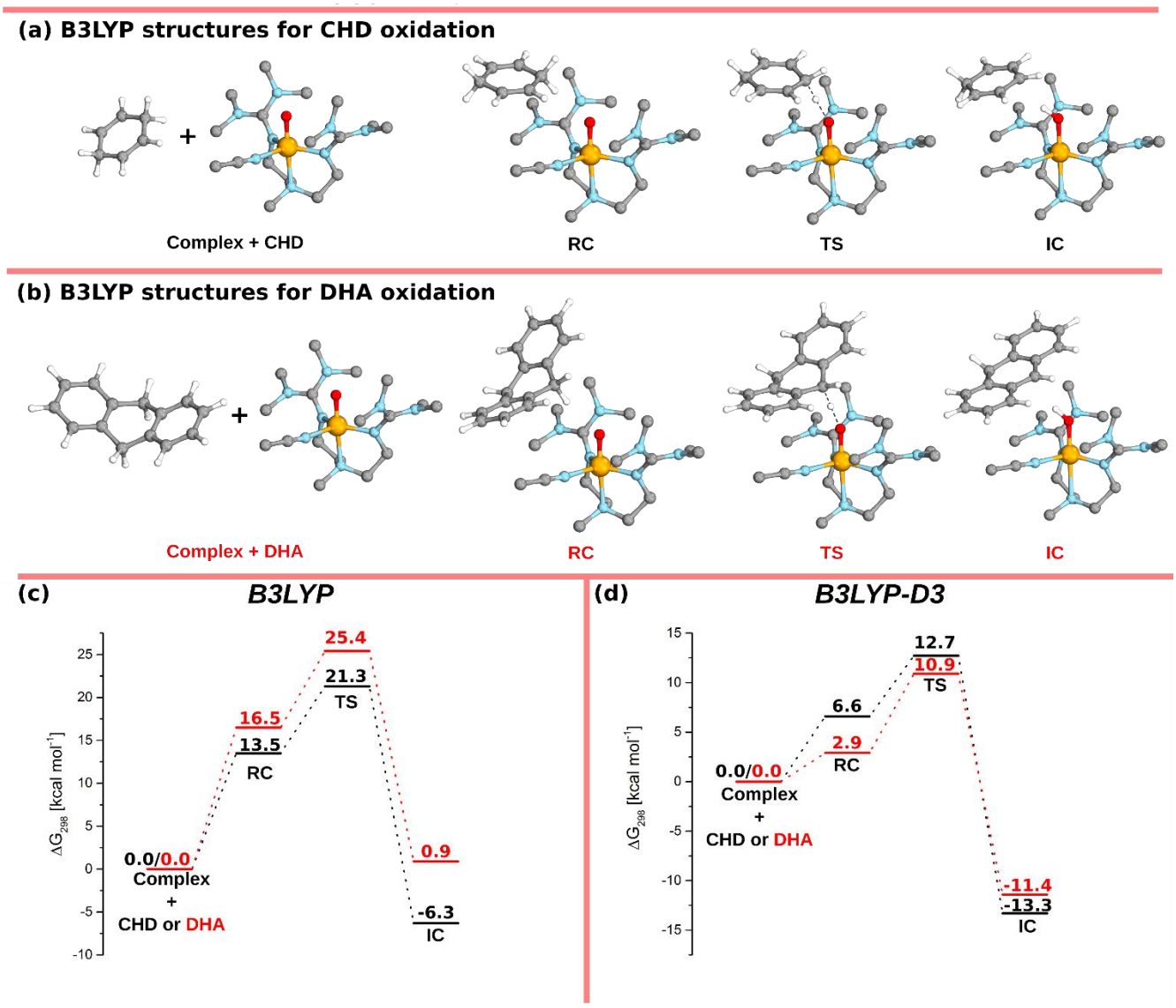

Figure S1: B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88) structures for HAT from CHD **(a)** and DHA **(b)** by $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ *via* a (σ) pathway; Free Energy Profiles (298.15 K) for HAT from CHD and DHA at the B3LYP-def2-TZVPP/B3LYP-def2-SVP(Fe:def2-TZVP) level of theory. COSMO (ε = 35.88) was used in all calculations. Data presented in section **(c)** was computed *without* Grimme's D3 correction and data presented in section **(d)** *with* the D3 correction.

2.2 $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (π) pathways

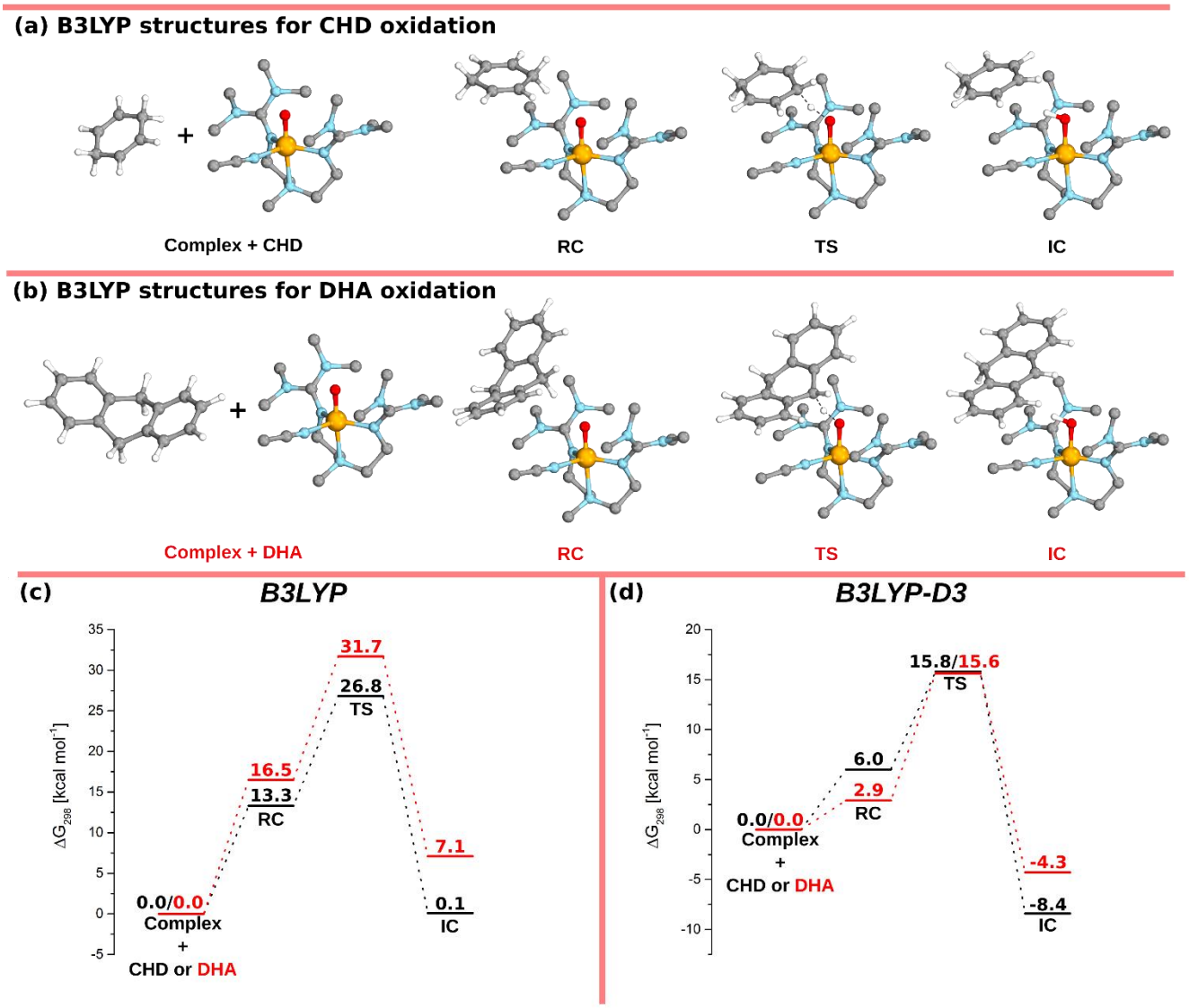

Figure S2: B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88) structures for HAT from CHD **(a)** and DHA **(b)** by $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ *via* a (π) pathway; Free Energy Profiles (298.15 K) for HAT from CHD and DHA at the B3LYP-def2-TZVPP/B3LYP-def2-SVP(Fe:def2-TZVP) level of theory. COSMO (ε = 35.88) was used in all calculations. Data presented in section **(c)** was computed *without* Grimme's D3 correction and data presented in section **(d)** *with* the D3 correction.

2.3 $[Fe^{IV}(O)TMG_3tren]^{2+}$ (σ) pathways

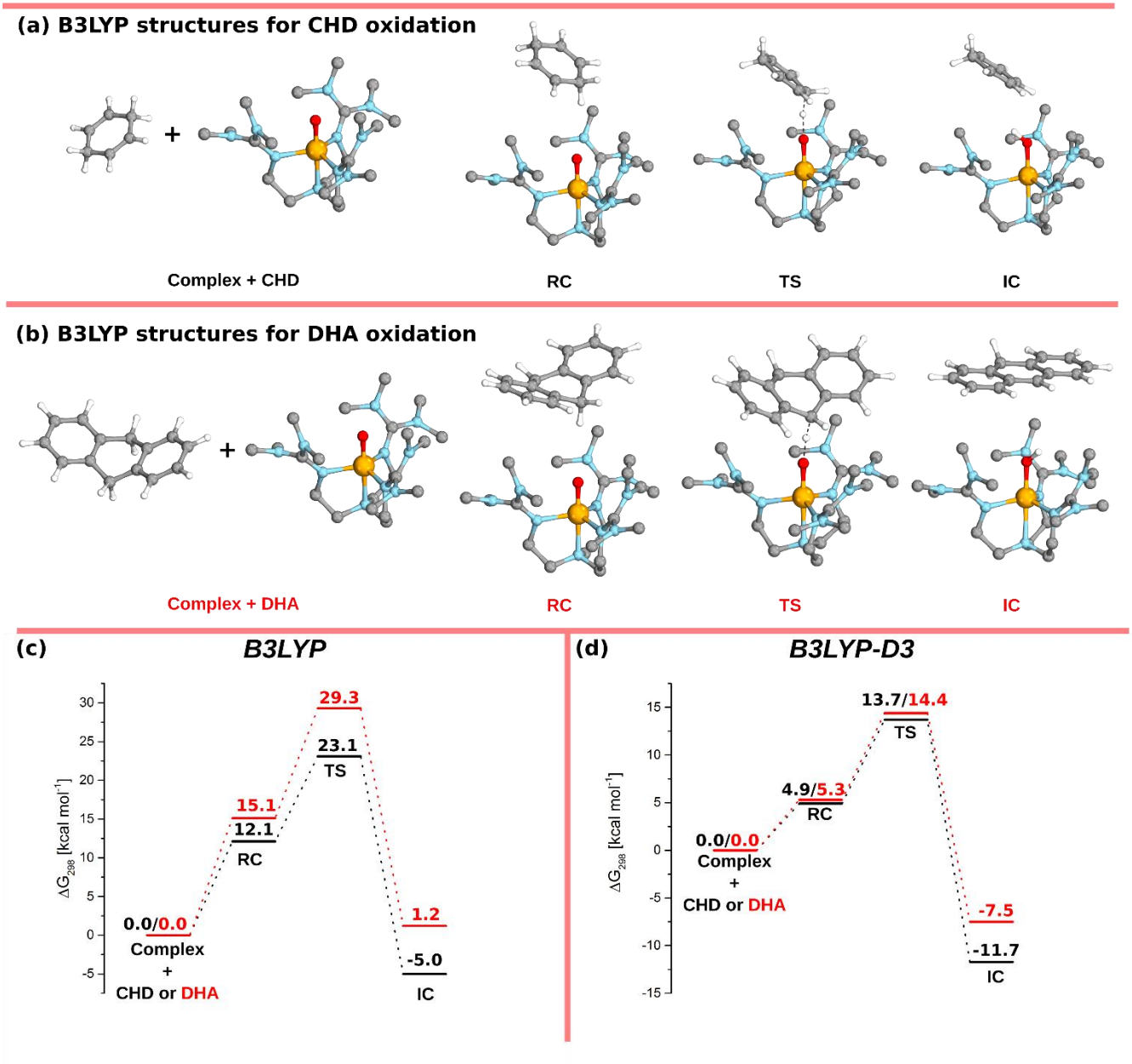

Figure S3: B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88) structures for HAT from CHD **(a)** and DHA **(b)** by $[Fe^{IV}(O)TMG_3tren]^{2+}$ *via* a (σ) pathway; Free Energy Profiles (298.15 K) for HAT from CHD and DHA at the B3LYP-def2-TZVPP/B3LYP-def2-SVP(Fe:def2-TZVP) level of theory. COSMO (ε = 35.88) was used in all calculations. Data presented in section **(c)** was computed *without* Grimme's D3 correction and data presented in section **(d)** *with* the D3 correction.

2.4 $Cu^{III}(OH)(L)$ pathways

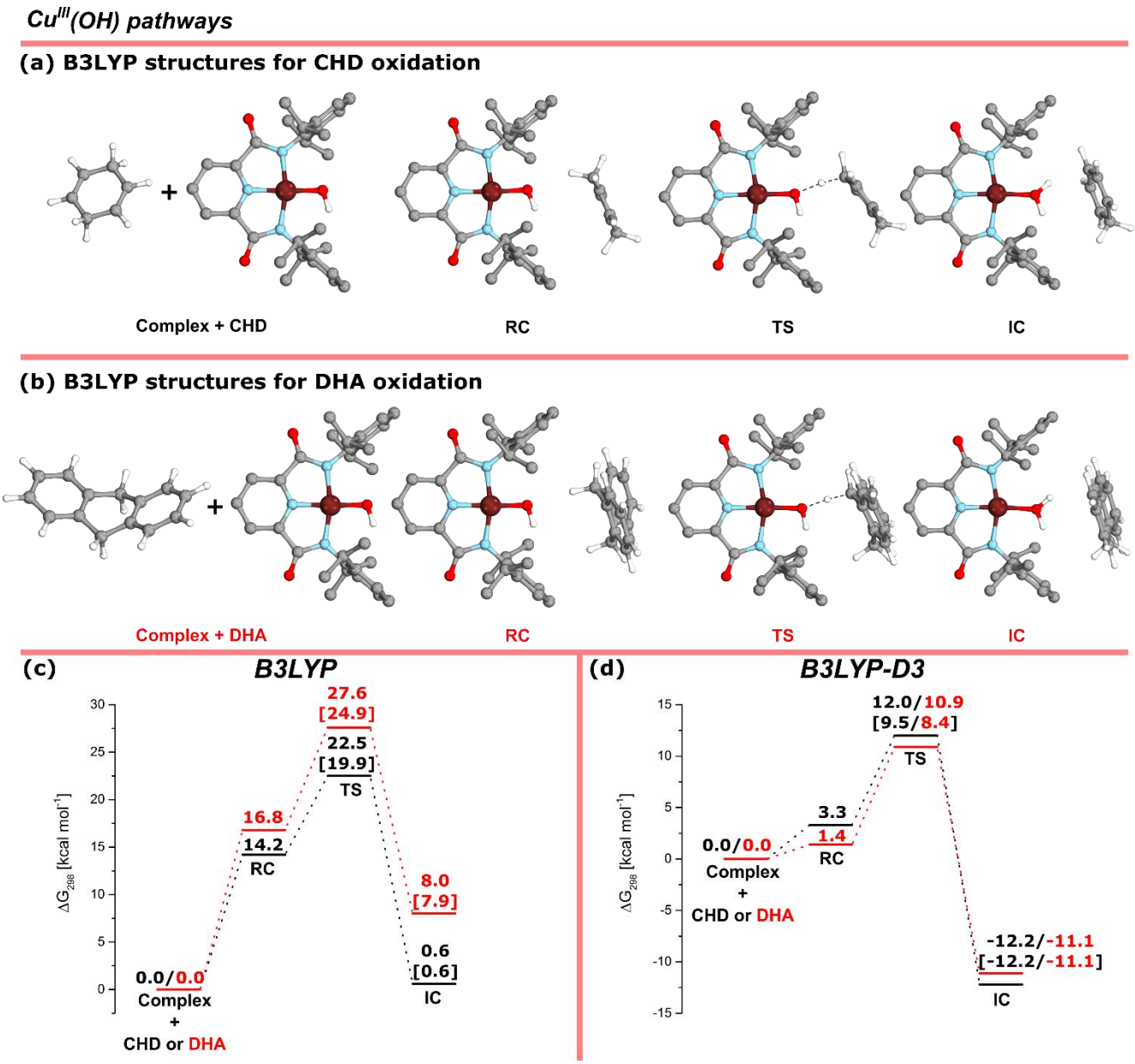

Figure S4: B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(ε = 8.51) structures for HAT from CHD **(a)** and DHA **(b)** by ***$Cu^{III}(OH)(L)$***; Free Energy Profiles (298.15 K) for HAT from CHD and DHA at the B3LYP-def2-TZVPP/B3LYP-def2-SVP(Cu:def2-TZVP) level of theory. COSMO (ε = 8.51) was used in all calculations. Data presented in section **(c)** was computed *without* Grimme's D3 correction and data presented in section **(d)** *with* the D3 correction. Values in brackets are spin purified.

3. Spin Density Plots of all Open-Shell Complexes

3.1 $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (σ) pathways

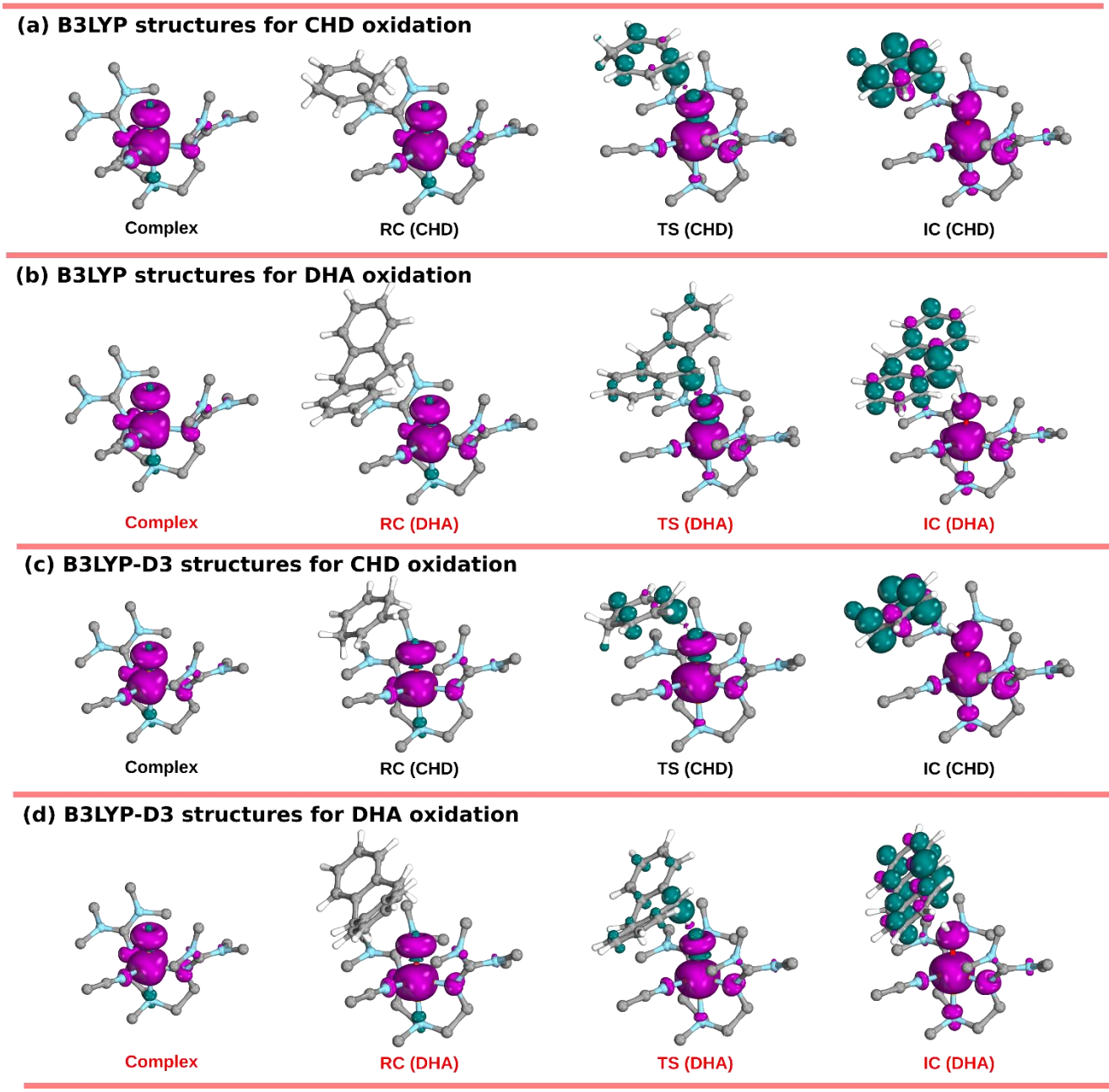

Figure S5: Spin density plots for all open shell complexes at the B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88) level of theory for HAT from CHD and DHA by **$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$** *via* (σ) pathways. Data presented in sections **(a)** and **(b)** is computed *without* Grimme's D3 correction and in sections **(c)** and **(d)** *with* the D3 correction. Positive spin density is depicted in purple and negative spin density in green (isosurface 0.005).

3.2 $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (π) pathways

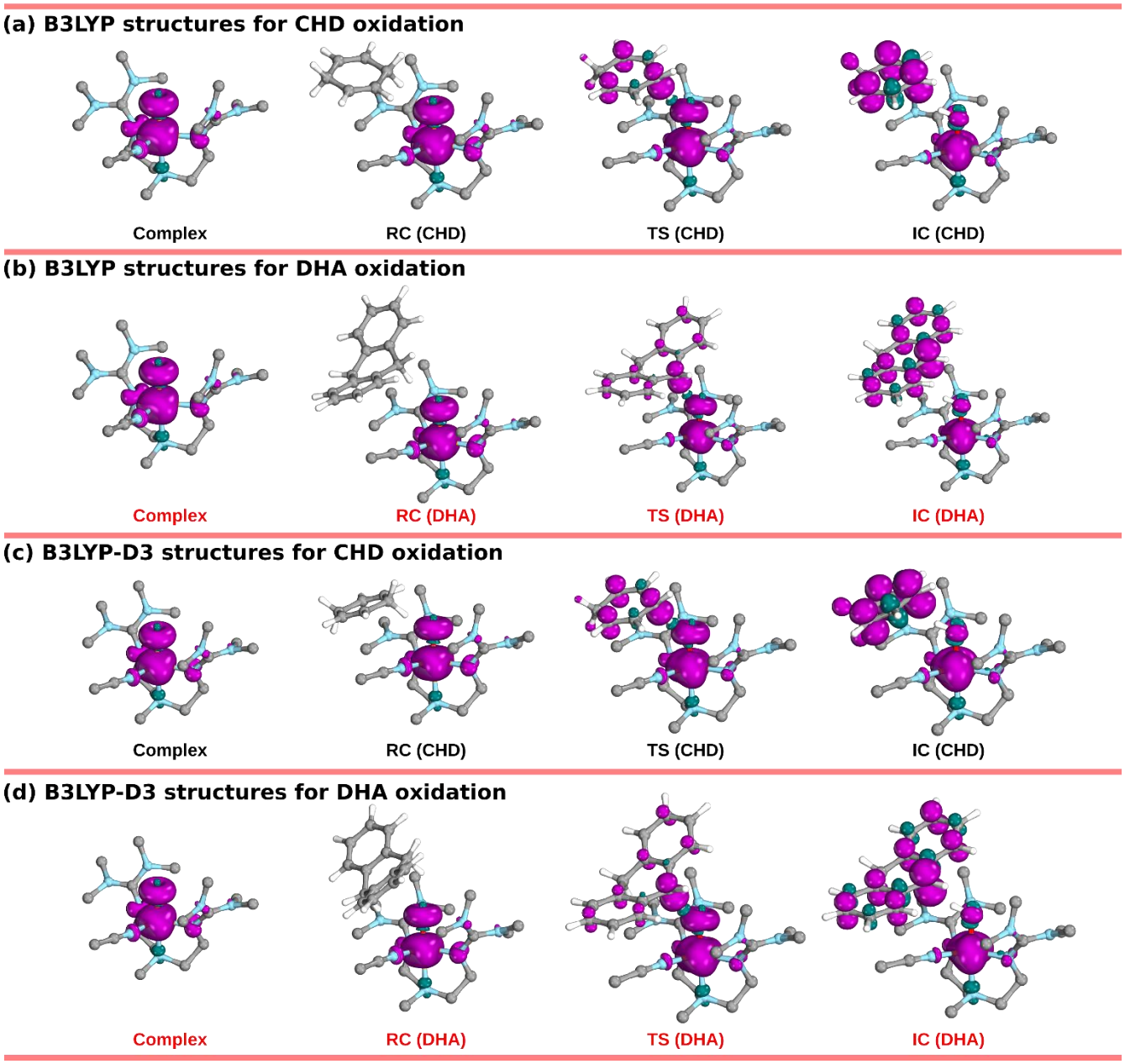

Figure S6: Spin density plots for all open shell complexes at the B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88) level of theory for HAT from CHD and DHA by **$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$** *via* (π) pathways. Data presented in sections **(a)** and **(b)** is computed *without* Grimme's D3 correction and in sections **(c)** and **(d)** *with* the D3 correction. Positive spin density is depicted in purple and negative spin density in green (isosurface 0.005).

3.3 $[Fe^{IV}(O)TMG_3tren]^{2+}$ (σ) pathways

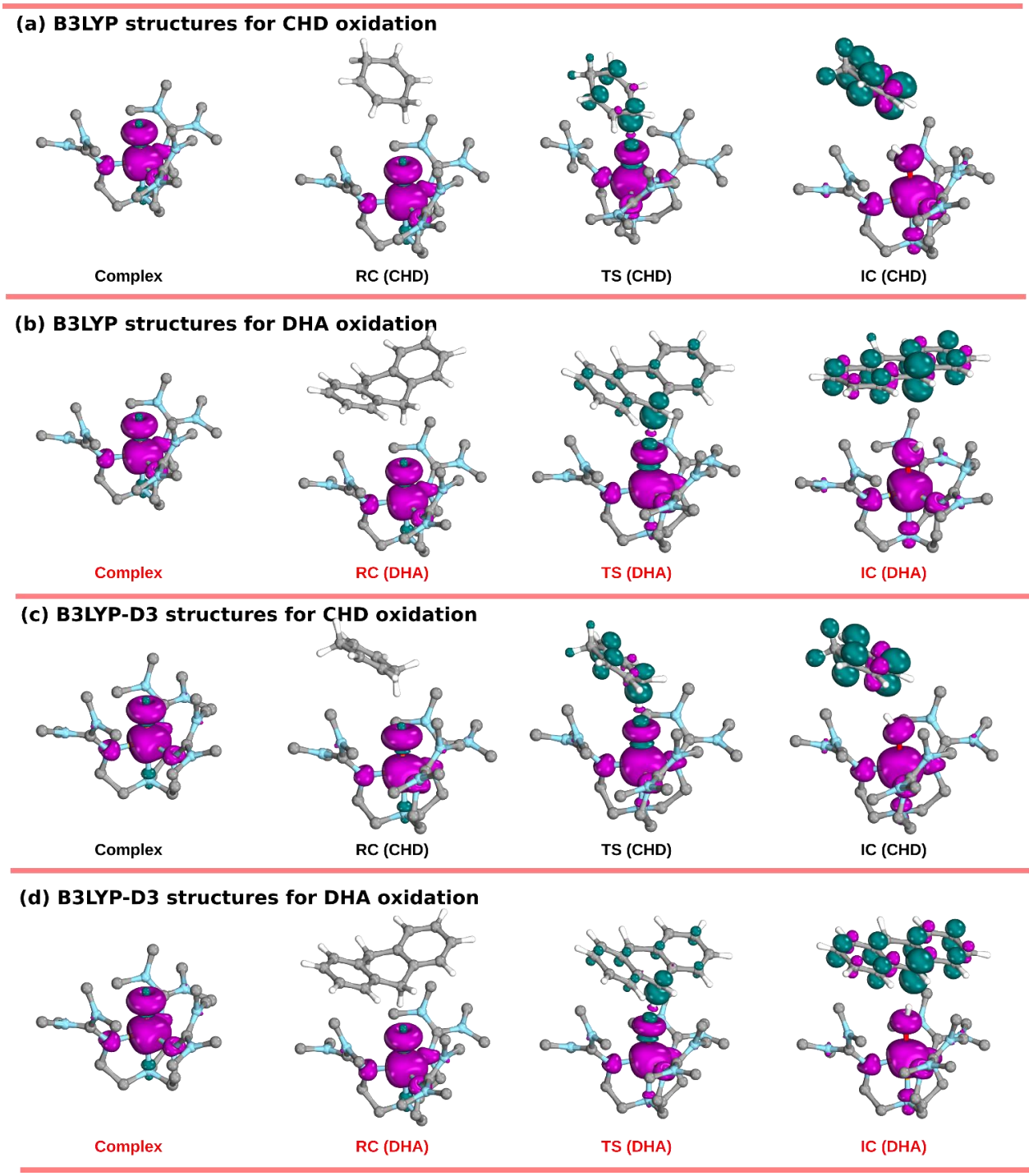

Figure S7: Spin density plots for all open shell complexes at the B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88) level of theory for HAT from CHD and DHA by **$[Fe^{IV}(O)TMG_3tren]^{2+}$** *via* (σ) pathways. Data presented in sections **(a)** and **(b)** is computed *without* Grimme's D3 correction and in sections **(c)** and **(d)** *with* the D3 correction. Positive spin density is depicted in purple and negative spin density in green (isosurface 0.005).

3.4 $Cu^{III}(OH)(L)$ pathways

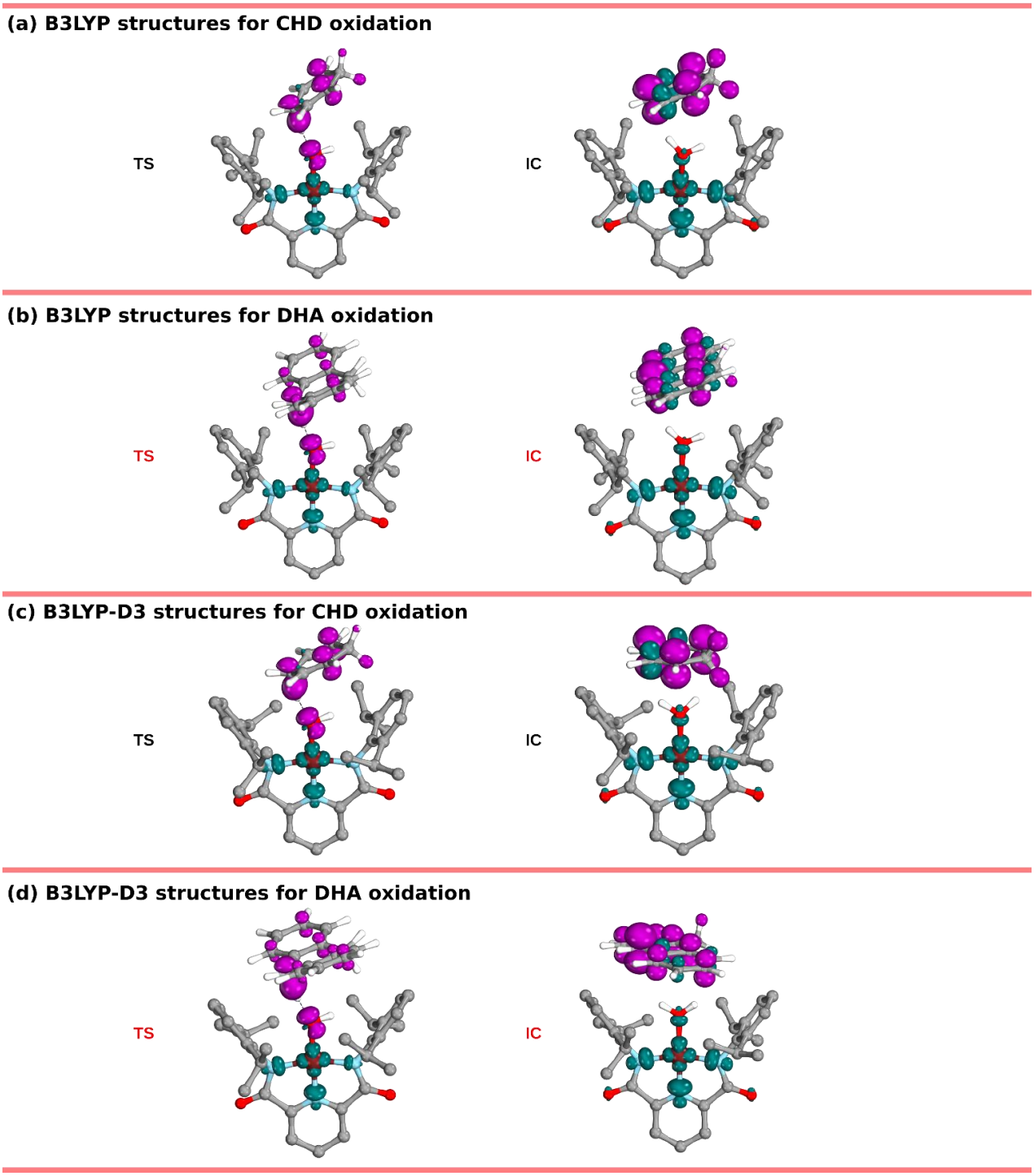

Figure S8: Spin density plots for all open shell complexes at the B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(ε = 8.51) level of theory for HAT from CHD and DHA by ***$Cu^{III}(OH)(L)$*** *via* (σ) pathways. Data presented in sections **(a)** and **(b)** is computed *without* Grimme's D3 correction and in sections **(c)** and **(d)** *with* the D3 correction. Positive spin density is depicted in purple and negative spin density in green (isosurface 0.005).

4. Experimental Determination of the Second Order Rate Constant for CHD Oxidation by $Cu^{III}(OH)(L)$

The following experiment was carried out by Mr. Debanjan Dhar in the laboratory of Professor William Tolman at the University of Minnesota and kindly provided for the comparison of CHD and DHA rates.

4.1 Materials and Methods

$[Bu_4N][Cu^{II}(OH)(L)]$ (L = *N*,*N′*-bis(2,6-diisopropylphenyl)-2,6-pyridinedicarboxamide)[32] and $[Fc][BAr^F{}_4]$[33] ($BAr^F{}_4$ = tetrakis(3,5bis(trifluoromethyl)phenyl)borate) were synthesized using previously reported procedures. 1,2-Difluorobenzene (DFB) was dried over calcium hydride and vacuum distilled and stored over 3 Å molecular sieves in a nitrogen atmosphere dry box. 1,4-cyclohexadiene (***CHD***) was purchased from Sigma-Aldrich and dried over 3 Å molecular sieves and vacuum distilled. UV-vis spectra were obtained using an HP8453 (190-1100) diode array spectrophotometer. Variable temperature UV-vis experiments were performed using a Unisoku low temperature cell holder.

4.2 General Procedure for Kinetic Studies of Reaction between $Cu^{III}(OH)(L)$ and 1,4-Cyclohexadiene in 1,2-Difluorobenzene.

Under an N_2 atmosphere, a 3.0 mL cuvette was charged with 1.8 mL of a known concentration of 1,4-cyclohexadiene solution in 1,2-difluorobenzene. The cuvette was cooled at -25 °C for approximately 10 min, after which 0.1 mL of a 2 mM stock solution of $[Bu_4N][Cu^{II}(OH)(L)]$ was added. After 2 min, to this was added 0.1 mL (2 mM solution) of [Fc][BArF4], which resulted in the immediate growth of an intense charge transfer band at 563 nm, consistent with the formation of the corresponding ***$Cu^{III}(OH)(L)$*** species. Decay of this feature was monitored over time by UV-vis spectroscopy. The decay traces were fit to a single exponential decay function to obtain the pseudo-first order rate constants (k_{obs}). Second order rate constants were extracted from linear fits of the plots of k_{obs} vs. substrate concentration (**Figure S1**).

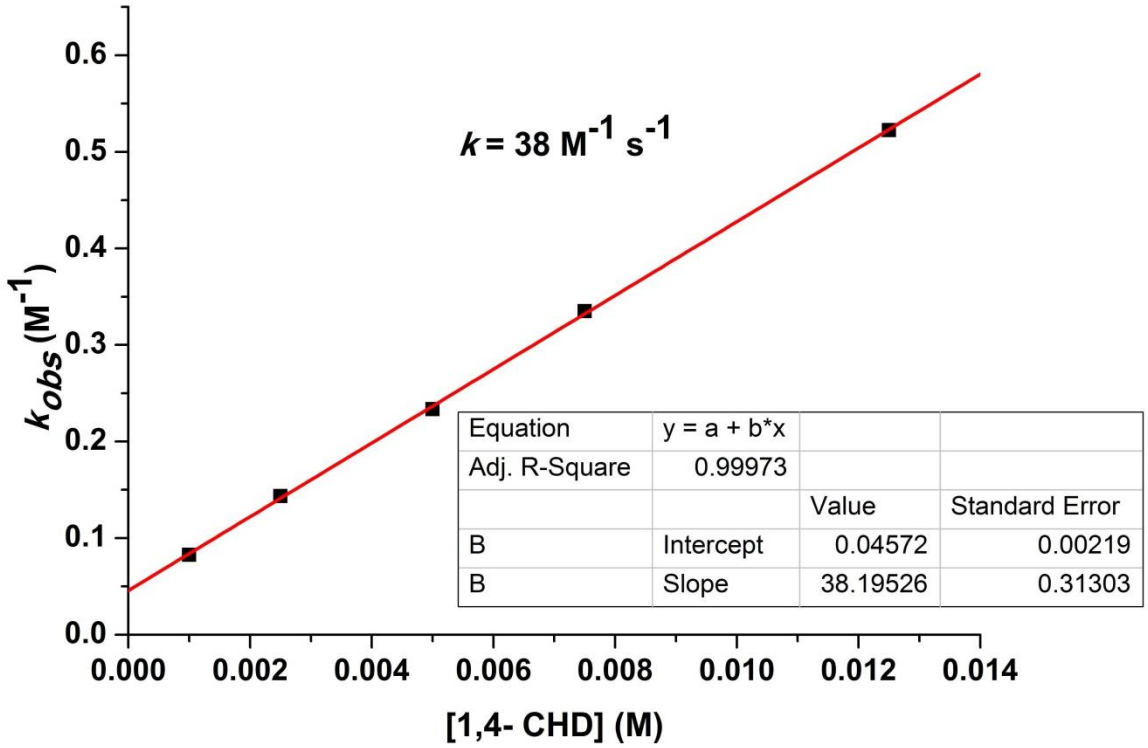

Figure S1: Determination of the second order rate constant (k_2) for CHD oxidation by the ***$Cu^{III}(OH)(L)$*** complex.

