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Supporting Information

Dramatic Influence of an Anionic Donor on the Oxygen-Atom Transfer Reactivity of an Mn^V–Oxo Complex

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Supporting Information

Materials. All reactions were performed under an argon atmosphere using dry solvents and standard Schlenk techniques. The $(TBP_8Cz)Mn^{III}$ and $(TBP_8Cz)Mn^{V}(O)$ complexes were synthesized according to published methods.[1] Solvents were purified via a Pure-Solv solvent purification system from Innovative Technologies, Inc. Dichloromethane and toluene were distilled under argon over calcium hydride. $H_2^{18}O$ (97% ^{18}O) was purchased from Cambridge Isotopes, Inc. All other reagents were purchased from Sigma-Aldrich at the highest level of purity and were used as received.

Instrumentation. UV-vis spectroscopy was performed on a Hewlett-Packard 8542 diode-array spectrophotometer equipped with HP Chemstation software. A 400 nm longpass filter was placed directly between the sample quartz cuvette and the spectrophotometer light source to prevent decomposition of the $[(TBP_8Cz)Mn^{V}(O)(CN)]^{-}$ complex. The temperature dependent kinetics were performed on a Hewlett Packard 8453 diode-array spectrophotometer, equipped with an Unisoku USP-203A cryostat, using a 1 cm modified Schlenk cuvette. Gas chromatography mass spectrometry (GC-MS) was carried out and recorded using a Hewlett-Packard 6890 series gas chromatograph system, equipped with a 5973N mass selective detector. Laser desorption ionization with a time-of-flight analyzer (LDI-TOF) was conducted on a Bruker Autoflex III TOF/TOF instrument, equipped with a nitrogen laser at 335 nm using an MTP 384 ground steel target plate.

X-ray Absorption Spectroscopy (XAS) Sample Preparation. A solution of $(TBP_8Cz)Mn^{V}(O)$ (10 mM) in benzonitrile (200 µL) at 25 °C was combined with $Bu_4N^{+}CN^{-}$ (10 or 100 equiv). Samples were loaded into 150 microliter Delrin XAS cells with 38 micron Kapton windows, immediately frozen in liquid nitrogen, and stored at 77 K until XAS measurements were performed.

X-ray Absorption Spectroscopy Data Collection. All XAS data were recorded at the Stanford Synchrotron Radiation Laboratory (SSRL) on focused beam line 9-3. A Si(220) monochromator was used for energy selection. A Rh-coated mirror (set to a cutoff of 10 keV) was used for harmonic rejection, in combination with 25% detuning of the monochromator. All data were measured in transmission mode to k = 12 Å^{-1}, stopping at the Fe K-edge. Internal energy calibration was performed by simultaneous measurement of the absorption of a Mn foil placed between a second and third ionization chamber. The first inflection point of the Mn foil was assigned to 6539.0 eV. Samples were monitored for photoreduction throughout the course of data collection. Only those scans that showed no evidence of photoreduction were used in the final averages. The averaged data were processed as described previously.[2] A second-order polynomial was fit to the pre-edge region and subtracted from the entire spectrum. A three-region cubic spline was used to model the background above the edge using the program PySpline.[3] Theoretical EXAFS spectra were calculated using FEFF.[4],[5] The resulting spectra were fit to the data using EXAFSPAK[6] as described previously.[2]

Product Analysis for Thioanisole Oxidation. In a typical reaction, a stirring solution of (TBP$_8$Cz)Mn^V(O) (5 mM) in toluene (1 mL) was combined with $Bu_4N^+CN^-$ (5 mM) at 25 °C. A stock solution of dodecane in toluene (0.1 M) was prepared and 20 µL of the stock solution was added to the reaction as an internal standard. To initiate the reaction, thioanisole (8 M) was added, and isosbestic conversion of [(TBP$_8$Cz)Mn^V(O)(CN)]$^-$ (λ_{max} = 419, 634 nm) to [(TBP$_8$Cz)Mn^{III}(CN)]$^-$ (λ_{max} = 443, 492, 694 nm) was observed by sampling of the reaction mixture and analysis by UV-vis spectroscopy. Upon completion of the reaction, the solution was concentrated to ~50 µL under vacuum, and immediately analyzed by GC-FID. The product methyl phenyl sulfoxide, (MPSO) was identified by comparison with an authentic sample. Yields were obtained by comparing the integration of the product peak with the integration of the internal standard peak and comparison with a dodecane calibration curve. The yield of 84% for MPSO is an average of two runs.