5. Coordinates and Absolute Energies

5.1 BDE calculations

Method: M06-2X/def2-TZVPP

C	-1.4046313	-0.5729506	0.1865345	***CHD***
C	-0.0446240	-1.2043565	0.1867505	**$E_{M06\text{-}2X/def2\text{-}TZVPP}$: -233.39460833711**
C	1.0638052	-0.1946436	0.1865059	**$H_{(298.15)M06\text{-}2X/def2\text{-}TZVPP}$: 0.127425**
C	0.8630094	1.1155965	0.1861086	**$E_{CCSD(T)\text{-}F12a/jun\text{-}cc\text{-}pV(D+d)Z}$: -233.02995965**
C	-0.4969980	1.7470028	0.1858907	**$E_{MP2\text{-}F12/jun\text{-}cc\text{-}pV(D+d)Z}$: -232.972719624611**
C	-1.6054273	0.7372893	0.1861467	**$E_{MP2\text{-}F12/jun\text{-}cc\text{-}pV(T+d)Z}$: -232.99822032**
H	-2.2567843	-1.2427789	0.1867285	
H	2.0774017	-0.5787197	0.1866752	
H	1.7151639	1.7854228	0.1859260	
H	-2.6190234	1.1213665	0.1859869	
H	-0.5983762	2.4074554	-0.6824256	
H	-0.5984238	2.4079425	1.0538316	
H	0.0567513	-1.8648160	1.0550623	
H	0.0568049	-1.8652921	-0.6811931	
C	-1.3784230	-0.5639650	0.3227757	***[CHD-H]$^{\cdot}$***
C	-0.0633745	-1.0822313	0.3816832	**$E_{M06\text{-}2X/def2\text{-}TZVPP}$: -232.76493438380**
C	1.0360570	-0.1940061	0.3222447	**$H_{(298.15)M06\text{-}2X/def2\text{-}TZVPP}$: 0.113821**
C	0.8582968	1.1447504	0.2092943	**$E_{RCCSD(T)\text{-}F12a/jun\text{-}cc\text{-}pV(D+d)Z}$: -232.39751727**
C	-0.4997089	1.7648306	0.1394156	**$E_{RMP2\text{-}F12/jun\text{-}cc\text{-}pV(D+d)Z}$: -232.344995096648**
C	-1.6096878	0.7665559	0.2096595	**$E_{RMP2\text{-}F12/jun\text{-}cc\text{-}pV(T+d)Z}$: -232.37029696**
H	-2.2163005	-1.2477576	0.3693563	
H	2.0402414	-0.5956586	0.3684931	
H	1.7151504	1.8044955	0.1663086	
H	-2.6247330	1.1396699	0.1666116	
H	-0.5917245	2.3630932	-0.7796361	
H	-0.6137877	2.5096723	0.9413216	
H	0.0998373	-2.1456388	0.4721938	
C	-3.5144132	-0.7611460	0.1517152	***DHA***
C	-3.5212029	0.6001798	0.4187428	**$E_{M06\text{-}2X/def2\text{-}TZVPP}$: -540.69848526566**
C	-2.3641503	-1.3615706	-0.3406861	**$H_{(298.15)M06\text{-}2X/def2\text{-}TZVPP}$: 0.226125**
C	-2.3777651	1.3532346	0.1916290	**$E_{RCCSD(T)\text{-}F12a/jun\text{-}cc\text{-}pV(D+d)Z}$: -539.83966492**
C	-1.2196695	-0.6109534	-0.5762761	**$E_{RMP2\text{-}F12/jun\text{-}cc\text{-}pV(D+d)Z}$: -539.755379227706**
C	-1.2265792	0.7583302	-0.3080083	**$E_{RMP2\text{-}F12/jun\text{-}cc\text{-}pV(T+d)Z}$: -539.80757449**
C	0.0448665	-1.2270745	-1.1196741	
C	0.0306146	1.5462042	-0.5776116	
C	1.2656009	0.7552321	-0.2266439	
C	1.2727226	-0.6140972	-0.4947006	
C	2.3833431	1.3472914	0.3469441	
C	2.3976503	-1.3675203	-0.1853477	
C	3.5078741	0.5914708	0.6474642	
C	3.5151780	-0.7698266	0.3804091	
H	-4.3993234	-1.3556102	0.3337349	
H	-4.4114880	1.0733890	0.8100464	

H	-2.3526379	-2.4259380	-0.5411878	
H	-2.3769647	2.4144880	0.4083343	
H	2.3708700	2.4084210	0.5638793	
H	2.3964233	-2.4319273	-0.3859711	
H	4.3721133	1.0625332	1.0955572	
H	4.3851218	-1.3663582	0.6190811	
H	0.0658117	1.7941054	-1.6457525	
H	0.0141446	2.4932599	-0.0387467	
H	0.0388176	-2.3072320	-0.9757588	
H	0.0804982	-1.0551186	-2.2025836	
C	-3.6689997	-0.7121762	0.0220328	***[DHA-H]•***
C	-3.6916643	0.6795956	-0.0535844	**$E_{M06\text{-}2X/def2\text{-}TZVPP}$: -540.06346911401**
C	-2.4637987	-1.3751681	0.0977193	**$H_{(298.15)M06\text{-}2X/def2\text{-}TZVPP}$: 0.212865**
C	-2.4985507	1.3879125	-0.0471438	**$E_{RCCSD(T)\text{-}F12a/jun\text{-}cc\text{-}pV(D+d)Z}$: -539.20079730**
C	-1.2439434	-0.6697467	0.1015060	**$E_{RMP2\text{-}F12/jun\text{-}cc\text{-}pV(D+d)Z}$: -539.117140429630**
C	-1.2751223	0.7394629	0.0320984	**$E_{RMP2\text{-}F12/jun\text{-}cc\text{-}pV(T+d)Z}$: -539.17021225**
C	-0.0000196	-1.3541940	0.1590610	
C	-0.0000127	1.5401553	0.0680441	
C	1.2750933	0.7394569	0.0320723	
C	1.2439046	-0.6697516	0.1015280	
C	2.4985187	1.3879001	-0.0472495	
C	2.4637645	-1.3751711	0.0978011	
C	3.6916318	0.6795806	-0.0536640	
C	3.6689653	-0.7121853	0.0220723	
H	-4.5952324	-1.2704868	0.0187659	
H	-4.6338210	1.2062145	-0.1168555	
H	-2.4380294	-2.4563028	0.1520493	
H	-2.5170961	2.4701042	-0.1034300	
H	2.5170727	2.4700880	-0.1035992	
H	2.4379953	-2.4563029	0.1521886	
H	4.6337844	1.2062005	-0.1169874	
H	4.5951939	-1.2705029	0.0188392	
H	-0.0000226	2.2557265	-0.7595464	
H	0.0000002	2.1530098	0.9770107	
H	-0.0000236	-2.4350306	0.2170268	
H	0	0	0	***H•***
				$E_{M06\text{-}2X/def2\text{-}TZVPP}$: -0.49814085117
				$E_{RCCSD(T)\text{-}F12a/jun\text{-}cc\text{-}pV(D+d)Z}$: -0.49933813
				$E_{RMP2\text{-}F12/jun\text{-}cc\text{-}pV(D+d)Z}$: -0.49933813
				$E_{RMP2\text{-}F12/jun\text{-}cc\text{-}pV(T+d)Z}$: -0.49982654
C	-0.6957042	-3.4845769	-1.2346887	***DHA-TS Inversion***
C	0.6956950	-3.4844783	-1.2349703	**$E_{M06\text{-}2X/def2\text{-}TZVPP}$: -540.69579592466**
C	-1.3751504	-2.3507977	-0.8330785	**$H_{(298.15)M06\text{-}2X/def2\text{-}TZVPP}$: 0.225142**
C	1.3751432	-2.3506025	-0.8336358	
C	-0.6948823	-1.2011816	-0.4259712	

C	0.6948772	-1.2010831	-0.4262524	
C	-1.4965466	0.0000647	0.0000670	
C	1.4965440	0.0002760	-0.0005364	
C	0.6948794	1.2014484	0.4257096	
C	-0.6948798	1.2013498	0.4259910	
C	1.3751475	2.3508821	0.8333321	
C	-1.3751462	2.3506861	0.8338899	
C	0.6957014	3.4844451	1.2355513	
C	-0.6956985	3.4843462	1.2358332	
H	-1.2420536	-4.3645289	-1.5458240	
H	1.2420432	-4.3643530	-1.5463261	
H	-2.4589758	-2.3447080	-0.8306766	
H	2.4589685	-2.3443587	-0.8316754	
H	2.4589728	2.3447809	0.8309648	
H	-2.4589715	2.3444299	0.8319644	
H	1.2420522	4.3642057	1.5472250	
H	-1.2420484	4.3640291	1.5477278	
H	2.1595528	-0.2906322	0.8197555	
H	2.1591274	0.2912926	-0.8211352	
H	-2.1594986	0.2909890	-0.8202666	
H	-2.1591867	-0.2909360	0.8206239	

5.2 HAT Calculations

5.2.1 $[Fe^{IV}(O)TMG_3tren]^{2+}$ (σ), $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (σ) and $[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (π) pathways (B3LYP)

Method: B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)

C	-1.4111774	-0.5812849	0.1866830	***CHD***
C	-0.0432947	-1.2131073	0.1865797	**$E_{B3LYP/def2-SVP/COSMO(\varepsilon = 35.88)}$:**
C	1.0725677	-0.2006139	0.1866134	**-233.0953243759**
C	0.8695532	1.1239299	0.1862949	**$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 35.88)}$:**
C	-0.4983290	1.7557522	0.1857224	**-233.3536128246**
C	-1.6141918	0.7432590	0.1862907	**$ZPE_{B3LYP/def2-SVP/COSMO(\varepsilon = 35.88)}$:**
H	-2.2712989	-1.2609750	0.1870781	**0.121841**
H	2.0967717	-0.5915000	0.1869724	**Chem. Pot.$_{(298.15)/B3LYP/def2-SVP/COSMO(\varepsilon = 35.88)}$:**
H	1.7296741	1.8036205	0.1864022	**0.094824 (σ = 4)**
H	-2.6383963	1.1341445	0.1864131	
H	-0.6019741	2.4319211	-0.6872346	
H	-0.6021373	2.4331810	1.0576689	
H	0.0604589	-1.8899700	1.0589738	
H	0.0604231	-1.8898398	-0.6859302	
C	-3.5649727	-0.7620845	0.1227423	***DHA***
C	-3.5720534	0.6113158	0.3916265	**$E_{B3LYP/def2-SVP/COSMO(\varepsilon = 35.88)}$:**
C	-2.3968395	-1.3720988	-0.3475023	**-540.0051075707**
C	-2.4109285	1.3651834	0.1885262	
C	-1.2318292	-0.6211688	-0.5609990	

C	-1.2389242	0.7618287	-0.2901190
C	0.0437069	-1.2497055	-1.0849793
C	0.0292922	1.5542064	-0.5358478
C	1.2768616	0.7587001	-0.2081356
C	1.2839046	-0.6243290	-0.4788309
C	2.4167616	1.3592284	0.3456654
C	2.4306561	-1.3781417	-0.1899994
C	3.5604072	0.6025407	0.6236470
C	3.5673290	-0.7709208	0.3550016
H	-4.4661176	-1.3599638	0.2854140
H	-4.4788239	1.0947386	0.7658700
H	-2.3880985	-2.4475928	-0.5503538
H	-2.4133122	2.4377919	0.4063001
H	2.4075452	2.4318207	0.5633344
H	2.4324083	-2.4536755	-0.3928329
H	4.4422596	1.0838161	1.0557318
H	4.4545330	-1.3709848	0.5758681
H	0.0645761	1.8375480	-1.6078281
H	0.0122184	2.5015903	0.0244303
H	0.0370663	-2.3385688	-0.9235728
H	0.0798299	-1.1073076	-2.1845682

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-540.5866247568

$ZPE_{B3LYP/def2\text{-}SVP/COSMO(\varepsilon = 35.88)}$:

0.217265

Chem. Pot.$_{(298.15)/B3LYP/def2\text{-}SVP/COSMO(\varepsilon = 35.88)}$:

0.182819 (σ = 2)

$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (σ) pathway

Fe	4.7688866	9.4501776	3.1777595
N	4.4657054	11.2878440	2.1549817
O	3.1678937	9.2340564	3.3921057
N	5.1825649	9.8456151	5.0580689
C	6.5890691	10.2129841	5.2979430
H	6.8828455	9.9712978	6.3320619
H	6.7774794	11.2907749	5.1582496
C	7.4309487	9.4063913	4.3252658
H	8.4971760	9.6820799	4.3854691
H	7.3439721	8.3376971	4.5662835
N	6.9239606	9.6226059	2.9371512
C	7.3325779	8.5225702	2.0160764
H	8.3959591	8.2715029	2.1696578
H	7.2165095	8.8951927	0.9886868
C	6.4380037	7.3145986	2.2172876
H	6.6326620	6.5749289	1.4248715
H	6.6702578	6.8204783	3.1755880
N	5.0450921	7.7885302	2.1608544
C	4.2853222	10.0102776	6.0614847
N	4.3239068	11.1098739	6.8557527
C	4.7336982	12.4162661	6.3486244
H	4.7412909	12.4131775	5.2523414
H	5.7293395	12.7071244	6.7227621

$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$

$E_{B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2445.7011101624 (<S^2> 6.05271312)

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2447.0153464804 (<S^2> 6.05510794)

$ZPE_{B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.572743

Chem. Pot.$_{(298.15)/B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.514953

H	4.0064646	13.1715858	6.6865287	
C	3.9789286	11.0732137	8.2766865	
H	3.9378121	10.0367438	8.6311348	
H	3.0154594	11.5677517	8.4816718	
H	4.7638517	11.6023252	8.8399915	
N	3.3563392	9.0637555	6.3064065	
C	2.0127476	9.3862676	6.7829070	
H	1.8351268	10.4661125	6.7270110	
H	1.8494797	9.0417491	7.8168824	
H	1.2821483	8.8818095	6.1308104	
C	3.5765358	7.6550197	5.9979898	
H	4.6414372	7.4723917	5.8149155	
H	2.9953725	7.3502467	5.1142463	
H	3.2553477	7.0494527	6.8605649	
C	7.4292424	10.9138974	2.4112479	
H	8.5299242	10.8838057	2.3456780	
H	7.1388580	11.7409151	3.0704542	
H	7.0171678	11.0960044	1.4119301	
C	4.0834601	6.9697067	1.6824469	
N	4.1471943	5.6230428	1.8569546	
C	4.6874751	5.0170077	3.0703655	
H	4.7808364	5.7665677	3.8639639	
H	5.6700607	4.5487644	2.8946239	
H	3.9921287	4.2356121	3.4163571	
C	3.6944682	4.6765401	0.8379478	
H	3.5384115	5.1917556	-0.1170177	
H	2.7633166	4.1652515	1.1325614	
H	4.4760242	3.9128722	0.6971182	
N	3.0459695	7.4781720	0.9823055	
C	1.7041787	6.9032841	1.0463718	
H	1.6429025	6.1594677	1.8487681	
H	1.4121671	6.4348119	0.0923431	
H	0.9881586	7.7106479	1.2680628	
C	3.1493896	8.7080732	0.2054660	
H	4.2016040	8.9745772	0.0559017	
H	2.6302674	9.5396602	0.7063742	
H	2.6806227	8.5453183	-0.7782137	
C	4.1404823	12.2782990	1.6555319	
C	3.7344875	13.5189803	1.0272112	
H	4.0389012	13.5112539	-0.0306102	
H	2.6411143	13.6252235	1.0948004	
H	4.2180567	14.3653572	1.5385425	
Fe	0.5428691	0.7317008	0.4951827	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-RC (σ)***
N	-0.3792568	-0.4090049	2.0295750	**E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
O	-0.4805130	0.1545360	-0.6341141	**-2678.7947971799 (<S^2> 6.05338439)**
N	2.1286857	-0.2440784	-0.1366422	
C	3.3140524	-0.0795066	0.7227011	

H	4.2387384	-0.2289907	0.1424330
H	3.3408044	-0.8033869	1.5546201
C	3.2746535	1.3379649	1.2663394
H	4.0921359	1.5203807	1.9839165
H	3.3877973	2.0499345	0.4368873
N	1.9545068	1.5785264	1.9221369
C	1.6328590	3.0320899	2.0150576
H	2.5161888	3.5975412	2.3578190
H	0.8431414	3.1453034	2.7710157
C	1.1271688	3.5421515	0.6792848
H	0.7356718	4.5645190	0.7991845
H	1.9556554	3.6035024	-0.0462018
N	0.0663529	2.6240114	0.2323354
C	2.1578716	-1.1773266	-1.1187360
N	2.7142910	-2.3972263	-0.9052092
C	2.6533885	-3.0572922	0.3957186
H	1.9137837	-2.5649486	1.0379883
H	3.6335381	-3.0593379	0.9008118
H	2.3427033	-4.1041299	0.2491391
C	3.4404264	-3.1295370	-1.9428519
H	3.6647323	-2.4685468	-2.7880421
H	2.8764933	-4.0050762	-2.3040122
H	4.3922849	-3.4853879	-1.5178347
N	1.6577183	-0.8968630	-2.3393964
C	1.0030943	-1.9045912	-3.1705822
H	0.8183352	-2.8164412	-2.5914341
H	1.5995307	-2.1546833	-4.0627150
H	0.0330492	-1.5034618	-3.5040878
C	1.6171255	0.4599171	-2.8740420
H	2.2719294	1.1142854	-2.2877255
H	0.5909572	0.8578820	-2.8580849
H	1.9746774	0.4405637	-3.9159204
C	1.9541512	0.9900555	3.2833171
H	2.7126685	1.4930202	3.9065997
H	2.1871338	-0.0808908	3.2423391
H	0.9689282	1.1209353	3.7457944
C	-0.9559153	3.1003268	-0.5094836
N	-0.7830350	4.1309749	-1.3791971
C	0.4446082	4.3065879	-2.1496269
H	1.0529029	3.3961086	-2.1138112
H	1.0422530	5.1579877	-1.7842136
H	0.1786785	4.5003737	-3.2010713
C	-1.8073309	5.1511498	-1.6011953
H	-2.5795908	5.0896488	-0.8255704
H	-2.2787795	5.0550381	-2.5930689
H	-1.3325424	6.1435510	-1.5412423
N	-2.1948063	2.5778266	-0.3730169
C	-3.1197396	2.4596444	-1.4976244

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2680.3651942219 (<S^2> 6.05578902)

$ZPE_{B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.695695

Chem. Pot.$_{(298.15)/B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.630469

H	-2.6103914	2.6894816	-2.4401858
H	-3.9919728	3.1236802	-1.3832002
H	-3.4809325	1.4198828	-1.5464153
C	-2.6591004	1.9717780	0.8689852
H	-2.0051241	2.2602255	1.6995647
H	-2.6831589	0.8737734	0.7908116
H	-3.6791276	2.3311958	1.0786453
C	-0.9565606	-1.1148437	2.7399073
C	-1.6849162	-2.0014613	3.6240474
H	-2.2090886	-1.4087569	4.3893369
H	-2.4187652	-2.5753296	3.0357896
H	-0.9823928	-2.6913132	4.1161752
C	-2.2987780	-5.1073081	-0.5961310
C	-3.1334050	-5.2573805	0.6492129
C	-3.8673117	-3.9950744	1.0212199
C	-3.7770872	-2.8537734	0.3223513
C	-2.9326591	-2.6995721	-0.9158943
C	-2.2122460	-3.9673423	-1.2948519
H	-1.7444057	-5.9916102	-0.9308970
H	-4.5103751	-4.0375362	1.9080990
H	-4.3472757	-1.9757692	0.6482225
H	-1.5903710	-3.9336808	-2.1968783
H	-2.2028082	-1.8756588	-0.7794907
H	-3.5654866	-2.3578584	-1.7601284
H	-3.8561095	-6.0886724	0.5222040
H	-2.4968681	-5.5886604	1.4946425
Fe	4.4308526	9.2851410	3.1850415
N	3.9038494	11.0430674	2.0864176
O	2.8132939	8.8720609	3.4892696
N	5.0156793	9.8042179	5.0408055
C	6.2803709	10.5573319	5.0665483
H	6.7077853	10.5652375	6.0821020
H	6.1461025	11.6123994	4.7714585
C	7.2493288	9.8764146	4.1126595
H	8.2218060	10.4000430	4.0970340
H	7.4314720	8.8504446	4.4620007
N	6.6672803	9.8243897	2.7470834
C	7.1833062	8.6798311	1.9594374
H	8.2805347	8.5944529	2.0644033
H	6.9649204	8.8797621	0.9002114
C	6.4989073	7.3848552	2.3689885
H	6.8228705	6.5791056	1.6918643
H	6.8169840	7.0890151	3.3836387
N	5.0448931	7.5856131	2.2875061
C	4.2821049	9.7441535	6.1686478
N	4.2008548	10.8052411	7.0194577
C	4.1908596	12.1805333	6.5322318

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-TS (σ)

E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

-2678.7771659493 (<S^2> 6.47328013)

E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:

-2680.3463477638 (<S^2> 6.46761236)

ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.689157

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.624082

H	3.9917096	12.2003448	5.4540298
H	5.1431152	12.6990517	6.7349408
H	3.3860508	12.7337792	7.0428540
C	4.1610916	10.6545565	8.4728034
H	4.4213294	9.6279513	8.7562515
H	3.1723227	10.9070589	8.8905645
H	4.9051964	11.3344913	8.9184690
N	3.6336194	8.6056126	6.5024109
C	2.3725261	8.6032109	7.2383643
H	1.9489040	9.6129732	7.2769703
H	2.4949320	8.2201128	8.2646976
H	1.6607166	7.9483009	6.7120427
C	4.0691947	7.2980398	6.0297095
H	5.1183879	7.3441123	5.7159737
H	3.4492706	6.9590317	5.1847545
H	3.9765857	6.5724019	6.8530534
C	6.9315340	11.0881505	2.0321098
H	8.0164862	11.2208418	1.8695388
H	6.5607808	11.9430392	2.6124635
H	6.4267438	11.0814789	1.0576651
C	4.2707049	6.5910660	1.8218772
N	4.5860505	5.2794061	2.0152361
C	5.2341324	4.8004529	3.2313217
H	5.2067885	5.5707247	4.0087940
H	6.2819200	4.5072510	3.0518024
H	4.6898172	3.9171328	3.6028983
C	4.3277239	4.2530856	1.0068692
H	4.0727488	4.7175579	0.0471850
H	3.5146309	3.5715860	1.3076904
H	5.2430189	3.6546050	0.8702108
N	3.1576606	6.8735821	1.1018658
C	1.9468458	6.0628435	1.1866080
H	2.0277952	5.3351468	2.0021620
H	1.7406660	5.5295880	0.2438978
H	1.0908112	6.7234790	1.3994873
C	3.0402336	8.0778148	0.2898541
H	4.0316682	8.5070718	0.1042842
H	2.4067649	8.8341113	0.7788109
H	2.5839856	7.8117797	-0.6770967
C	3.4568590	11.9695012	1.5592788
C	2.8921522	13.1288706	0.8991307
H	3.2440820	13.1686764	-0.1430309
H	1.7937327	13.0575980	0.9111174
H	3.2062396	14.0430992	1.4255775
C	-0.6574007	11.0568062	4.9238442
C	-0.7497750	12.0650310	3.8165097
C	-0.4672174	11.4920718	2.4584639
C	-0.0545598	10.2212477	2.2732216

C	0.1932010	9.2915236	3.4000411
C	-0.2492947	9.7871810	4.7229678
H	-0.9602755	11.3817258	5.9248239
H	-0.6371324	12.1427281	1.5936478
H	0.1162464	9.8509516	1.2569806
H	-0.2234809	9.0868234	5.5631681
H	1.3938658	9.1086716	3.4634510
H	-0.1220484	8.2538476	3.1923562
H	-1.7497681	12.5442795	3.8237375
H	-0.0633882	12.9149626	4.0202543
Fe	0.2946972	0.5358629	0.4576258
N	-0.5586012	-0.4551866	2.1462471
O	-0.9330809	-0.1875874	-0.6815360
N	1.9922772	-0.4153338	-0.0916437
C	3.1068106	-0.3020920	0.8621215
H	4.0640131	-0.5438237	0.3726425
H	3.0016339	-0.9982611	1.7119079
C	3.1477999	1.1290737	1.3766939
H	3.9733782	1.2609839	2.0989377
H	3.3387619	1.8049404	0.5314912
N	1.8503006	1.4901820	1.9986911
C	1.5807509	2.9444916	1.9304135
H	2.4653890	3.5244996	2.2532615
H	0.7649734	3.1636853	2.6351039
C	1.1510238	3.3622536	0.5303706
H	0.8513292	4.4217956	0.5520491
H	2.0033485	3.2923404	-0.1670241
N	0.0306722	2.5091166	0.1121066
C	2.0896427	-1.3077974	-1.0972425
N	2.6898682	-2.5172349	-0.9226641
C	2.6062326	-3.2444102	0.3397758
H	1.8117738	-2.8255433	0.9691600
H	3.5584247	-3.2212572	0.8956255
H	2.3611613	-4.2979067	0.1285362
C	3.4839694	-3.1635192	-1.9665313
H	3.6989600	-2.4543503	-2.7744314
H	2.9779904	-4.0489847	-2.3859940
H	4.4409022	-3.4909878	-1.5293182
N	1.6046660	-1.0064724	-2.3236972
C	1.0071642	-2.0104669	-3.1998021
H	0.8584304	-2.9517629	-2.6584678
H	1.6244294	-2.1992591	-4.0931678
H	0.0228879	-1.6437053	-3.5321469
C	1.4889264	0.3668539	-2.7982151
H	2.1355993	1.0239629	-2.2052746
H	0.4466331	0.7181196	-2.7352880
H	1.8120542	0.4087275	-3.8504045

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-IC (σ)

$E_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:

-2678.8195904194 (<S^2> 7.03662745)

$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 35.88)}$:

-2680.3907041148 (<S^2> 7.03398300)

$ZPE_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:

0.691013

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:

0.624496

C	1.8056154	1.0309555	3.3987201	
H	2.5660943	1.5550548	4.0060494	
H	2.0015801	-0.0480450	3.4560187	
H	0.8152986	1.2299171	3.8283776	
C	-0.9795159	3.0506997	-0.5947618	
N	-0.7739218	4.0555816	-1.4896434	
C	0.4457879	4.1579008	-2.2842867	
H	1.0127016	3.2223033	-2.2363940	
H	1.0890215	4.9873551	-1.9466723	
H	0.1725088	4.3412835	-3.3358611	
C	-1.7484207	5.1229653	-1.7101494	
H	-2.5055130	5.1163810	-0.9173959	
H	-2.2470645	5.0329827	-2.6894717	
H	-1.2225868	6.0908720	-1.6809006	
N	-2.2503549	2.6189098	-0.4074335	
C	-3.2057911	2.5078357	-1.5056649	
H	-2.7122434	2.6967022	-2.4657071	
H	-4.0506414	3.2061297	-1.3877131	
H	-3.6052796	1.4806027	-1.5215332	
C	-2.7180826	2.0887542	0.8667417	
H	-2.0186061	2.3532716	1.6682490	
H	-2.8296523	0.9938243	0.8257276	
H	-3.7014037	2.5298015	1.0967939	
C	-1.0805846	-1.0647719	2.9786351	
C	-1.7348395	-1.8300839	4.0189662	
H	-2.4140623	-1.1747519	4.5856423	
H	-2.3121799	-2.6480399	3.5608948	
H	-0.9788728	-2.2507627	4.6995272	
C	-1.9003835	-4.4416560	-0.9916887	
C	-2.2481093	-4.9497718	0.3770538	
C	-3.2314727	-4.0849853	1.1115343	
C	-3.7405443	-2.9359143	0.5640368	
C	-3.3608248	-2.5053992	-0.7409305	
C	-2.4427084	-3.2877508	-1.4982154	
H	-1.2034521	-5.0330493	-1.5936173	
H	-3.5529433	-4.4113369	2.1057792	
H	-4.4647509	-2.3414617	1.1297914	
H	-2.1739834	-2.9624050	-2.5077767	
H	-1.4732821	-0.9907046	-0.6072284	
H	-3.8094260	-1.6089843	-1.1755799	
H	-2.6351772	-5.9911902	0.3085843	
H	-1.3243686	-5.0833788	0.9842471	
Fe	1.7468852	0.4623730	0.2216486	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-RC (σ)***
N	0.7442064	2.0637573	-0.7479917	**E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
O	0.5933707	-0.6065980	-0.2061384	**-2985.7042212119 (<S^2> 6.05358326)**
N	1.3165638	0.4765539	2.1386781	
C	2.0900990	1.4586550	2.9187750	

H	2.1675992	1.1448009	3.9720543
H	1.6287654	2.4607258	2.9189706
C	3.4757217	1.5218912	2.3004483
H	4.1005112	2.2929716	2.7815612
H	3.9767564	0.5523253	2.4287595
N	3.3507844	1.8029852	0.8389062
C	4.5631492	1.3774930	0.0811845
H	5.4765758	1.6939521	0.6132109
H	4.5402173	1.8924178	-0.8895209
C	4.5402831	-0.1221563	-0.1441731
H	5.3449098	-0.4020197	-0.8421155
H	4.7413372	-0.6546864	0.8004648
N	3.2208762	-0.4630712	-0.7020662
C	0.2831045	-0.1649008	2.7381368
N	-0.5713541	0.5046850	3.5540107
C	-0.9153224	1.9055353	3.3284358
H	-0.6127846	2.2151410	2.3210183
H	-0.4420825	2.5690480	4.0711214
H	-2.0073508	2.0231675	3.4162839
C	-1.1750731	-0.1021486	4.7404949
H	-0.6655474	-1.0401722	4.9891474
H	-2.2514534	-0.2973408	4.6045966
H	-1.0565496	0.5926068	5.5868718
N	0.1068828	-1.4887182	2.5565050
C	-1.2133196	-2.1157852	2.5332589
H	-2.0012418	-1.3570992	2.4708569
H	-1.3831091	-2.7486516	3.4190795
H	-1.2811144	-2.7492482	1.6358521
C	1.2144268	-2.3876971	2.2503570
H	2.1693170	-1.8953048	2.4656907
H	1.1891553	-2.6952608	1.1937555
H	1.1267088	-3.2850319	2.8832885
C	3.1249205	3.2529511	0.6248391
H	3.9962714	3.8229765	0.9888074
H	2.2333725	3.5902116	1.1674754
H	2.9884468	3.4554337	-0.4436919
C	3.1095045	-1.5008844	-1.5580387
N	3.9130824	-2.5931932	-1.4605009
C	4.3610386	-3.1244370	-0.1765071
H	3.7758703	-2.6922035	0.6423902
H	5.4318166	-2.9291250	-0.0009574
H	4.2058072	-4.2151456	-0.1705610
C	4.4030486	-3.3139982	-2.6351569
H	4.2309710	-2.7236853	-3.5427038
H	3.9227119	-4.3000966	-2.7453656
H	5.4877613	-3.4708902	-2.5228124
N	2.2085063	-1.4572062	-2.5647840
C	1.5105244	-2.6496536	-3.0388777

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2987.5970827314 (<S^2> 6.05599834)

$ZPE_{B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.791331

Chem. Pot.$_{(298.15)/B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.722174

H	1.6974246	-3.4966251	-2.3692215
H	1.8115405	-2.9217140	-4.0636589
H	0.4279705	-2.4444505	-3.0402656
C	1.7679859	-0.2070133	-3.1714712
H	2.4522370	0.6060221	-2.9042381
H	0.7489448	0.0550277	-2.8472947
H	1.7677962	-0.3255817	-4.2667723
C	0.1070105	2.8506973	-1.3056340
C	-0.6838581	3.8413484	-2.0067830
H	-0.1623227	4.1380890	-2.9297491
H	-1.6696207	3.4218686	-2.2610902
H	-0.8166767	4.7257132	-1.3649323
C	-3.7527357	2.0917802	-3.9113866
C	-4.3395962	2.9998155	-3.0220891
C	-3.2659213	0.8690123	-3.4359447
C	-4.4320174	2.6797189	-1.6625961
C	-3.3506477	0.5429329	-2.0741417
C	-3.9373811	1.4598544	-1.1783263
C	-2.8303736	-0.7719818	-1.5295677
C	-4.0104816	1.0915630	0.2898046
C	-4.2652465	-0.3877439	0.5000804
C	-3.6889140	-1.3054424	-0.4007131
C	-5.0488630	-0.8609768	1.5628182
C	-3.9128170	-2.6783381	-0.2227013
C	-5.2582017	-2.2330056	1.7406396
C	-4.6895058	-3.1443682	0.8437096
H	-3.6820422	2.3310968	-4.9759619
H	-4.7310794	3.9534229	-3.3866956
H	-2.8200148	0.1536526	-4.1338847
H	-4.8971408	3.3857270	-0.9678079
H	-5.5045192	-0.1465963	2.2555634
H	-3.4747899	-3.3908088	-0.9285853
H	-5.8722835	-2.5886833	2.5725960
H	-4.8561427	-4.2177585	0.9697904
H	-3.0434793	1.3552031	0.7657573
H	-4.7712125	1.6964120	0.8063162
H	-2.7430255	-1.5169723	-2.3356035
H	-1.8010589	-0.6189987	-1.1436558
Fe	4.5431323	9.1291806	2.8522580
N	4.1036280	10.4664865	1.2482468
O	2.9048843	8.9064313	3.2657224
N	5.1707084	10.2112008	4.4272551
C	6.4576091	10.8890933	4.1943714
H	6.8909234	11.2367717	5.1456273
H	6.3506301	11.7790217	3.5505171
C	7.4006293	9.8918956	3.5412084
H	8.3896785	10.3471822	3.3553167

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-TS (σ)

E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

-2985.6843261097 (<S^2> 6.49026349)

E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:

-2987.5758563751 (<S^2> 6.48683816)

ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

H	7.5501237	9.0433360	4.2234183
N	6.8132034	9.3932337	2.2719853
C	7.2785998	8.0265709	1.9389830
H	8.3692313	7.9348547	2.0947519
H	7.0800298	7.8571483	0.8706531
C	6.5258692	6.9841756	2.7512170
H	6.8183554	5.9812552	2.4038341
H	6.8137020	7.0445612	3.8151975
N	5.0850381	7.2072496	2.5614029
C	4.4655898	10.5490176	5.5252269
N	4.4352358	11.8350909	5.9761469
C	4.4460850	12.9694276	5.0582017
H	4.2196778	12.6361822	4.0381196
H	5.4157254	13.4951669	5.0600434
H	3.6695350	13.6874909	5.3685997
C	4.4521449	12.1787079	7.3970699
H	4.6921607	11.2952301	8.0000755
H	3.4902916	12.5985216	7.7355040
H	5.2348348	12.9356664	7.5675588
N	3.7991867	9.6071538	6.2274718
C	2.5761002	9.8935968	6.9729093
H	2.1874957	10.8825971	6.7081530
H	2.7398931	9.8478955	8.0618868
H	1.8154904	9.1452150	6.7046725
C	4.1776132	8.2002311	6.1943326
H	5.2129898	8.0985916	5.8495677
H	3.5115396	7.6300185	5.5277546
H	4.1006024	7.7868311	7.2121303
C	7.1300232	10.3175602	1.1661374
H	8.2185687	10.3349596	0.9766205
H	6.8056181	11.3370883	1.4121530
H	6.6178094	9.9975976	0.2496533
C	4.2779869	6.1459487	2.3917240
N	4.5232552	4.9506297	2.9982469
C	5.1069179	4.8570683	4.3321349
H	5.0887451	5.8336945	4.8265301
H	6.1455100	4.4877237	4.3024705
H	4.5100507	4.1541498	4.9356487
C	4.2646256	3.6687788	2.3444292
H	4.0710871	3.8178486	1.2757888
H	3.4118550	3.1365439	2.7975554
H	5.1592391	3.0336793	2.4484881
N	3.2051336	6.2309320	1.5684279
C	1.9662778	5.5010430	1.8199389
H	1.9710042	5.0720891	2.8285622
H	1.8032205	4.6961285	1.0845682
H	1.1199181	6.2021738	1.7471451
C	3.1711197	7.1336666	0.4242080

0.784392

Chem. Pot.(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88):

0.715142

H	4.1867952	7.4541830	0.1650045
H	2.5544949	8.0228169	0.6287867
H	2.7397479	6.5999443	-0.4375134
C	3.7578835	11.2120961	0.4355629
C	3.3329581	12.1478189	-0.5854916
H	3.6167432	11.7629791	-1.5770192
H	2.2402259	12.2724397	-0.5404556
H	3.8203725	13.1205323	-0.4185276
C	-0.3685074	10.7176297	-0.3200550
C	-0.5233787	12.0608046	0.0511364
C	-0.0948256	9.7575576	0.6550700
C	-0.4009135	12.4319937	1.3951121
C	0.0267230	10.1197037	2.0107490
C	-0.1232854	11.4764053	2.3811375
C	0.2996187	9.1066288	3.0646954
C	0.0284357	11.8598972	3.8363507
C	-0.4080314	10.7715266	4.7922665
C	-0.2520310	9.4193033	4.4083601
C	-0.9449435	11.0706363	6.0510029
C	-0.6261414	8.3985918	5.3041022
C	-1.3155285	10.0492987	6.9328857
C	-1.1546891	8.7082181	6.5577346
H	-0.4718551	10.4202635	-1.3668747
H	-0.7488424	12.8174391	-0.7052058
H	0.0073467	8.7067482	0.3693986
H	-0.5311917	13.4793631	1.6832158
H	-1.0786694	12.1162997	6.3439600
H	-0.5090425	7.3530594	5.0041990
H	-1.7361164	10.2994729	7.9105385
H	-1.4483643	7.9069098	7.2409025
H	1.1004293	12.0786920	4.0249217
H	-0.5031979	12.8001954	4.0480534
H	0.0726594	8.0802558	2.7405350
H	1.5288274	9.0430166	3.1873587
Fe	1.4706147	0.4120464	0.2147883
N	0.5786991	2.1364768	-0.6693640
O	0.0613122	-0.6567263	-0.2174985
N	1.3060805	0.5623444	2.2236161
C	2.1124345	1.6280819	2.8391072
H	2.2324957	1.4496616	3.9197995
H	1.6422412	2.6207097	2.7325983
C	3.4792364	1.6366417	2.1720560
H	4.1211296	2.4236552	2.6070349
H	3.9710295	0.6715891	2.3576628
N	3.3370224	1.8317889	0.7084480
C	4.4595419	1.2315849	-0.0473445
H	5.4306375	1.5119193	0.4016195

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-IC (σ)

E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

-2985.7220368753 (<S^2> 7.03807160)

E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:

-2987.6160271672 (<S^2> 7.03583511)

ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.78681

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

H	4.4330507	1.6459184	-1.0660689	**0.716232**
C	4.3244894	-0.2829282	-0.1257160	
H	5.1119768	-0.6762409	-0.7874499	
H	4.4955548	-0.7339095	0.8668325	
N	2.9904471	-0.6036727	-0.6499433	
C	0.3673302	-0.0502526	2.9727865	
N	-0.3620831	0.6306130	3.8993550	
C	-0.7615823	2.0198364	3.6988045	
H	-0.6322377	2.3063476	2.6480904	
H	-0.1870959	2.7127587	4.3360312	
H	-1.8278563	2.1247823	3.9568830	
C	-0.7752355	0.0375006	5.1702878	
H	-0.2398601	-0.9036071	5.3422221	
H	-1.8610932	-0.1509002	5.2075543	
H	-0.5206234	0.7352819	5.9842573	
N	0.1429510	-1.3763766	2.8323454	
C	-1.1856722	-1.9660622	2.9730375	
H	-1.9476083	-1.1829516	3.0550625	
H	-1.2509531	-2.6280873	3.8518518	
H	-1.4045487	-2.5597091	2.0718322	
C	1.1711161	-2.2945155	2.3583396	
H	2.1618261	-1.8400530	2.4753102	
H	1.0060446	-2.5570270	1.3012730	
H	1.1313209	-3.2152268	2.9617324	
C	3.2215405	3.2662568	0.3897919	
H	4.1516285	3.8012559	0.6554509	
H	2.3917130	3.7190924	0.9484705	
H	3.0351333	3.3991005	-0.6838298	
C	2.8545484	-1.6273756	-1.5135524	
N	3.6234550	-2.7471063	-1.4296590	
C	4.0876781	-3.2824906	-0.1539284	
H	3.5417311	-2.8212342	0.6756942	
H	5.1686699	-3.1211886	-0.0085455	
H	3.8961498	-4.3673366	-0.1312632	
C	4.0647569	-3.4885029	-2.6100414	
H	3.8911506	-2.8979008	-3.5171141	
H	3.5512577	-4.4596119	-2.7048708	
H	5.1462867	-3.6798444	-2.5212272	
N	1.9527004	-1.5516160	-2.5227372	
C	1.1886994	-2.7104269	-2.9734816	
H	1.3685957	-3.5694682	-2.3175346	
H	1.4346922	-2.9872806	-4.0116967	
H	0.1151420	-2.4642136	-2.9268050	
C	1.5633515	-0.2855324	-3.1296597	
H	2.2867735	0.4972020	-2.8736886	
H	0.5599231	0.0264031	-2.7986149	
H	1.5469325	-0.4052186	-4.2249203	
C	0.0197421	3.0385489	-1.1285608	

C	-0.6722433	4.1748392	-1.6992675
H	-0.0526391	4.6188257	-2.4935504
H	-1.6329803	3.8483430	-2.1267828
H	-0.8548140	4.9253496	-0.9149267
C	-3.2746422	2.4237485	-3.9614968
C	-4.1347507	3.1777004	-3.1440056
C	-2.8747329	1.1543227	-3.5598846
C	-4.5790211	2.6486737	-1.9252772
C	-3.3248234	0.5986247	-2.3311541
C	-4.1879516	1.3747455	-1.5005532
C	-2.9630315	-0.7289683	-1.9408279
C	-4.6477453	0.8354156	-0.1639685
C	-4.3888725	-0.6353085	0.0785900
C	-3.5230853	-1.3663409	-0.7899843
C	-4.9704895	-1.2891456	1.1695456
C	-3.2674822	-2.7366970	-0.5084623
C	-4.7145963	-2.6415757	1.4275274
C	-3.8554776	-3.3649042	0.5825086
H	-2.9254151	2.8316616	-4.9137971
H	-4.4590908	4.1733501	-3.4575537
H	-2.2170446	0.5584627	-4.1993964
H	-5.2472395	3.2406802	-1.2922447
H	-5.6404196	-0.7311247	1.8310762
H	-2.6059469	-3.2976505	-1.1747835
H	-5.1845918	-3.1321357	2.2838677
H	-3.6538785	-4.4212142	0.7796442
H	-4.1455293	1.4161022	0.6372545
H	-5.7206671	1.0536995	-0.0228362
H	-2.3212015	-1.3143351	-2.6054465
H	-0.8643775	-0.5213988	-0.4669635

$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (π) pathway

Fe	0.5950928	0.6550936	0.5563116
N	-0.4898703	-0.4313406	2.0220278
O	-0.4168192	0.1828271	-0.6306163
N	2.1244200	-0.4380607	-0.0201422
C	3.2783225	-0.3827889	0.8942791
H	4.2139457	-0.5962543	0.3528600
H	3.2095180	-1.1198497	1.7120498
C	3.3263609	1.0242655	1.4636484
H	4.1214900	1.1288602	2.2208326
H	3.5340484	1.7383134	0.6545349
N	2.0004357	1.3593932	2.0637167
C	1.7923221	2.8324057	2.1729174
H	2.7005237	3.3181293	2.5688039
H	0.9785649	2.9957555	2.8933698
C	1.3943925	3.4055062	0.8262575

$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$-CHD-RC (π)

$E_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:

-2678.7948298231 (<S^2> 6.05337167)

$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 35.88)}$:

-2680.3652325018 (<S^2> 6.05576575)

$ZPE_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:

0.69563

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:

0.63033

H	1.0802048	4.4538026	0.9499097
H	2.2593819	3.4129132	0.1420307
N	0.2866611	2.5840701	0.3102385
C	2.1230658	-1.3572377	-1.0159439
N	2.5670352	-2.6216788	-0.7985122
C	2.3926194	-3.2917556	0.4869458
H	1.6664470	-2.7491689	1.1035730
H	3.3449814	-3.3806814	1.0355212
H	2.0052125	-4.3076253	0.3087065
C	3.2773023	-3.3978023	-1.8150818
H	3.5945886	-2.7463052	-2.6375381
H	2.6600588	-4.2180375	-2.2166177
H	4.1756406	-3.8377650	-1.3538775
N	1.7052684	-1.0198787	-2.2530515
C	1.0091699	-1.9584591	-3.1302813
H	0.7207166	-2.8584574	-2.5754241
H	1.6245205	-2.2468889	-3.9976719
H	0.0933174	-1.4725486	-3.5020291
C	1.8019600	0.3425972	-2.7655436
H	2.4794782	0.9325865	-2.1380962
H	0.8123917	0.8240249	-2.7905593
H	2.2062183	0.3076387	-3.7898067
C	1.8884278	0.7489675	3.4105251
H	2.6547530	1.1773324	4.0783830
H	2.0359371	-0.3364827	3.3572309
H	0.8962075	0.9515086	3.8302238
C	-0.6555690	3.1540289	-0.4705571
N	-0.3565426	4.1797147	-1.3113318
C	0.9180737	4.2651954	-2.0181192
H	1.4474970	3.3071942	-1.9705356
H	1.5643078	5.0587804	-1.6080165
H	0.7213193	4.4962469	-3.0772140
C	-1.2821315	5.2838045	-1.5632132
H	-2.0941681	5.2745592	-0.8268356
H	-1.7102744	5.2413683	-2.5782037
H	-0.7316664	6.2328201	-1.4619839
N	-1.9381342	2.7333248	-0.4035489
C	-2.8128805	2.7079147	-1.5733209
H	-2.2405743	2.9089491	-2.4858558
H	-3.6329053	3.4394889	-1.4886365
H	-3.2544694	1.7020946	-1.6587754
C	-2.5108972	2.1492923	0.8032130
H	-1.8773381	2.3706650	1.6694284
H	-2.6203645	1.0582375	0.7034726
H	-3.5073963	2.5881972	0.9704140
C	-1.1578802	-1.1014905	2.6859130
C	-2.0000296	-1.9430178	3.5110935
H	-2.5106007	-1.3254737	4.2658600

H	-2.7487167	-2.4403349	2.8739192
H	-1.3824443	-2.7004400	4.0175841
C	-2.7242650	-4.8416207	-0.9101160
C	-3.5937595	-4.9755386	0.3130312
C	-4.2200798	-3.6717406	0.7352010
C	-4.0125735	-2.5105851	0.0966651
C	-3.1299000	-2.3730851	-1.1166158
C	-2.5204251	-3.6814194	-1.5485731
H	-2.2459611	-5.7555543	-1.2807532
H	-4.8842285	-3.6991860	1.6070192
H	-4.5093525	-1.6016261	0.4561541
H	-1.8796693	-3.6603014	-2.4376538
H	-2.3302889	-1.6289522	-0.9240617
H	-3.7093017	-1.9318131	-1.9529915
H	-4.3846789	-5.7317183	0.1338586
H	-3.0061399	-5.4023399	1.1510369
Fe	0.4653340	0.6314797	0.5668364
N	-0.3773204	-0.4196315	2.1898100
O	-0.6400653	0.0205103	-0.5870524
N	2.0676240	-0.4218714	-0.0108930
C	3.1760447	-0.2880030	0.9467549
H	4.1327249	-0.5857210	0.4884847
H	3.0420970	-0.9214911	1.8407019
C	3.2385507	1.1754432	1.3501080
H	4.0355335	1.3592975	2.0907899
H	3.4560766	1.7849825	0.4619437
N	1.9195190	1.5966099	1.9057674
C	1.7088500	3.0667141	1.7733993
H	2.6413054	3.6092688	2.0062948
H	0.9531927	3.3617273	2.5150332
C	1.1956358	3.3992396	0.3849306
H	0.9070286	4.4612556	0.3458055
H	1.9942163	3.2598305	-0.3645069
N	0.0428208	2.5242403	0.1311492
C	2.1963124	-1.3101225	-1.0142162
N	2.8093218	-2.5114186	-0.8128765
C	2.6782377	-3.2331081	0.4481085
H	1.8562611	-2.8140506	1.0408066
H	3.6066818	-3.2001590	1.0429730
H	2.4492572	-4.2899246	0.2341086
C	3.6838781	-3.1343359	-1.8043815
H	3.9293502	-2.4196241	-2.5986151
H	3.2310099	-4.0340010	-2.2535319
H	4.6218111	-3.4343733	-1.3094224
N	1.7608461	-1.0132147	-2.2586052
C	1.2864395	-2.0281262	-3.1948080
H	1.1071492	-2.9754095	-2.6746391

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-TS (π)

E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

-2678.7696620860 (<S^2> 6.06685088)

E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:

-2680.3378005802 (<S^2> 6.06849822)

ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.689043

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.624368

H	1.9989902	-2.1930274	-4.0196104
H	0.3345672	-1.6866455	-3.6299762
C	1.6313823	0.3598792	-2.7302300
H	2.2237768	1.0300975	-2.0969214
H	0.5781386	0.6796825	-2.7148579
H	2.0115872	0.4188250	-3.7624061
C	1.8411693	1.2221521	3.3370782
H	2.5916505	1.7884432	3.9147718
H	2.0370549	0.1507153	3.4662878
H	0.8434403	1.4520686	3.7305028
C	-1.0229189	3.0024511	-0.5303718
N	-0.9040393	3.9651460	-1.4877800
C	0.2394458	4.0340449	-2.3909689
H	0.8225378	3.1088413	-2.3403903
H	0.8973730	4.8883878	-2.1597715
H	-0.1266386	4.1533497	-3.4236625
C	-1.9000742	5.0197298	-1.6673741
H	-2.5876272	5.0431350	-0.8137841
H	-2.4798009	4.8883809	-2.5962616
H	-1.3811571	5.9905059	-1.7220808
N	-2.2687630	2.5646320	-0.2270595
C	-3.3057487	2.4030303	-1.2415863
H	-2.8863822	2.5403601	-2.2446417
H	-4.1380863	3.1111869	-1.0956847
H	-3.7109094	1.3801070	-1.1765994
C	-2.6189008	2.0726012	1.0975112
H	-1.8830468	2.4128727	1.8352828
H	-2.6685570	0.9724815	1.1201550
H	-3.6082703	2.4697142	1.3753055
C	-0.8335628	-1.0316376	3.0575414
C	-1.4016754	-1.7919931	4.1526716
H	-2.4712926	-1.5529665	4.2534996
H	-1.2841430	-2.8681096	3.9556366
H	-0.8836451	-1.5352690	5.0892674
C	-1.6179141	-4.1400735	-1.1354906
C	-1.9148783	-4.6230115	0.2545827
C	-2.6471490	-3.6156921	1.0929444
C	-2.8878224	-2.3547413	0.6746549
C	-2.4244678	-1.8531423	-0.6326622
C	-1.8782506	-2.8785707	-1.5397137
H	-1.1962490	-4.8647572	-1.8400411
H	-3.0155297	-3.9485295	2.0691442
H	-3.4524088	-1.6694629	1.3158784
H	-1.6694454	-2.5843679	-2.5722625
H	-1.4890286	-0.9918185	-0.4687026
H	-3.1197386	-1.1484730	-1.1176774
H	-2.4909762	-5.5694424	0.2121721
H	-0.9728376	-4.9257511	0.7611561

Fe	0.4285230	0.6192748	0.6001255
N	-0.7148046	-0.4484004	2.0177602
O	-0.7026364	0.1633923	-0.7251009
N	1.8967972	-0.6620971	0.1339692
C	2.9198026	-0.6891152	1.1888410
H	3.8732000	-1.0888613	0.8076523
H	2.6301955	-1.3210774	2.0458300
C	3.1156218	0.7477568	1.6425089
H	3.8405622	0.8213320	2.4701952
H	3.4968914	1.3446977	0.8023785
N	1.8019209	1.3209795	2.0720520
C	1.8054802	2.8147951	1.9954689
H	2.7751393	3.2087900	2.3428742
H	1.0260766	3.1821458	2.6774488
C	1.4802718	3.2594201	0.5823231
H	1.3185418	4.3485821	0.5663183
H	2.3291196	3.0537008	-0.0928350
N	0.2676099	2.5309918	0.1834576
C	1.9770202	-1.5495008	-0.8734198
N	2.3963277	-2.8279029	-0.6552651
C	2.0874580	-3.5369250	0.5819213
H	1.2978970	-3.0126464	1.1334631
H	2.9726396	-3.6416730	1.2316233
H	1.7264197	-4.5485662	0.3345467
C	3.2211869	-3.5645839	-1.6111176
H	3.6119593	-2.8860453	-2.3784278
H	2.6633955	-4.3811153	-2.0993266
H	4.0751735	-4.0073758	-1.0735264
N	1.6741449	-1.1834121	-2.1398186
C	1.0738678	-2.1015223	-3.1033338
H	0.7317555	-3.0136826	-2.6013125
H	1.7756114	-2.3717634	-3.9093206
H	0.2002831	-1.6100664	-3.5602743
C	1.8077241	0.1915977	-2.6048076
H	2.4536581	0.7558826	-1.9222042
H	0.8234602	0.6801794	-2.6644958
H	2.2692240	0.1854651	-3.6051640
C	1.5128598	0.9095328	3.4684103
H	2.2560893	1.3585137	4.1481955
H	1.5608249	-0.1814254	3.5659048
H	0.5120816	1.2514737	3.7591484
C	-0.6680910	3.1412718	-0.5631739
N	-0.3424751	4.0970000	-1.4778186
C	0.8886806	4.0456584	-2.2589448
H	1.3535497	3.0577018	-2.1759173
H	1.6126610	4.8134448	-1.9387236
H	0.6473350	4.2236146	-3.3194278
C	-1.1901240	5.2605057	-1.7314206

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-IC (π)

E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

-2678.8130470238 (<S^2> 6.08665171)

E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:

-2680.3838297758 (<S^2> 6.08556742)

ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.693289

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.627817

H	-1.9544839	5.3511481	-0.9507215
H	-1.6830109	5.2069561	-2.7164636
H	-0.5625453	6.1662075	-1.7112423
N	-1.9791680	2.8517505	-0.3905871
C	-2.9187457	2.8101643	-1.5069902
H	-2.3906582	2.9331533	-2.4591342
H	-3.6947791	3.5881627	-1.4186368
H	-3.4148870	1.8258345	-1.5153797
C	-2.5102058	2.3656631	0.8742825
H	-1.8159277	2.5942275	1.6912670
H	-2.6894094	1.2793805	0.8420437
H	-3.4691566	2.8696282	1.0749427
C	-1.3751166	-1.0537769	2.7489695
C	-2.1974269	-1.8038916	3.6771874
H	-3.2233607	-1.4055372	3.6677647
H	-2.2153239	-2.8636388	3.3818321
H	-1.7823949	-1.7138136	4.6926394
C	-2.1381616	-4.1187016	-1.4853968
C	-2.5596493	-4.7885294	-0.2096627
C	-3.4322425	-3.9320518	0.6618905
C	-3.7873778	-2.6564966	0.3058668
C	-3.3425373	-2.0763505	-0.9171574
C	-2.5226767	-2.8388864	-1.7962151
H	-1.5178542	-4.6920583	-2.1813939
H	-3.7970680	-4.3648441	1.5987094
H	-4.4375659	-2.0725798	0.9651901
H	-2.2032088	-2.3939736	-2.7433841
H	-1.1518071	-0.6790737	-0.5412463
H	-3.6570293	-1.0678570	-1.1947645
H	-3.0745649	-5.7491611	-0.4361689
H	-1.6656589	-5.1310201	0.3593395
Fe	1.6778791	0.5836997	0.3596301
N	0.5530954	2.2253560	-0.3808925
O	0.6393553	-0.4993540	-0.2766485
N	1.2029140	0.2500286	2.2368001
C	1.8616121	1.1589031	3.1914747
H	1.9425307	0.6882183	4.1843580
H	1.3084584	2.1030265	3.3314084
C	3.2497782	1.4433750	2.6453504
H	3.7876385	2.1793379	3.2661958
H	3.8362067	0.5140898	2.6382684
N	3.1344934	1.9437955	1.2428104
C	4.3992246	1.7544249	0.4750439
H	5.2659692	2.0604977	1.0854559
H	4.3518880	2.4147552	-0.4022510
C	4.5218356	0.3145170	0.0148514
H	5.3657139	0.2227154	-0.6867856

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-RC (π)

E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

-2985.7042299745 (<S^2> 6.05361025)

E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:

-2987.5970932176 (<S^2> 6.05600842)

ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.791332

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.722209

H	4.7487666	-0.3432311	0.8705500
N	3.2538780	-0.0472991	-0.6407085
C	0.2208934	-0.5694648	2.6871654
N	-0.7114776	-0.1195459	3.5660183
C	-1.1807110	1.2629161	3.5528623
H	-0.8856355	1.7570792	2.6195826
H	-0.7893878	1.8372942	4.4088723
H	-2.2806987	1.2667134	3.6168617
C	-1.2822779	-0.9615111	4.6175359
H	-0.6925147	-1.8780894	4.7330462
H	-2.3321315	-1.2274445	4.4119911
H	-1.2490126	-0.4048699	5.5673465
N	0.1744761	-1.8569509	2.2911682
C	-1.0797770	-2.5875910	2.1189665
H	-1.9341792	-1.9024358	2.1483247
H	-1.2091885	-3.3679234	2.8860119
H	-1.0670691	-3.0711717	1.1304216
C	1.3686135	-2.5920024	1.8882980
H	2.2675736	-2.0576059	2.2151301
H	1.3968570	-2.7256472	0.7960696
H	1.3512278	-3.5840981	2.3667834
C	2.7797145	3.3836920	1.2519125
H	3.5852201	3.9623534	1.7346233
H	1.8479260	3.5493967	1.8063009
H	2.6506169	3.7425178	0.2243267
C	3.2608773	-0.9391924	-1.6539325
N	4.1607150	-1.9573545	-1.6995110
C	4.6254060	-2.6469313	-0.4994870
H	3.9828454	-2.4058960	0.3542612
H	5.6686560	-2.3884358	-0.2538501
H	4.5728462	-3.7337290	-0.6723489
C	4.7444471	-2.4327821	-2.9535766
H	4.5397782	-1.7213511	-3.7620894
H	4.3615655	-3.4268482	-3.2372813
H	5.8360619	-2.5088814	-2.8253686
N	2.3843420	-0.8136764	-2.6752807
C	1.8129000	-1.9710901	-3.3591704
H	2.0621454	-2.8950802	-2.8254756
H	2.1627909	-2.0464144	-4.4016292
H	0.7162330	-1.8651304	-3.3701275
C	1.8433464	0.4740173	-3.0927665
H	2.4417561	1.2906638	-2.6736684
H	0.7967222	0.5889687	-2.7709342
H	1.8806870	0.5342503	-4.1921829
C	-0.1426359	3.0320701	-0.8296940
C	-1.0073593	4.0484510	-1.3933236
H	-0.4950676	4.5368491	-2.2365007
H	-1.9427665	3.5890752	-1.7487991

H	-1.2382237	4.8011870	-0.6240368	
C	-3.8530971	2.3619723	-3.6647630	
C	-4.5433840	3.0561085	-2.6640309	
C	-3.2635634	1.1266540	-3.3737712	
C	-4.6359098	2.5112128	-1.3780348	
C	-3.3479221	0.5761880	-2.0861829	
C	-4.0390735	1.2780228	-1.0775940	
C	-2.7179592	-0.7579309	-1.7404104	
C	-4.1102844	0.6696615	0.3084944	
C	-4.2288441	-0.8409011	0.2685749	
C	-3.5477828	-1.5436103	-0.7453766	
C	-4.9882827	-1.5497813	1.2109834	
C	-3.6447116	-2.9416101	-0.7987811	
C	-5.0708300	-2.9456036	1.1580650	
C	-4.3980123	-3.6434089	0.1486839	
H	-3.7812005	2.7773582	-4.6736600	
H	-5.0150826	4.0174045	-2.8853329	
H	-2.7361648	0.5779378	-4.1602018	
H	-5.1814948	3.0495041	-0.5969620	
H	-5.5251919	-1.0020022	1.9916985	
H	-3.1251293	-3.4869346	-1.5927643	
H	-5.6673632	-3.4860827	1.8981886	
H	-4.4651173	-4.7335357	0.0943392	
H	-3.1834760	0.9374238	0.8566489	
H	-4.9362075	1.1113565	0.8865184	
H	-2.5417765	-1.3502588	-2.6517007	
H	-1.7169606	-0.5781642	-1.2959619	
Fe	1.7562054	0.5694450	0.3014995	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-TS (π)***
N	0.8544378	2.2694508	-0.5603767	**E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
O	0.4406693	-0.4877354	-0.0126906	**-2985.6755525812 (<S^2> 6.06687451)**
N	1.4482759	0.7886504	2.2684366	**E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:**
C	2.2960473	1.8462268	2.8396475	**-2987.5661503117 (<S^2> 6.06864081)**
H	2.3541807	1.7572761	3.9361077	**ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
H	1.9131365	2.8586307	2.6232312	**0.784396**
C	3.6800653	1.6731011	2.2399596	**Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
H	4.3794784	2.4473111	2.5987419	**0.715554**
H	4.0805106	0.6932613	2.5351680	
N	3.5872544	1.7211754	0.7517831	
C	4.7181542	0.9915615	0.1098528	
H	5.6562625	1.1838284	0.6582081	
H	4.8359169	1.3875732	-0.9085341	
C	4.4028979	-0.4899192	0.0301502	
H	5.1764741	-0.9976219	-0.5664226	
H	4.4256426	-0.9463618	1.0351516	
N	3.0803951	-0.6094704	-0.5992725	
C	0.5046788	0.2352346	3.0532268	
N	-0.1981017	0.9904683	3.9455227	

C	-0.5652350	2.3726403	3.6576601
H	-0.4313923	2.5873848	2.5905826
H	0.0301171	3.0908726	4.2463627
H	-1.6270513	2.5229643	3.9128135
C	-0.5728791	0.5070640	5.2732259
H	-0.0492883	-0.4291316	5.4994621
H	-1.6598163	0.3457377	5.3658000
H	-0.2737155	1.2594743	6.0209691
N	0.2616269	-1.0924004	3.0070483
C	-1.0540393	-1.6662055	3.2738922
H	-1.8141854	-0.8796494	3.3224259
H	-1.0665209	-2.2404344	4.2147924
H	-1.3170295	-2.3446033	2.4483147
C	1.2646702	-2.0530151	2.5653229
H	2.2625211	-1.6022217	2.6138637
H	1.0612732	-2.3821707	1.5349120
H	1.2377008	-2.9273881	3.2347601
C	3.5992326	3.1311934	0.2972807
H	4.5748266	3.5914498	0.5292725
H	2.8148364	3.7060416	0.8045179
H	3.4339684	3.1778232	-0.7862142
C	2.8633599	-1.5771214	-1.5046853
N	3.4883853	-2.7850570	-1.4279882
C	3.7865935	-3.4286877	-0.1530641
H	3.2406063	-2.9369793	0.6585507
H	4.8653859	-3.4126383	0.0750695
H	3.4614674	-4.4807031	-0.1986475
C	3.9493526	-3.5086825	-2.6116767
H	3.9175827	-2.8574734	-3.4929742
H	3.3477836	-4.4122053	-2.8055991
H	4.9938237	-3.8206705	-2.4496688
N	2.0397075	-1.3526374	-2.5562175
C	1.2236135	-2.4078417	-3.1494333
H	1.2208863	-3.2965283	-2.5078702
H	1.5764515	-2.6876860	-4.1555965
H	0.1872610	-2.0468242	-3.2438254
C	1.8260769	-0.0183660	-3.1010316
H	2.6391262	0.6501714	-2.7951542
H	0.8672850	0.4094242	-2.7679484
H	1.8143390	-0.0799942	-4.2005884
C	0.3780795	3.2451752	-0.9571034
C	-0.1917087	4.4856970	-1.4432812
H	-0.0296791	4.5646223	-2.5287729
H	-1.2714484	4.5064420	-1.2346448
H	0.2972352	5.3339114	-0.9398759
C	-2.8023174	2.6325434	-3.1562124
C	-3.6818488	3.2709516	-2.2704468
C	-2.1936690	1.4338094	-2.7839675

C	-3.9443018	2.7025960	-1.0188239	
C	-2.4531597	0.8492621	-1.5271588	
C	-3.3395920	1.4984245	-0.6349051	
C	-1.8610460	-0.4519996	-1.1443267	
C	-3.6170079	0.8654594	0.7103232	
C	-3.5566908	-0.6461759	0.6816786	
C	-2.6638706	-1.2787640	-0.2159477	
C	-4.3483740	-1.4294308	1.5308779	
C	-2.5701814	-2.6853605	-0.2177855	
C	-4.2539383	-2.8255856	1.5141271	
C	-3.3578136	-3.4548597	0.6388714	
H	-2.6013685	3.0652236	-4.1398148	
H	-4.1694563	4.2061480	-2.5582381	
H	-1.5249150	0.9244131	-3.4838186	
H	-4.6405057	3.1957226	-0.3339001	
H	-5.0509098	-0.9407913	2.2127026	
H	-1.8802939	-3.1742528	-0.9115492	
H	-4.8819590	-3.4227659	2.1806189	
H	-3.2815780	-4.5452737	0.6200650	
H	-2.8552398	1.2302290	1.4313315	
H	-4.5834002	1.2094483	1.1094233	
H	-1.4757580	-1.0203013	-2.0021018	
H	-0.7099134	-0.2839663	-0.5366111	
Fe	1.6771061	0.6351167	0.3850702	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-IC (π)*** **$E_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:** **-2985.7154660033 (<S^2> 6.08206800)** **$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 35.88)}$:** **-2987.6096878526 (<S^2> 6.08160453)** **$ZPE_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:** **0.789187** **Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:** **0.719821**
N	0.4347516	2.2576450	-0.1576925	
O	0.4961989	-0.5492498	-0.2868702	
N	1.2287536	0.3861479	2.3236306	
C	1.9243524	1.3789647	3.1548402	
H	1.9980270	1.0393792	4.2004680	
H	1.4085157	2.3542257	3.1742601	
C	3.3182449	1.5392904	2.5727786	
H	3.8996027	2.3082989	3.1081007	
H	3.8583257	0.5858650	2.6550017	
N	3.2184591	1.9020440	1.1244039	
C	4.4717343	1.5507504	0.3871099	
H	5.3531104	1.7928695	1.0040501	
H	4.5085368	2.1739229	-0.5172232	
C	4.4379199	0.0891715	-0.0150889	
H	5.2742633	-0.1256786	-0.6984935	
H	4.5741636	-0.5584988	0.8682902	
N	3.1404936	-0.1327787	-0.6697645	
C	0.3123398	-0.4149394	2.8963591	
N	-0.5097513	0.0438400	3.8818806	
C	-1.0067071	1.4154972	3.8962315	
H	-0.8517283	1.8864712	2.9180829	
H	-0.5162771	2.0266516	4.6724106	
H	-2.0883790	1.4020574	4.1065262	

C	-0.9238426	-0.7833638	5.0139302
H	-0.3226152	-1.6991777	5.0552218
H	-1.9919613	-1.0523911	4.9620204
H	-0.7579056	-0.2173241	5.9447658
N	0.2031801	-1.7117729	2.5275349
C	-1.0761717	-2.4149811	2.4975492
H	-1.9042559	-1.7154096	2.6588507
H	-1.1253926	-3.2122970	3.2571961
H	-1.2053078	-2.8740226	1.5048743
C	1.3318645	-2.4719442	2.0040538
H	2.2703095	-1.9569938	2.2406126
H	1.2470270	-2.5950479	0.9139113
H	1.3426901	-3.4648774	2.4816826
C	2.9716102	3.3593495	0.9904292
H	3.8453247	3.9187795	1.3640310
H	2.0902437	3.6560959	1.5709174
H	2.8091609	3.6153135	-0.0637138
C	3.0551114	-0.9648613	-1.7220810
N	3.8595316	-2.0580801	-1.8346123
C	4.2814026	-2.8400572	-0.6772969
H	3.6849195	-2.5743731	0.2019414
H	5.3498601	-2.6928921	-0.4473386
H	4.1211094	-3.9092638	-0.8907132
C	4.3818067	-2.5193249	-3.1196601
H	4.2227011	-1.7560827	-3.8904515
H	3.9125306	-3.4636012	-3.4423595
H	5.4655413	-2.6922234	-3.0190264
N	2.1911407	-0.7073744	-2.7314246
C	1.4875020	-1.7714365	-3.4402837
H	1.6859641	-2.7423133	-2.9731808
H	1.7729026	-1.8136746	-4.5041123
H	0.4037331	-1.5794221	-3.3799925
C	1.7422202	0.6403596	-3.0484183
H	2.4282528	1.3804828	-2.6203079
H	0.7256764	0.8241065	-2.6655848
H	1.7298838	0.7633988	-4.1431267
C	-0.2932265	3.1045777	-0.4589390
C	-1.1955389	4.1743924	-0.8333285
H	-0.6401750	4.9384674	-1.3989086
H	-2.0081428	3.7766037	-1.4610052
H	-1.6208684	4.6319144	0.0730864
C	-3.2110676	2.4489784	-3.6868318
C	-4.2230598	3.0441323	-2.9132661
C	-2.7626906	1.1707018	-3.3743393
C	-4.7684024	2.3481300	-1.8264321
C	-3.3129057	0.4460030	-2.2811695
C	-4.3308179	1.0624284	-1.4922405
C	-2.8941160	-0.8888647	-1.9899376

C	-4.9078064	0.3434600	-0.2923814
C	-4.5369464	-1.1171941	-0.1550781
C	-3.5205928	-1.6840793	-0.9813865
C	-5.1659428	-1.9212785	0.8010574
C	-3.1758345	-3.0517339	-0.8011538
C	-4.8163642	-3.2675366	0.9633880
C	-3.8146398	-3.8318448	0.1553047
H	-2.7817496	2.9870015	-4.5362946
H	-4.5860652	4.0456392	-3.1583243
H	-1.9866805	0.6977787	-3.9832368
H	-5.5542386	2.8169487	-1.2259830
H	-5.9479523	-1.4872944	1.4320574
H	-2.4002930	-3.4877837	-1.4374821
H	-5.3247975	-3.8767924	1.7152576
H	-3.5399270	-4.8832093	0.2763503
H	-4.5826973	0.8763267	0.6246626
H	-6.0070823	0.4494549	-0.2897079
H	-2.1185435	-1.3445435	-2.6114763
H	-0.4141488	-0.2156491	-0.2474446

$[Fe^{IV}(O)TMG_3tren]^{2+}$ (σ) pathway

Fe	2.5117018	4.4181172	6.3729970
O	3.7856860	4.4762431	5.3634522
N	0.8376096	4.3408896	7.6998255
N	3.3996394	3.3598908	7.8688171
N	1.2267776	3.4411268	5.1319592
N	2.2705373	6.4247226	6.6231261
N	5.4174789	2.8833960	9.0175080
N	5.1485192	2.2104059	6.8108823
N	0.9952763	1.8631068	3.3784508
N	2.0330505	3.9020819	2.9786947
N	2.4798754	8.5734282	5.6443585
N	4.3785529	7.3302291	6.1379706
C	1.1423972	3.3106159	8.7316161
H	0.9251675	2.3225646	8.3044188
H	0.4897329	3.4491437	9.6102170
C	2.6116462	3.3851722	9.1106972
H	2.7967175	4.2964612	9.7039923
H	2.8670056	2.5319683	9.7595431
C	4.6376789	2.8424106	7.8973964
C	5.4208518	4.0104015	9.9430001
H	4.9126374	4.8732837	9.5013807
H	6.4641388	4.2980861	10.1521015
H	4.9369490	3.7591235	10.9017205
C	6.3101908	1.7854999	9.3845520
H	6.0824739	0.8938410	8.7888343
H	6.1528416	1.5424603	10.4479815

$[Fe^{IV}(O)TMG_3tren]^{2+}$

$E_{B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2713.2952880582 (<S^2> 6.05191598)

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2714.8951214215 (<S^2> 6.05445028)

$ZPE_{B3LYP/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.724368

Chem. Pot.(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88):

0.662954 (σ = 3)

H	7.3719928	2.0508657	9.2479043
C	6.5567653	2.3080172	6.4409240
H	7.0676207	3.0515976	7.0636676
H	6.6254732	2.6328240	5.3897081
H	7.0759950	1.3397344	6.5369533
C	4.3135149	1.4780553	5.8713301
H	3.3297970	1.2983867	6.3186245
H	4.7878904	0.5069090	5.6539949
H	4.1878340	2.0326703	4.9288125
C	-0.3521384	3.9684707	6.8844570
H	-0.7187983	4.8722496	6.3797558
H	-1.1590108	3.5967615	7.5386210
C	0.0437652	2.9343300	5.8443610
H	0.2361069	1.9663456	6.3370342
H	-0.7967795	2.7710231	5.1508370
C	1.4263722	3.0663725	3.8587730
C	1.0037607	0.6405771	4.1734577
H	1.5989065	0.7757663	5.0819734
H	1.4626824	-0.1678199	3.5811430
H	-0.0145861	0.3230238	4.4537663
C	0.4771906	1.7081148	2.0202830
H	0.2805254	2.6895566	1.5732014
H	-0.4723128	1.1503717	2.0656892
H	1.1722573	1.1478542	1.3725966
C	2.9393355	3.4199663	1.9415056
H	3.1499834	2.3531355	2.0799694
H	3.8905704	3.9719617	2.0172354
H	2.5290100	3.5777809	0.9300222
C	1.9137422	5.3490736	3.0693708
H	1.0839365	5.6069155	3.7363984
H	1.7020214	5.7533973	2.0658337
H	2.8404039	5.8055183	3.4497662
C	0.6907691	5.6958125	8.3010630
H	1.4134335	5.7867004	9.1229356
H	-0.3202555	5.8145506	8.7263904
C	0.9825757	6.7553263	7.2521285
H	0.1578596	6.7910685	6.5205881
H	1.0187317	7.7465862	7.7319752
C	3.0246795	7.4192830	6.1297594
C	1.2191301	8.6111872	4.9123612
H	0.9138067	7.6021915	4.6181122
H	1.3556939	9.2080583	3.9958211
H	0.4115332	9.0737455	5.5041945
C	3.1193622	9.8745508	5.8320633
H	3.9183922	9.8021671	6.5791324
H	2.3648980	10.5896344	6.1983178
H	3.5377685	10.2706565	4.8915706
C	5.2027113	7.8602057	5.0565735

H	4.5751923	8.1883973	4.2197910	
H	5.8696939	7.0606306	4.6945270	
H	5.8276762	8.7051161	5.3911093	
C	5.1053028	6.6048807	7.1685091	
H	4.4415098	6.4134100	8.0186636	
H	5.9516809	7.2229685	7.5105399	
H	5.4931964	5.6474729	6.7881964	
Fe	-0.9688324	-0.0315295	0.8179396	***[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-CHD-RC (σ)***
O	0.1979603	-0.1264185	-0.3125066	
N	-2.5090601	0.0904373	2.3006792	**E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	0.1677664	0.7266144	2.3335927	**-2946.3902236849 (<S^2> 6.05271281)**
N	-1.4577365	-2.0087079	0.8721029	
N	-2.2042811	1.2473725	-0.1749975	**E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:**
N	2.0178712	2.0722175	2.9544539	**-2948.2464037180 (<S^2> 6.05539672)**
N	2.3610514	0.0829862	1.8061970	
N	-0.7088069	-4.2430079	0.6245967	**ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-0.8160128	-2.8407245	-1.2244556	**0.847527**
N	-2.9912216	2.0141562	-2.2749183	
N	-0.7924028	2.4126069	-1.6407206	**Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
C	-1.8393787	0.3025512	3.6138021	
H	-1.4843444	-0.6701724	3.9793988	**0.777683**
H	-2.5620636	0.6956894	4.3488512	
C	-0.6565519	1.2387486	3.4393641	
H	-1.0182766	2.2632619	3.2489878	
H	-0.0801704	1.2794589	4.3774452	
C	1.4879574	0.9665204	2.3520084	
C	1.3701456	3.3785495	2.9326698	
H	0.5560182	3.3934758	2.2015221	
H	2.1101245	4.1396776	2.6356266	
H	0.9706759	3.6582562	3.9219434	
C	3.2828674	2.0278392	3.6857751	
H	3.5874807	0.9889655	3.8581658	
H	3.1427120	2.5154465	4.6642570	
H	4.0895875	2.5578324	3.1520839	
C	3.5763631	0.5100734	1.1203772	
H	3.5829546	1.5987811	0.9929754	
H	3.6059060	0.0482772	0.1199471	
H	4.4853580	0.2062995	1.6662775	
C	2.1067532	-1.3490846	1.7791468	
H	1.2980445	-1.5904612	2.4776368	
H	3.0195483	-1.8800830	2.0956580	
H	1.8255067	-1.6887172	0.7705991	
C	-3.2552868	-1.1979205	2.2679394	
H	-3.9729782	-1.1586912	1.4376214	
H	-3.8271907	-1.3287637	3.2022837	
C	-2.2841616	-2.3435534	2.0423354	
H	-1.6773847	-2.5023696	2.9497393	

H	-2.8481741	-3.2751820	1.8755669
C	-0.9875951	-3.0090514	0.1104845
C	-0.1472087	-4.4391105	1.9560690
H	0.2195209	-3.4913853	2.3627140
H	0.7053633	-5.1342026	1.8857686
H	-0.8829849	-4.8703766	2.6554138
C	-0.9719632	-5.4743063	-0.1182954
H	-1.6017385	-5.2658955	-0.9910685
H	-1.5114843	-6.1752240	0.5392657
H	-0.0419861	-5.9648611	-0.4513385
C	0.2771045	-3.4700628	-1.9576021
H	0.9886463	-3.9338657	-1.2646355
H	0.8091706	-2.6955810	-2.5332431
H	-0.0862102	-4.2337551	-2.6653280
C	-1.6521393	-1.9464017	-2.0106126
H	-2.5497245	-1.6874257	-1.4385123
H	-1.9566165	-2.4632209	-2.9354232
H	-1.1138243	-1.0240280	-2.2772725
C	-3.3818887	1.2406589	1.9352927
H	-2.8996202	2.1630592	2.2853307
H	-4.3560653	1.1547122	2.4459526
C	-3.5459203	1.2982020	0.4262008
H	-4.1854725	0.4650457	0.0888042
H	-4.0695112	2.2272237	0.1494218
C	-1.9988470	1.8651705	-1.3487660
C	-4.0108518	0.9999990	-2.5167645
H	-3.7350016	0.0545775	-2.0394525
H	-4.0906910	0.8248450	-3.6020879
H	-5.0015195	1.3140718	-2.1474913
C	-3.1201302	3.2204336	-3.0906665
H	-2.4822078	4.0189041	-2.6940956
H	-4.1673158	3.5620716	-3.0530595
H	-2.8577490	3.0375783	-4.1461947
C	-0.2389881	2.4113261	-2.9907594
H	-0.8422923	1.7796406	-3.6532011
H	0.7827787	1.9991389	-2.9559427
H	-0.1834022	3.4278008	-3.4150769
C	0.0848982	2.9564519	-0.6155811
H	-0.4811571	3.1013581	0.3109159
H	0.4680324	3.9328578	-0.9546816
H	0.9361637	2.2867117	-0.4192507
C	5.4637405	-0.0058737	-2.7034625
C	5.4418424	1.2213368	-3.5766161
C	4.1636154	1.3634327	-4.3609893
C	3.1392140	0.5044747	-4.2673160
C	3.1438013	-0.6993783	-3.3610423
C	4.4393903	-0.8650254	-2.6097235
H	6.3772537	-0.1875285	-2.1256271

H	4.0914666	2.2200706	-5.0410385	
H	2.2412326	0.6653797	-4.8747854	
H	4.5273129	-1.7419187	-1.9579273	
H	2.9265057	-1.6147206	-3.9475355	
H	2.3010827	-0.6307012	-2.6427220	
H	5.6101139	2.1275351	-2.9597196	
H	6.3087785	1.2081139	-4.2676670	
Fe	2.6250481	4.3115403	6.3260195	***[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-CHD-TS (σ)***
O	3.9939871	4.1845170	5.3146118	**E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	0.7846524	4.4270370	7.7131244	**-2946.3671746049 (<S^2> 6.52206113)**
N	3.3365789	3.3425791	8.0261986	**E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:**
N	1.1981471	3.3070016	5.1778735	**-2948.2217801537 (<S^2> 6.51430048)**
N	2.3655618	6.3850560	6.4641382	**ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	5.2166375	2.6803943	9.3108912	**0.840466**
N	4.8511197	1.7497729	7.2141463	**Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	0.7135970	1.7614003	3.4449074	**0.770718**
N	1.7639613	3.7757298	2.9517124	
N	2.6903610	8.5537968	5.5548459	
N	4.5179153	7.2845313	6.2191236	
C	1.0801394	3.5718230	8.8828083	
H	0.8365280	2.5313781	8.6258926	
H	0.4501796	3.8568720	9.7448608	
C	2.5575097	3.6617104	9.2311350	
H	2.7902623	4.6692035	9.6182558	
H	2.7793148	2.9547186	10.0458672	
C	4.4540047	2.6199437	8.1763494	
C	5.4211488	3.9146880	10.0583816	
H	5.0786140	4.7760750	9.4770437	
H	6.4981762	4.0412915	10.2575451	
H	4.8935624	3.9045804	11.0271800	
C	5.8521698	1.4986834	9.8892474	
H	5.4626538	0.5874647	9.4203674	
H	5.6173853	1.4603757	10.9657889	
H	6.9496523	1.5205144	9.7799267	
C	6.2568445	1.4804773	6.9322323	
H	6.8979616	2.2035500	7.4493512	
H	6.4217537	1.5833378	5.8493553	
H	6.5499729	0.4598146	7.2304016	
C	3.9063796	1.0955537	6.3223928	
H	2.8984928	1.1526985	6.7487766	
H	4.1874130	0.0348907	6.2188232	
H	3.9044157	1.5625394	5.3256536	
C	-0.3656732	3.9265366	6.9299190	
H	-0.7674108	4.7544185	6.3292157	
H	-1.1740583	3.5811889	7.5995076	
C	0.0817348	2.8118374	5.9963716	
H	0.3675718	1.9228540	6.5857670	

H	-0.7694328	2.5093901	5.3666944
C	1.2378739	2.9458504	3.8897312
C	0.8007233	0.5248037	4.2112956
H	1.5030108	0.6373717	5.0428437
H	1.1716928	-0.2804936	3.5557166
H	-0.1796151	0.2149894	4.6113236
C	-0.0281180	1.6565864	2.1902679
H	-0.2532063	2.6537697	1.7941898
H	-0.9829663	1.1403809	2.3841959
H	0.5222076	1.0801643	1.4274879
C	2.4238721	3.2869805	1.7462272
H	2.6268085	2.2128132	1.8271368
H	3.3815320	3.8169847	1.6227868
H	1.8207234	3.4696745	0.8411570
C	1.7654598	5.2211020	3.1113102
H	1.0274803	5.5049713	3.8694570
H	1.4882660	5.6884305	2.1526969
H	2.7561045	5.5936066	3.4160783
C	0.6338074	5.8492690	8.0877993
H	1.3045376	6.0613244	8.9320703
H	-0.3978577	6.0580590	8.4245919
C	1.0136024	6.7436585	6.9188748
H	0.2683539	6.6369612	6.1112705
H	0.9715902	7.7943096	7.2455128
C	3.1709873	7.3791510	6.0715612
C	1.5414766	8.6178497	4.6606259
H	1.2636477	7.6171451	4.3176192
H	1.8061428	9.2208843	3.7760698
H	0.6665092	9.0854290	5.1431839
C	3.2748363	9.8493385	5.8936986
H	3.9741108	9.7464832	6.7317576
H	2.4669238	10.5338638	6.2012541
H	3.8010230	10.3059326	5.0382667
C	5.4498556	7.9114756	5.2885347
H	4.9238218	8.2573163	4.3913604
H	6.2028505	7.1698761	4.9808418
H	5.9822325	8.7625422	5.7452748
C	5.1298934	6.4967065	7.2780414
H	4.3885025	6.2999630	8.0607861
H	5.9635079	7.0699376	7.7151346
H	5.5133728	5.5368978	6.8988905
C	7.0476580	1.7878396	3.1059738
C	8.3349531	2.1938748	3.7601219
C	8.3251196	3.6020126	4.2759692
C	7.2495496	4.4102856	4.1769005
C	5.9649956	3.9730633	3.5883996
C	5.9803967	2.6087113	3.0158606
H	7.0011289	0.7852977	2.6678932

H	9.2500152	3.9793107	4.7246795
H	7.3199330	5.4379020	4.5456775
H	5.0793315	2.2592650	2.5037111
H	5.5128860	4.7265823	2.9183513
H	5.0804316	4.0241957	4.4579639
H	8.5881707	1.4879165	4.5793250
H	9.1768115	2.0593133	3.0494990
Fe	-0.8533561	0.0043579	0.5570301
O	0.3516320	-0.0341391	-0.8223623
N	-2.3963177	0.0724741	2.3000065
N	0.2868408	0.8611248	2.0913675
N	-1.3019818	-2.0149712	0.7813779
N	-2.3492210	1.1914381	-0.2635538
N	2.1390036	2.2301026	2.6594882
N	2.4754389	0.1894000	1.5911382
N	-0.5457068	-4.2454063	0.4728242
N	-0.9064695	-2.8709968	-1.3636009
N	-3.3587665	1.9435761	-2.2759030
N	-1.1758174	2.5515829	-1.7688422
C	-1.6356943	0.4200705	3.5175969
H	-1.1831663	-0.4969935	3.9202931
H	-2.3041664	0.8285183	4.2972025
C	-0.5302753	1.4121032	3.1824944
H	-0.9748726	2.3849119	2.9104635
H	0.0794956	1.5874327	4.0827190
C	1.6042443	1.1009102	2.1085876
C	1.4870728	3.5323182	2.5800376
H	0.6777674	3.5120977	1.8436941
H	2.2265793	4.2828061	2.2562806
H	1.0788959	3.8513027	3.5536259
C	3.3901265	2.2146058	3.4157633
H	3.6916573	1.1841914	3.6367775
H	3.2306138	2.7385684	4.3722842
H	4.2065581	2.7249833	2.8780499
C	3.7332529	0.5734497	0.9553631
H	3.7388103	1.6475298	0.7357358
H	3.8377576	0.0242927	0.0054450
H	4.6066958	0.3300153	1.5831629
C	2.2255410	-1.2438321	1.6590340
H	1.3964993	-1.4390934	2.3478005
H	3.1284207	-1.7517403	2.0358225
H	1.9775905	-1.6633463	0.6706675
C	-2.9951554	-1.2774234	2.3679606
H	-3.7976562	-1.3398793	1.6198459
H	-3.4526847	-1.4551422	3.3581382
C	-1.9482552	-2.3392763	2.0603934
H	-1.2193189	-2.3885519	2.8876896

[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-CHD-IC (σ)

E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

-2946.4108672118 (<S^2> 7.04650544)

E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:

-2948.2674955056 (<S^2> 7.04388757)

ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.842558

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.771514

H	-2.4381532	-3.3249780	2.0168036
C	-0.9123488	-3.0215135	-0.0131345
C	0.1743310	-4.4199673	1.7285068
H	0.5577247	-3.4611787	2.0897907
H	1.0333265	-5.0899190	1.5594807
H	-0.4608825	-4.8688610	2.5104729
C	-0.8627531	-5.4876816	-0.2289012
H	-1.5938988	-5.3006240	-1.0240281
H	-1.3049756	-6.1972614	0.4894518
H	0.0339987	-5.9586316	-0.6658296
C	0.1232616	-3.4620615	-2.2103238
H	0.9158083	-3.9084998	-1.5983185
H	0.5695704	-2.6688815	-2.8328192
H	-0.2878561	-4.2334548	-2.8828399
C	-1.8395133	-1.9925953	-2.0516809
H	-2.6836227	-1.7653334	-1.3907519
H	-2.2221528	-2.5082316	-2.9476047
H	-1.3523061	-1.0548611	-2.3616950
C	-3.3845723	1.1092628	1.9346534
H	-2.9797676	2.0912733	2.2166694
H	-4.3276404	0.9677800	2.4933112
C	-3.6387101	1.0909403	0.4333184
H	-4.1837272	0.1705904	0.1612691
H	-4.2972075	1.9335797	0.1689893
C	-2.2976559	1.8675884	-1.4196755
C	-4.2969506	0.8456963	-2.4774120
H	-3.9077500	-0.0787517	-2.0406284
H	-4.4316936	0.6833799	-3.5593316
H	-5.2852167	1.0616285	-2.0380446
C	-3.6501697	3.1479290	-3.0513111
H	-3.0623611	3.9941081	-2.6769222
H	-4.7194053	3.3907884	-2.9389862
H	-3.4422148	3.0100457	-4.1257378
C	-0.6977887	2.6161514	-3.1447429
H	-1.2922704	1.9596388	-3.7904071
H	0.3483867	2.2684307	-3.1743377
H	-0.7301642	3.6430673	-3.5453789
C	-0.2993521	3.1595069	-0.7817446
H	-0.8164565	3.2243410	0.1822357
H	-0.0360100	4.1777803	-1.1120779
H	0.6306754	2.5826840	-0.6565031
C	5.2447370	-1.1077620	-2.5256498
C	5.9390780	0.2118695	-2.7010181
C	5.0113592	1.3411945	-3.0450300
C	3.6608557	1.1541976	-3.1891437
C	3.0656787	-0.1273517	-3.0119166
C	3.8890080	-1.2417362	-2.6813876
H	5.8584828	-1.9778487	-2.2728047

H	5.4478266	2.3346927	-3.1869590
H	3.0249714	2.0065390	-3.4494474
H	3.4276405	-2.2259643	-2.5518215
H	1.9891493	-0.2579209	-3.1426825
H	1.3003122	0.1326979	-0.8844993
H	6.5261616	0.4613575	-1.7884693
H	6.7350458	0.1233474	-3.4750242

Fe	-2.0382242	-0.2003816	0.0104925
O	-0.4536177	0.1732540	0.0025980
N	-4.1234282	-0.6929268	0.0178722
N	-2.2045879	-0.6689593	1.9885224
N	-1.9678812	-1.7213700	-1.3433414
N	-2.7522734	1.6064611	-0.6102194
N	-1.4414704	-0.2872002	4.1992861
N	-0.0377152	-1.2868058	2.6420230
N	-0.6972182	-3.4833258	-2.2895878
N	-0.0709300	-1.2753378	-2.6486084
N	-2.3616590	3.5680935	-1.8822065
N	-1.0944838	3.1416733	0.0169804
C	-4.4058590	-1.3935773	1.3012249
H	-4.1013708	-2.4432370	1.1943303
H	-5.4885784	-1.3762180	1.5121220
C	-3.6088589	-0.7481101	2.4208418
H	-4.0292565	0.2448807	2.6530683
H	-3.7079590	-1.3524148	3.3366299
C	-1.2427842	-0.7303998	2.9227182
C	-2.2423259	0.8895582	4.5165076
H	-2.4532358	1.4677405	3.6115432
H	-1.6743342	1.5325709	5.2085751
H	-3.1952667	0.6218630	5.0029646
C	-0.8763981	-0.9751314	5.3589535
H	-0.4955941	-1.9614415	5.0692810
H	-1.6724599	-1.1170313	6.1079101
H	-0.0635776	-0.3966904	5.8291502
C	1.2059064	-0.7887195	3.2204154
H	1.0331854	0.1565159	3.7475903
H	1.9291368	-0.6016411	2.4103999
H	1.6548582	-1.5137490	3.9195503
C	0.1174077	-2.3661880	1.6792803
H	-0.8623268	-2.8034688	1.4582312
H	0.7632283	-3.1453546	2.1163880
H	0.5710217	-2.0073503	0.7424550
C	-4.3721963	-1.5762164	-1.1550989
H	-4.4708289	-0.9437841	-2.0474293
H	-5.3209265	-2.1235244	-1.0228993
C	-3.2003558	-2.5250213	-1.3358951
H	-3.2017773	-3.2779446	-0.5296844

[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-DHA-RC (σ)

$E_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:

-3253.2990426887 (<S^2> 6.05301605)

$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 35.88)}$:

-3255.4782627353 (<S^2> 6.05554972)

$ZPE_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(\varepsilon = 35.88)}$:

0.943034

Chem. Pot.(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88):

0.869432

H	-3.3187383	-3.0778168	-2.2814514
C	-0.9232449	-2.1552457	-2.0664062
C	-0.9628681	-4.5123414	-1.2909265
H	-1.1345577	-4.0608008	-0.3088484
H	-0.0835113	-5.1725897	-1.2151574
H	-1.8342449	-5.1330051	-1.5590527
C	-0.1881834	-3.9833516	-3.5656319
H	-0.2412747	-3.2000935	-4.3307530
H	-0.8173189	-4.8281263	-3.8900974
H	0.8516355	-4.3421164	-3.4857165
C	1.3568562	-1.5434647	-2.7863594
H	1.6369977	-2.4342140	-2.2121128
H	1.9219829	-0.6844487	-2.3905422
H	1.6500080	-1.6888099	-3.8394052
C	-0.4980432	0.0398982	-3.1003510
H	-1.5915858	0.0706364	-3.1556737
H	-0.0863350	0.2235978	-4.1062420
H	-0.1482477	0.8314290	-2.4200561
C	-4.8794252	0.5859612	-0.0873095
H	-4.9284559	1.0398423	0.9114552
H	-5.9128810	0.3890738	-0.4194178
C	-4.1585714	1.5284132	-1.0351595
H	-4.2606712	1.1648188	-2.0715954
H	-4.6382797	2.5196402	-1.0018416
C	-2.0741588	2.7425220	-0.8332596
C	-2.7771915	3.0764741	-3.1908808
H	-2.6030088	1.9990981	-3.2712474
H	-2.1782437	3.5787492	-3.9679873
H	-3.8414290	3.2850326	-3.3913972
C	-2.2909436	5.0240515	-1.7686570
H	-2.2081570	5.3209900	-0.7166514
H	-3.2181103	5.4557881	-2.1793290
H	-1.4400614	5.4430370	-2.3315590
C	0.1114532	3.8194815	-0.4450888
H	0.1605119	3.8148477	-1.5401389
H	0.9915636	3.2801766	-0.0582137
H	0.1630428	4.8610653	-0.0867362
C	-1.1255664	2.8374057	1.4392073
H	-2.1351108	2.5213753	1.7236892
H	-0.8651958	3.7469091	2.0049539
H	-0.4116976	2.0395978	1.6956708
C	5.6064148	-0.1890937	3.5335034
C	5.0622806	1.1002484	3.5511934
C	5.5049887	-0.9703167	2.3777236
C	4.4199887	1.5988387	2.4130380
C	4.8551220	-0.4801238	1.2355048
C	4.3062370	0.8175583	1.2536747
C	4.7158964	-1.3112670	-0.0239197

C	3.5970613	1.3242928	0.0138887
C	4.2376477	0.8244946	-1.2654690
C	4.7889654	-0.4722149	-1.2835675
C	4.2851673	1.6107872	-2.4260411
C	5.3763840	-0.9555737	-2.4618926
C	4.8647609	1.1187580	-3.6002015
C	5.4123968	-0.1689062	-3.6181110
H	6.1166395	-0.5837032	4.4165792
H	5.1445264	1.7206706	4.4479424
H	5.9386528	-1.9749947	2.3598819
H	4.0030278	2.6106993	2.4235247
H	3.8666854	2.6219017	-2.4089299
H	5.8123543	-1.9593487	-2.4726720
H	4.8955187	1.7431168	-4.4974490
H	5.8743028	-0.5584150	-4.5295718
H	2.5434837	0.9751898	0.0408312
H	3.5506203	2.4244142	0.0181164
H	5.4689769	-2.1136951	-0.0461020
H	3.7330793	-1.8262939	-0.0004826
Fe	2.5858680	4.3344305	6.2945104
O	3.9076802	4.2107058	5.2128329
N	0.8053033	4.5191126	7.7676867
N	3.3835543	3.4434447	8.0033378
N	1.1200721	3.2211056	5.3048594
N	2.3148657	6.4161873	6.3613351
N	5.2685455	2.7454774	9.2638980
N	4.8025235	1.7486532	7.2182400
N	0.5288696	1.5645567	3.7103882
N	1.5459624	3.5340203	3.0205756
N	2.6108182	8.5544600	5.3807981
N	4.4482181	7.3778641	6.1849859
C	1.1798207	3.7545860	8.9765396
H	0.9228590	2.6980971	8.8172867
H	0.6071036	4.1055480	9.8538363
C	2.6759981	3.8650728	9.2221379
H	2.9342192	4.8999788	9.5083308
H	2.9443074	3.2271926	10.0780300
C	4.4718466	2.6755956	8.1513120
C	5.5735376	4.0002323	9.9391425
H	5.2540422	4.8516128	9.3310501
H	6.6635719	4.0752939	10.0891963
H	5.0885886	4.0671212	10.9277830
C	5.8277411	1.5542972	9.8992821
H	5.3716558	0.6484944	9.4829470
H	5.6025939	1.5884212	10.9781817
H	6.9229222	1.4935914	9.7814313
C	6.1816784	1.3542731	6.9512858

[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-DHA-TS (σ)

E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

-3253.2719808009 (<S^2> 6.51805389)

E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:

-3255.4489572209 (<S^2> 6.51339206)

ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.936232

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:

0.862698

H	6.8799748	2.0446224	7.4355814
H	6.3611471	1.3967561	5.8666431
H	6.3885471	0.3272258	7.2954391
C	3.8106223	1.1308934	6.3540632
H	2.8157258	1.2483304	6.7970719
H	4.0343614	0.0560263	6.2631449
H	3.8132532	1.5835929	5.3499533
C	-0.3700408	3.9405328	7.0830938
H	-0.8185112	4.7127817	6.4426606
H	-1.1371910	3.6324700	7.8163498
C	0.0576462	2.7687445	6.2162113
H	0.3938602	1.9330047	6.8547793
H	-0.8157646	2.4025145	5.6554237
C	1.0814994	2.7730384	4.0425985
C	0.6605742	0.3739571	4.5403887
H	1.3996741	0.5342715	5.3301180
H	1.0047627	-0.4663632	3.9146810
H	-0.2982819	0.0848652	5.0029650
C	-0.2832343	1.3846567	2.5089025
H	-0.5313594	2.3559825	2.0653542
H	-1.2243818	0.8831884	2.7891356
H	0.2234601	0.7610784	1.7530904
C	2.1484321	2.9538861	1.8242311
H	2.3563488	1.8888360	1.9793082
H	3.0990860	3.4663582	1.6202755
H	1.4996018	3.0672690	0.9396411
C	1.5390883	4.9875963	3.0727344
H	0.8318879	5.3231523	3.8398520
H	1.2127470	5.3791117	2.0958559
H	2.5379609	5.3883254	3.3014278
C	0.6303495	5.9599512	8.0458874
H	1.3204648	6.2495553	8.8507772
H	-0.3959978	6.1682481	8.3985664
C	0.9564566	6.7703309	6.8018384
H	0.2053233	6.5741337	6.0165768
H	0.8830992	7.8412792	7.0449367
C	3.1082386	7.4209252	5.9677355
C	1.4938631	8.5261927	4.4450407
H	1.2859785	7.4997709	4.1278735
H	1.7567137	9.1162903	3.5514479
H	0.5764201	8.9574851	4.8802926
C	3.0948871	9.8913792	5.7198184
H	3.7469661	9.8518447	6.6001338
H	2.2297554	10.5298349	5.9642020
H	3.6408899	10.3615867	4.8847555
C	5.4075520	8.0838867	5.3412044
H	4.9505506	8.3535714	4.3816821
H	6.2677145	7.4261418	5.1452573

H	5.7939699	8.9970087	5.8231636
C	5.0264424	6.6146903	7.2808310
H	4.2548646	6.4075554	8.0306344
H	5.8261211	7.2086544	7.7507265
H	5.4481505	5.6593931	6.9307735
C	9.3321240	2.1852941	4.9766153
C	9.0548105	3.3842273	5.6473986
C	8.5213092	1.7790774	3.9111944
C	7.9702588	4.1652649	5.2478472
C	7.4268440	2.5537950	3.5046672
C	7.1464809	3.7670841	4.1762942
C	6.5321721	2.1218010	2.3643706
C	6.0117543	4.6099738	3.7186707
C	5.6730584	4.4916955	2.2770424
C	5.9464110	3.2835942	1.5940154
C	5.1077433	5.5699193	1.5673241
C	5.6612748	3.1870225	0.2256733
C	4.8215742	5.4610497	0.2062293
C	5.1002541	4.2645602	-0.4684518
H	10.1848092	1.5711044	5.2781510
H	9.6898404	3.7120748	6.4745958
H	8.7457352	0.8480310	3.3822305
H	7.7641825	5.1089877	5.7608754
H	4.9069309	6.5092715	2.0906864
H	5.8855668	2.2569171	-0.3049733
H	4.3896944	6.3090076	-0.3316363
H	4.8863906	4.1733693	-1.5366808
H	4.9955282	4.3154996	4.3995729
H	6.1140534	5.6564504	4.0348213
H	7.0684170	1.4385943	1.6880913
H	5.6957081	1.5236752	2.7826847

Fe	-1.8127432	-0.2905016	0.0960943	***[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-DHA-IC (σ)***
O	0.0004281	-0.0032504	0.1461586	**E$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-4.1068001	-0.6371153	0.0075940	**-3253.3137521106 (<S^2> 7.04498858)**
N	-2.2023798	-0.8809774	2.0494702	**E$_{B3LYP/def2-TZVPP/COSMO(ε = 35.88)}$:**
N	-1.9438937	-1.7658131	-1.3576835	**-3255.4941296469 (<S^2> 7.04338375)**
N	-2.5001365	1.6160516	-0.4301522	**ZPE$_{B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-1.4884421	-0.7577163	4.3121643	**0.938204**
N	-0.1394064	-1.7691502	2.7165508	**Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-0.7974189	-3.5549772	-2.4147266	**0.86304**
N	-0.0463456	-1.3732947	-2.6764070	
N	-1.9778145	3.6751976	-1.4859237	
N	-0.8580541	3.0337285	0.4527106	
C	-4.4597928	-1.3418639	1.2589332	
H	-4.2546306	-2.4128467	1.1235423	
H	-5.5379402	-1.2375589	1.4778201	
C	-3.6229655	-0.8196427	2.4189153	

H	-3.9388696	0.2084876	2.6658769
H	-3.8249996	-1.4311858	3.3127956
C	-1.2952130	-1.1157119	3.0074726
C	-2.1873941	0.4583277	4.7105893
H	-2.3268162	1.1226761	3.8526113
H	-1.5799377	0.9916166	5.4601244
H	-3.1713947	0.2416101	5.1591034
C	-1.0014987	-1.5749056	5.4217759
H	-0.6964913	-2.5641647	5.0609824
H	-1.8182070	-1.7060994	6.1503323
H	-0.1515583	-1.1028519	5.9430940
C	1.1384739	-1.3892625	3.3082838
H	1.0217820	-0.5023928	3.9416438
H	1.8455607	-1.1394459	2.4996615
H	1.5701921	-2.2063250	3.9101738
C	-0.0550940	-2.7698455	1.6646459
H	-1.0617050	-3.1215979	1.4111878
H	0.5347242	-3.6256823	2.0318464
H	0.4307450	-2.3634016	0.7635565
C	-4.3510360	-1.4652395	-1.1926716
H	-4.3812370	-0.8050600	-2.0707257
H	-5.3303861	-1.9731304	-1.1270250
C	-3.2285684	-2.4787185	-1.3723590
H	-3.2872261	-3.2405265	-0.5761638
H	-3.3728909	-3.0118781	-2.3255898
C	-0.9444956	-2.2296227	-2.1218859
C	-1.1343770	-4.6178777	-1.4750216
H	-1.2873487	-4.2105853	-0.4710297
H	-0.2982367	-5.3346890	-1.4302786
H	-2.0402570	-5.1674204	-1.7811283
C	-0.2989065	-4.0168268	-3.7088704
H	-0.2950284	-3.1928947	-4.4319286
H	-0.9695448	-4.8065935	-4.0848039
H	0.7177589	-4.4382009	-3.6351858
C	1.3721811	-1.6943730	-2.7881552
H	1.5913652	-2.6432899	-2.2854297
H	1.9590391	-0.9020626	-2.2949852
H	1.6979822	-1.7605266	-3.8393743
C	-0.4058658	-0.0228846	-3.0744463
H	-1.4966253	0.0732445	-3.1179117
H	0.0077838	0.1804205	-4.0760238
H	-0.0035805	0.7259823	-2.3739111
C	-4.7287843	0.6994823	-0.0902092
H	-4.8015786	1.1250174	0.9204908
H	-5.7552376	0.6284880	-0.4935931
C	-3.8735864	1.6169090	-0.9543712
H	-3.9121358	1.2789367	-2.0041238
H	-4.3024821	2.6313059	-0.9359741

C	-1.7931573	2.7501564	-0.5002401
C	-2.3102550	3.3103564	-2.8586920
H	-2.1430183	2.2412699	-3.0229163
H	-1.6537019	3.8697471	-3.5446750
H	-3.3559630	3.5536082	-3.1102707
C	-1.9011653	5.1135263	-1.2334892
H	-1.8890992	5.3134024	-0.1558178
H	-2.7950876	5.5948481	-1.6623169
H	-1.0108877	5.5688286	-1.6983951
C	0.3674027	3.7706604	0.1589615
H	0.5295257	3.8307835	-0.9238906
H	1.2232302	3.2412837	0.6115234
H	0.3514958	4.7913269	0.5763158
C	-1.0345666	2.6507987	1.8472950
H	-2.0626848	2.3080178	2.0056822
H	-0.8481605	3.5262519	2.4908793
H	-0.3391358	1.8480228	2.1418069
C	4.4849201	1.1848826	3.3361602
C	4.1555714	2.4715586	2.8776736
C	4.7624098	0.1683567	2.4137898
C	4.1057736	2.7277849	1.5125053
C	4.7164156	0.4021458	1.0352496
C	4.3798380	1.7057916	0.5616166
C	5.0244097	-0.7156047	0.0624219
C	4.3280464	1.9663583	-0.8417371
C	4.6104944	0.9631839	-1.8185514
C	4.9596370	-0.3579143	-1.4067085
C	4.5576682	1.2537782	-3.2097024
C	5.2428435	-1.3229832	-2.3792527
C	4.8416979	0.2786670	-4.1579044
C	5.1880292	-1.0193428	-3.7449744
H	4.5292325	0.9771102	4.4084796
H	3.9427357	3.2710586	3.5926158
H	5.0247781	-0.8308363	2.7759177
H	3.8614154	3.7309741	1.1507379
H	4.2901953	2.2664955	-3.5254363
H	5.5135236	-2.3352936	-2.0624870
H	4.7971510	0.5216436	-5.2231312
H	5.4152060	-1.7905342	-4.4857723
H	0.4987674	0.8191096	0.0764495
H	4.0715016	2.9737507	-1.1814312
H	6.0271468	-1.1247653	0.2899780
H	4.3375812	-1.5617054	0.2569019

5.2.2 Cu^{III}(OH)(L) pathway (B3LYP)

Method: B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(ε = 8.51)

C	-1.4110746	-0.5811711	0.1864074
C	-0.0433063	-1.2130284	0.1868696
C	1.0724370	-0.2005383	0.1863025
C	0.8694511	1.1238161	0.1860749
C	-0.4983167	1.7556738	0.1860713
C	-1.6140606	0.7431835	0.1860358
H	-2.2715345	-1.2603502	0.1863915
H	2.0968129	-0.5908306	0.1862730
H	1.7299106	1.8029953	0.1856497
H	-2.6384368	1.1334754	0.1856475
H	-0.6019635	2.4320887	-0.6867080
H	-0.6020100	2.4321149	1.0588273
H	0.0603226	-1.8888584	1.0601106
H	0.0604170	-1.8900523	-0.6854244

CHD

$E_{B3LYP/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:

-233.0949079571

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-233.3530859463

$ZPE_{B3LYP/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:

0.121605

Chem. Pot.$_{(298.15)/B3LYP/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:

0.094502 (σ = 4)

C	-3.5664355	-0.7614063	0.1200915
C	-3.5736524	0.6118827	0.3884271
C	-2.3977057	-1.3717106	-0.3475301
C	-2.4120217	1.3650768	0.1874918
C	-1.2321748	-0.6213765	-0.5592466
C	-1.2393415	0.7614569	-0.2886968
C	0.0435691	-1.2507224	-1.0816461
C	0.0291973	1.5539064	-0.5323394
C	1.2771470	0.7582663	-0.2065563
C	1.2842735	-0.6244828	-0.4775173
C	2.4176903	1.3588879	0.3454258
C	2.4318457	-1.3776383	-0.1910000
C	3.5620006	0.6028503	0.6211548
C	3.5691151	-0.7702789	0.3519436
H	-4.4680029	-1.3589856	0.2812141
H	-4.4809344	1.0956988	0.7607854
H	-2.3887716	-2.4473304	-0.5496337
H	-2.4143916	2.4376698	0.4052765
H	2.4083347	2.4313698	0.5635672
H	2.4336276	-2.4531365	-0.3939530
H	4.4442286	1.0843407	1.0521171
H	4.4569512	-1.3700171	0.5709218
H	0.0645358	1.8406524	-1.6034748
H	0.0120213	2.4997593	0.0306666
H	0.0368911	-2.3392022	-0.9171586
H	0.0794599	-1.1117635	-2.1817432

DHA

$E_{B3LYP/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:

-540.0041012622

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-540.5854693574

$ZPE_{B3LYP/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:

0.217078

Chem. Pot.$_{(298.15)/B3LYP/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:

0.18259 (σ = 2)

H	-4.5384713	4.4455857	0.1230360
C	-4.5011574	3.3613687	0.0047112
C	-4.3053119	0.6109200	-0.2907882
C	-5.6595963	2.5825155	-0.1348635
C	-3.2693878	2.7098386	-0.0110868

$Cu^{III}(OH)(L)$

$E_{B3LYP/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

-3232.5271394185

N	-3.2319618	1.3866339	-0.1556621
C	-5.5727999	1.1906173	-0.2850839
H	-6.6396552	3.0652816	-0.1264349
H	-6.4564683	0.5598756	-0.3954661
C	-1.8959393	3.3287386	0.1200227
O	-1.7411495	4.5362527	0.2632464
C	-3.9583511	-0.8538149	-0.4360971
O	-4.8260501	-1.7103426	-0.5719179
N	-2.6101321	-1.0473585	-0.3928425
N	-0.9168332	2.3798501	0.0565301
Cu	-1.5548637	0.5667085	-0.1705336
H	0.7226318	0.3856141	-0.0956722
O	0.0250762	-0.2822635	-0.1947284
C	0.4531476	2.7332760	0.1550860
C	3.1646180	3.4006060	0.3473044
C	1.0829180	2.7424222	1.4302739
C	1.1840220	3.0388826	-1.0262794
C	2.5391725	3.3745286	-0.9003629
C	2.4406264	3.0849348	1.4981544
H	3.1179791	3.6233459	-1.7933155
H	2.9426552	3.1084610	2.4686121
H	4.2229045	3.6653022	0.4227506
C	-2.0336675	-2.3300892	-0.5033063
C	-0.9031739	-4.8790225	-0.7241638
C	-1.8016548	-3.0962054	0.6718471
C	-1.6687032	-2.8243360	-1.7854002
C	-1.1127853	-4.1074146	-1.8689865
C	-1.2425458	-4.3729260	0.5323538
H	-0.8374745	-4.5145667	-2.8450585
H	-1.0680256	-4.9864150	1.4197287
H	-0.4684789	-5.8787921	-0.8112133
C	0.5196601	3.0512578	-2.3987991
H	-0.4678797	2.5790379	-2.2893633
C	0.2823605	4.4974423	-2.8772255
H	-0.2623816	4.5040859	-3.8361801
H	1.2378491	5.0276045	-3.0290503
H	-0.3078361	5.0645313	-2.1407143
C	1.2979543	2.2309734	-3.4412205
H	0.7406856	2.1969025	-4.3917640
H	1.4497057	1.1944874	-3.0991318
H	2.2875565	2.6664776	-3.6565874
C	0.3102105	2.4332189	2.7080804
H	-0.6662857	2.0236196	2.4101300
C	0.0372772	3.7225731	3.5075815
H	-0.4939341	4.4642065	2.8906784
H	0.9776909	4.1814243	3.8569890
H	-0.5810223	3.5051458	4.3945577
C	1.0016068	1.3652267	3.5722813

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-3234.2848324600

$ZPE_{B3LYP/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.632973

Chem. Pot.$_{(298.15)/B3LYP/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.569457

H	1.9732787	1.7119948	3.9608413
H	1.1749304	0.4414461	2.9970577
H	0.3719302	1.1118407	4.4409373
C	-1.9121337	-2.0111146	-3.0514083
H	-2.1296970	-0.9791227	-2.7384960
C	-3.1515935	-2.5308772	-3.8072263
H	-4.0398369	-2.5346154	-3.1563994
H	-2.9917114	-3.5608565	-4.1690533
H	-3.3676398	-1.8960661	-4.6830619
C	-0.6778895	-1.9522977	-3.9663116
H	-0.4226993	-2.9406618	-4.3829365
H	0.2012471	-1.5747134	-3.4202370
H	-0.8672116	-1.2778054	-4.8176700
C	-2.1898322	-2.5761796	2.0511276
H	-2.3752373	-1.4963268	1.9512106
C	-3.5043755	-3.2241503	2.5308458
H	-3.8218655	-2.7919370	3.4947883
H	-3.3800269	-4.3111205	2.6737277
H	-4.3125609	-3.0688531	1.7994547
C	-1.0684577	-2.7455068	3.0892580
H	-1.3565140	-2.2690292	4.0408646
H	-0.1330858	-2.2777597	2.7428673
H	-0.8597466	-3.8062868	3.3053501

H	-5.5803086	1.2058615	0.1766970
C	-4.9216556	0.3363665	0.1448668
C	-3.1678702	-1.8101797	0.0604182
C	-5.4137480	-0.9773528	0.1520271
C	-3.5406274	0.5169150	0.0943567
N	-2.7430688	-0.5485328	0.0557023
C	-4.5362356	-2.0708111	0.1093192
H	-6.4917929	-1.1505210	0.1910434
H	-4.8902332	-3.1030584	0.1135439
C	-2.7813989	1.8244680	0.0745854
O	-3.3602275	2.9053857	0.1058598
C	-2.0365027	-2.8124692	0.0100681
O	-2.2472962	-4.0213639	0.0065338
N	-0.8271535	-2.1870119	-0.0271103
N	-1.4336896	1.6177770	0.0191787
Cu	-0.9011259	-0.2444082	-0.0153063
H	1.0984475	0.8993084	-0.1013566
O	0.8804857	-0.0465559	-0.0919416
H	3.2204559	-0.5641291	0.0532580
C	-0.5319431	2.7128730	-0.0137769
C	1.2442930	4.8742412	-0.0776002
C	-0.0116704	3.2269239	1.2059141
C	-0.1417996	3.2609009	-1.2666456
C	0.7443832	4.3466433	-1.2691423

Cu^{III}(OH)(L)-CHD-RC

$E_{B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:

-3465.6207230790

$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 8.51)}$:

-3467.6334689277

$ZPE_{B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:

0.755861

Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:

0.685164

C	0.8710982	4.3138610	1.1452094
H	1.0492009	4.7911254	-2.2196572
H	1.2744452	4.7327396	2.0701551
H	1.9320329	5.7240903	-0.1021952
C	0.3866448	-2.9035150	-0.0670465
C	2.7889431	-4.3336427	-0.1470948
C	1.0240177	-3.2684239	1.1502620
C	0.9685461	-3.2231798	-1.3238173
C	2.1669177	-3.9478065	-1.3361083
C	2.2209996	-3.9919071	1.0820141
H	2.6258341	-4.2167377	-2.2909500
H	2.7219018	-4.2955928	2.0047330
H	3.7241549	-4.8999451	-0.1783196
C	4.7268647	2.0276548	-1.0984641
C	4.4120127	0.7274350	-1.1754319
C	4.9701554	2.7472442	0.2031006
H	4.2477459	3.5825112	0.3083488
H	5.9595106	3.2480514	0.1821565
C	4.2546643	-0.1655360	0.0264675
H	4.8957955	-1.0638621	-0.0788183
C	4.8758014	1.8394685	1.4022963
C	4.5599856	0.5394997	1.3210956
C	-0.6953522	2.7245586	-2.5825124
H	-1.1744991	1.7580723	-2.3657098
C	-1.7869738	3.6602974	-3.1393357
H	-2.2359870	3.2333651	-4.0518759
H	-1.3669887	4.6465688	-3.4004701
H	-2.5879877	3.8173412	-2.4005423
C	0.4040217	2.4589715	-3.6246063
H	-0.0269981	1.9762889	-4.5171567
H	1.1843828	1.7949968	-3.2196425
H	0.8907204	3.3899630	-3.9589081
C	-0.4274682	2.6533500	2.5563949
H	-0.9020787	1.6792854	2.3644896
C	-1.4852857	3.5513508	3.2291266
H	-2.3546565	3.7026735	2.5707075
H	-1.0653927	4.5428429	3.4699745
H	-1.8384969	3.0974684	4.1703055
C	0.7680301	2.3972382	3.4889927
H	1.2539797	3.3348688	3.8055782
H	1.5296548	1.7701752	2.9985683
H	0.4321900	1.8792153	4.4023680
C	0.2990360	-2.8304904	-2.6353013
H	-0.4980405	-2.1126983	-2.3917051
C	-0.3716493	-4.0500623	-3.2980790
H	-1.0900467	-4.5270025	-2.6128492
H	0.3766965	-4.8079176	-3.5860885
H	-0.9134081	-3.7486963	-4.2105163

C	1.2634695	-2.1193624	-3.5989794
H	2.0692440	-2.7871927	-3.9461429
H	1.7268467	-1.2460671	-3.1132727
H	0.7207888	-1.7688994	-4.4926320
C	0.4134894	-2.9263289	2.5042307
H	-0.3857119	-2.1919615	2.3247733
C	-0.2410152	-4.1680441	3.1420038
H	-0.7434059	-3.9012675	4.0871848
H	0.5126227	-4.9414699	3.3683806
H	-0.9891089	-4.6110929	2.4662849
C	1.4227376	-2.2663333	3.4585133
H	0.9188181	-1.9508041	4.3871831
H	1.8780710	-1.3765003	2.9956053
H	2.2339066	-2.9560995	3.7447858
H	5.0752775	2.2890166	2.3820712
H	4.8110008	2.6206957	-2.0165660
H	4.2412816	0.2706276	-2.1572680
H	4.5039441	-0.0599566	2.2373520
H	-4.4832955	4.4323747	0.1393451
C	-4.4480563	3.3482342	0.0206623
C	-4.2582986	0.5969737	-0.2772458
C	-5.6088601	2.5721612	-0.1164453
C	-3.2175157	2.6911251	0.0013291
N	-3.1834949	1.3689417	-0.1435751
C	-5.5261942	1.1801894	-0.2682340
H	-6.5878483	3.0575931	-0.1051239
H	-6.4121943	0.5526833	-0.3772995
C	-1.8441067	3.3213935	0.1291796
O	-1.7200628	4.5385409	0.2697961
C	-3.9298633	-0.8767962	-0.4274199
O	-4.8325462	-1.7063864	-0.5630719
N	-2.5947178	-1.1007617	-0.3905040
N	-0.8524492	2.3953894	0.0671681
Cu	-1.4680191	0.5262229	-0.1627610
H	0.8721667	0.4445082	-0.0856064
O	0.2261068	-0.2781346	-0.1753039
H	1.1903943	-1.3375600	-0.1939390
C	0.5082026	2.7886743	0.1651605
C	3.2190656	3.4865159	0.3499874
C	1.1437379	2.8113375	1.4377549
C	1.2375193	3.0977673	-1.0166979
C	2.5900130	3.4477773	-0.8955156
C	2.4984909	3.1677785	1.5023221
H	3.1636101	3.6984450	-1.7912948
H	3.0008386	3.2007427	2.4721717
H	4.2738810	3.7658749	0.4228649
C	-2.0836662	-2.4177947	-0.5059687

Cu^{III}(OH)(L)-CHD-TS

$E_{B3LYP/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

-3465.6053997020 (<S^2> 0.48079694)

$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-3467.6148183357 (*S* = 0; <S^2> 0.49509705)

-3467.6021338349 (*S* = 1; <S^2> 2.01516229)

-3467.6189914014 (spin purified)

$ZPE_{B3LYP/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.749835

Chem. Pot.(298.15)/B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(ε = 8.51):

0.679808

C	-1.0227474	-5.0045089	-0.7333170
C	-1.9074829	-3.2097187	0.6601915
C	-1.7125028	-2.9153311	-1.7840236
C	-1.1876734	-4.2127835	-1.8715325
C	-1.3792838	-4.5012495	0.5189788
H	-0.9064878	-4.6164211	-2.8475280
H	-1.2473549	-5.1293977	1.4038457
H	-0.6144433	-6.0153023	-0.8225786
C	4.2034082	-1.0941764	-1.0955593
C	3.0209564	-1.7127364	-1.3063402
C	4.7339983	-0.8170370	0.2799462
H	4.7958653	0.2834305	0.4387561
H	5.7921139	-1.1401507	0.3562495
C	2.1383244	-2.1201209	-0.1964201
H	1.5485950	-3.0326410	-0.3897319
C	3.9211215	-1.4360177	1.3781809
C	2.7406121	-2.0521001	1.1482147
C	0.5660131	3.0990694	-2.3864854
H	-0.3808421	2.5479625	-2.2828593
C	0.2108961	4.5364923	-2.8177517
H	-0.3421926	4.5313274	-3.7721759
H	1.1225048	5.1419046	-2.9597560
H	-0.4127114	5.0331745	-2.0587368
C	1.3937546	2.3794566	-3.4639263
H	0.8197777	2.3128890	-4.4027814
H	1.6542400	1.3553963	-3.1509564
H	2.3313272	2.9126832	-3.6925073
C	0.3701701	2.5049986	2.7163536
H	-0.5551829	1.9890853	2.4183650
C	-0.0447513	3.8095216	3.4267667
H	-0.6172588	4.4627039	2.7505365
H	0.8418292	4.3690395	3.7712667
H	-0.6691578	3.5908370	4.3094593
C	1.1267094	1.5651795	3.6692603
H	2.0310454	2.0375829	4.0872023
H	1.4344227	0.6391423	3.1572482
H	0.4823019	1.2872853	4.5194758
C	-1.9287490	-2.0863344	-3.0462988
H	-2.0519214	-1.0406178	-2.7261913
C	-3.2344401	-2.5033097	-3.7537261
H	-4.0928684	-2.4418749	-3.0672860
H	-3.1675282	-3.5416886	-4.1215299
H	-3.4354046	-1.8510545	-4.6205940
C	-0.7346149	-2.1256807	-4.0128912
H	-0.5787744	-3.1289246	-4.4428485
H	0.1969905	-1.8230861	-3.5080757
H	-0.9036543	-1.4340975	-4.8547796
C	-2.3265391	-2.7012959	2.0362657

H	-2.4637703	-1.6129081	1.9497906	
C	-3.6852287	-3.3021064	2.4500517	
H	-4.0253093	-2.8754905	3.4090533	
H	-3.6105153	-4.3959448	2.5761589	
H	-4.4526644	-3.0984162	1.6878669	
C	-1.2601425	-2.9369921	3.1183103	
H	-1.5718742	-2.4722871	4.0683762	
H	-0.2927856	-2.4963932	2.8278101	
H	-1.0992499	-4.0094117	3.3175717	
H	4.3224606	-1.3811538	2.3953468	
H	4.8178480	-0.7801974	-1.9456160	
H	2.6765937	-1.8957752	-2.3293280	
H	2.1842428	-2.4920024	1.9820490	
H	-5.5211098	1.1594075	0.2487648	***Cu^{III}(OH)(L)-CHD-IC***
C	-4.8343946	0.3125671	0.2064854	**$E_{B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
C	-3.0157199	-1.7813600	0.0958674	**-3465.6440302639 (<S^2> 1.03881585)**
C	-5.2851671	-1.0163807	0.2193615	**$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 8.51)}$:**
C	-3.4578258	0.5345404	0.1362709	**-3467.6525467610 (*S* = 0; <S^2> 1.03693909)**
N	-2.6333372	-0.5080237	0.0855123	**-3467.6525079370 (*S* = 1; <S^2> 2.03876534)**
C	-4.3770196	-2.0845967	0.1637848	**-3467.6525885633 (spin purified)**
H	-6.3572259	-1.2218907	0.2734805	**$ZPE_{B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
H	-4.7030933	-3.1257802	0.1725857	**0.753768**
C	-2.7487408	1.8810225	0.1097251	**Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
O	-3.4034115	2.9271800	0.1491789	**0.682639**
C	-1.8602512	-2.7693331	0.0324975	
O	-2.0869125	-3.9833739	0.0292950	
N	-0.6599306	-2.1464330	-0.0133332	
N	-1.4051914	1.7413719	0.0432491	
Cu	-0.7375902	-0.1492849	-0.0414510	
H	1.3640647	1.3087108	-0.2955772	
O	1.1700985	0.3637644	-0.4128194	
H	1.9912683	-0.1315900	-0.2248331	
C	-0.5563495	2.8801243	0.0127255	
C	1.2345234	5.0447071	-0.0536130	
C	-0.0413166	3.4085352	1.2300356	
C	-0.1615788	3.4323885	-1.2378471	
C	0.7321279	4.5148166	-1.2428808	
C	0.8484686	4.4915603	1.1688123	
H	1.0380362	4.9555411	-2.1949715	
H	1.2458621	4.9145932	2.0945550	
H	1.9270763	5.8906337	-0.0789190	
C	0.5384431	-2.9106608	-0.0553486	
C	2.9614997	-4.3287994	-0.1403246	
C	1.1587969	-3.3188553	1.1568487	
C	1.1370950	-3.2090648	-1.3093771	
C	2.3472607	-3.9189250	-1.3249608	
C	2.3673172	-4.0285317	1.0865613	

H	2.8163639	-4.1633571	-2.2813123
H	2.8524490	-4.3581187	2.0089235
H	3.9029101	-4.8844511	-0.1733653
C	4.6960576	1.5671234	-1.2010321
C	4.4523105	0.2181625	-1.1750032
C	4.7028097	2.3995203	0.0481129
H	3.9868786	3.2469441	-0.0499931
H	5.6781187	2.9273888	0.1480675
C	4.1804533	-0.4644998	0.0477572
H	4.0224438	-1.5460581	0.0522243
C	4.4128764	1.6189527	1.2969122
C	4.1750139	0.2685017	1.2713153
C	-0.7300696	2.9031831	-2.5515350
H	-1.1666299	1.9154066	-2.3394393
C	-1.8763978	3.8067046	-3.0491141
H	-2.3387870	3.3852591	-3.9576705
H	-1.5040396	4.8155169	-3.2969673
H	-2.6564849	3.9102538	-2.2793824
C	0.3394847	2.7039048	-3.6377561
H	-0.1044076	2.2239520	-4.5253580
H	1.1596045	2.0602961	-3.2796488
H	0.7792265	3.6588726	-3.9696332
C	-0.4823577	2.8515635	2.5806947
H	-0.8900064	1.8456190	2.3954397
C	-1.6260527	3.7020933	3.1707612
H	-2.4651172	3.7810066	2.4630953
H	-1.2755785	4.7230173	3.4005438
H	-2.0009113	3.2553898	4.1071709
C	0.6706123	2.7000809	3.5860434
H	1.0759822	3.6749001	3.9037593
H	1.5021019	2.1120216	3.1640545
H	0.3168039	2.1847055	4.4939526
C	0.4551189	-2.8257739	-2.6199655
H	-0.2798726	-2.0412521	-2.3832677
C	-0.3311057	-4.0238601	-3.1904888
H	-1.0457202	-4.4147806	-2.4500073
H	0.3520581	-4.8442869	-3.4699991
H	-0.8922092	-3.7295467	-4.0936472
C	1.4202220	-2.2438491	-3.6649116
H	2.1505384	-2.9898223	-4.0193998
H	1.9814025	-1.3863784	-3.2592004
H	0.8594551	-1.8936634	-4.5471425
C	0.5100724	-3.0483983	2.5121496
H	-0.2515987	-2.2693236	2.3554292
C	-0.2227973	-4.3046652	3.0256288
H	-0.7568789	-4.0877784	3.9663448
H	0.4913531	-5.1221632	3.2247891
H	-0.9542641	-4.6615569	2.2851119

C	1.4959793	-2.5152022	3.5646051	
H	0.9580983	-2.2480622	4.4891106	
H	2.0205376	-1.6136458	3.2080826	
H	2.2590607	-3.2629516	3.8366414	
H	4.4065620	2.1600945	2.2477552	
H	4.9021239	2.0702144	-2.1505729	
H	4.4654673	-0.3514879	-2.1091918	
H	3.9808838	-0.2628446	2.2079519	
H	-4.6826027	4.4246884	0.3184253	***Cu^{III}(OH)(L)-DHA-RC***
C	-4.6093688	3.3401413	0.2220337	**$E_{B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
C	-4.3217347	0.5930211	-0.0225875	**-3772.5299617668**
C	-5.7423697	2.5163338	0.1458920	**$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 8.51)}$:**
C	-3.3555543	2.7340960	0.1698412	**-3774.8654251167**
N	-3.2737793	1.4100379	0.0532428	**$ZPE_{B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
C	-5.6090721	1.1256610	0.0212697	**0.851331**
H	-6.7388239	2.9627906	0.1836285	**Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
H	-6.4717442	0.4602261	-0.0408551	**0.776904**
C	-2.0025767	3.4064855	0.2295375	
O	-1.8895208	4.6218779	0.3461041	
C	-3.9271638	-0.8609320	-0.1510652	
O	-4.7695914	-1.7487858	-0.2392066	
N	-2.5725486	-1.0074719	-0.1507480	
N	-0.9912866	2.4950995	0.1375819	
Cu	-1.5678663	0.6520862	-0.0178174	
H	0.7194220	0.5613483	-0.0919678	
O	0.0450310	-0.1363955	-0.1009638	
H	1.7949655	-1.7075173	-0.0023538	
C	0.3666944	2.9024086	0.1756557	
C	3.0558371	3.6734733	0.2484265	
C	1.0439914	2.9604506	1.4248612	
C	1.0397747	3.2093451	-1.0394706	
C	2.3849196	3.5975275	-0.9731682	
C	2.3890886	3.3549364	1.4329002	
H	2.9199003	3.8464688	-1.8926851	
H	2.9266043	3.4171911	2.3823295	
H	4.1052118	3.9793506	0.2773355	
C	-1.9601569	-2.2743717	-0.2527097	
C	-0.7761693	-4.7994839	-0.4571400	
C	-1.6698992	-3.0079147	0.9303972	
C	-1.6238880	-2.7868081	-1.5351608	
C	-1.0404645	-4.0578640	-1.6102905	
C	-1.0851196	-4.2735612	0.7992039	
H	-0.7875551	-4.4792730	-2.5863879	
H	-0.8668083	-4.8629528	1.6930536	
H	-0.3222158	-5.7913559	-0.5374812	
H	5.9974257	0.4921229	-1.7987438	
C	5.2665815	-0.2940776	-2.0130966	

C	3.4178578	-2.3085713	-2.5506520
C	4.4774199	-0.8021654	-0.9712848
C	5.1313552	-0.7807118	-3.3172530
C	4.2025138	-1.7919172	-3.5868565
C	3.5429021	-1.8216877	-1.2410596
H	5.7543206	-0.3756999	-4.1198181
H	4.0935980	-2.1834800	-4.6022955
H	2.6962040	-3.1042543	-2.7590387
C	4.5895618	-0.2764473	0.4453642
H	3.8229501	0.5124147	0.5902427
H	5.5596985	0.2212903	0.5996421
C	2.6924414	-2.3526576	-0.1062562
H	2.3021190	-3.3527394	-0.3494120
C	4.3725481	-1.3584401	1.4835883
C	3.4372212	-2.3770562	1.2117421
C	5.0677600	-1.3651358	2.7014520
H	5.8005814	-0.5780536	2.9058599
C	4.8376567	-2.3646934	3.6523608
H	5.3883500	-2.3581415	4.5973111
C	3.2161676	-3.3784968	2.1688093
H	2.4934142	-4.1718495	1.9554979
C	3.9071489	-3.3748734	3.3848426
H	3.7242081	-4.1639854	4.1197723
C	0.3211785	3.1688811	-2.3839403
H	-0.6258513	2.6297038	-2.2320653
C	-0.0357522	4.5936724	-2.8533441
H	-0.6195848	4.5591586	-3.7884597
H	0.8747002	5.1862069	-3.0462510
H	-0.6309507	5.1232510	-2.0934526
C	1.1095465	2.4026271	-3.4590686
H	0.5100526	2.3181139	-4.3803845
H	1.3614498	1.3847093	-3.1211394
H	2.0495744	2.9127263	-3.7261551
C	0.3340294	2.6465682	2.7374029
H	-0.6343516	2.1897107	2.4851454
C	0.0358188	3.9402412	3.5209132
H	-0.5496360	4.6454473	2.9104213
H	0.9681943	4.4457555	3.8246058
H	-0.5385397	3.7160913	4.4353790
C	1.1023321	1.6273972	3.5955488
H	2.0707132	2.0242457	3.9419793
H	1.2968467	0.7005764	3.0325661
H	0.5155792	1.3653654	4.4913870
C	-1.9258187	-2.0062811	-2.8088681
H	-2.1578417	-0.9733547	-2.5097759
C	-3.1754602	-2.5695739	-3.5151260
H	-4.0431952	-2.5802971	-2.8371906
H	-3.0026501	-3.6029484	-3.8611813

H	-3.4331963	-1.9584532	-4.3966274
C	-0.7213829	-1.9377135	-3.7619296
H	-0.4617037	-2.9275851	-4.1725715
H	0.1664754	-1.5381389	-3.2471937
H	-0.9497073	-1.2797266	-4.6168318
C	-2.0263609	-2.4659586	2.3098352
H	-2.2089222	-1.3867037	2.1964825
C	-3.3337050	-3.1008894	2.8263943
H	-3.6310472	-2.6512095	3.7888844
H	-3.2074595	-4.1853691	2.9863444
H	-4.1560608	-2.9583743	2.1085965
C	-0.8871210	-2.6255753	3.3296325
H	-1.1505674	-2.1207442	4.2738780
H	0.0500952	-2.1854185	2.9544407
H	-0.6922575	-3.6837639	3.5702604

H	-4.1902480	4.7419690	-0.0685681	***Cu^{III}(OH)(L)-DHA-TS***
C	-4.2157155	3.6560142	-0.1720485	**$E_{B3LYP/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:**
C	-4.1766053	0.8955007	-0.4213409	**-3772.5111701159 (<S^2> 0.50062830)**
C	-5.4121869	2.9500565	-0.3666348	**$E_{B3LYP/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:**
C	-3.0286570	2.9254320	-0.1116144	**-3774.8423596806 (*S* = 0; <S^2> 0.51836229)**
N	-3.0648973	1.6015146	-0.2372606	**-3774.8300055974 (*S* = 1; <S^2> 2.01602640)**
C	-5.4052856	1.5534581	-0.4940066	**-3774.8466818511 (spin purified)**
H	-6.3587170	3.4936762	-0.4188390	**$ZPE_{B3LYP/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:**
H	-6.3196322	0.9774632	-0.6448742	**0.845117**
C	-1.6322623	3.4767051	0.0923176	**Chem. Pot.$_{(298.15)/B3LYP/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:**
O	-1.4470179	4.6860485	0.2330746	**0.771166**
C	-3.9350734	-0.5970693	-0.5251618	
O	-4.8815023	-1.3707967	-0.6928135	
N	-2.6220693	-0.9063486	-0.4064891	
N	-0.6933662	2.4954453	0.0970391	
Cu	-1.3982117	0.6542855	-0.1611991	
H	0.9317541	0.5142321	-0.0067432	
O	0.2911303	-0.2081232	-0.1336511	
H	1.2174668	-1.2266136	-0.2180778	
C	0.6757511	2.8211002	0.2808793	
C	3.3985669	3.3864846	0.6401297	
C	1.2279034	2.8148767	1.5924216	
C	1.4920570	3.0968885	-0.8515111	
C	2.8496360	3.3796146	-0.6432114	
C	2.5909845	3.1049527	1.7443527	
H	3.4907748	3.6017478	-1.4995949	
H	3.0315606	3.1152559	2.7442611	
H	4.4591430	3.6124163	0.7810450	
C	-2.2007012	-2.2583180	-0.4621461	
C	-1.2684741	-4.9007102	-0.5551253	
C	-2.0757929	-3.0010176	0.7435857	
C	-1.8759955	-2.8437256	-1.7152819	

C	-1.4088708	-4.1662411	-1.7342157
C	-1.6064642	-4.3203767	0.6696368
H	-1.1600721	-4.6367834	-2.6890656
H	-1.5115815	-4.9114481	1.5840294
H	-0.9038817	-5.9312715	-0.5912587
H	5.9560835	0.2938269	-1.5672795
C	5.1034291	-0.3178902	-1.8769976
C	2.9454448	-1.8971253	-2.6734163
C	4.2006722	-0.7768140	-0.9092473
C	4.9322398	-0.6356074	-3.2278673
C	3.8480264	-1.4305445	-3.6268783
C	3.1050643	-1.5809400	-1.3079347
H	5.6480114	-0.2703998	-3.9692488
H	3.7147130	-1.6903265	-4.6803540
H	2.1079296	-2.5301755	-2.9773273
C	4.3623199	-0.4136126	0.5484752
H	3.8628866	0.5646415	0.7193277
H	5.4231445	-0.2338903	0.7848857
C	2.1516102	-2.0722513	-0.2879100
H	1.5455100	-2.9273720	-0.6244670
C	3.7724296	-1.4241146	1.5046295
C	2.6799601	-2.2227340	1.0853729
C	4.2733232	-1.5750675	2.8039518
H	5.1244202	-0.9668359	3.1247615
C	3.7050817	-2.4954729	3.6904316
H	4.1108681	-2.6022773	4.7000555
C	2.1144614	-3.1467523	1.9888356
H	1.2737534	-3.7627839	1.6590682
C	2.6216328	-3.2854876	3.2791930
H	2.1788456	-4.0111543	3.9665220
C	0.9085352	3.1396166	-2.2603368
H	-0.0739738	2.6457404	-2.2188755
C	0.6668890	4.5973963	-2.7020603
H	0.1732628	4.6279933	-3.6881012
H	1.6201546	5.1469995	-2.7855569
H	0.0296844	5.1278491	-1.9781682
C	1.7574938	2.3752935	-3.2891239
H	1.2427942	2.3548803	-4.2639515
H	1.9321751	1.3339016	-2.9750836
H	2.7403072	2.8482428	-3.4497182
C	0.3585417	2.5522046	2.8182285
H	-0.5723132	2.0868594	2.4604223
C	-0.0302423	3.8789940	3.5017763
H	-0.5208947	4.5610407	2.7905690
H	0.8609199	4.3901882	3.9045884
H	-0.7220796	3.6962082	4.3412514
C	1.0000721	1.5750990	3.8167215
H	1.9034559	1.9961696	4.2880635

H	1.2833545	0.6288416	3.3282594	
H	0.2900375	1.3403059	4.6266991	
C	-2.1010103	-2.0903788	-3.0235167	
H	-2.2345355	-1.0288750	-2.7669447	
C	-3.4037269	-2.5645870	-3.7002750	
H	-4.2595206	-2.4656080	-3.0154815	
H	-3.3277939	-3.6225907	-4.0049075	
H	-3.6119581	-1.9683502	-4.6049562	
C	-0.9109601	-2.1718348	-3.9916790	
H	-0.7190987	-3.2029687	-4.3320373	
H	0.0090421	-1.7893131	-3.5235750	
H	-1.1092485	-1.5638898	-4.8899275	
C	-2.5175586	-2.4105975	2.0802272	
H	-2.5309377	-1.3166366	1.9591372	
C	-3.9591875	-2.8513782	2.4112334	
H	-4.3155757	-2.3589173	3.3319983	
H	-4.0063374	-3.9421391	2.5728946	
H	-4.6500055	-2.5992005	1.5926857	
C	-1.5669294	-2.7255873	3.2448716	
H	-1.8973658	-2.1977518	4.1547447	
H	-0.5368686	-2.4070475	3.0226603	
H	-1.5455878	-3.8016270	3.4854439	
H	-4.4491619	4.3797665	0.2388911	***Cu^{III}(OH)(L)-DHA-IC***
C	-4.3870423	3.2948284	0.1411394	**$E_{B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
C	-4.1347184	0.5417916	-0.1032575	**-3772.5449710456 (<S^2> 1.03125625)**
C	-5.5292542	2.4887846	0.0192521	**$E_{B3LYP/def2-TZVPP/COSMO(\varepsilon = 8.51)}$:**
C	-3.1404424	2.6662457	0.1346068	**-3774.8762104980 (*S* = 0; <S^2> 1.02955312)**
N	-3.0802163	1.3430137	0.0146545	**-3774.8760477380 (*S* = 1; <S^2> 2.03491663)**
C	-5.4163674	1.0957092	-0.1051156	**-3774.8763831711 (spin purified)**
H	-6.5191700	2.9519317	0.0211293	**$ZPE_{B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
H	-6.2891773	0.4480523	-0.2011505	**0.84896**
C	-1.7790514	3.3353771	0.2513539	**Chem. Pot.$_{(298.15)/B3LYP/def2-SVP(Cu:def2-TZVP)/COSMO(\varepsilon = 8.51)}$:**
O	-1.6999143	4.5618079	0.3697821	**0.773707**
C	-3.7741949	-0.9308599	-0.2263444	
O	-4.6667157	-1.7771708	-0.3380704	
N	-2.4366203	-1.1304071	-0.1953250	
N	-0.7690842	2.4366601	0.2050094	
Cu	-1.3302412	0.5169003	0.0361546	
H	1.2376796	0.4636615	0.2683474	
O	0.5373583	-0.2098871	0.2799136	
H	0.9362029	-1.0675525	0.0454926	
C	0.5837172	2.8632450	0.2888742	
C	3.2966871	3.5769019	0.4432572	
C	1.2285065	2.9176174	1.5565182	
C	1.3053338	3.1577406	-0.9024887	
C	2.6582302	3.5139203	-0.7967710	
C	2.5839593	3.2790670	1.6057958	

H	3.2243598	3.7507073	-1.7006803
H	3.0911790	3.3342930	2.5719996
H	4.3510917	3.8603451	0.5036873
C	-1.9008281	-2.4424858	-0.3063339
C	-0.6938277	-4.9686595	-0.5137775
C	-1.6214511	-3.1878509	0.8713523
C	-1.5892701	-2.9701492	-1.5892616
C	-0.9851932	-4.2345761	-1.6650156
C	-1.0159216	-4.4469470	0.7405721
H	-0.7448356	-4.6590010	-2.6430898
H	-0.7998381	-5.0366734	1.6349769
H	-0.2234192	-5.9526601	-0.5947222
H	5.5461232	0.6660553	-2.2094884
C	4.8186560	-0.1445520	-2.3158003
C	2.9686443	-2.2161512	-2.6115921
C	4.3020928	-0.7513899	-1.1663541
C	4.4244236	-0.5541391	-3.5946441
C	3.4926079	-1.5958933	-3.7388786
C	3.3583434	-1.8130730	-1.3050306
H	4.8430592	-0.0648025	-4.4778332
H	3.1838186	-1.9215850	-4.7357140
H	2.2521758	-3.0352384	-2.7169155
C	4.7182331	-0.2702840	0.2060853
H	4.3317385	0.7602315	0.3498644
H	5.8160866	-0.1524786	0.2392950
C	2.8466306	-2.4733623	-0.1424263
H	2.1451556	-3.3033837	-0.2735565
C	4.2650514	-1.1216328	1.3715703
C	3.3249354	-2.1768939	1.1740524
C	4.7433562	-0.8676832	2.6612317
H	5.4673873	-0.0609885	2.8121329
C	4.3156898	-1.6248133	3.7578091
H	4.7046647	-1.4077798	4.7560323
C	2.9022128	-2.9365417	2.2986944
H	2.1876418	-3.7495637	2.1448522
C	3.3892277	-2.6645152	3.5710048
H	3.0548101	-3.2609355	4.4240041
C	0.6179908	3.1464613	-2.2651237
H	-0.2979867	2.5449071	-2.1578763
C	0.1804445	4.5717293	-2.6618156
H	-0.3883663	4.5554466	-3.6068777
H	1.0589957	5.2233946	-2.8082044
H	-0.4525660	5.0224624	-1.8827211
C	1.4635415	2.4994768	-3.3736186
H	0.8719561	2.4169888	-4.3001844
H	1.8004843	1.4880049	-3.0950653
H	2.3592563	3.0957896	-3.6136946
C	0.4593499	2.6485401	2.8469818

H	-0.4586116	2.1086632	2.5684402
C	0.0227463	3.9749901	3.5019244
H	-0.5580588	4.5895246	2.7973248
H	0.9003422	4.5613101	3.8242728
H	-0.6002633	3.7835050	4.3919109
C	1.2265835	1.7612188	3.8403209
H	2.1236571	2.2626823	4.2393234
H	1.5489686	0.8163950	3.3735716
H	0.5839996	1.5122812	4.7007625
C	-1.9635554	-2.2195756	-2.8653048
H	-2.1315549	-1.1686425	-2.5836918
C	-3.2935185	-2.7558188	-3.4348233
H	-4.0917491	-2.7111184	-2.6789316
H	-3.1854652	-3.8052454	-3.7590184
H	-3.6093109	-2.1637146	-4.3105850
C	-0.8621146	-2.2324042	-3.9367715
H	-0.6759818	-3.2455845	-4.3300171
H	0.0908607	-1.8422199	-3.5454693
H	-1.1585914	-1.6026518	-4.7917274
C	-2.0343658	-2.6701123	2.2469684
H	-2.1814490	-1.5833205	2.1513300
C	-3.3909887	-3.2756237	2.6635089
H	-3.7345324	-2.8431453	3.6185730
H	-3.3070712	-4.3677378	2.7987230
H	-4.1595556	-3.0847562	1.8993094
C	-0.9727519	-2.8902788	3.3353087
H	-1.2903833	-2.4119136	4.2764515
H	-0.0019253	-2.4572649	3.0467214
H	-0.8147620	-3.9596443	3.5529864

5.2.3 [Fe^{IV}(O)TMG$_3$tren]$^{2+}$ (σ), [Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$ (σ) and [Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$ (π) pathways (B3LYP-D3)

Method: B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)

C	-1.4119613	-0.5813402	0.1866777
C	-0.0433912	-1.2124765	0.1865911
C	1.0733326	-0.2004321	0.1866015
C	0.8703374	1.1239852	0.1862897
C	-0.4982323	1.7551214	0.1857342
C	-1.6149565	0.7430773	0.1862790
H	-2.2710082	-1.2622791	0.1870593
H	2.0968857	-0.5928307	0.1869418
H	1.7293838	1.8049247	0.1863825
H	-2.6385100	1.1354753	0.1863816
H	-0.6017571	2.4305300	-0.6876950
H	-0.6019217	2.4317505	1.0581859
H	0.0602426	-1.8885396	1.0594899

CHD

$E_{B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 35.88)}$:

-233.1023616359

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-233.3606579473

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 35.88)}$:

0.121825

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 35.88)}$:

H	0.0602054	-1.8884489	-0.6863914	**0.094797 (σ = 4)**
C	-3.5492648	-0.7666814	0.1461993	***DHA***
C	-3.5563323	0.6068804	0.4151635	**$E_{B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 35.88)}$:**
C	-2.3863934	-1.3741389	-0.3417281	**-540.0255643803**
C	-2.4005063	1.3650163	0.1946140	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:**
C	-1.2284241	-0.6189383	-0.5718221	**-540.6071353248**
C	-1.2355248	0.7638963	-0.3010167	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 35.88)}$:**
C	0.0446237	-1.2364957	-1.1126839	**0.217425**
C	0.0302879	1.5524300	-0.5665943	**Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 35.88)}$:**
C	1.2742013	0.7607970	-0.2193002	**0.182998 (σ = 2)**
C	1.2812650	-0.6220544	-0.4899937	
C	2.4059580	1.3590973	0.3510587	
C	2.4199155	-1.3801091	-0.1850918	
C	3.5431270	0.5981354	0.6462273	
C	3.5501154	-0.7754653	0.3773877	
H	-4.4463858	-1.3667970	0.3222208	
H	-4.4590021	1.0873287	0.8028613	
H	-2.3765914	-2.4494525	-0.5450393	
H	-2.4018306	2.4376609	0.4117981	
H	2.3957653	2.4317408	0.5680144	
H	2.4207036	-2.4554130	-0.3886897	
H	4.4199033	1.0764022	1.0917333	
H	4.4324295	-1.3777518	0.6113241	
H	0.0657789	1.8006762	-1.6468147	
H	0.0141195	2.5149337	-0.0329980	
H	0.0389850	-2.3292727	-0.9815508	
H	0.0805332	-1.0586584	-2.2066907	

$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (σ) pathway

Fe	4.7858346	9.4737996	3.1601846	***$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$***
N	4.5058367	11.2995332	2.1430726	
O	3.1813417	9.2752017	3.3759226	**$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
N	5.1974233	9.8797429	5.0214387	**-2445.7971144150 (<S^2> 6.05144800)**
C	6.5859842	10.3032311	5.2500544	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:**
H	6.8823165	10.1247002	6.2956532	**-2447.1111691153 (<S^2> 6.05369072)**
H	6.7372338	11.3771086	5.0515443	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
C	7.4442208	9.4719154	4.3130614	**0.574404**
H	8.5073130	9.7595677	4.3606283	**Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
H	7.3616913	8.4138386	4.5960367	**0.517299**
N	6.9321335	9.6273521	2.9184544	
C	7.3384553	8.4889439	2.0443167	
H	8.4020532	8.2453166	2.2048116	
H	7.2123248	8.8153486	1.0028657	
C	6.4376160	7.2970625	2.3036750	
H	6.6279360	6.5115593	1.5562195	
H	6.6549998	6.8597248	3.2919791	

N	5.0545573	7.7845267	2.2160839
C	4.2918628	9.9813281	6.0203387
N	4.2734472	11.0654903	6.8312801
C	4.6405282	12.3902427	6.3397272
H	4.6384907	12.3996548	5.2426977
H	5.6313476	12.7026174	6.7086875
H	3.8939510	13.1181639	6.6939393
C	3.9083838	10.9931617	8.2449041
H	3.9082969	9.9501662	8.5832911
H	2.9194327	11.4395937	8.4379297
H	4.6594191	11.5489214	8.8281074
N	3.4089638	8.9854417	6.2293526
C	2.0426353	9.2323320	6.6838702
H	1.8166209	10.3043127	6.6521408
H	1.8761009	8.8528384	7.7047059
H	1.3511948	8.7148229	6.0003757
C	3.6925503	7.6091376	5.8400210
H	4.7685313	7.4827075	5.6734555
H	3.1523176	7.3490557	4.9169828
H	3.3715535	6.9355120	6.6496127
C	7.4215700	10.8985670	2.3349693
H	8.5213372	10.8770740	2.2581391
H	7.1233717	11.7461830	2.9631273
H	6.9916929	11.0341296	1.3360066
C	4.0779223	6.9856626	1.7458411
N	4.1086751	5.6412066	1.9298252
C	4.6519921	5.0346654	3.1408781
H	4.7665324	5.7888071	3.9264608
H	5.6256480	4.5520677	2.9563361
H	3.9473136	4.2684315	3.5005939
C	3.6155671	4.7014168	0.9244578
H	3.4660424	5.2142208	-0.0331886
H	2.6704449	4.2262061	1.2342067
H	4.3703162	3.9115302	0.7833112
N	3.0516993	7.5200355	1.0507821
C	1.6921480	6.9955157	1.1475916
H	1.6214127	6.2612623	1.9584585
H	1.3651984	6.5292466	0.2041425
H	1.0123031	7.8305486	1.3795664
C	3.1831250	8.7635994	0.3013197
H	4.2420306	8.9951149	0.1377217
H	2.7146024	9.5986770	0.8436585
H	2.6856079	8.6453204	-0.6737902
C	4.2049469	12.2959388	1.6414617
C	3.8287404	13.5431651	1.0091718
H	4.1399946	13.5258513	-0.0467248
H	2.7371206	13.6709684	1.0700966
H	4.3267878	14.3799541	1.5227180

Fe	-0.3355169	0.4206954	-0.6869580
N	0.8703801	-0.5983625	-2.0734470
O	0.5539672	-0.0359018	0.5989927
N	-1.8730262	-0.6812882	-0.2521932
C	-2.8876247	-0.7361389	-1.3129924
H	-3.8641379	-1.0440361	-0.9073347
H	-2.6271953	-1.4553798	-2.1078252
C	-2.9755791	0.6707629	-1.8813653
H	-3.6810364	0.7338578	-2.7261132
H	-3.3224940	1.3522721	-1.0927898
N	-1.6136583	1.1047420	-2.3151695
C	-1.4777682	2.5895866	-2.3504802
H	-2.3697938	3.0443545	-2.8131727
H	-0.6075515	2.8224922	-2.9793910
C	-1.2327210	3.1236322	-0.9518188
H	-0.9794401	4.1938857	-0.9997356
H	-2.1479382	3.0364175	-0.3430554
N	-0.1279294	2.3428996	-0.3812813
C	-1.9756052	-1.5013234	0.8187911
N	-2.3072022	-2.8043895	0.6549960
C	-1.8890549	-3.5414126	-0.5331967
H	-1.1134225	-2.9815987	-1.0698429
H	-2.7356327	-3.7357015	-1.2121758
H	-1.4659791	-4.5093183	-0.2208970
C	-3.1163989	-3.5544979	1.6131112
H	-3.5914063	-2.8710704	2.3268960
H	-2.5185471	-4.2992459	2.1633131
H	-3.9079845	-4.0859276	1.0614692
N	-1.7721321	-1.0112088	2.0549436
C	-1.2186944	-1.8099552	3.1443532
H	-0.8605302	-2.7716112	2.7671715
H	-1.9588522	-1.9724757	3.9437280
H	-0.3570323	-1.2700686	3.5667447
C	-1.9098053	0.4098191	2.3507051
H	-2.5068104	0.8997613	1.5732826
H	-0.9190233	0.8868695	2.3979429
H	-2.4142946	0.5256386	3.3219474
C	-1.3149462	0.5523661	-3.6571518
H	-2.0197236	0.9647824	-4.3982490
H	-1.4055139	-0.5403274	-3.6484340
H	-0.2921238	0.8190550	-3.9464121
C	0.7561096	2.9079872	0.4594084
N	0.4139227	3.9396767	1.2741164
C	-0.9098471	4.0555461	1.8771154
H	-1.4552715	3.1110025	1.7872075
H	-1.5024408	4.8609318	1.4132847
H	-0.7933914	4.2829511	2.9485737
C	1.3455009	5.0177032	1.6005728

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-RC (σ)

E$_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2678.9113164419 (<S^2> 6.05193047)

E$_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2680.4803982992 (<S^2> 6.05439593)

ZPE$_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.698111

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.634162

H	2.2090209	4.9904817	0.9253109
H	1.6978379	4.9549275	2.6432544
H	0.8280574	5.9811545	1.4677766
N	2.0318464	2.4632870	0.4881829
C	2.7978033	2.3912042	1.7289535
H	2.1518293	2.5917460	2.5915938
H	3.6409958	3.1007631	1.7323837
H	3.1988639	1.3705592	1.8323081
C	2.6676103	1.8394453	-0.6665045
H	2.1097787	2.0807880	-1.5788436
H	2.7068798	0.7464310	-0.5473317
H	3.6932405	2.2292874	-0.7600516
C	1.5653184	-1.1960519	-2.7756089
C	2.4325305	-1.9489149	-3.6571936
H	2.0521599	-1.8899743	-4.6884264
H	3.4496812	-1.5304453	-3.6186701
H	2.4549895	-3.0017485	-3.3366990
C	1.6204945	-3.8184402	1.1469413
C	2.2028800	-3.5290016	-0.2120810
C	3.2197694	-2.4167331	-0.1886035
C	3.4476703	-1.6514014	0.8861557
C	2.7172379	-1.8206734	2.1906201
C	1.8637309	-3.0602612	2.2238941
H	0.9761512	-4.7007490	1.2348276
H	3.7937525	-2.2424798	-1.1051435
H	4.1989383	-0.8555988	0.8343020
H	1.4226522	-3.3321877	3.1885184
H	2.0759040	-0.9328171	2.3623219
H	3.4345421	-1.8260146	3.0334611
H	2.6516456	-4.4481763	-0.6357676
H	1.3832339	-3.2779138	-0.9161421
Fe	4.3756530	9.2653301	3.2261156
N	3.7415840	10.9940120	2.1774938
O	2.8215059	8.6991906	3.5766177
N	4.9247984	9.7609767	5.0634175
C	6.1319040	10.5944551	5.1218437
H	6.5462388	10.6140674	6.1424595
H	5.9316139	11.6412801	4.8362474
C	7.1390391	9.9778391	4.1613933
H	8.0858443	10.5452820	4.1490199
H	7.3631876	8.9558802	4.4967612
N	6.5528487	9.9146495	2.7966514
C	7.1223794	8.8131445	1.9817522
H	8.2219125	8.7791934	2.0833722
H	6.8864744	9.0258738	0.9292491
C	6.4942688	7.4803793	2.3618970
H	6.8411029	6.7004760	1.6662593

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-TS (σ)

E$_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2678.8956380853 (<S^2> 6.42237422)

E$_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2680.4640206190 (<S^2> 6.41717159)

ZPE$_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.691413

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.627566

H	6.8221893	7.1780075	3.3708400
N	5.0383125	7.6380224	2.2962661
C	4.1601451	9.6131469	6.1603334
N	3.9184643	10.6606233	6.9914041
C	3.7962663	12.0175388	6.4692135
H	3.6378927	11.9902868	5.3837572
H	4.6868295	12.6280247	6.6940464
H	2.9213406	12.4998081	6.9335265
C	3.8136347	10.5255057	8.4420214
H	4.1381701	9.5259834	8.7554880
H	2.7855357	10.7019816	8.7996535
H	4.4748389	11.2695953	8.9149557
N	3.6391396	8.4037276	6.4534845
C	2.3562367	8.2322051	7.1263342
H	1.8676249	9.1993163	7.2773753
H	2.4764559	7.7316277	8.1002817
H	1.7047753	7.6103903	6.4909823
C	4.2069414	7.1763746	5.9109678
H	5.2516413	7.3425006	5.6239463
H	3.6380566	6.8534058	5.0251996
H	4.1628117	6.3901882	6.6798195
C	6.7306135	11.2044074	2.1025997
H	7.8025367	11.4092876	1.9322447
H	6.3072270	12.0201226	2.7023614
H	6.2137163	11.1800603	1.1351727
C	4.2525565	6.6502275	1.8451573
N	4.5768244	5.3384189	1.9929138
C	5.3037568	4.8384549	3.1545342
H	5.3212599	5.5918498	3.9475864
H	6.3392464	4.5584622	2.9006726
H	4.7874009	3.9453778	3.5411858
C	4.2246593	4.3301118	0.9957672
H	3.9112747	4.8129677	0.0624467
H	3.4175934	3.6669891	1.3489556
H	5.1135058	3.7126329	0.7896440
N	3.1019187	6.9513776	1.1966535
C	1.8799109	6.1794458	1.3948797
H	2.0196512	5.4345544	2.1868172
H	1.5603047	5.6721757	0.4700412
H	1.0779126	6.8656194	1.7124100
C	2.9330681	8.1931359	0.4541711
H	3.9115298	8.6328512	0.2270393
H	2.3402022	8.9201410	1.0297690
H	2.4102547	7.9765557	-0.4906411
C	3.3197317	11.8932323	1.5877551
C	2.7987723	13.0155281	0.8357654
H	3.3497317	13.1067444	-0.1130324
H	1.7327221	12.8493016	0.6202743

H	2.9203553	13.9407940	1.4191998
C	0.2122362	11.5440573	4.7362128
C	0.1534151	12.2009583	3.3869176
C	-0.0617447	11.2330270	2.2571700
C	-0.0195865	9.8968881	2.4271074
C	0.2824758	9.2779182	3.7379945
C	0.2368286	10.2057049	4.8898386
H	0.2143812	12.1985921	5.6139471
H	-0.2801311	11.6504641	1.2684307
H	-0.1884618	9.2325625	1.5736662
H	0.2548131	9.7730316	5.8930187
H	1.4427800	8.9209815	3.6717659
H	-0.2220331	8.3133082	3.9106362
H	-0.6351289	12.9789788	3.3766529
H	1.0848215	12.7841439	3.2196255
Fe	-0.1292200	0.4258964	-0.4874836
N	1.1289945	-0.5225680	-1.8945332
O	0.9208811	-0.0203652	0.9350118
N	-1.7525742	-0.6995014	-0.1700348
C	-2.6566605	-0.8359068	-1.3187948
H	-3.6436417	-1.2066015	-0.9997140
H	-2.2704754	-1.5514725	-2.0640054
C	-2.8020864	0.5392353	-1.9553962
H	-3.4806222	0.5036520	-2.8261095
H	-3.2442333	1.2211406	-1.2162464
N	-1.4706122	1.0592202	-2.3509608
C	-1.4171484	2.5386759	-2.3482033
H	-2.2905476	2.9661651	-2.8742359
H	-0.5132061	2.8373600	-2.8989443
C	-1.3225290	3.0807259	-0.9273238
H	-1.1717405	4.1707229	-0.9657254
H	-2.2699955	2.9094528	-0.3890394
N	-0.2000542	2.4147932	-0.2617661
C	-1.9346934	-1.4683469	0.9181694
N	-2.3413634	-2.7610245	0.8150977
C	-1.9559529	-3.5899771	-0.3208571
H	-1.1103619	-3.1340336	-0.8494401
H	-2.7892886	-3.7353436	-1.0277905
H	-1.6422363	-4.5789365	0.0488215
C	-3.2226934	-3.3963321	1.7922474
H	-3.6570747	-2.6419806	2.4590164
H	-2.6926054	-4.1518502	2.3955024
H	-4.0426851	-3.8979619	1.2538631
N	-1.7261756	-0.9490976	2.1482540
C	-1.1846227	-1.7329193	3.2534423
H	-0.8675918	-2.7208132	2.9033558
H	-1.9186920	-1.8534795	4.0661536

$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$-CHD-IC (σ)

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2678.9369866803 (<S^2> 7.03885069)

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2680.5065384748 (<S^2> 7.03646759)

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.69354

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.628654

H	-0.3017301	-1.2090540	3.6531200
C	-1.8210088	0.4826303	2.4023503
H	-2.4161670	0.9610195	1.6157920
H	-0.8178864	0.9365195	2.4264717
H	-2.3143074	0.6427351	3.3733365
C	-1.0771145	0.5323368	-3.6686815
H	-1.7600388	0.8952482	-4.4581635
H	-1.1007840	-0.5653242	-3.6621143
H	-0.0556509	0.8549347	-3.9081033
C	0.6065793	3.0971730	0.5659598
N	0.1553375	4.1220455	1.3360671
C	-1.1985638	4.1546324	1.8781462
H	-1.6691597	3.1707287	1.7911428
H	-1.8273179	4.9005132	1.3649122
H	-1.1488515	4.4186419	2.9464886
C	0.9890889	5.2740854	1.6721306
H	1.8830329	5.2935815	1.0374041
H	1.2968295	5.2637100	2.7308655
H	0.4094430	6.1932102	1.4901317
N	1.9219757	2.7799567	0.6369160
C	2.6431406	2.7581805	1.9050725
H	1.9625708	2.9674338	2.7383658
H	3.4689663	3.4879641	1.9173756
H	3.0585068	1.7476535	2.0517022
C	2.6447293	2.2043797	-0.4889816
H	2.0842611	2.3616367	-1.4184010
H	2.8022070	1.1245274	-0.3421888
H	3.6254060	2.6984283	-0.5753858
C	1.8676089	-1.0313175	-2.6228059
C	2.7850123	-1.6465063	-3.5577497
H	2.7801176	-1.0763739	-4.4998251
H	3.8001403	-1.6453036	-3.1338915
H	2.4687010	-2.6815006	-3.7565233
C	1.3492135	-3.8464969	1.1243481
C	1.8255127	-4.2387496	-0.2435164
C	3.0753238	-3.5287172	-0.6749194
C	3.6848391	-2.5847144	0.1085151
C	3.1715207	-2.2486156	1.3951393
C	2.0103589	-2.9134819	1.8825352
H	0.4600624	-4.3473442	1.5182077
H	3.5012605	-3.7987139	-1.6452587
H	4.5922655	-2.0871793	-0.2474028
H	1.6405483	-2.6669580	2.8813072
H	1.4760831	-0.8063732	1.0647913
H	3.6857590	-1.5128630	2.0174280
H	1.9750622	-5.3397811	-0.2928729
H	1.0195418	-4.0776877	-0.9945039

Fe	1.3092622	0.7546715	0.3784955
N	0.4968548	2.2172917	-0.9004615
O	0.2617650	-0.4118909	-0.0680376
N	0.6218800	0.9296301	2.1808556
C	1.1989532	2.0432533	2.9466026
H	1.0983848	1.8684039	4.0292424
H	0.7067453	3.0057006	2.7277767
C	2.6677225	2.0988090	2.5601784
H	3.1923602	2.9403934	3.0413996
H	3.1548827	1.1657676	2.8741463
N	2.7726369	2.2095645	1.0740570
C	4.0919440	1.7402023	0.5603604
H	4.9090217	2.1371707	1.1858423
H	4.2076296	2.1439533	-0.4548193
C	4.1174273	0.2251586	0.4955560
H	5.0260016	-0.1111034	-0.0271102
H	4.1559363	-0.1995222	1.5121289
N	2.9076198	-0.1987986	-0.2220658
C	-0.4100749	0.2206323	2.7030259
N	-1.4624801	0.8607787	3.2630637
C	-1.8750131	2.1817230	2.7968938
H	-1.4330023	2.3926959	1.8157115
H	-1.5841476	2.9724498	3.5077079
H	-2.9707678	2.1936284	2.6955502
C	-2.2255907	0.3262987	4.3900056
H	-1.6837074	-0.5036880	4.8580572
H	-3.2257520	-0.0167059	4.0792181
H	-2.3479789	1.1257410	5.1372020
N	-0.3689576	-1.1230275	2.6808776
C	-1.5623214	-1.9606771	2.5923959
H	-2.4441283	-1.3549198	2.3697052
H	-1.7266912	-2.5305325	3.5202760
H	-1.4239721	-2.6716178	1.7648028
C	0.8900569	-1.8492971	2.5598892
H	1.7290252	-1.2011982	2.8361809
H	1.0295390	-2.1981831	1.5253366
H	0.8663642	-2.7181796	3.2347276
C	2.5580771	3.6171839	0.6631868
H	3.3373481	4.2593963	1.1059002
H	1.5740562	3.9673247	0.9968080
H	2.6103227	3.6951188	-0.4282139
C	2.9206180	-1.3014919	-0.9941903
N	3.7458694	-2.3481504	-0.7286329
C	4.0702253	-2.7635176	0.6321056
H	3.3890779	-2.2932594	1.3484080
H	5.1090152	-2.5118296	0.9014121
H	3.9464808	-3.8554164	0.7089687
C	4.3759408	-3.1329901	-1.7887069

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-RC (σ)

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2985.8471857051 (<S^2> 6.05269199)

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2987.7376222869 (<S^2> 6.05486530)

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.794496

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.727192

H	4.2834310	-2.6147657	-2.7506393	
H	3.9343038	-4.1394119	-1.8741462	
H	5.4465450	-3.2436281	-1.5536926	
N	2.1168805	-1.3781081	-2.0764364	
C	1.5110772	-2.6375538	-2.4997071	
H	1.6451291	-3.4066076	-1.7303015	
H	1.9328924	-2.9967282	-3.4523390	
H	0.4325882	-2.4712071	-2.6382861	
C	1.6563984	-0.2002520	-2.8034741	
H	2.2713455	0.6673235	-2.5388548	
H	0.6034177	0.0158167	-2.5711795	
H	1.7496957	-0.3921160	-3.8836459	
C	0.1340480	3.0027422	-1.6655548	
C	-0.2789999	4.0060348	-2.6241696	
H	-0.3764452	3.5440685	-3.6179389	
H	-1.2458263	4.4345972	-2.3205188	
H	0.4777516	4.8050264	-2.6617012	
C	-1.7777066	-0.3236608	-4.7369769	
C	-2.0399477	1.0115904	-4.4115693	
C	-1.8688875	-1.3091532	-3.7476552	
C	-2.3805786	1.3495712	-3.0968220	
C	-2.1904580	-0.9733008	-2.4250912	
C	-2.4379730	0.3732597	-2.0939098	
C	-2.2688845	-2.0143238	-1.3307645	
C	-2.7367907	0.7242628	-0.6542207	
C	-3.5464930	-0.3436954	0.0461514	
C	-3.3279561	-1.6916936	-0.2993359	
C	-4.4783651	-0.0286999	1.0452749	
C	-4.0558340	-2.6965677	0.3527058	
C	-5.1852115	-1.0382544	1.7085339	
C	-4.9755503	-2.3772719	1.3575016	
H	-1.5178445	-0.6005943	-5.7621578	
H	-1.9942610	1.7865176	-5.1818844	
H	-1.6901054	-2.3569248	-4.0075878	
H	-2.6181156	2.3869261	-2.8458306	
H	-4.6530005	1.0192722	1.3067007	
H	-3.8889725	-3.7430341	0.0800285	
H	-5.9041370	-0.7789934	2.4903678	
H	-5.5291373	-3.1721794	1.8644429	
H	-1.7654017	0.8123582	-0.1329059	
H	-3.2290354	1.7058269	-0.5789059	
H	-2.4239736	-3.0186941	-1.7535266	
H	-1.2894167	-2.0329795	-0.8138236	
Fe	4.3753654	9.3435691	3.0739493	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-TS (σ)***
N	3.8809601	10.9614759	1.8085704	**E$_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
O	2.7786474	8.9173661	3.4869516	**-2985.8279795301 (<S^2> 6.48039190)**
N	4.9737964	10.0130883	4.8395343	

C	6.2233615	10.7838150	4.8050529
H	6.6410591	10.8983291	5.8178030
H	6.0732900	11.7997888	4.4023256
C	7.1968298	10.0133290	3.9245572
H	8.1720611	10.5263360	3.8575337
H	7.3675445	9.0249946	4.3728266
N	6.6108747	9.8313056	2.5713036
C	7.1112000	8.6123970	1.8918799
H	8.2079132	8.5273741	1.9965843
H	6.8812390	8.7136502	0.8215031
C	6.4140870	7.3687562	2.4227773
H	6.7221675	6.4979264	1.8239371
H	6.7268171	7.1687499	3.4616010
N	4.9670296	7.5876397	2.3333637
C	4.2486979	9.9627154	5.9738294
N	4.0842659	11.0628744	6.7523217
C	4.0579059	12.4039703	6.1791152
H	3.9185220	12.3515555	5.0935306
H	4.9847462	12.9596064	6.3971437
H	3.2103870	12.9590436	6.6114104
C	3.9687653	11.0012759	8.2074180
H	4.2820517	10.0163193	8.5730447
H	2.9396885	11.2054295	8.5468019
H	4.6346458	11.7617154	8.6449577
N	3.6931837	8.7960440	6.3591935
C	2.4202152	8.7217759	7.0681539
H	1.9228403	9.6957299	7.0657557
H	2.5481475	8.3745254	8.1059146
H	1.7693112	8.0115179	6.5386554
C	4.2086444	7.5143740	5.8980565
H	5.2499076	7.6222870	5.5734108
H	3.6050936	7.1416009	5.0560511
H	4.1629467	6.7910996	6.7263621
C	6.8748381	11.0191568	1.7379760
H	7.9591531	11.1398919	1.5654568
H	6.4954530	11.9232549	2.2315138
H	6.3728735	10.9122151	0.7682500
C	4.1461945	6.5959084	1.9593315
N	4.4202773	5.2887459	2.2166277
C	5.1158908	4.8543794	3.4229366
H	5.1689189	5.6695253	4.1500948
H	6.1372666	4.5035316	3.2019396
H	4.5546534	4.0233327	3.8793634
C	4.0514096	4.2178718	1.2931534
H	3.7697857	4.6358426	0.3193497
H	3.2181274	3.6088755	1.6810263
H	4.9233744	3.5593913	1.1515483
N	3.0119299	6.8839780	1.2770271

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2987.7176740604 (<S^2> 6.47641129)

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.787387

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.720003

C	1.7676531	6.1566571	1.5022069	
H	1.8645139	5.4856480	2.3636537	
H	1.4660405	5.5725093	0.6175428	
H	0.9711654	6.8837809	1.7258146	
C	2.8956810	8.0595072	0.4239609	
H	3.8919592	8.4417623	0.1719725	
H	2.3210203	8.8552614	0.9207437	
H	2.3765205	7.7766054	-0.5052271	
C	3.6647968	11.8281047	1.0759266	
C	3.4431009	12.9116668	0.1419095	
H	2.6817327	12.6125576	-0.5930592	
H	3.0944696	13.8020491	0.6854406	
H	4.3880352	13.1427953	-0.3742495	
C	-0.4008820	10.8160194	0.0577751	
C	-0.0405944	12.1472876	0.3024065	
C	-0.3212862	9.8747723	1.0874212	
C	0.4180288	12.5277298	1.5711706	
C	0.1264550	10.2515359	2.3648113	
C	0.5221779	11.5883269	2.6007300	
C	0.2227605	9.2897903	3.4915155	
C	1.0925262	11.9259359	3.9587976	
C	0.3920111	11.1919986	5.0791723	
C	-0.0451310	9.8701984	4.8306290	
C	0.1769623	11.7642404	6.3373636	
C	-0.7019669	9.1538327	5.8459683	
C	-0.4737861	11.0412494	7.3461545	
C	-0.9202270	9.7364163	7.0963252	
H	-0.7553548	10.5153562	-0.9314569	
H	-0.1171697	12.8917475	-0.4946272	
H	-0.6186466	8.8380822	0.9055813	
H	0.7003378	13.5677709	1.7593357	
H	0.5124384	12.7875273	6.5299446	
H	-1.0416663	8.1330923	5.6488222	
H	-0.6383032	11.4998825	8.3246489	
H	-1.4346209	9.1732070	7.8791900	
H	2.1496784	11.5950575	3.9507635	
H	1.1026560	13.0115022	4.1344016	
H	-0.2752185	8.3274288	3.3098201	
H	1.4330769	9.0076992	3.5146695	
Fe	1.1965026	0.6823128	0.2364298	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-IC (σ)***
N	0.4947346	2.2484576	-0.9887124	**E$_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
O	-0.0131880	-0.5394677	-0.3489013	**-2985.8627953930 (<S^2> 7.04023782)**
N	0.5995574	0.9006264	2.1196818	**E$_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:**
C	1.1127522	2.0813877	2.8232547	**-2987.7538662395 (<S^2> 7.03845116)**
H	0.9721820	1.9812047	3.9112802	
H	0.5939054	3.0049953	2.5155617	
C	2.5963770	2.1914647	2.4990198	

H	3.0518454	3.0597020	3.0073168
H	3.1012997	1.2876974	2.8664434
N	2.7892891	2.2854304	1.0307762
C	4.0943507	1.7417791	0.5934714
H	4.9154132	2.1298608	1.2241297
H	4.2680653	2.0887560	-0.4356304
C	4.0850337	0.2183931	0.5976222
H	5.0288984	-0.1481054	0.1651274
H	4.0413086	-0.1603073	1.6327433
N	2.9324611	-0.2341510	-0.1858794
C	-0.3959133	0.1690884	2.6568521
N	-1.4400345	0.7560746	3.2950604
C	-1.9161467	2.0797370	2.9088122
H	-1.5587117	2.3326720	1.9027786
H	-1.5886225	2.8592887	3.6162784
H	-3.0163434	2.0693042	2.8930918
C	-2.1368567	0.1373076	4.4205718
H	-1.5626257	-0.7165120	4.7994138
H	-3.1477294	-0.2006783	4.1383739
H	-2.2315901	0.8805673	5.2280631
N	-0.3541417	-1.1770243	2.5671240
C	-1.5516743	-1.9866868	2.3697571
H	-2.4307148	-1.3486053	2.2509385
H	-1.7138545	-2.6825022	3.2080989
H	-1.4304650	-2.5662069	1.4418139
C	0.8998157	-1.8897341	2.3648649
H	1.7417111	-1.2745535	2.7030761
H	1.0321135	-2.1366058	1.2993646
H	0.8789157	-2.8228224	2.9483685
C	2.6358836	3.6784978	0.5789466
H	3.4209520	4.3226708	1.0149442
H	1.6548811	4.0704139	0.8785242
H	2.7098593	3.7254185	-0.5150269
C	3.0365438	-1.2995842	-0.9942220
N	3.8528496	-2.3491335	-0.7126106
C	4.1244725	-2.7847276	0.6529532
H	3.4147599	-2.3274338	1.3486137
H	5.1500859	-2.5308437	0.9670746
H	4.0047571	-3.8784011	0.7089199
C	4.5341997	-3.1119809	-1.7564464
H	4.4869080	-2.5753768	-2.7114895
H	4.0982047	-4.1167178	-1.8828291
H	5.5924905	-3.2278802	-1.4729883
N	2.3210578	-1.3423567	-2.1453153
C	1.7103374	-2.5748623	-2.6318702
H	1.8049496	-3.3714316	-1.8848218
H	2.1597851	-2.9105446	-3.5807995
H	0.6376689	-2.3896931	-2.8012358

ZPE$_{\text{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}}$:

0.789606

Chem. Pot.$_{\text{(298.15)/B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}}$:

0.720699

C	1.9542856	-0.1387651	-2.8795680
H	2.5559027	0.7109489	-2.5361600
H	0.8879347	0.1008712	-2.7511856
H	2.1438926	-0.3007085	-3.9526212
C	0.1428601	3.0898859	-1.6977100
C	-0.2784657	4.1508851	-2.5867207
H	-0.3409242	3.7642723	-3.6153376
H	-1.2629737	4.5290440	-2.2719304
H	0.4552100	4.9711498	-2.5500118
C	-1.4575658	-0.5769421	-4.4928002
C	-1.6369244	0.7938808	-4.2398823
C	-1.8975479	-1.5161584	-3.5674297
C	-2.2339486	1.2057656	-3.0423119
C	-2.5141809	-1.1139995	-2.3495744
C	-2.6515439	0.2823419	-2.0803638
C	-3.0211875	-2.0711320	-1.4178457
C	-3.1699304	0.7455751	-0.7398955
C	-3.8830127	-0.3033270	0.0807362
C	-3.7534077	-1.6839793	-0.2548205
C	-4.6182246	0.0596987	1.2125358
C	-4.3706486	-2.6517918	0.5827816
C	-5.2184124	-0.9071222	2.0297668
C	-5.0887030	-2.2697033	1.7098483
H	-0.9827322	-0.9050802	-5.4208644
H	-1.3134433	1.5351138	-4.9752357
H	-1.7868202	-2.5844810	-3.7732093
H	-2.3855496	2.2712916	-2.8504675
H	-4.7241280	1.1194311	1.4625772
H	-4.2683046	-3.7105269	0.3286577
H	-5.7864015	-0.6002394	2.9116154
H	-5.5523788	-3.0279786	2.3461244
H	-2.2947160	1.0942911	-0.1531694
H	-3.8063335	1.6380981	-0.8608613
H	-2.9048644	-3.1352305	-1.6396109
H	-0.6473454	-0.6703819	-1.0659405

$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$ (π) pathway

Fe	0.2332221	0.5161617	0.5395806	***$[Fe^{IV}(O)TMG_2dien(MeCN)]^{2+}$-CHD-RC (π)***
N	-1.2133050	-0.5579767	1.6335486	**$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
O	-0.4531600	0.2009692	-0.9034446	**-2678.9124553028 (<S^2> 6.05188503)**
N	1.7505529	-0.6901609	0.3308932	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:**
C	2.5590672	-0.8304180	1.5503829	**-2680.4812635465 (<S^2> 6.05421978)**
H	3.5710466	-1.1928449	1.3111736	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
H	2.1201434	-1.5470904	2.2640380	
C	2.6329621	0.5506173	2.1774311	
H	3.1879340	0.5426456	3.1299896	
H	3.1483585	1.2306635	1.4856776	

N	1.2464404	1.0602929	2.3946654
C	1.2053385	2.5493285	2.4767512
H	2.0358547	2.9202192	3.1004893
H	0.2596459	2.8247575	2.9633907
C	1.2332162	3.1426807	1.0813972
H	1.0443440	4.2261110	1.1293461
H	2.2284019	3.0089333	0.6256222
N	0.1876189	2.4569180	0.3127937
C	1.9996823	-1.4959963	-0.7251508
N	2.2800232	-2.8090634	-0.5379263
C	1.6836601	-3.5597313	0.5623178
H	0.8060679	-3.0267022	0.9473821
H	2.4036372	-3.7299032	1.3796409
H	1.3546790	-4.5398166	0.1848567
C	3.2339063	-3.5477239	-1.3633953
H	3.8266604	-2.8554373	-1.9727850
H	2.7319956	-4.2756799	-2.0214835
H	3.9188570	-4.0976017	-0.6988192
N	2.0046507	-0.9863318	-1.9717603
C	1.6254602	-1.7606284	-3.1499818
H	1.1663987	-2.7098484	-2.8558863
H	2.4910886	-1.9615413	-3.8010230
H	0.8861255	-1.1812522	-3.7245108
C	2.2588104	0.4270505	-2.2267269
H	2.7211762	0.8880437	-1.3465837
H	1.3187611	0.9512578	-2.4554848
H	2.9438359	0.5181058	-3.0837111
C	0.6849238	0.4861305	3.6395486
H	1.2658549	0.8350290	4.5094581
H	0.7200017	-0.6089653	3.6046426
H	-0.3582634	0.8033431	3.7532519
C	-0.5221837	3.1099396	-0.6246839
N	0.0126788	4.1221669	-1.3523369
C	1.4180840	4.1399115	-1.7452304
H	1.8648232	3.1501932	-1.6068266
H	1.9950060	4.8818682	-1.1695059
H	1.4846679	4.4004911	-2.8132208
C	-0.7740819	5.2756646	-1.7854144
H	-1.7275367	5.3089156	-1.2448595
H	-0.9714130	5.2541295	-2.8696861
H	-0.2087672	6.1924205	-1.5543951
N	-1.8131131	2.7723394	-0.8372239
C	-2.4078618	2.7768597	-2.1707110
H	-1.6382422	2.9443682	-2.9329972
H	-3.1907754	3.5463727	-2.2668474
H	-2.8614274	1.7895213	-2.3534855
C	-2.6420382	2.1883886	0.2088845
H	-2.1954508	2.3728893	1.1927192

0.698061

Chem. Pot.(298.15)/B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88):

0.634122

H	-2.7492711	1.1027335	0.0654072	
H	-3.6405031	2.6507341	0.1733159	
C	-1.9680213	-1.1778934	2.2506221	
C	-2.8922985	-1.9278100	3.0760689	
H	-3.9195144	-1.7723114	2.7163496	
H	-2.6495499	-2.9988642	3.0180924	
H	-2.8068346	-1.5832069	4.1185062	
C	-1.2313077	-3.6733301	-1.2606446	
C	-1.9520566	-4.4750352	-0.2081869	
C	-3.2419613	-3.8364594	0.2370905	
C	-3.6852300	-2.6610539	-0.2309807	
C	-2.9425449	-1.8434004	-1.2524162	
C	-1.6741868	-2.4979289	-1.7244160	
H	-0.2985340	-4.0964966	-1.6490868	
H	-3.8322433	-4.3815449	0.9824188	
H	-4.6359702	-2.2561312	0.1349679	
H	-1.0999625	-1.9521431	-2.4765489	
H	-2.6910451	-0.8480051	-0.8399908	
H	-3.6015834	-1.6233357	-2.1155382	
H	-2.1484593	-5.5011770	-0.5776821	
H	-1.2892432	-4.6323882	0.6673864	
Fe	0.4056101	0.6590079	0.5594121	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-TS (π)***
N	-0.4651455	-0.3920442	2.1430184	**E$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
O	-0.7186543	0.1106939	-0.6065010	**-2678.8928803855 (<S^2> 6.06219379)**
N	1.9240975	-0.4688210	-0.0031066	**E$_{B3LYP-D3/def2-TZVPP/COSMO(ε = 35.88)}$:**
C	3.0094800	-0.4336800	0.9836119	**-2680.4600743158 (<S^2> 6.06368298)**
H	3.9516697	-0.8108847	0.5558522	**ZPE$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
H	2.7870424	-1.0525576	1.8694601	**0.691699**
C	3.1689458	1.0240828	1.3872765	**Chem. Pot.$_{(298.15)/B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
H	3.9568620	1.1601226	2.1466943	**0.62848**
H	3.4433633	1.6095184	0.4991779	
N	1.8655101	1.5356433	1.9056099	
C	1.7472306	3.0161171	1.7600966	
H	2.7058590	3.5023316	2.0073264	
H	0.9940098	3.3583314	2.4831006	
C	1.2736549	3.3637050	0.3610308	
H	1.0419656	4.4383333	0.3030127	
H	2.0702436	3.1646790	-0.3761604	
N	0.0871241	2.5421373	0.1052712	
C	2.0135075	-1.3058991	-1.0503448	
N	2.5253893	-2.5571376	-0.8942390	
C	2.2998103	-3.3066397	0.3356313	
H	1.4849638	-2.8477900	0.9090994	
H	3.2049176	-3.3518528	0.9643040	
H	2.0078793	-4.3371413	0.0774285	
C	3.3821842	-3.2033535	-1.8845987	
H	3.6993060	-2.4794396	-2.6446782	

H	2.8782149	-4.0509287	-2.3780881
H	4.2825615	-3.5860295	-1.3771419
N	1.6293576	-0.9006318	-2.2777578
C	1.1408769	-1.8150532	-3.3044847
H	0.9361847	-2.8006368	-2.8747585
H	1.8622021	-1.9184297	-4.1311443
H	0.2015181	-1.4129487	-3.7145076
C	1.5451460	0.5113211	-2.6287513
H	2.1507451	1.1047015	-1.9340127
H	0.5011394	0.8547278	-2.5752338
H	1.9285663	0.6508540	-3.6510722
C	1.7179656	1.1743516	3.3344057
H	2.4710338	1.7083947	3.9377914
H	1.8552874	0.0952889	3.4702020
H	0.7152173	1.4492589	3.6831748
C	-0.9668510	3.0304232	-0.5603112
N	-0.8400744	3.9953636	-1.5106490
C	0.3182580	4.0772717	-2.3930501
H	0.9095853	3.1587982	-2.3340966
H	0.9628509	4.9367057	-2.1454700
H	-0.0308972	4.1937926	-3.4315930
C	-1.8536120	5.0275892	-1.7148678
H	-2.5579956	5.0391496	-0.8744943
H	-2.4126889	4.8747786	-2.6530186
H	-1.3538483	6.0082993	-1.7670128
N	-2.2129485	2.5852337	-0.2708214
C	-3.2103551	2.3600642	-1.3117823
H	-2.7753864	2.5270528	-2.3038105
H	-4.0881109	3.0143322	-1.1842569
H	-3.5436338	1.3104802	-1.2595026
C	-2.5565154	2.0463783	1.0362235
H	-1.8318603	2.3834552	1.7871717
H	-2.5642378	0.9454384	1.0204055
H	-3.5586117	2.4043552	1.3192970
C	-0.9261835	-1.0042624	3.0069616
C	-1.4979246	-1.7641789	4.0987865
H	-2.5902737	-1.8185349	3.9785573
H	-1.0781892	-2.7812694	4.0963337
H	-1.2585905	-1.2729822	5.0544731
C	-1.1084659	-4.0501765	-0.9194788
C	-1.3480777	-4.4825301	0.4993081
C	-2.2824115	-3.5776898	1.2506383
C	-2.7289658	-2.4086870	0.7453952
C	-2.3180118	-1.9189530	-0.5824321
C	-1.5910751	-2.8922790	-1.4156267
H	-0.5427644	-4.7307912	-1.5644773
H	-2.6125583	-3.9103950	2.2399097
H	-3.4159495	-1.7873336	1.3295721

H	-1.4233489	-2.6323317	-2.4631069	
H	-1.5032757	-0.9525114	-0.4556075	
H	-3.0916522	-1.3449551	-1.1168569	
H	-1.7306705	-5.5224851	0.5186028	
H	-0.3819214	-4.5590210	1.0424449	
Fe	0.2575793	0.4910479	0.6374487	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-CHD-IC (π)***
N	-1.1288167	-0.6683211	1.7057837	**$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
O	-0.5428539	0.1463387	-0.9332727	**-2678.9331937799 (<S^2> 6.08368116)**
N	1.7596037	-0.7694925	0.4006762	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:**
C	2.5174245	-0.9187666	1.6467992	**-2680.5021632039 (<S^2> 6.08275989)**
H	3.5178865	-1.3402415	1.4605359	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
H	2.0140519	-1.5867783	2.3656806	**0.695919**
C	2.6434879	0.4803263	2.2305225	**Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
H	3.1734745	0.4829448	3.1969844	**0.631999**
H	3.2045640	1.1107273	1.5273674	
N	1.2780891	1.0691604	2.4002573	
C	1.3154802	2.5646449	2.4159601	
H	2.1896225	2.9160703	2.9882691	
H	0.4074798	2.9091362	2.9293821	
C	1.3046451	3.0920168	0.9934444	
H	1.1635864	4.1838684	0.9997044	
H	2.2722291	2.8935793	0.5015837	
N	0.2022807	2.4069623	0.3118378	
C	2.0474014	-1.5393992	-0.6600865	
N	2.3711051	-2.8514513	-0.5048305	
C	1.7917344	-3.6488230	0.5699227	
H	0.9079434	-3.1437424	0.9782453	
H	2.5126562	-3.8295335	1.3844809	
H	1.4801105	-4.6245730	0.1645102	
C	3.3611834	-3.5314197	-1.3366901	
H	3.9237778	-2.8016146	-1.9310440	
H	2.8959440	-4.2683033	-2.0121085	
H	4.0690008	-4.0631920	-0.6807383	
N	2.0394968	-1.0112324	-1.9028924	
C	1.6602759	-1.7736206	-3.0876349	
H	1.2368437	-2.7428907	-2.8034711	
H	2.5181920	-1.9386982	-3.7590814	
H	0.8933995	-1.2068749	-3.6390125	
C	2.2414386	0.4139830	-2.1328686	
H	2.7122034	0.8700038	-1.2540224	
H	1.2763837	0.9076095	-2.3190882	
H	2.9013366	0.5462768	-3.0042009	
C	0.6769157	0.5855481	3.6664230	
H	1.2441405	0.9814587	4.5247377	
H	0.6948169	-0.5095634	3.7015270	
H	-0.3634257	0.9260364	3.7330521	
C	-0.5646580	3.0380602	-0.5863988	

N	-0.0863667	4.0513836	-1.3578054
C	1.2899120	4.0836459	-1.8390223
H	1.7666976	3.1087244	-1.6989437
H	1.8871781	4.8540023	-1.3238660
H	1.2866385	4.3114387	-2.9170445
C	-0.9151914	5.1852342	-1.7592712
H	-1.8431177	5.2018083	-1.1750421
H	-1.1653088	5.1517240	-2.8328250
H	-0.3598337	6.1167320	-1.5635869
N	-1.8677513	2.6975486	-0.7217597
C	-2.5080211	2.6230508	-2.0309200
H	-1.7873142	2.8459247	-2.8257200
H	-3.3600351	3.3180662	-2.1060367
H	-2.8725436	1.5939113	-2.1837018
C	-2.6215039	2.0824134	0.3600525
H	-2.1400022	2.2905243	1.3233199
H	-2.6883973	0.9922711	0.2200436
H	-3.6389842	2.5035433	0.3712357
C	-1.8983473	-1.2692715	2.3239431
C	-2.8440567	-1.9970365	3.1451795
H	-3.8662653	-1.8208912	2.7804134
H	-2.6191309	-3.0730556	3.1029380
H	-2.7594142	-1.6493295	4.1867012
C	-1.3027690	-3.5360613	-1.3057700
C	-2.0402208	-4.0580134	-0.1071632
C	-3.3528009	-3.3709412	0.1380746
C	-3.7949188	-2.3390115	-0.6494766
C	-3.0396415	-1.8855390	-1.7663569
C	-1.8030487	-2.5195849	-2.0794453
H	-0.3526936	-4.0118673	-1.5647912
H	-3.9643484	-3.7275411	0.9713402
H	-4.7541332	-1.8618020	-0.4267850
H	-1.2442583	-2.1821676	-2.9561482
H	-0.9067859	-0.7537071	-0.9615449
H	-3.4075348	-1.0654829	-2.3862694
H	-2.1943320	-5.1551301	-0.2046380
H	-1.3959347	-3.9926924	0.7995783

Fe	1.2513539	0.8269348	0.3732368	***[Fe^{IV}(O)TMG_2dien(MeCN)]$^{2+}$-DHA-RC (π)***
N	0.1555888	2.3978191	-0.5031940	**$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
O	0.2605622	-0.3486169	-0.1689369	**-2985.8471964201 (<S^2> 6.05268463)**
N	0.7947884	0.5966206	2.2415925	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:**
C	1.3707516	1.6087150	3.1380776	**-2987.7376292103 (<S^2> 6.05485736)**
H	1.4305125	1.2296980	4.1703270	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
H	0.7728820	2.5350326	3.1682377	**0.79455**
C	2.7647197	1.8945415	2.6045120	
H	3.2742065	2.6870044	3.1768422	
H	3.3679910	0.9792159	2.6734873	

N	2.6609756	2.2845744	1.1661873
C	3.9362432	2.0660697	0.4240622
H	4.7912064	2.4317678	1.0171167
H	3.8797041	2.6573810	-0.5001279
C	4.0860824	0.6002752	0.0645950
H	4.9426912	0.4677277	-0.6139656
H	4.2975770	0.0056091	0.9684334
N	2.8333073	0.1808877	-0.5780306
C	-0.0932464	-0.3044019	2.7314751
N	-1.1127702	0.1041490	3.5218612
C	-1.6958124	1.4344648	3.3711623
H	-1.4084661	1.8672775	2.4054208
H	-1.3817145	2.1099761	4.1836494
H	-2.7922116	1.3444076	3.4006068
C	-1.6693997	-0.7058325	4.6045424
H	-1.0003751	-1.5421885	4.8379056
H	-2.6688602	-1.0945966	4.3506069
H	-1.7591156	-0.0730091	5.5011316
N	0.0605451	-1.6090617	2.4454090
C	-1.0567845	-2.5434557	2.3354751
H	-2.0096602	-2.0085229	2.3372026
H	-1.0451375	-3.2859460	3.1486843
H	-0.9696128	-3.0738688	1.3760104
C	1.3502778	-2.1587377	2.0432898
H	2.1591397	-1.4817139	2.3393312
H	1.3795974	-2.2998669	0.9521106
H	1.4929665	-3.1313103	2.5379785
C	2.2712144	3.7106960	1.0637213
H	3.0423485	4.3442395	1.5324114
H	1.3125763	3.8824801	1.5673953
H	2.1725568	3.9913774	0.0095138
C	2.8397041	-0.7570464	-1.5437492
N	3.7803599	-1.7372325	-1.5794297
C	4.3169932	-2.3514424	-0.3694005
H	3.6983421	-2.0951329	0.4964806
H	5.3564136	-2.0391675	-0.1769418
H	4.3000103	-3.4462978	-0.4895959
C	4.3297153	-2.2456839	-2.8349830
H	4.0659219	-1.5769267	-3.6629915
H	3.9692810	-3.2627902	-3.0603669
H	5.4275509	-2.2785631	-2.7493211
N	1.9096327	-0.7259892	-2.5221113
C	1.3634488	-1.9477684	-3.1063524
H	1.6643739	-2.8229082	-2.5190189
H	1.6840177	-2.0820831	-4.1521304
H	0.2657866	-1.8782225	-3.0857892
C	1.2572358	0.5054733	-2.9530716
H	1.8244125	1.3735733	-2.5987358

Chem. Pot.(298.15)/B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88):

0.727264

H	0.2294297	0.5596811	-2.5656272
H	1.2234183	0.5217979	-4.0534833
C	-0.3671640	3.2624655	-1.0627316
C	-0.9822954	4.3687590	-1.7655031
H	-1.1874064	4.0727692	-2.8050866
H	-1.9238857	4.6470853	-1.2689196
H	-0.2968116	5.2304434	-1.7559668
C	-2.3858366	0.3658038	-4.4617920
C	-2.7173596	1.5823625	-3.8554566
C	-2.2583067	-0.7870599	-3.6788827
C	-2.9072953	1.6361811	-2.4698514
C	-2.4287547	-0.7347721	-2.2883633
C	-2.7453461	0.4935743	-1.6758551
C	-2.2707911	-1.9596109	-1.4152455
C	-2.8779247	0.5416986	-0.1707571
C	-3.4931913	-0.7178188	0.3964819
C	-3.2076084	-1.9482176	-0.2270471
C	-4.3084332	-0.6937951	1.5369248
C	-3.7539424	-3.1284679	0.2956399
C	-4.8321535	-1.8783909	2.0672460
C	-4.5566139	-3.0999876	1.4412228
H	-2.2420512	0.3103020	-5.5441313
H	-2.8425517	2.4845008	-4.4608420
H	-2.0254581	-1.7438747	-4.1560103
H	-3.1975858	2.5781346	-1.9964499
H	-4.5364570	0.2635690	2.0150053
H	-3.5355115	-4.0831243	-0.1924146
H	-5.4610128	-1.8460153	2.9610112
H	-4.9680193	-4.0295929	1.8435994
H	-1.8565479	0.6384497	0.2423758
H	-3.4372227	1.4336124	0.1502340
H	-2.3930397	-2.8812919	-2.0043990
H	-1.2334752	-1.9637288	-1.0268089

Fe	1.7525801	0.5343741	0.2757682	***[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-TS (π)***
N	0.7580960	2.1833744	-0.5474474	**$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
O	0.4765436	-0.5763362	-0.0152960	**-2985.8205751957 (<S^2> 6.06140423)**
N	1.4058162	0.7858405	2.2021017	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:**
C	2.1976129	1.8807149	2.7718327	**-2987.7100429454 (<S^2> 6.06299607)**
H	2.2318825	1.8191077	3.8710036	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
H	1.7868469	2.8730142	2.5184726	**0.787135**
C	3.5956497	1.7324472	2.1956748	**Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
H	4.2734055	2.5319542	2.5378542	
H	4.0114545	0.7678744	2.5167960	
N	3.5129882	1.7360115	0.7044711	
C	4.6739343	1.0295482	0.0872075	
H	5.6010508	1.2727890	0.6325531	
H	4.7760528	1.3979035	-0.9427852	

C	4.4048884	-0.4626168	0.0471124	**0.719866**
H	5.1911313	-0.9676559	-0.5344713	
H	4.4288929	-0.8898413	1.0641408	
N	3.0872774	-0.6256788	-0.5740001	
C	0.4491411	0.1990726	2.9410350	
N	-0.3495915	0.9356091	3.7605602	
C	-0.7254715	2.3024412	3.4177363	
H	-0.5344951	2.4890382	2.3536610	
H	-0.1755345	3.0458735	4.0186219	
H	-1.8022072	2.4361076	3.6080980	
C	-0.8188490	0.4575123	5.0588996	
H	-0.2869656	-0.4587302	5.3414172	
H	-1.9037671	0.2613043	5.0580123	
H	-0.6081903	1.2288175	5.8171287	
N	0.2873219	-1.1382166	2.8970244	
C	-1.0089488	-1.7854408	3.0660135	
H	-1.8105799	-1.0423736	3.0927193	
H	-1.0433099	-2.3919409	3.9852671	
H	-1.1905357	-2.4408870	2.2015602	
C	1.3612653	-2.0300037	2.4788074	
H	2.3270632	-1.5175175	2.5579632	
H	1.2068578	-2.3456868	1.4361773	
H	1.3667125	-2.9149689	3.1336993	
C	3.4701284	3.1291368	0.2041274	
H	4.4307705	3.6320082	0.4047847	
H	2.6704585	3.6882480	0.7037432	
H	3.2818101	3.1277310	-0.8764400	
C	2.8559679	-1.6115739	-1.4505053	
N	3.5018308	-2.8057755	-1.3755563	
C	3.8616649	-3.4132226	-0.0991199	
H	3.3377049	-2.9129278	0.7213824	
H	4.9476085	-3.3686175	0.0858202	
H	3.5547196	-4.4713136	-0.1081742	
C	3.9116298	-3.5511270	-2.5635869	
H	3.8388920	-2.9158210	-3.4544756	
H	3.3013349	-4.4571045	-2.7130243	
H	4.9626200	-3.8586147	-2.4413980	
N	1.9801109	-1.4174102	-2.4631254	
C	1.1399650	-2.4944821	-2.9771530	
H	1.1751346	-3.3604029	-2.3056032	
H	1.4416855	-2.8063897	-3.9900773	
H	0.0990626	-2.1403741	-3.0251414	
C	1.6797912	-0.0871863	-2.9744029	
H	2.4930685	0.6053322	-2.7260715	
H	0.7436554	0.3041435	-2.5477423	
H	1.5755257	-0.1382617	-4.0687737	
C	0.2835764	3.1788543	-0.8921997	
C	-0.2644237	4.4543945	-1.3019256	

H	-0.3286858	4.4909623	-2.3990580
H	-1.2722311	4.5757251	-0.8798106
H	0.3917364	5.2618718	-0.9413007
C	-2.6695835	2.7331119	-3.0539074
C	-3.4573727	3.3939291	-2.1009549
C	-2.1065008	1.4934379	-2.7490850
C	-3.6647322	2.8149830	-0.8431107
C	-2.3260607	0.8930927	-1.4937716
C	-3.1043771	1.5714397	-0.5268118
C	-1.7963211	-0.4470931	-1.1746496
C	-3.3048665	0.9211266	0.8229695
C	-3.3725346	-0.5875740	0.7495509
C	-2.5858953	-1.2514078	-0.2200299
C	-4.1501581	-1.3390623	1.6373308
C	-2.5663637	-2.6590447	-0.2496069
C	-4.1345124	-2.7382189	1.5926902
C	-3.3342858	-3.3993783	0.6504176
H	-2.5023878	3.1823980	-4.0362685
H	-3.9067504	4.3622029	-2.3361938
H	-1.5063000	0.9676255	-3.4969391
H	-4.2800531	3.3319313	-0.1009668
H	-4.7692468	-0.8248295	2.3784518
H	-1.9478506	-3.1697960	-0.9931200
H	-4.7449968	-3.3127234	2.2942089
H	-3.3150605	-4.4917550	0.6158934
H	-2.4379774	1.1844551	1.4626076
H	-4.1886879	1.3334159	1.3325306
H	-1.4649420	-1.0111036	-2.0559214
H	-0.6460321	-0.3371512	-0.5768350
Fe	1.4866935	0.5817235	0.2174032
N	0.1629969	1.9477617	-0.6670555
O	0.4440772	-0.8348841	-0.1785290
N	0.8796597	0.7993043	2.0810200
C	1.3498021	2.0673473	2.6416375
H	1.2820569	2.0709395	3.7410907
H	0.7662321	2.9314953	2.2800052
C	2.8018947	2.1957362	2.2051711
H	3.2595687	3.1395075	2.5432728
H	3.3756019	1.3608135	2.6297832
N	2.8773134	2.1032397	0.7123650
C	4.2223799	1.6346999	0.2514707
H	5.0127291	2.0780989	0.8786423
H	4.3596646	1.9930111	-0.7777619
C	4.2632134	0.1179639	0.2502675
H	5.1820221	-0.2314840	-0.2450433
H	4.2821205	-0.2706800	1.2828505
N	3.0608287	-0.3178524	-0.4660481

[Fe^{IV}(O)TMG$_2$dien(MeCN)]$^{2+}$-DHA-IC (π)

E$_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2985.8538807335 (<S^2> 6.07905533)

E$_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2987.7452109988 (<S^2> 6.07861123)

ZPE$_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.791536

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.723438

C	-0.0157465	0.0459360	2.7376556
N	-1.0671420	0.6110744	3.3888220
C	-1.6805349	1.8402588	2.8993167
H	-1.3926651	2.0110971	1.8543592
H	-1.3918989	2.7181361	3.5009679
H	-2.7764838	1.7382405	2.9485181
C	-1.6227568	0.0687794	4.6262614
H	-0.9413076	-0.6776224	5.0516712
H	-2.6114981	-0.3927652	4.4670961
H	-1.7370789	0.8893925	5.3521972
N	0.1231294	-1.2947255	2.7600132
C	-1.0215066	-2.1995854	2.7497169
H	-1.9432351	-1.6514477	2.5262105
H	-1.1366048	-2.7334783	3.7065807
H	-0.8740203	-2.9376486	1.9490124
C	1.4144664	-1.9325043	2.5365605
H	2.2255110	-1.2277271	2.7546336
H	1.4936583	-2.2604230	1.4893098
H	1.5036650	-2.8031645	3.2038529
C	2.5974754	3.4300140	0.1119018
H	3.4216295	4.1250662	0.3409634
H	1.6670228	3.8419302	0.5180060
H	2.4982815	3.3298116	-0.9759981
C	3.0811489	-1.3555167	-1.3119891
N	3.9274710	-2.4056891	-1.1436257
C	4.3178495	-2.8869010	0.1769311
H	3.6692152	-2.4577397	0.9470158
H	5.3666563	-2.6398060	0.4100326
H	4.2052394	-3.9825157	0.2056670
C	4.5187681	-3.1219863	-2.2713064
H	4.3736625	-2.5548917	-3.1986334
H	4.0854270	-4.1287853	-2.3914354
H	5.6006125	-3.2307657	-2.0927082
N	2.2647524	-1.3579933	-2.3917750
C	1.6083573	-2.5760813	-2.8547061
H	1.8027293	-3.4039844	-2.1634088
H	1.9392161	-2.8600534	-3.8667277
H	0.5204719	-2.4029091	-2.8784855
C	1.7562804	-0.1243800	-2.9729603
H	2.4149847	0.7148668	-2.7177052
H	0.7404031	0.0965192	-2.6088071
H	1.7251059	-0.2311417	-4.0680723
C	-0.5645143	2.7779888	-1.0104828
C	-1.4465266	3.8556918	-1.4013532
H	-1.3207139	4.0629109	-2.4738698
H	-2.4915220	3.5677784	-1.2140016
H	-1.1987855	4.7566992	-0.8190733
C	-3.4567860	2.3635630	-3.7401564

C	-4.4842067	2.8066678	-2.8906248
C	-2.7083626	1.2419865	-3.3987498
C	-4.7366973	2.1301789	-1.6883912
C	-2.9754891	0.5235634	-2.2023831
C	-3.9952819	1.0023369	-1.3254425
C	-2.3026765	-0.7019333	-1.9047648
C	-4.2199107	0.3067797	-0.0020999
C	-3.7588846	-1.1320926	0.0460805
C	-2.7480111	-1.5727617	-0.8614367
C	-4.2713042	-2.0279213	0.9876349
C	-2.2568550	-2.9012020	-0.7473465
C	-3.8003562	-3.3459522	1.0630424
C	-2.7825307	-3.7766268	0.1956584
H	-3.2472068	2.8973683	-4.6707480
H	-5.0795188	3.6830943	-3.1584481
H	-1.9189079	0.8835160	-4.0655662
H	-5.5272202	2.4876167	-1.0218163
H	-5.0550801	-1.6929102	1.6737259
H	-1.4693739	-3.2333726	-1.4288620
H	-4.2185914	-4.0327521	1.8031461
H	-2.4031530	-4.7996046	0.2620505
H	-3.6591100	0.8693381	0.7748686
H	-5.2755913	0.3859399	0.3028167
H	-1.5255917	-1.0531308	-2.5877669
H	-0.4959377	-0.6010244	-0.2394521

$[Fe^{IV}(O)TMG_3tren]^{2+}$ (σ) pathway

Fe	2.4730594	4.4164800	6.4042077
O	3.7467882	4.4752947	5.3929296
N	0.8063533	4.3387685	7.7277133
N	3.3678259	3.4035539	7.8927996
N	1.2203695	3.4181598	5.1890624
N	2.2161133	6.3991232	6.6183398
N	5.4309717	2.9273049	8.9512330
N	5.0559889	2.2579811	6.7587528
N	1.0678659	1.8809671	3.3953222
N	2.0530512	3.9601989	3.0768357
N	2.5094666	8.5168141	5.6017818
N	4.3532101	7.2209683	6.1645824
C	1.1346861	3.3388362	8.7820634
H	0.9419915	2.3381842	8.3739867
H	0.4813983	3.4830515	9.6585579
C	2.6062085	3.4514390	9.1458925
H	2.7831469	4.3882216	9.6997122
H	2.8895403	2.6261024	9.8181326
C	4.6012775	2.8847683	7.8721272
C	5.4488454	4.0398789	9.8932817

$[Fe^{IV}(O)TMG_3tren]^{2+}$

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2713.4279427064 ($<S^2>$ 6.04963931)

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2715.0272346409 ($<S^2>$ 6.05198125)

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.726585

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.666116 (σ = 3)

H	4.9081674	4.8987680	9.4857612
H	6.4935128	4.3444203	10.0663780
H	5.0037292	3.7624838	10.8631247
C	6.3672772	1.8467878	9.2534164
H	6.1231523	0.9558415	8.6627004
H	6.2800226	1.5926811	10.3220038
H	7.4114825	2.1389844	9.0524876
C	6.4306955	2.4009179	6.2944354
H	6.9631865	3.1473257	6.8960112
H	6.4144052	2.7512208	5.2493570
H	6.9799697	1.4456912	6.3362376
C	4.1648402	1.5429257	5.8598736
H	3.2021940	1.3827288	6.3571162
H	4.6101073	0.5662536	5.6103648
H	3.9938066	2.1123091	4.9338431
C	-0.3729977	3.9235618	6.9177147
H	-0.7506471	4.8077822	6.3880306
H	-1.1744373	3.5512185	7.5772096
C	0.0546938	2.8797420	5.8988958
H	0.2864881	1.9313087	6.4111111
H	-0.7754080	2.6719961	5.2052563
C	1.4494715	3.0807867	3.9144432
C	1.0644969	0.6470693	4.1718733
H	1.6214473	0.7768288	5.1040876
H	1.5582570	-0.1448562	3.5861074
H	0.0401093	0.3150545	4.4086875
C	0.6207881	1.7411033	2.0111194
H	0.4133666	2.7264852	1.5771422
H	-0.3093450	1.1505446	1.9985828
H	1.3676927	1.2215121	1.3880004
C	3.0352579	3.5385025	2.0852395
H	3.2715661	2.4746854	2.2075984
H	3.9616827	4.1154441	2.2403003
H	2.6808209	3.7130638	1.0557737
C	1.8924889	5.3975283	3.2241048
H	1.0497568	5.6002686	3.8936177
H	1.6852948	5.8414115	2.2369587
H	2.7984027	5.8572472	3.6471103
C	0.6365454	5.7061964	8.2938962
H	1.3620114	5.8299387	9.1083874
H	-0.3755875	5.8191179	8.7166513
C	0.9199484	6.7394086	7.2156359
H	0.1083307	6.7324119	6.4695054
H	0.9359976	7.7477059	7.6588219
C	3.0048779	7.3611136	6.1249518
C	1.2488984	8.5796393	4.8719702
H	0.9073235	7.5754815	4.6053789
H	1.4037892	9.1466049	3.9399790

H	0.4616585	9.0832956	5.4569889	
C	3.2063028	9.7936291	5.7422168	
H	3.9949763	9.7150477	6.4999558	
H	2.4820024	10.5569216	6.0690728	
H	3.6517135	10.1262407	4.7898058	
C	5.2108683	7.6508296	5.0666336	
H	4.6058512	7.9760438	4.2118133	
H	5.8262911	6.7946865	4.7450232	
H	5.8818805	8.4726970	5.3669380	
C	5.0192543	6.4806052	7.2236609	
H	4.3173389	6.3202296	8.0489947	
H	5.8790611	7.0655155	7.5883946	
H	5.3710155	5.5019923	6.8637199	
Fe	-0.9133655	-0.0077933	0.7188512	***$[Fe^{IV}(O)TMG_3tren]^{2+}$-CHD-RC (σ)***
O	0.1830448	-0.0062660	-0.4843244	
N	-2.3449025	-0.0309893	2.3012602	**$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
N	0.3312123	0.5019202	2.2080771	**-2946.5429520195 (<S^2> 6.05142420)**
N	-1.4771641	-1.9279584	0.5351077	
N	-2.1598778	1.3952061	-0.0291854	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:**
N	2.3330557	1.6052280	2.8099672	**-2948.3981139061 (<S^2> 6.05373523)**
N	2.4010030	-0.3028267	1.4840447	
N	-0.8459804	-4.0893136	-0.1968571	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
N	-1.0518557	-2.3487038	-1.7210590	**0.850417**
N	-3.0023495	2.4813976	-1.9570207	
N	-0.7470982	2.6275372	-1.4237537	**Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:**
C	-1.5818271	0.0181242	3.5790207	
H	-1.2254411	-0.9956663	3.8038158	**0.781968**
H	-2.2407985	0.3404920	4.4022554	
C	-0.3849383	0.9391901	3.4126525	
H	-0.7229781	1.9858104	3.3329528	
H	0.2582823	0.8794109	4.3045115	
C	1.6667455	0.6106001	2.1595103	
C	1.7905601	2.9507771	2.9520876	
H	0.9373783	3.0934750	2.2823580	
H	2.5683778	3.6811756	2.6768514	
H	1.4723875	3.1573985	3.9874708	
C	3.6290470	1.3880079	3.4487964	
H	3.8341431	0.3145988	3.5387344	
H	3.5986333	1.8204990	4.4617477	
H	4.4504771	1.8689296	2.8922650	
C	3.6364591	0.0432336	0.7894339	
H	3.7200247	1.1295440	0.6704311	
H	3.6096338	-0.4082261	-0.2114224	
H	4.5277177	-0.3354161	1.3166458	
C	1.9556542	-1.6763652	1.3112437	
H	1.1362378	-1.8818240	2.0081450	
H	2.7938959	-2.3581109	1.5260795	

H	1.5981370	-1.8496465	0.2853121
C	-3.1241699	-1.2936177	2.1673350
H	-3.8976648	-1.1381312	1.4041346
H	-3.6260616	-1.5321918	3.1196317
C	-2.2007170	-2.4134111	1.7153193
H	-1.5136404	-2.6860413	2.5337335
H	-2.7916199	-3.3129966	1.4817502
C	-1.1194237	-2.7768738	-0.4360014
C	-0.2182123	-4.5575396	1.0330257
H	0.2020532	-3.7194285	1.5953184
H	0.6048660	-5.2431765	0.7752041
H	-0.9317506	-5.0989003	1.6759235
C	-1.1830218	-5.1393871	-1.1559556
H	-1.8743347	-4.7541909	-1.9149135
H	-1.6799181	-5.9620900	-0.6173159
H	-0.2869106	-5.5448544	-1.6544457
C	-0.0204877	-2.8086018	-2.6427903
H	0.7473960	-3.3785641	-2.1059096
H	0.4577486	-1.9270766	-3.0979327
H	-0.4353988	-3.4337152	-3.4506186
C	-1.9102654	-1.2907706	-2.2277440
H	-2.7264256	-1.1169777	-1.5188896
H	-2.3318678	-1.5995576	-3.1977935
H	-1.3485816	-0.3534773	-2.3567255
C	-3.2040028	1.1730397	2.1293471
H	-2.6662577	2.0371908	2.5404234
H	-4.1426209	1.0534494	2.6955279
C	-3.4604628	1.4060124	0.6508757
H	-4.1316644	0.6230138	0.2610541
H	-3.9779925	2.3679232	0.5101433
C	-1.9778118	2.1428507	-1.1230351
C	-4.1140644	1.5872961	-2.2572724
H	-3.8959371	0.5707106	-1.9185770
H	-4.2635364	1.5577975	-3.3487226
H	-5.0522617	1.9277545	-1.7886846
C	-3.0673027	3.7858994	-2.6125837
H	-2.3419498	4.4746283	-2.1633349
H	-4.0776909	4.2023006	-2.4707752
H	-2.8735957	3.7129191	-3.6958185
C	-0.2698684	2.7222535	-2.7976459
H	-0.9783913	2.2460124	-3.4852797
H	0.6881406	2.1866250	-2.8756399
H	-0.1125264	3.7684584	-3.1079153
C	0.2254229	2.9697214	-0.3979390
H	-0.2727919	2.9926479	0.5771910
H	0.6436127	3.9663165	-0.6141017
H	1.0406357	2.2318886	-0.3581137
C	4.7648208	-1.2127639	-2.5561386

C	5.5887033	0.0189556	-2.2846540
C	4.7921859	1.2939838	-2.3812571
C	3.4768371	1.3244624	-2.6333278
C	2.6386930	0.0901098	-2.8437781
C	3.4488206	-1.1796094	-2.8082879
H	5.2894317	-2.1746454	-2.5359709
H	5.3376527	2.2319659	-2.2279147
H	2.9635946	2.2912669	-2.6832898
H	2.9125575	-2.1168060	-2.9919837
H	2.0907796	0.1619482	-3.8051076
H	1.8381147	0.0448584	-2.0776030
H	6.0566796	-0.0563298	-1.2814788
H	6.4523725	0.0573998	-2.9779840
Fe	2.6034545	4.4018110	6.2897386
O	3.9355685	4.3882740	5.2258933
N	0.8329856	4.3412420	7.7514161
N	3.4485246	3.4455948	7.8869959
N	1.2398864	3.3491648	5.1818485
N	2.2009444	6.4181251	6.4853617
N	5.4736552	2.8274200	8.9451081
N	4.9269087	1.9657793	6.8570863
N	0.8689160	1.8924682	3.3475614
N	1.7947713	3.9964401	3.0108092
N	2.3983660	8.6160477	5.6178658
N	4.2971041	7.3900693	6.1564474
C	1.2511029	3.4805659	8.8791782
H	1.0785076	2.4322161	8.5990977
H	0.6460953	3.6922540	9.7787487
C	2.7373736	3.6737813	9.1484997
H	2.9213809	4.6889395	9.5408596
H	3.0634945	2.9672269	9.9275500
C	4.6024123	2.7708142	7.8968294
C	5.6608924	4.0342312	9.7399340
H	5.2101434	4.8952571	9.2384912
H	6.7400851	4.2273595	9.8524288
H	5.2204395	3.9367391	10.7463381
C	6.2489624	1.6688846	9.3808206
H	5.8588712	0.7540621	8.9188551
H	6.1554736	1.5713480	10.4746067
H	7.3189922	1.7705133	9.1338596
C	6.2975479	1.7905921	6.3947065
H	6.9559351	2.5421841	6.8444106
H	6.3091880	1.9347643	5.3056466
H	6.6848657	0.7828068	6.6183661
C	3.9131365	1.3495173	6.0179579
H	2.9526250	1.3505332	6.5450011
H	4.2047293	0.3090897	5.8039654

[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-CHD-TS (σ)

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

-2946.5236426768 (<S^2> 6.50946640)

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 35.88)}$:

-2948.3775944569 (<S^2> 6.50015134)

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.843587

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Fe:def2\text{-}TZVP)/COSMO(\varepsilon = 35.88)}$:

0.775481

H	3.7992050	1.8984162	5.0708812
C	-0.3063874	3.7780464	6.9946180
H	-0.7891018	4.5918884	6.4368228
H	-1.0591603	3.3503584	7.6803280
C	0.1893588	2.7363176	6.0011132
H	0.5657558	1.8519167	6.5437337
H	-0.6547057	2.3944981	5.3822741
C	1.3082601	3.0717266	3.8773288
C	0.9914411	0.6163535	4.0407867
H	1.6459412	0.7107478	4.9104660
H	1.4368947	-0.1236847	3.3559985
H	0.0114485	0.2344695	4.3722634
C	0.2046701	1.8253890	2.0481782
H	-0.0822080	2.8294954	1.7136520
H	-0.7106745	1.2200231	2.1501689
H	0.8430815	1.3567331	1.2805092
C	2.5711267	3.6338514	1.8323828
H	2.8836936	2.5838776	1.8859797
H	3.4722686	4.2655867	1.7989744
H	2.0087114	3.7951965	0.8977894
C	1.6925228	5.4220114	3.2717968
H	0.9298599	5.5952491	4.0385372
H	1.3970248	5.9401322	2.3456810
H	2.6505327	5.8301202	3.6290238
C	0.5975884	5.7388076	8.1707129
H	1.2995849	5.9814450	8.9801666
H	-0.4261439	5.8626065	8.5668309
C	0.8544365	6.6814597	7.0055933
H	0.0861774	6.5324506	6.2274423
H	0.7558441	7.7210661	7.3539037
C	2.9433060	7.4502526	6.0801622
C	1.1965833	8.6603157	4.7953145
H	0.9305243	7.6597247	4.4450902
H	1.3886846	9.2910205	3.9116916
H	0.3386761	9.0854760	5.3427367
C	2.9647039	9.9205538	5.9511844
H	3.7068451	9.8216509	6.7524096
H	2.1548575	10.5768629	6.3099385
H	3.4369959	10.4028432	5.0788090
C	5.1573892	8.0546841	5.1849058
H	4.5700523	8.3945554	4.3238284
H	5.9103788	7.3415823	4.8207094
H	5.6873572	8.9167041	5.6230071
C	4.9721714	6.5974903	7.1728519
H	4.2688752	6.3793804	7.9852083
H	5.8201010	7.1731273	7.5765367
H	5.3360348	5.6434846	6.7649295
C	7.2741475	2.5730138	2.9168805

C	8.4455687	2.8011654	3.8270367	
C	8.3265904	4.0480566	4.6523472	
C	7.2532123	4.8624243	4.5975103	
C	6.0745226	4.5831137	3.7488023	
C	6.2076365	3.3984540	2.8742991	
H	7.3166048	1.7031559	2.2533043	
H	9.1670152	4.2974507	5.3083284	
H	7.2424968	5.7657773	5.2134637	
H	5.3955658	3.1880479	2.1735951	
H	5.6765691	5.4730746	3.2297695	
H	5.0841989	4.4153898	4.4875601	
H	8.5928961	1.9208870	4.4879629	
H	9.3835987	2.8285436	3.2353089	
Fe	-0.7990526	-0.0044602	0.5325437	***[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-CHD-IC (σ)***
O	0.3974778	0.0141229	-0.8413424	**E$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-2.3462975	-0.0382943	2.2882572	**-2946.5636030582 (<S^2> 7.04129636)**
N	0.3709819	0.5481969	2.1339950	**E$_{B3LYP-D3/def2-TZVPP/COSMO(ε = 35.88)}$:**
N	-1.4139584	-1.9622216	0.5010343	**-2948.4186051997 (<S^2> 7.03867054)**
N	-2.1785248	1.3734919	-0.1083423	**ZPE$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	2.3922544	1.5955055	2.7927576	**0.845622**
N	2.4322012	-0.3394482	1.5029401	**Chem. Pot.$_{(298.15)/B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-0.8249427	-4.1460702	-0.2198070	**0.776052**
N	-1.1187806	-2.4365285	-1.7627350	
N	-3.0308013	2.5125041	-2.0062463	
N	-0.8123998	2.7782291	-1.3743386	
C	-1.5599527	0.1113781	3.5282681	
H	-1.1700180	-0.8752836	3.8144158	
H	-2.1933693	0.4739911	4.3578373	
C	-0.3820058	1.0481508	3.2883883	
H	-0.7489153	2.0747509	3.1174455	
H	0.2466019	1.0808890	4.1918522	
C	1.7054679	0.6143680	2.1428618	
C	1.8950904	2.9614887	2.9037767	
H	1.0603195	3.1231522	2.2163315	
H	2.7034583	3.6596445	2.6327167	
H	1.5638792	3.1953246	3.9291176	
C	3.6646752	1.3423964	3.4650816	
H	3.8321655	0.2639619	3.5713254	
H	3.6251968	1.7869264	4.4725345	
H	4.5146187	1.7898747	2.9234823	
C	3.6904750	-0.0487080	0.8262137	
H	3.8201596	1.0324839	0.6999914	
H	3.6634382	-0.5099225	-0.1718145	
H	4.5594472	-0.4577193	1.3678530	
C	1.9553146	-1.7070682	1.3709213	
H	1.1287535	-1.8724373	2.0704423	
H	2.7748023	-2.4035305	1.6093014	

H	1.5983941	-1.9112099	0.3492400
C	-3.0332891	-1.3426245	2.1937245
H	-3.8369588	-1.2578163	1.4494015
H	-3.4990134	-1.6146851	3.1579606
C	-2.0574908	-2.4196830	1.7351774
H	-1.3167563	-2.6108825	2.5306234
H	-2.6022661	-3.3634888	1.5758921
C	-1.1143886	-2.8363701	-0.4640761
C	-0.1374008	-4.5991925	0.9830467
H	0.2884353	-3.7531271	1.5275348
H	0.6879470	-5.2697721	0.6936625
H	-0.8133029	-5.1521611	1.6561388
C	-1.1928641	-5.2083998	-1.1530615
H	-1.9152866	-4.8355981	-1.8889314
H	-1.6621410	-6.0291079	-0.5869382
H	-0.3145130	-5.6139519	-1.6827028
C	-0.1051788	-2.8750655	-2.7128996
H	0.6747645	-3.4536988	-2.2032831
H	0.3638230	-1.9832288	-3.1593940
H	-0.5355795	-3.4861039	-3.5236170
C	-1.9973880	-1.3807497	-2.2376199
H	-2.8022987	-1.2238916	-1.5106741
H	-2.4381899	-1.6820794	-3.2014737
H	-1.4450104	-0.4378582	-2.3718075
C	-3.2521570	1.1026600	2.0464260
H	-2.7765398	2.0122433	2.4382957
H	-4.2086588	0.9685844	2.5829578
C	-3.4840258	1.2811466	0.5512620
H	-4.0737623	0.4336040	0.1623602
H	-4.0825898	2.1896113	0.3805388
C	-2.0188270	2.1942873	-1.1500963
C	-4.0868148	1.5755886	-2.3694149
H	-3.8297254	0.5620308	-2.0511577
H	-4.2003136	1.5715002	-3.4656165
H	-5.0548002	1.8560726	-1.9221157
C	-3.1404181	3.8327542	-2.6225928
H	-2.4706937	4.5431699	-2.1235276
H	-4.1765417	4.1907435	-2.5095655
H	-2.9011342	3.8060103	-3.6989037
C	-0.2683705	2.9398285	-2.7158190
H	-0.9169324	2.4562916	-3.4556124
H	0.7163838	2.4485136	-2.7569255
H	-0.1411378	4.0016249	-2.9840350
C	0.0958562	3.1054357	-0.2889774
H	-0.4506518	3.0913575	0.6609612
H	0.5093592	4.1137614	-0.4514204
H	0.9254220	2.3840462	-0.2297242
C	4.6960928	-1.2059539	-2.5163037

C	5.5360931	-0.0073289	-2.1809186
C	4.7924062	1.2941769	-2.2627926
C	3.4783815	1.3565986	-2.6492580
C	2.7445292	0.1812128	-2.9778083
C	3.3834565	-1.0896844	-2.8947437
H	5.1670915	-2.1916702	-2.4574962
H	5.3365079	2.2093041	-2.0110636
H	2.9842239	2.3312201	-2.7076322
H	2.8121088	-1.9901714	-3.1376846
H	1.7077376	0.2522956	-3.3129288
H	1.3379334	0.0820455	-1.0500092
H	5.9922349	-0.1271225	-1.1729964
H	6.4313409	0.0252218	-2.8424235

Fe	-0.1565893	-0.1381174	1.8265869	***[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-DHA-RC (σ)***
O	0.1418367	-0.0613245	0.2268001	**E$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-0.5316348	-0.2267944	3.9373856	**-3253.4702932659 (<S^2> 6.05235696)**
N	-0.6234681	-2.1028349	1.9416610	**E$_{B3LYP-D3/def2-TZVPP/COSMO(ε = 35.88)}$:**
N	-1.6626080	1.2000614	1.8972868	**-3255.6479784981 (<S^2> 6.05471527)**
N	1.6753600	0.4127600	2.4511587	**ZPE$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-0.4462782	-4.2771957	1.0203246	**0.946335**
N	-1.4401318	-2.5696810	-0.1977466	**Chem. Pot.$_{(298.15)/B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-3.4101584	2.3211415	0.7666062	**0.87412**
N	-1.1998052	2.6675083	0.1385724	
N	3.7130170	1.5077645	1.9591704	
N	3.0831398	-0.3854900	0.7665612	
C	-1.1813700	-1.5370581	4.2138069	
H	-2.2502241	-1.4453741	3.9813466	
H	-1.0846367	-1.7901587	5.2826335	
C	-0.5716320	-2.6020259	3.3208402	
H	0.4636451	-2.8110782	3.6387721	
H	-1.1345222	-3.5419785	3.4294839	
C	-0.8184618	-2.9667127	0.9380958	
C	0.7646366	-4.7225574	1.6986080	
H	1.4109137	-3.8739541	1.9369405	
H	1.3223560	-5.3976240	1.0291901	
H	0.5356278	-5.2691074	2.6284874	
C	-1.2529915	-5.3475647	0.4385062	
H	-2.2469206	-4.9720810	0.1676260	
H	-1.3753154	-6.1447356	1.1895529	
H	-0.7764184	-5.7855083	-0.4544101	
C	-1.0715176	-3.0940750	-1.5074443	
H	-0.1438753	-3.6735037	-1.4442757	
H	-0.8941531	-2.2500943	-2.1872932	
H	-1.8654848	-3.7265347	-1.9371541	
C	-2.4421224	-1.5169131	-0.2093933	
H	-2.7628128	-1.3111670	0.8174198	
H	-3.3105662	-1.8506241	-0.7999428	

H	-2.0386441	-0.5885994	-0.6418501
C	-1.4324860	0.9094879	4.2711631
H	-0.8214380	1.8167213	4.3655709
H	-1.9288698	0.7285070	5.2390653
C	-2.4315177	1.1013609	3.1445336
H	-3.1427302	0.2587473	3.1205896
H	-3.0222829	2.0126328	3.3247149
C	-2.0873879	2.0375400	0.9411891
C	-4.4594306	1.3274975	0.9578624
H	-4.0311466	0.3231300	1.0214503
H	-5.1411808	1.3552556	0.0924239
H	-5.0490811	1.5232066	1.8689245
C	-3.8818423	3.6620246	0.4274579
H	-3.0801707	4.3962271	0.5709356
H	-4.7132392	3.9230764	1.1019192
H	-4.2476680	3.7222512	-0.6109680
C	-1.5091563	3.0241416	-1.2417664
H	-2.3848340	2.4667072	-1.5952959
H	-0.6519832	2.7565054	-1.8715127
H	-1.6971060	4.1033183	-1.3618242
C	0.1573567	2.9647058	0.5686912
H	0.2211309	2.8710082	1.6582414
H	0.4105824	3.9966120	0.2787529
H	0.8782766	2.2688339	0.1141284
C	0.7846728	-0.1055606	4.6219545
H	1.2607048	-1.0947992	4.6293319
H	0.6404416	0.2125096	5.6678231
C	1.6664634	0.8603713	3.8490279
H	1.2779043	1.8883276	3.9451112
H	2.6803856	0.8601460	4.2779187
C	2.7993576	0.5220101	1.7310347
C	3.3324859	2.8562028	2.3623746
H	2.2591089	3.0108155	2.2229501
H	3.8685283	3.5831775	1.7311269
H	3.5889603	3.0571093	3.4157633
C	5.1526667	1.2713840	1.8715382
H	5.3616564	0.1954005	1.8409890
H	5.6328847	1.6904802	2.7703616
H	5.5980969	1.7536864	0.9857121
C	3.8205572	-0.0412347	-0.4427788
H	3.8417256	1.0461869	-0.5854479
H	3.3055332	-0.4929542	-1.3022096
H	4.8541167	-0.4237317	-0.4243355
C	2.6016414	-1.7561490	0.8282129
H	2.2466852	-1.9688807	1.8416985
H	3.4280521	-2.4418594	0.5827635
H	1.7710844	-1.9149663	0.1240563
C	-0.0978718	-3.1667485	-4.9766905

C	1.1731809	-3.1267792	-4.3914114
C	-0.9123937	-2.0299779	-4.9470606
C	1.6228292	-1.9482713	-3.7871218
C	-0.4745187	-0.8518686	-4.3256680
C	0.8083297	-0.8079441	-3.7453788
C	-1.3617396	0.3692294	-4.2177748
C	1.2558389	0.4641010	-3.0609718
C	0.7026468	1.7097361	-3.7150733
C	-0.5840762	1.6649625	-4.2851804
C	1.4181003	2.9158518	-3.7179290
C	-1.1317593	2.8270323	-4.8456767
C	0.8613524	4.0750746	-4.2679953
C	-0.4182367	4.0303292	-4.8339449
H	-0.4540688	-4.0818503	-5.4574257
H	1.8167178	-4.0104338	-4.4111596
H	-1.9072887	-2.0597997	-5.4014827
H	2.6209148	-1.9139621	-3.3396776
H	2.4187354	2.9482763	-3.2760075
H	-2.1319826	2.7903533	-5.2878872
H	1.4267232	5.0108899	-4.2581976
H	-0.8593496	4.9311669	-5.2691694
H	0.9084531	0.4305475	-2.0070546
H	2.3537825	0.5139504	-3.0203986
H	-2.1570204	0.3469902	-4.9782188
H	-1.8820770	0.3315978	-3.2376354

Fe	-0.3796608	0.0235024	1.7190311	***[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-DHA-TS (σ)***
O	-0.0226506	-0.0187595	0.0529880	**E$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-0.8343958	0.0459205	3.9630135	**-3253.4513279768 (<S^2> 6.48938568)**
N	0.1980091	-1.8707445	2.2318231	**E$_{B3LYP-D3/def2-TZVPP/COSMO(ε = 35.88)}$:**
N	-2.4063868	0.3555470	1.6890283	**-3255.6272794767 (<S^2> 6.48416285)**
N	0.8269976	1.5865924	2.3359179	**ZPE$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	1.4122343	-3.8227552	1.6560787	**0.939819**
N	-0.3651072	-3.1155416	0.3380448	**Chem. Pot.$_{(298.15)/B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-4.4491429	0.3191213	0.4842329	**0.868057**
N	-2.6821414	1.6362075	-0.2435044	
N	2.0939944	3.5211689	1.8377364	
N	2.7629720	1.4411107	1.0324567	
C	-0.6295343	-1.3395045	4.4408592	
H	-1.5529873	-1.9077471	4.2642436	
H	-0.4304274	-1.3525819	5.5269123	
C	0.5007534	-1.9975428	3.6617379	
H	1.4620303	-1.5176722	3.9155551	
H	0.5828022	-3.0528680	3.9638972	
C	0.4236141	-2.9096077	1.4193792	
C	2.7016853	-3.4582163	2.2274489	
H	2.8208782	-2.3723329	2.2477067	
H	3.5066299	-3.8806593	1.6034966	

H	2.8210028	-3.8467383	3.2526430
C	1.2318406	-5.2496312	1.4008733
H	0.1728906	-5.4762299	1.2290101
H	1.5657682	-5.8122844	2.2878148
H	1.8201600	-5.5942207	0.5337665
C	0.1258797	-3.7186003	-0.8947074
H	1.2204642	-3.7339782	-0.9092532
H	-0.2089934	-3.1043967	-1.7416545
H	-0.2581991	-4.7421363	-1.0358673
C	-1.7364447	-2.6404214	0.2840530
H	-2.0893934	-2.4341922	1.2998569
H	-2.3712230	-3.4188560	-0.1673988
H	-1.8113751	-1.7165458	-0.3099443
C	-2.2387098	0.4896009	4.0999555
H	-2.2606257	1.5874729	4.0739689
H	-2.6569095	0.1693391	5.0705338
C	-3.0648084	-0.0397735	2.9395498
H	-3.1590069	-1.1368341	3.0156305
H	-4.0834667	0.3719584	3.0036100
C	-3.1628599	0.7471514	0.6586246
C	-4.8886167	-1.0358712	0.7907248
H	-4.0334802	-1.6844562	0.9940950
H	-5.4279196	-1.4451422	-0.0794644
H	-5.5671278	-1.0594851	1.6597874
C	-5.4996248	1.2085579	-0.0047975
H	-5.1604171	2.2509680	0.0212399
H	-6.3778490	1.1136786	0.6545357
H	-5.8117939	0.9558570	-1.0320373
C	-3.0510711	1.5874425	-1.6541032
H	-3.5518376	0.6397703	-1.8855442
H	-2.1379953	1.6502028	-2.2577680
H	-3.7117632	2.4231720	-1.9378626
C	-1.6835183	2.6309876	0.1124927
H	-1.6650017	2.7523850	1.2017588
H	-1.9504117	3.5929362	-0.3528603
H	-0.6823223	2.3296831	-0.2267563
C	0.1113879	1.0059717	4.5697366
H	1.0640401	0.4902785	4.7536086
H	-0.2680745	1.3677419	5.5418530
C	0.3605120	2.1573464	3.6064508
H	-0.5625735	2.7467246	3.4694683
H	1.1091207	2.8348352	4.0440076
C	1.8656808	2.1759233	1.7348657
C	1.0064033	4.4906423	1.8430951
H	0.0741709	4.0194300	1.5184539
H	1.2456122	5.3041958	1.1387659
H	0.8509092	4.9342576	2.8410934
C	3.4226909	4.0760704	2.0861015

H	4.1274710	3.2794844	2.3529175	
H	3.3602491	4.7727377	2.9382369	
H	3.8121698	4.6303195	1.2159432	
C	3.6017407	2.0111985	-0.0180265	
H	3.1362976	2.9136932	-0.4333098	
H	3.7171833	1.2753633	-0.8257579	
H	4.6115991	2.2617930	0.3439747	
C	2.9507215	0.0223875	1.2976907	
H	2.6065558	-0.2043156	2.3130636	
H	4.0199893	-0.2242690	1.2186544	
H	2.3742371	-0.5951995	0.5930133	
C	2.3019571	-3.5164464	-3.7723572	
C	3.1119931	-2.9033422	-2.8061588	
C	1.1398148	-2.8763591	-4.2163859	
C	2.7535641	-1.6562756	-2.2940723	
C	0.7658944	-1.6285809	-3.7013229	
C	1.5850188	-1.0045514	-2.7333103	
C	-0.5213752	-0.9549184	-4.1190693	
C	1.1929910	0.3184733	-2.1960471	
C	0.3591492	1.1648237	-3.0783816	
C	-0.4716144	0.5537674	-4.0442183	
C	0.3671874	2.5681511	-2.9605573	
C	-1.2594130	1.3569714	-4.8787578	
C	-0.4295540	3.3586910	-3.7887483	
C	-1.2446283	2.7506767	-4.7540589	
H	2.5779356	-4.4916481	-4.1818817	
H	4.0231771	-3.3966083	-2.4579998	
H	0.5093178	-3.3560685	-4.9707994	
H	3.3901797	-1.1724977	-1.5487291	
H	1.0112263	3.0381361	-2.2114918	
H	-1.8970785	0.8850572	-5.6320263	
H	-0.4147140	4.4467594	-3.6865423	
H	-1.8687978	3.3631727	-5.4099190	
H	0.5352610	0.1101342	-1.1518773	
H	2.0306912	0.8690154	-1.7557378	
H	-0.8279081	-1.2866344	-5.1230344	
H	-1.3251627	-1.3020198	-3.4358449	
Fe	-0.1551138	-0.0868732	1.5385494	***[Fe^{IV}(O)TMG$_3$tren]$^{2+}$-DHA-IC (σ)***
O	0.0154277	-0.0160009	-0.2588974	**E$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-0.4131187	-0.2463606	3.8728323	**-3253.4855233643 (<S^2> 7.03286810)**
N	-0.6182836	-2.0736601	1.7827963	**E$_{B3LYP-D3/def2-TZVPP/COSMO(ε = 35.88)}$:**
N	-1.7206047	1.2127330	1.8898245	**-3255.6626558995 (<S^2> 7.03084143)**
N	1.7088470	0.5132768	2.2117708	**ZPE$_{B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88)}$:**
N	-0.5646674	-4.2074008	0.7439212	**0.941853**
N	-1.7881188	-2.4731804	-0.1949378	
N	-3.5615222	2.3775064	0.9451452	
N	-1.4150805	2.7212408	0.1359269	

N	3.7588499	1.6113297	1.7769765
N	3.1993812	-0.3301192	0.6195447
C	-0.9455831	-1.5989224	4.1332681
H	-2.0372406	-1.5713570	4.0117634
H	-0.7335328	-1.9138551	5.1708513
C	-0.3723827	-2.5931390	3.1301073
H	0.7062152	-2.7335475	3.3195497
H	-0.8504039	-3.5744061	3.2758587
C	-0.9687018	-2.9052886	0.7969226
C	0.7309428	-4.6571706	1.2362505
H	1.3788034	-3.8048982	1.4535810
H	1.2191382	-5.2704706	0.4610218
H	0.6319385	-5.2692845	2.1479549
C	-1.4135857	-5.2622056	0.1955150
H	-2.4438351	-4.9035068	0.0856410
H	-1.4125014	-6.1158577	0.8923499
H	-1.0502084	-5.6176243	-0.7835938
C	-1.5920990	-2.8522854	-1.5869471
H	-0.6655363	-3.4227366	-1.7079095
H	-1.4963553	-1.9369621	-2.1901423
H	-2.4364204	-3.4433694	-1.9779024
C	-2.7730554	-1.4286943	0.0219937
H	-2.9542538	-1.3157132	1.0963993
H	-3.7154689	-1.7106185	-0.4742771
H	-2.4237093	-0.4673394	-0.3854905
C	-1.3576178	0.8218677	4.2543393
H	-0.7970646	1.7605372	4.3616747
H	-1.8292645	0.6028593	5.2292198
C	-2.4066474	1.0055749	3.1681668
H	-3.0637041	0.1195437	3.1325307
H	-3.0460361	1.8648639	3.4230103
C	-2.2314722	2.0742619	1.0069196
C	-4.6171826	1.4041038	1.1943133
H	-4.2079248	0.3927459	1.2501276
H	-5.3381172	1.4343011	0.3607957
H	-5.1604199	1.6203997	2.1291807
C	-4.0324702	3.7192711	0.6108755
H	-3.2052746	4.4372325	0.6615457
H	-4.7998848	4.0176928	1.3435746
H	-4.4832752	3.7600227	-0.3950842
C	-1.8027839	2.9595869	-1.2487125
H	-2.7614865	2.4755855	-1.4680778
H	-1.0404601	2.5221647	-1.9069733
H	-1.8800175	4.0352598	-1.4756128
C	-0.0389981	3.0511572	0.4647497
H	0.1016701	2.9893603	1.5502259
H	0.1774970	4.0786343	0.1309022
H	0.6661312	2.3618212	-0.0239075

Chem. Pot.(298.15)/B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 35.88):

0.868414

C	0.9307288	-0.0337062	4.4405191
H	1.4785704	-0.9860182	4.4124818
H	0.8694221	0.2854846	5.4968110
C	1.6888728	0.9867630	3.6020585
H	1.2077630	1.9766802	3.6821509
H	2.7074256	1.0941160	4.0043785
C	2.8628268	0.6056372	1.5424036
C	3.3307336	2.9713887	2.0783851
H	2.2692890	3.0977765	1.8447170
H	3.9073364	3.6757353	1.4568119
H	3.4948308	3.2326834	3.1374041
C	5.1982820	1.3771240	1.8695691
H	5.4098075	0.3021645	1.9156042
H	5.5707258	1.8362175	2.7999944
H	5.7476545	1.8205820	1.0225360
C	4.1220529	-0.0589110	-0.4776030
H	4.1574921	1.0158879	-0.6949543
H	3.7726424	-0.5872829	-1.3746187
H	5.1424393	-0.4159497	-0.2653918
C	2.6575170	-1.6801427	0.6677117
H	2.2701027	-1.8783495	1.6730094
H	3.4564223	-2.4025548	0.4416350
H	1.8346539	-1.8056719	-0.0532202
C	0.1106971	-3.4359698	-4.5798263
C	1.2537234	-3.3856055	-3.7635896
C	-0.5867156	-2.2585659	-4.8759508
C	1.6933720	-2.1658333	-3.2637270
C	-0.1679881	-1.0222681	-4.3750692
C	1.0029620	-0.9600637	-3.5627610
C	-0.9763756	0.2273029	-4.6380242
C	1.4762659	0.3060223	-3.0969852
C	0.8791678	1.5413145	-3.4955849
C	-0.2989486	1.5346662	-4.2987379
C	1.4489445	2.7879996	-3.1204957
C	-0.8460890	2.7516815	-4.7162348
C	0.8830453	3.9861853	-3.5386334
C	-0.2671704	3.9718916	-4.3461337
H	-0.2369832	-4.3918507	-4.9795081
H	1.7992965	-4.3024972	-3.5259204
H	-1.4820993	-2.3036029	-5.5031788
H	2.5914029	-2.1246615	-2.6420709
H	2.3495182	2.7924973	-2.4994749
H	-1.7479326	2.7463585	-5.3357747
H	1.3323634	4.9369479	-3.2406421
H	-0.7145516	4.9113004	-4.6804850
H	0.4644855	0.0947860	-1.1075480
H	2.3960006	0.3444327	-2.5128604
H	-1.3242127	0.2404863	-5.6850261

H	-1.9081809	0.1620059	-4.0381194	

5.2.4 Cu^{III}(OH) pathway (B3LYP-D3)

Method: B3LYP-D3/def2-SVP(Fe:def2-TZVP)/COSMO(ε = 8.51)

C	-1.4118919	-0.5812107	0.1864666	***CHD***
C	-0.0434186	-1.2122965	0.1868101	**$E_{B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:**
C	1.0732293	-0.2003316	0.1863369	**-233.1019473762**
C	0.8702683	1.1238559	0.1861765	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:**
C	-0.4982046	1.7549418	0.1859693	**-233.3601352119**
C	-1.6148530	0.7429767	0.1861132	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:**
H	-2.2710917	-1.2618718	0.1865000	**0.121586**
H	2.0968466	-0.5924153	0.1862660	**Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:**
H	1.7294676	1.8045174	0.1860200	**0.094467 (σ = 4)**
H	-2.6384705	1.1350598	0.1859017	
H	-0.6016943	2.4304723	-0.6874051	
H	-0.6018452	2.4309050	1.0589932	
H	0.0601441	-1.8875561	1.0603892	
H	0.0601620	-1.8885284	-0.6860088	
C	-3.5497633	-0.7663013	0.1449849	***DHA***
C	-3.5567773	0.6070146	0.4140184	**$E_{B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:**
C	-2.3868223	-1.3737445	-0.3421200	**-540.0245562672**
C	-2.4008192	1.3647660	0.1943482	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:**
C	-1.2286556	-0.6189297	-0.5713775	**-540.6059779633**
C	-1.2357311	0.7636913	-0.3005658	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:**
C	0.0445716	-1.2368234	-1.1114020	**0.217245**
C	0.0302477	1.5522147	-0.5652714	**Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP/COSMO(\varepsilon = 8.51)}$:**
C	1.2744365	0.7606115	-0.2189928	**0.182779 (σ = 2)**
C	1.2815052	-0.6220344	-0.4896593	
C	2.4063801	1.3588709	0.3505875	
C	2.4203645	-1.3797285	-0.1854719	
C	3.5436581	0.5982478	0.6450835	
C	3.5506576	-0.7751246	0.3762814	
H	-4.4469757	-1.3663159	0.3205997	
H	-4.4595339	1.0875520	0.8012734	
H	-2.3769879	-2.4490740	-0.5452558	
H	-2.4020015	2.4373138	0.4119243	
H	2.3960999	2.4314566	0.5677378	
H	2.4210664	-2.4550667	-0.3887981	
H	4.4205132	1.0765845	1.0902460	
H	4.4330148	-1.3773518	0.6099908	
H	0.0656300	1.8023954	-1.6451127	
H	0.0140610	2.5139343	-0.0301347	
H	0.0388879	-2.3294541	-0.9785348	
H	0.0804298	-1.0609377	-2.2057912	

H	-4.5914508	4.4682746	0.2429564
C	-4.5581195	3.3890409	0.0851513
C	-4.3662518	0.6501713	-0.3108641
C	-5.7173026	2.6171264	-0.0899855
C	-3.3281719	2.7365423	0.0513946
N	-3.2938140	1.4197824	-0.1414757
C	-5.6322476	1.2308514	-0.2914234
H	-6.6965836	3.1009054	-0.0689424
H	-6.5145150	0.6036505	-0.4290559
C	-1.9516227	3.3429931	0.2045465
O	-1.7838337	4.5402012	0.4017165
C	-4.0152393	-0.8087789	-0.4963697
O	-4.8728425	-1.6664626	-0.6719352
N	-2.6674297	-0.9940607	-0.4351969
N	-0.9843573	2.3888821	0.0891948
Cu	-1.6215001	0.6003844	-0.1780624
H	0.6721552	0.3861681	-0.0965633
O	-0.0405143	-0.2586881	-0.2355506
C	0.3909803	2.7024101	0.1739082
C	3.1194402	3.2436886	0.3364864
C	1.0556346	2.5391942	1.4166303
C	1.0870836	3.0976284	-0.9979980
C	2.4564370	3.3721116	-0.8871868
C	2.4264497	2.8246563	1.4746113
H	3.0204027	3.6828425	-1.7691043
H	2.9635035	2.7184764	2.4195280
H	4.1889976	3.4619111	0.4005928
C	-2.0644009	-2.2601409	-0.5324236
C	-0.8354024	-4.7514183	-0.7305059
C	-1.9437727	-3.0646455	0.6306780
C	-1.5322088	-2.6712047	-1.7809318
C	-0.9282154	-3.9319097	-1.8585125
C	-1.3328299	-4.3177168	0.5022249
H	-0.5201042	-4.2825443	-2.8088083
H	-1.2319138	-4.9657575	1.3752792
H	-0.3611057	-5.7337053	-0.8095369
C	0.3734658	3.1450718	-2.3430791
H	-0.6957686	3.3088856	-2.1426101
C	0.8440411	4.2904071	-3.2494858
H	0.2140580	4.3390503	-4.1523873
H	1.8841485	4.1493974	-3.5862968
H	0.7810405	5.2620788	-2.7337295
C	0.5006751	1.7813151	-3.0527414
H	-0.1026087	1.7621602	-3.9753663
H	0.1713858	0.9556340	-2.4039756
H	1.5513411	1.5869687	-3.3274455

Cu^{III}(OH)(L)

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

-3232.6379302794

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-3234.3954435859

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.635055

Chem. Pot.(298.15)/B3LYP-D3/def2-SVP(Cu:def2-TZVP)/COSMO(ε = 8.51):

0.572492

C	0.2798924	2.1009260	2.6511548
H	-0.6109085	1.5593712	2.2963247
C	-0.2169240	3.3326637	3.4326384
H	-0.7985010	4.0061723	2.7845030
H	0.6368493	3.9039550	3.8350562
H	-0.8526470	3.0261983	4.2800274
C	1.0606598	1.1351232	3.5519104
H	1.9236974	1.6228458	4.0338986
H	1.4302220	0.2694522	2.9793539
H	0.4069098	0.7574201	4.3544211
C	-1.6614556	-1.7702508	-2.9997942
H	-1.7296640	-0.7370125	-2.6268178
C	-2.9710355	-2.0742426	-3.7534197
H	-3.8416994	-2.0121265	-3.0824724
H	-2.9448436	-3.0928462	-4.1767686
H	-3.1178449	-1.3633650	-4.5838925
C	-0.4467585	-1.8256602	-3.9343416
H	-0.3542652	-2.8016763	-4.4386186
H	0.4856053	-1.6334128	-3.3804633
H	-0.5412170	-1.0590580	-4.7204253
C	-2.4018099	-2.5379158	1.9844609
H	-3.2071825	-1.8111545	1.8002221
C	-2.9757067	-3.6191162	2.9095309
H	-3.3896804	-3.1553805	3.8196286
H	-2.2043266	-4.3370187	3.2333532
H	-3.7818047	-4.1847469	2.4150344
C	-1.2462756	-1.7753649	2.6647697
H	-1.5926638	-1.2773194	3.5855903
H	-0.8149187	-1.0200316	1.9910059
H	-0.4352141	-2.4720281	2.9369674
H	-5.6005232	0.6614407	0.2148683
C	-4.8489285	-0.1264355	0.1436797
C	-2.8623194	-2.0551515	-0.0356155
C	-5.1883214	-1.4860209	0.0608206
C	-3.4974280	0.2103917	0.1315114
N	-2.5860223	-0.7556419	0.0436161
C	-4.1920219	-2.4704215	-0.0304670
H	-6.2401345	-1.7812832	0.0675964
H	-4.4243659	-3.5346193	-0.0952409
C	-2.8829185	1.5905829	0.2004972
O	-3.5671122	2.6032761	0.2880538
C	-1.6192813	-2.9132927	-0.1174323
O	-1.6786894	-4.1346263	-0.2072969
N	-0.4973678	-2.1437184	-0.0774817
N	-1.5215597	1.5233419	0.1476124
Cu	-0.7945695	-0.2439196	0.0387739
H	1.1307696	1.0722061	0.2067431

Cu^{III}(OH)(L)-CHD-RC

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

-3465.7587837766

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-3467.7693930849

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.758544

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.689108

O	0.9556485	0.1361354	0.0202690
H	3.1936322	-0.9129435	0.5173071
C	-0.7267257	2.6930260	0.1683935
C	0.8412114	4.9955490	0.2193820
C	-0.2059165	3.1468405	1.4056055
C	-0.4262975	3.3501397	-1.0524983
C	0.3542616	4.5120854	-0.9980263
C	0.5722423	4.3122234	1.4069009
H	0.6004226	5.0433925	-1.9197405
H	0.9785789	4.6918646	2.3467320
H	1.4517035	5.9023670	0.2394281
C	0.8011765	-2.6816459	-0.1177931
C	3.3776113	-3.7368357	-0.2110623
C	1.4198975	-3.1018905	1.0882904
C	1.4851544	-2.7282865	-1.3591252
C	2.7747593	-3.2724520	-1.3824460
C	2.7087972	-3.6429038	1.0127590
H	3.3224945	-3.3312527	-2.3251565
H	3.2101382	-3.9814034	1.9219182
H	4.3865044	-4.1571150	-0.2482168
C	3.9621855	1.3190852	-1.6142119
C	4.1791510	0.1138851	-1.0725277
C	3.5319794	2.5200527	-0.8133457
H	2.5358850	2.8618097	-1.1565427
H	4.1967232	3.3819331	-1.0230074
C	4.0122305	-0.1819012	0.3923445
H	4.9148225	-0.6878062	0.7886821
C	3.4837299	2.2533309	0.6689928
C	3.7003799	1.0444127	1.2053455
C	-0.8712302	2.7553911	-2.3822411
H	-1.7491327	2.1232287	-2.1820056
C	-1.2954685	3.8068160	-3.4161029
H	-1.7073159	3.3116890	-4.3104754
H	-0.4446960	4.4236627	-3.7492998
H	-2.0671190	4.4806193	-3.0101424
C	0.2342094	1.8335172	-2.9379697
H	-0.1168514	1.3024452	-3.8381858
H	0.5525981	1.0878138	-2.1939624
H	1.1242743	2.4224441	-3.2167223
C	-0.5168760	2.3960423	2.6933208
H	-0.7689150	1.3621848	2.4088177
C	-1.7586774	2.9975152	3.3786935
H	-2.6167197	3.0292376	2.6898268
H	-1.5532609	4.0295792	3.7104557
H	-2.0412881	2.4043766	4.2644993
C	0.6782445	2.3167675	3.6525213
H	0.9440499	3.3031879	4.0665457
H	1.5641813	1.9066397	3.1437754

H	0.4362519	1.6583734	4.5023565
C	0.8047694	-2.2327707	-2.6265627
H	0.0583780	-1.4857471	-2.3159161
C	0.0459078	-3.3858467	-3.3118802
H	-0.6518417	-3.8761130	-2.6155588
H	0.7535603	-4.1515212	-3.6733047
H	-0.5270036	-3.0155547	-4.1787102
C	1.7590211	-1.5265648	-3.5974564
H	2.4956514	-2.2212518	-4.0341902
H	2.3026328	-0.7162835	-3.0890509
H	1.1880136	-1.0890960	-4.4325366
C	0.7298217	-2.8858578	2.4283124
H	-0.3532419	-2.8429072	2.2387393
C	0.9680368	-4.0176498	3.4366701
H	0.3570337	-3.8542197	4.3393720
H	2.0204434	-4.0656144	3.7614914
H	0.6976590	-4.9977573	3.0115945
C	1.1442131	-1.5175974	3.0084660
H	0.5716753	-1.2898910	3.9231998
H	0.9866487	-0.7132251	2.2749186
H	2.2167638	-1.5196299	3.2673384
H	3.2312435	3.1000798	1.3153772
H	4.0755677	1.4584822	-2.6954852
H	4.4657886	-0.7269278	-1.7127782
H	3.6277427	0.9129575	2.2910086
H	-4.5541131	4.2849085	0.2774878
C	-4.4939981	3.2048436	0.1344291
C	-4.2434479	0.4614889	-0.2264294
C	-5.6361690	2.4022472	-0.0188835
C	-3.2490776	2.5778272	0.0977112
N	-3.1911410	1.2607997	-0.0764908
C	-5.5235564	1.0148506	-0.2029209
H	-6.6261676	2.8641844	0.0046877
H	-6.3947608	0.3694422	-0.3258161
C	-1.8813646	3.2247618	0.2334747
O	-1.7625064	4.4347713	0.4150628
C	-3.8648500	-0.9997946	-0.4127346
O	-4.7276992	-1.8610856	-0.5865600
N	-2.5230059	-1.1647042	-0.3624197
N	-0.8847735	2.3070777	0.1301551
Cu	-1.4684010	0.4654045	-0.1186066
H	0.8897979	0.3446085	-0.0388912
O	0.2105170	-0.3424093	-0.1587056
H	1.1184765	-1.4230456	-0.1712464
C	0.4790496	2.6608034	0.2241937
C	3.2079509	3.2346487	0.4009475
C	1.1480276	2.4940109	1.4663929

Cu^{III}(OH)(L)-CHD-TS

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

-3465.7410374778 (<S^2> 0.43940638)

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-3467.7497649775 (*S* = 0; <S^2> 0.45695148)

-3467.7361455118 (*S* = 1; <S^2> 2.01530241)

-3467.7537981851 (spin purified)

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.75227

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.683264

C	1.1811552	3.0660101	-0.9417729
C	2.5463169	3.3573109	-0.8247179
C	2.5146104	2.7963539	1.5320598
H	3.1097518	3.6772378	-1.7036365
H	3.0500277	2.6846584	2.4769820
H	4.2721551	3.4747139	0.4723679
C	-1.8976127	-2.4204931	-0.5240804
C	-0.5184284	-4.8304938	-0.8315628
C	-1.6908182	-3.2504120	0.6054380
C	-1.3834659	-2.7701502	-1.7977267
C	-0.7011348	-3.9867598	-1.9301743
C	-1.0030901	-4.4588166	0.4249888
H	-0.3012646	-4.2823056	-2.9026409
H	-0.8317730	-5.1180356	1.2788883
H	0.0178074	-5.7760209	-0.9522149
C	3.9046477	-0.8295338	-1.2914355
C	2.8887211	-1.7189776	-1.3364154
C	4.3759009	-0.2148280	-0.0062814
H	4.1320325	0.8731416	-0.0099595
H	5.4824135	-0.2270727	0.0497969
C	2.1393062	-2.1048591	-0.1274066
H	1.6763987	-3.1030909	-0.1558318
C	3.7771308	-0.8396076	1.2194376
C	2.7627838	-1.7290395	1.1547580
C	0.4762533	3.1001787	-2.2922811
H	-0.5926844	3.2756450	-2.1001090
C	0.9618066	4.2265832	-3.2143180
H	0.3338969	4.2702848	-4.1189438
H	2.0006354	4.0682675	-3.5478264
H	0.9103648	5.2063824	-2.7128274
C	0.5992008	1.7262057	-2.9822357
H	0.0216970	1.7044223	-3.9211141
H	0.2385570	0.9122106	-2.3362815
H	1.6536442	1.5079172	-3.2218893
C	0.3755118	2.0252260	2.6919969
H	-0.4734614	1.4272934	2.3238857
C	-0.2137772	3.2325654	3.4469305
H	-0.8136361	3.8674903	2.7772379
H	0.5951254	3.8545071	3.8669336
H	-0.8542004	2.8974479	4.2799173
C	1.1913421	1.1195309	3.6232279
H	2.0025527	1.6684309	4.1293647
H	1.6400249	0.2820494	3.0665460
H	0.5398872	0.7016562	4.4075613
C	-1.5997358	-1.8440067	-2.9866112
H	-1.7055899	-0.8257792	-2.5802982
C	-2.9212492	-2.1877392	-3.7008986
H	-3.7658284	-2.1859834	-2.9948392

H	-2.8629591	-3.1917381	-4.1552848
H	-3.1338345	-1.4619718	-4.5040211
C	-0.4208384	-1.8110978	-3.9668735
H	-0.2900887	-2.7701767	-4.4945628
H	0.5194191	-1.5732140	-3.4451529
H	-0.5883048	-1.0366310	-4.7328506
C	-2.1298979	-2.7896636	1.9900276
H	-2.9679450	-2.0903683	1.8521069
C	-2.6326528	-3.9258397	2.8907509
H	-3.0396983	-3.5135366	3.8284976
H	-1.8240556	-4.6226504	3.1669174
H	-3.4284643	-4.5067976	2.3972778
C	-0.9871922	-2.0063701	2.6674600
H	-1.3180838	-1.5757658	3.6272999
H	-0.6212779	-1.1930382	2.0237834
H	-0.1315217	-2.6733050	2.8693421
H	4.1861918	-0.5405394	2.1895885
H	4.4142297	-0.5279306	-2.2122288
H	2.5653095	-2.1367205	-2.2946642
H	2.3383734	-2.1472372	2.0726452
H	-5.6350037	0.6334916	0.1156344
C	-4.8692619	-0.1428896	0.0786549
C	-2.8542054	-2.0556115	-0.0111695
C	-5.1884272	-1.5102788	0.0397452
C	-3.5192094	0.2106216	0.0683501
N	-2.6022805	-0.7508767	0.0244800
C	-4.1811119	-2.4881283	-0.0063115
H	-6.2370244	-1.8181983	0.0456792
H	-4.4057748	-3.5553945	-0.0372022
C	-2.9266706	1.6155589	0.1060172
O	-3.6615417	2.6043589	0.1660961
C	-1.5963731	-2.9173352	-0.0569374
O	-1.6805845	-4.1458426	-0.1217785
N	-0.4780473	-2.1588385	-0.0212242
N	-1.5763965	1.5812960	0.0708124
Cu	-0.7548346	-0.2089510	0.0128192
H	1.4682021	1.1775018	0.3428811
O	1.1539774	0.3582065	-0.0774911
H	1.8799707	-0.2876683	-0.0122448
C	-0.7819774	2.7505807	0.1080625
C	0.9593918	4.9413607	0.1753610
C	-0.1815063	3.1298579	1.3365637
C	-0.4910960	3.4466413	-1.0929370
C	0.3782957	4.5451369	-1.0322705
C	0.6840149	4.2343193	1.3469217
H	0.6171057	5.0983089	-1.9429559
H	1.1516102	4.5483058	2.2824917

Cu^{III}(OH)(L)-CHD-IC

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

-3465.7828945679 (<S^2> 1.04071524)

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-3467.7910857678 (*S* = 0, <S^2> 1.03901619)

-3467.7911092310 (*S* = 1; <S^2> 2.03915370)

-3467.7910603994 (spin purified)

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.756091

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.686013

H	1.6381916	5.7981312	0.2002059
C	0.8189780	-2.7213181	-0.0781296
C	3.4462317	-3.6798236	-0.1900442
C	1.4646362	-3.1279323	1.1180256
C	1.4988630	-2.7542876	-1.3225686
C	2.8119630	-3.2467655	-1.3555036
C	2.7780722	-3.6115099	1.0354141
H	3.3498977	-3.2908345	-2.3050466
H	3.2955255	-3.9339153	1.9413139
H	4.4708486	-4.0591400	-0.2334089
C	4.0010692	1.1896667	-1.5107372
C	4.2698093	0.0022139	-0.8774553
C	3.6393911	2.4332795	-0.7525086
H	2.6660503	2.8370654	-1.1111942
H	4.3430664	3.2563071	-1.0097701
C	4.2120292	-0.1128215	0.5403641
H	4.4107972	-1.0729660	1.0198438
C	3.6017745	2.2419689	0.7381035
C	3.8842402	1.0328688	1.3236043
C	-1.0528976	2.9503446	-2.4205177
H	-2.0233507	2.4776199	-2.2074101
C	-1.3096918	4.0666702	-3.4415785
H	-1.8321928	3.6593979	-4.3222654
H	-0.3717783	4.5205834	-3.8020505
H	-1.9327289	4.8680477	-3.0129868
C	-0.1298793	1.8673427	-3.0142204
H	-0.5595015	1.4448585	-3.9374661
H	0.0384252	1.0429091	-2.3063165
H	0.8581831	2.2925489	-3.2593044
C	-0.5154492	2.3670149	2.6131197
H	-0.7527012	1.3322559	2.3154390
C	-1.7880679	2.9449353	3.2620266
H	-2.6206129	2.9780970	2.5428975
H	-1.6040891	3.9745149	3.6137023
H	-2.0965372	2.3375000	4.1294226
C	0.6426793	2.2929445	3.6160682
H	0.8758251	3.2769172	4.0546485
H	1.5599477	1.9069131	3.1430053
H	0.3802898	1.6182336	4.4466082
C	0.7912366	-2.2944587	-2.5910062
H	0.0159126	-1.5754693	-2.2813235
C	0.0624465	-3.4785423	-3.2544151
H	-0.6134936	-3.9749797	-2.5410629
H	0.7904220	-4.2278882	-3.6097378
H	-0.5292608	-3.1394906	-4.1213773
C	1.7094751	-1.5637118	-3.5791713
H	2.4647967	-2.2349611	-4.0199253
H	2.2365610	-0.7301462	-3.0880692

H	1.1157735	-1.1489922	-4.4098237
C	0.7596175	-2.9631073	2.4599307
H	-0.3191445	-3.0825025	2.2782565
C	1.1619327	-4.0095138	3.5073605
H	0.5261672	-3.9117375	4.4021568
H	2.2068187	-3.8842205	3.8362220
H	1.0490142	-5.0331778	3.1159412
C	0.9816089	-1.5366490	3.0012402
H	0.4188942	-1.3732510	3.9348769
H	0.6592041	-0.7741826	2.2766138
H	2.0506439	-1.3615641	3.2087538
H	3.3433192	3.1068464	1.3537257
H	4.0382725	1.2510515	-2.6022171
H	4.5130410	-0.8845504	-1.4679371
H	3.8436239	0.9377076	2.4129548
H	-4.5464764	4.1601746	0.7504300
C	-4.4415490	3.0858214	0.5908648
C	-4.0679394	0.3690299	0.1734432
C	-5.5429190	2.2157674	0.5705728
C	-3.1750766	2.5397722	0.3975705
N	-3.0520745	1.2277236	0.2068730
C	-5.3658864	0.8399240	0.3585056
H	-6.5490532	2.6145147	0.7194862
H	-6.2015569	0.1386964	0.3331436
C	-1.8467382	3.2600583	0.3809792
O	-1.7589486	4.4683799	0.5693154
C	-3.6222695	-1.0532647	-0.0789864
O	-4.4185185	-1.9812769	-0.1488699
N	-2.2666396	-1.1209924	-0.2050834
N	-0.8235390	2.3906748	0.1468223
Cu	-1.3385886	0.5615692	-0.1017983
H	0.9195291	0.5606700	-0.6555938
O	0.2678481	-0.1411951	-0.5025869
H	1.2664654	-2.2732157	-0.5511717
C	0.5269902	2.8011906	0.1953676
C	3.1844199	3.6269011	0.2844596
C	1.1940017	2.8427182	1.4459793
C	1.2002163	3.0938063	-1.0181529
C	2.5324816	3.5186861	-0.9461696
C	2.5246003	3.2791013	1.4653716
H	3.0748639	3.7591864	-1.8623849
H	3.0594674	3.3399638	2.4159711
H	4.2243861	3.9625233	0.3211905
C	-1.6019392	-2.3387459	-0.4366067
C	-0.3444976	-4.7793637	-0.9067792
C	-1.2476261	-3.1580556	0.6699511
C	-1.2775472	-2.7050916	-1.7656093

Cu^{III}(OH)(L)-DHA-RC

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

-3772.6905852519

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-3775.0223000453

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.854417

Chem. Pot.(298.15)/B3LYP-D3/def2-SVP(Cu:def2-TZVP)/COSMO(ε = 8.51):

0.781454

C	-0.6541352	-3.9414808	-1.9782999
C	-0.6302060	-4.3846160	0.4045153
H	-0.3988277	-4.2496556	-2.9954129
H	-0.3538488	-5.0428544	1.2290998
H	0.1436081	-5.7407197	-1.0895835
H	4.6859693	1.4498864	-0.8672130
C	4.2969817	0.5722047	-1.3886505
C	3.2936027	-1.6634311	-2.7091318
C	3.5951042	-0.3996016	-0.6607491
C	4.4873874	0.4396345	-2.7667638
C	3.9777361	-0.6816676	-3.4317125
C	3.0957629	-1.5354812	-1.3263613
H	5.0281321	1.2117830	-3.3208600
H	4.1174300	-0.7937578	-4.5105984
H	2.8988859	-2.5440653	-3.2245228
C	3.3254596	-0.2322284	0.8186576
H	2.3563560	0.2866314	0.9316357
H	4.0720589	0.4326372	1.2793945
C	2.3290021	-2.5748543	-0.5452103
H	2.3761038	-3.5530072	-1.0459778
C	3.2381257	-1.5434534	1.5660122
C	2.7660680	-2.6879182	0.8957219
C	3.5769610	-1.6297058	2.9245960
H	3.9430074	-0.7376735	3.4421684
C	3.4486807	-2.8349819	3.6218386
H	3.7116884	-2.8848933	4.6821704
C	2.6596421	-3.8980438	1.5966976
H	2.2962653	-4.7859625	1.0725610
C	2.9911214	-3.9763152	2.9526602
H	2.8939283	-4.9263055	3.4856989
C	0.4664402	2.9789145	-2.3474937
H	-0.3617858	2.2687138	-2.1954734
C	-0.1601599	4.3340414	-2.7276762
H	-0.7703104	4.2398180	-3.6414945
H	0.6277346	5.0825049	-2.9184978
H	-0.7995342	4.7174225	-1.9172605
C	1.3396245	2.4159850	-3.4766575
H	0.7246073	2.2381347	-4.3737527
H	1.8076290	1.4626210	-3.1864272
H	2.1445858	3.1123702	-3.7636404
C	0.4763260	2.4523494	2.7315031
H	-0.4296767	1.8973748	2.4416359
C	0.0243064	3.7093597	3.4989612
H	-0.5946622	4.3581404	2.8608429
H	0.8985028	4.2925016	3.8352582
H	-0.5622186	3.4314698	4.3905914
C	1.3060135	1.5147400	3.6221541
H	2.2220781	2.0014818	3.9947888

H	1.5994057	0.6011451	3.0838029
H	0.7147725	1.2104404	4.5010658
C	-1.5814483	-1.7825133	-2.9360256
H	-2.0384764	-0.8708217	-2.5240173
C	-2.6026665	-2.4118982	-3.8985588
H	-3.5317424	-2.6767366	-3.3680092
H	-2.2041509	-3.3290580	-4.3639471
H	-2.8564428	-1.7081478	-4.7088364
C	-0.2914186	-1.3515072	-3.6541852
H	0.2195616	-2.2108177	-4.1196559
H	0.4020805	-0.8829606	-2.9408323
H	-0.5196569	-0.6252196	-4.4524135
C	-1.4999174	-2.6768153	2.0938905
H	-2.4274763	-2.0832784	2.0748997
C	-1.7097027	-3.8112269	3.1050605
H	-2.0113026	-3.3945764	4.0796754
H	-0.7832411	-4.3852608	3.2710338
H	-2.4925052	-4.5126210	2.7740434
C	-0.3616693	-1.7435134	2.5570955
H	-0.6142257	-1.2726506	3.5214678
H	-0.1566232	-0.9524069	1.8222657
H	0.5745732	-2.3081925	2.6833516
H	-4.3875996	4.4701506	0.2489433
C	-4.3593110	3.3876107	0.1150968
C	-4.1860775	0.6369454	-0.2203201
C	-5.5252901	2.6099770	0.0289681
C	-3.1319236	2.7322152	0.0251228
N	-3.1094614	1.4123869	-0.1359735
C	-5.4514278	1.2184342	-0.1402512
H	-6.5025811	3.0942085	0.0956312
H	-6.3406513	0.5898146	-0.2089130
C	-1.7469194	3.3484558	0.0989489
O	-1.5897588	4.5535414	0.2757332
C	-3.8543843	-0.8333286	-0.4030641
O	-4.7487977	-1.6751256	-0.5051181
N	-2.5176383	-1.0352918	-0.4418602
N	-0.7767173	2.4064244	-0.0484987
Cu	-1.4024211	0.5727944	-0.2317894
H	0.9630622	0.4262429	-0.2232260
O	0.2786995	-0.2657232	-0.2465541
H	1.1085046	-1.3457375	-0.2381851
C	0.5916628	2.7557385	0.0288514
C	3.3197325	3.3579891	0.1709745
C	1.2145185	2.8702342	1.2983607
C	1.3392494	2.8946390	-1.1686916
C	2.7064147	3.1932184	-1.0712686
C	2.5771422	3.1909457	1.3438947

Cu^{III}(OH)(L)-DHA-TS

$E_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

-3772.6706428579 (<S^2> 0.47252884)

$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:

-3775.0009736851 (*S* = 0; <S^2> 0.49819223)

-3774.9891593620 (*S* = 1; <S^2> 2.01620343)

-3775.0048928311 (spin purified)

$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.84792

Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:

0.775156

H	3.3019439	3.2902012	-1.9822314
H	3.0762396	3.2847765	2.3117835
H	4.3860725	3.5922905	0.2280792
C	-1.9472513	-2.3157400	-0.6129496
C	-0.6670144	-4.7740402	-0.9514674
C	-1.8455493	-3.2000167	0.4912270
C	-1.4098002	-2.6519099	-1.8822813
C	-0.7687214	-3.8893162	-2.0277836
C	-1.2045756	-4.4314522	0.2919062
H	-0.3450672	-4.1735168	-2.9930191
H	-1.1172263	-5.1393880	1.1178494
H	-0.1631693	-5.7359476	-1.0807186
H	5.4782808	0.8938576	-1.0772452
C	4.8056130	0.1311232	-1.4798665
C	3.0911677	-1.8156170	-2.5129431
C	3.9221763	-0.5281009	-0.6170322
C	4.8336009	-0.1715452	-2.8453935
C	3.9760392	-1.1533944	-3.3622337
C	3.0493363	-1.5118073	-1.1381068
H	5.5271227	0.3550124	-3.5064170
H	3.9988129	-1.3981489	-4.4273604
H	2.4230557	-2.5858908	-2.9062237
C	3.8457932	-0.1777227	0.8505654
H	3.1643232	0.6905501	0.9598909
H	4.8192091	0.1888455	1.2128590
C	2.0715245	-2.1513848	-0.2343413
H	1.5815444	-3.0448247	-0.6436449
C	3.3296589	-1.2874976	1.7342622
C	2.4428079	-2.2471557	1.1896450
C	3.6656693	-1.3575326	3.0909689
H	4.3548973	-0.6194548	3.5120224
C	3.1278233	-2.3548036	3.9120077
H	3.3988335	-2.3941822	4.9704511
C	1.9036244	-3.2456777	2.0251358
H	1.2086154	-3.9724923	1.5982332
C	2.2435071	-3.3023090	3.3755486
H	1.8207706	-4.0825773	4.0140310
C	0.6923138	2.6847593	-2.5313398
H	-0.3847121	2.5384330	-2.3604293
C	0.8506551	3.9152598	-3.4389015
H	0.3115458	3.7637844	-4.3886765
H	1.9088473	4.1052225	-3.6843850
H	0.4467763	4.8189134	-2.9544379
C	1.2281305	1.4068600	-3.2019374
H	0.7300606	1.2378484	-4.1707294
H	1.0487962	0.5234922	-2.5715690
H	2.3134278	1.4689127	-3.3823158
C	0.4555361	2.5515993	2.5793645

H	-0.6063092	2.4408627	2.3184644	
C	0.5534047	3.6733751	3.6231110	
H	0.1916201	4.6265908	3.2054640	
H	1.5895307	3.8219308	3.9698538	
H	-0.0590372	3.4299270	4.5069383	
C	0.9240983	1.1943702	3.1387363	
H	1.9820172	1.2321859	3.4464990	
H	0.8268792	0.3995188	2.3829522	
H	0.3254262	0.9036978	4.0177239	
C	-1.5921123	-1.6992917	-3.0572062	
H	-1.5436308	-0.6757534	-2.6508112	
C	-2.9938900	-1.8810294	-3.6743214	
H	-3.7858657	-1.8125032	-2.9141181	
H	-3.0739338	-2.8735312	-4.1498927	
H	-3.1826369	-1.1169621	-4.4470593	
C	-0.5060986	-1.8055115	-4.1329061	
H	-0.5385631	-2.7728270	-4.6607672	
H	0.4979971	-1.6800347	-3.7027381	
H	-0.6487714	-1.0166917	-4.8888500	
C	-2.4094107	-2.7969637	1.8515980	
H	-3.3632389	-2.2820513	1.6562425	
C	-2.7288065	-3.9868625	2.7663685	
H	-3.2533885	-3.6354466	3.6694203	
H	-1.8140754	-4.5028548	3.1029198	
H	-3.3717689	-4.7269965	2.2635762	
C	-1.4779878	-1.8057778	2.5761186	
H	-1.9415331	-1.4506468	3.5113813	
H	-1.2491281	-0.9289364	1.9559796	
H	-0.5179396	-2.2824931	2.8265151	
H	-4.6723683	4.0474041	0.6974681	***Cu^{III}(OH)(L)-DHA-IC***
C	-4.5037916	2.9818076	0.5345273	**$E_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:**
C	-3.9803716	0.2848904	0.1196655	**-3772.7083616292 (<S^2> 1.03681583)**
C	-5.5498094	2.0448019	0.5538607	**$E_{B3LYP\text{-}D3/def2\text{-}TZVPP/COSMO(\varepsilon = 8.51)}$:**
C	-3.2117318	2.5100331	0.2989386	**-3775.0388727157 (*S* = 0; <S^2> 1.03541793)**
N	-3.0243584	1.2081759	0.1064914	**-3775.0388596882 (*S* = 1; <S^2> 2.03599411)**
C	-5.3000477	0.6784949	0.3464467	**-3775.0388866999 (spin purified)**
H	-6.5729445	2.3836702	0.7348453	**$ZPE_{B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:**
H	-6.0952281	-0.0684806	0.3591341	**0.852027**
C	-1.9226786	3.3208905	0.2531043	**Chem. Pot.$_{(298.15)/B3LYP\text{-}D3/def2\text{-}SVP(Cu:def2\text{-}TZVP)/COSMO(\varepsilon = 8.51)}$:**
O	-1.9344673	4.5323307	0.4816730	**0.778106**
C	-3.4666691	-1.1270265	-0.1306893	
O	-4.2494364	-2.0806569	-0.1623821	
N	-2.1275140	-1.1428436	-0.3069058	
N	-0.8582290	2.5393705	-0.0400871	
Cu	-1.2162489	0.6084766	-0.2015379	
H	1.4278080	0.5328603	-0.5709435	
O	0.6674398	-0.0415967	-0.3744494	

H	0.8830765	-0.9371731	-0.6832474
C	0.4569529	3.0608384	-0.0399043
C	3.0961804	3.9874720	-0.0468659
C	1.2326561	2.9661319	1.1418901
C	1.0062118	3.5883485	-1.2372085
C	2.3299005	4.0490910	-1.2148863
C	2.5517512	3.4435553	1.1172716
H	2.7757266	4.4661248	-2.1200091
H	3.1609778	3.3922548	2.0235894
H	4.1256092	4.3562952	-0.0497952
C	-1.4237614	-2.3370140	-0.5898623
C	0.0828548	-4.6191952	-1.1747057
C	-1.0563071	-3.2152635	0.4624393
C	-1.0148275	-2.5817522	-1.9270631
C	-0.2552065	-3.7303156	-2.1961636
C	-0.3152990	-4.3601540	0.1391281
H	0.0674978	-3.9416477	-3.2177145
H	-0.0315342	-5.0602040	0.9255036
H	0.6672986	-5.5153236	-1.4010732
H	4.1942935	1.5044484	-0.3112321
C	3.8654907	0.5983675	-0.8244352
C	2.9835951	-1.6991534	-2.1534294
C	3.7548061	-0.5942101	-0.1046343
C	3.5440153	0.6566985	-2.1888155
C	3.1140894	-0.5034404	-2.8536352
C	3.2871173	-1.7718999	-0.7654518
H	3.6246357	1.6054536	-2.7234278
H	2.8654059	-0.4631039	-3.9169232
H	2.6169694	-2.5960820	-2.6591719
C	4.1565565	-0.6658566	1.3479373
H	3.9540973	0.2927788	1.8499898
H	5.2604569	-0.7805513	1.3839516
C	3.0551065	-2.9625768	-0.0116484
H	2.7052148	-3.8548656	-0.5340635
C	3.5522042	-1.8149993	2.1196575
C	3.1066470	-2.9735670	1.4153530
C	3.4806824	-1.7913106	3.5140917
H	3.8027346	-0.8936543	4.0500649
C	3.0080040	-2.8970030	4.2331835
H	2.9540915	-2.8557895	5.3241100
C	2.6585514	-4.0960784	2.1609521
H	2.3284948	-4.9876994	1.6226760
C	2.6096252	-4.0578112	3.5495972
H	2.2489528	-4.9258896	4.1076831
C	0.1667352	3.6079409	-2.5109818
H	-0.8744961	3.7921120	-2.2034969
C	0.5544552	4.7199664	-3.4940696
H	-0.1707621	4.7605223	-4.3227600

H	1.5479374	4.5471170	-3.9402482
H	0.5696571	5.7059328	-3.0026412
C	0.2038157	2.2342354	-3.2090742
H	-0.4706985	2.2158571	-4.0807104
H	-0.1027530	1.4241711	-2.5310206
H	1.2225607	2.0008802	-3.5581085
C	0.6325011	2.4022485	2.4241096
H	-0.3254397	1.9325750	2.1547516
C	0.3138333	3.5375709	3.4131533
H	-0.3525109	4.2804553	2.9465599
H	1.2355282	4.0549920	3.7297327
H	-0.1818664	3.1431914	4.3160837
C	1.4998267	1.3051493	3.0565702
H	2.4824084	1.6866457	3.3802814
H	1.6666122	0.4805150	2.3481559
H	1.0009052	0.8831555	3.9438920
C	-1.4641355	-1.6443318	-3.0419587
H	-1.5574567	-0.6380795	-2.6016077
C	-2.8680392	-2.0455764	-3.5360314
H	-3.5817969	-2.1164651	-2.7015014
H	-2.8305973	-3.0313403	-4.0304561
H	-3.2513321	-1.3121152	-4.2651786
C	-0.4742238	-1.5341002	-4.2072837
H	-0.4009114	-2.4730755	-4.7800315
H	0.5336570	-1.2715944	-3.8514689
H	-0.8022425	-0.7489546	-4.9073536
C	-1.4311861	-2.8827303	1.9039575
H	-2.4472175	-2.4579277	1.8803392
C	-1.4742459	-4.1048337	2.8309381
H	-1.8796553	-3.8156014	3.8138831
H	-0.4676886	-4.5194376	3.0042083
H	-2.1102321	-4.9056428	2.4207217
C	-0.4834481	-1.8126785	2.4822828
H	-0.7841531	-1.5383396	3.5068133
H	-0.4849416	-0.8956191	1.8776503
H	0.5518896	-2.1841424	2.5186830

6. References

1. (a) *TURBOMOLE V6.6 2014, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from* http://www.turbomole.com; (b) F. Furche, R. Ahlrichs, C. Hättig, W. Klopper, M. Sierka and F. Weigend, *WIREs Comput. Mol. Sci.*, 2014, **4**, 91-100.
2. Y. Zhao and D. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
3. Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A*, 2008, **112**, 1095-1099.
4. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
5. M. Sierka, A. Hogekamp and R. Ahlrichs, *J. Chem. Phys.*, 2003, **118**, 9136-9148.
6. F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057-1065.

7. I. M. Alecu, J. Zheng, Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput.*, 2010, **6**, 2872-2887.
8. B. B. Averkiev and D. G. Truhlar, *Catal. Sci. Technol.*, 2011, **1**, 1526-1529.
9. H.-J. Werner, P. J. Knowles, G. Knizia, F. R. Manby and M. Schütz, *WIREs Comput. Mol. Sci.*, 2012, **2**, 242-253.
10. (a) E. Papajak and D. G. Truhlar, *J. Chem. Phys.*, 2012, **137**, 064110; (b) J. Zheng, P. Seal and D. G. Truhlar, *Chem. Sci.*, 2013, **4**, 200-212.
11. (a) T. B. Adler, G. Knizia and H.-J. Werner, *J. Chem. Phys.*, 2007, **127**, 221106; (b) G. Knizia, T. B. Adler and H.-J. Werner, *J. Chem. Phys.*, 2009, **130**, 054104.
12. (a) G. Knizia and H.-J. Werner, *J. Chem. Phys.*, 2008, **128**, 154103; (b) H.-J. Werner, T. B. Adler and F. R. Manby, *J. Chem. Phys.*, 2007, **126**, 164102.
13. (a) E. Papajak, J. Zheng, X. Xu, H. R. Leverentz and D. G. Truhlar, *J. Chem. Theory Comput.*, 2011, **7**, 3027-3034; (b) E. Papajak and D. G. Truhlar, *J. Chem. Theory Comput.*, 2010, **6**, 597-601; (c) E. Papajak and D. G. Truhlar, *J. Chem. Theory Comput.*, 2011, **7**, 10-18.
14. F. Weigend, *Phys. Chem. Chem. Phys.*, 2002, **4**, 4285-4291.
15. F. Weigend, A. Köhn and C. Hättig, *J. Chem. Phys.*, 2002, **116**, 3175-3183.
16. (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652; (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.
17. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
18. L. G. Gagliardi, C. B. Castells, C. Ràfols, M. Rosés and E. Bosch, *J. Chem. Eng. Data*, 2007, **52**, 1103-1107.
19. (a) T. M. Lowry and S. T. Henderson, *Proc. R. Soc. London Ser. A*, 1932, **136**, 471-487; (b) http://www.sigmaaldrich.com/chemistry/solvents/acetonitrile-center.html, Accessed June 7th 2016.
20. V. P. Pawar, *J. Chem. Eng. Data*, 2006, **51**, 882-885.
21. S. H. Canzonieri, M. A. Postigo, J. A. Salas and M. Katz, *J. Argent. Chem. Soc.*, 2002, **90**, 31-48.
22. A. Klamt and G. Schüürmann, *J. Chem. Soc., Perkin Trans. 2*, 1993, 799-805.
23. A. Klamt and V. Jonas, *J. Chem. Phys.*, 1996, **105**, 9972-9981.
24. (a) A. J. Johansson, M. R. A. Blomberg and P. E. M. Siegbahn, *J. Chem. Phys.*, 2008, **129**, 154301; (b) A. J. Johansson, M. R. A. Blomberg and P. E. M. Siegbahn, *J. Phys. Chem. C*, 2007, **111**, 12397-12406.
25. V. S. Bryantsev, M. S. Diallo and W. A. Goddard III, *J. Phys. Chem. B*, 2008, **112**, 9709-9719.
26. (a) T. Ziegler, A. Rauk and E. J. Baerends, *Theor. Chim. Acta*, 1977, **43**, 261-271; (b) L. Noodleman and J. G. Norman, *J. Chem. Phys.*, 1979, **70**, 4903-4906; (c) K. Yamaguchi, F. Jensen, A. Dorigo and K. N. Houk, *Chem. Phys. Lett.*, 1988, **149**, 537-542; (d) L. Noodleman and D. A. Case, in *Advances in Inorganic Chemistry*, ed. C. Richard, Academic Press, 1992, vol. Volume 38, pp. 423-470; (e) M. H. Lim, S. E. Worthington, F. J. Dulles and C. J. Cramer, in *Chemical Applications of Density-Functional Theory*, American Chemical Society, 1996, vol. 629, ch. 27, pp. 402-422; (f) H. Isobe, Y. Takano, Y. Kitagawa, T. Kawakami, S. Yamanaka, K. Yamaguchi and K. N. Houk, *Molecular Physics*, 2002, **100**, 717-727; (g) S. M. Huber, M. Z. Ertem, F. Aquilante, L. Gagliardi, W. B. Tolman and C. J. Cramer, *Chem. Eur. J.*, 2009, **15**, 4886-4895.
27. A. Hellweg, *J. Comput. Chem.*, 2013, **34**, 1835-1841.
28. J. England, Y. Guo, K. M. Van Heuvelen, M. A. Cranswick, G. T. Rohde, E. L.

Bominaar, E. Münck and L. Que, Jr., *J. Am. Chem. Soc.*, 2011, **133**, 11880-11883.
29. J. England, Y. Guo, E. R. Farquhar, V. G. Young, Jr., E. Münck and L. Que, Jr., *J. Am. Chem. Soc.*, 2010, **132**, 8635-8644.
30. D. Dhar, G. M. Yee, A. D. Spaeth, D. W. Boyce, H. Zhang, B. Dereli, C. J. Cramer and W. B. Tolman, *J. Am. Chem. Soc.*, 2016, **138**, 356-368.
31. (a) G. Knizia and J. E. M. N. Klein, *Angew. Chem. Int. Ed.*, 2015, **54**, 5518-5522; (b) G. Knizia, *http://www.iboview.org/*.
32. P. J. Donoghue, J. Tehranchi, C. J. Cramer, R. Sarangi, E. I. Solomon and W. B. Tolman, *J. Am. Chem. Soc.*, 2011, **133**, 17602-17605.
33. J. Le Bras, H. Jiao, W. E. Meyer, F. Hampel and J. A. Gladysz, *J. Organomet. Chem.*, 2000, **616**, 54-66.