Preparation of [$(TBP_8Cz)Mn^V(^{18}O)(CN)]^-$ and Reaction with Thioanisole. Following an earlier report,[7] 30 μL of $H_2{}^{18}O$ was added to a solution of $(TBP_8Cz)Mn^V(O)$ (3 mM) in dry CH_2Cl_2 (5 mL). The solution was then stirred vigorously for 48 h to ensure complete exchange of the terminal oxo group with $H_2{}^{18}O$. The reaction was analyzed by LDI-MS (LDI-TOF: isotopic cluster centered at *m/z* 1427.8) and fitting of the isotopic distribution pattern gave an ^{18}O incorporation of 78%. The ^{18}O labeled sample was dried under vacuum for 48 h. The solid $(TBP_8Cz)Mn^V(^{18}O)$ was then dissolved in dry toluene (1.6 mL) and $Bu_4N^+CN^-$ (1 equiv) was added. A mass spectrometry sample was taken out and analyzed by LDI-MS (LDI-TOF: isotopic cluster centered at *m/z* 1453.4) and fitting of the isotopic distribution pattern gave an ^{18}O incorporation of 35%. The addition of $Bu_4N^+CN^-$ likely introduces residual H_2O, accounting for lower ^{18}O incorporation in the 6-coordinate complex. The OAT reaction was initiated by the addition of excess thioanisole (1.6 M) and progress was monitored by thin layer chromatography (TLC), showing complete conversion of $[(TBP_8Cz)Mn^V(O)(CN)]^-$ (R_f = 0.9, CH_2Cl_2 neat on silica) to $[(TBP_8Cz)Mn^{III}(CN)]^-$ (R_f = 0.2, CH_2Cl_2 neat on silica) after stirring for 19 h. The solution was then concentrated to ~50 μL under vacuum and analyzed directly by GC-MS. Peaks for the labeled and unlabeled product methyl phenyl sulfoxide were observed at *m/z* 140.2 and 142.2, and their area ratio gave an ^{18}O incorporation of 71% based on total ^{18}O label in the starting complex. The ^{18}O incorporation percentage is an average of two runs.

Kinetic Measurements. In a typical reaction, a solution of $(TBP_8Cz)Mn^V(O)$ (11 μM) in dry toluene (2 mL) was combined with $Bu_4N^+CN^-$ (11 mM) at 25 °C and excess dibutyl sulfide

(DBS) was added immediately to initiate the reaction. In the absence of substrate, the $[(TBP_8Cz)Mn^V(O)(CN)]^-$ complex decays to $[(TBP_8Cz)Mn^{III}(CN)]^-$ after ~25 min under the same conditions. Thus the concentration of DBS was maintained such that the OAT reactions were completed in 5-15 minutes. The changes in absorbance were monitored by UV-vis spectroscopy, and showed isosbestic decay of $[(TBP_8Cz)Mn^V(O)(CN)]^-$ (λ_{max} = 419, 634 nm) and the formation of $[(TBP_8Cz)Mn^{III}(CN)]^-$ (λ_{max} = 443, 492, 694 nm). The pseudo-first-order rate constants, k_{obs}, were obtained by nonlinear least-squares fitting of plots of the growth in absorbance of $[(TBP_8Cz)Mn^{III}(CN)]^-$ at (694 nm) or decay of $[(TBP_8Cz)Mn^V(O)(CN)]^-$ (634 nm) versus time to eq. 1:

$$Abs_t = Abs_f + (Abs_0 - Abs_f)\exp(-k_{obs}t) \qquad \text{Eq. 1}$$

where Abs_f = final absorbance, Abs_0 = initial absorbance and Abs_t = absorbance at time (t). Second-order rate constants were obtained from the slope of the best-fit line of the linear plot of k_{obs} versus substrate concentration.

Temperature Dependence of the Rate Constants. A solution of $(TBP_8Cz)Mn^V(O)$ (13 μM) in dry toluene (2 mL) was combined with DBS (21 mM), and brought to the desired temperature. The reaction was then initiated by the addition of $Bu_4N^+CN^-$ (13 mM) and the temperature was maintained at ±0.1°C throughout the reaction. The changes in absorbance were monitored by UV-vis spectroscopy showing the isosbestic decay of $[(TBP_8Cz)Mn^V(O)(CN)]^-$ (λ_{max} = 419, 634 nm) and formation of $[(TBP_8Cz)Mn^{III}(CN)]^-$ (λ_{max} = 443, 492, 694 nm). The pseudo-first-order (k_{obs}) rate constants were obtained over a sixty-degree temperature range (40 to -20 °C). The pseudo-first-order rate constant at each temperature was divided by the concentration of substrate to yield a second-order rate constant (*k*). Activation parameters were determined from the plot of ln(*k*/T) vs 1/T.

Computational Methods. All calculations were performed using the Orca or Gaussian-09 program packages.[8],[9]

TD-DFT Calculations for XAS Pre-edge Transitions. Optimized geometries of $^{1}[(H_8Cz)Mn^{V}(O)]$ and $^{1}[(H_8Cz)Mn^{V}(O)(CN)]^{-}$ were obtained using the unrestricted hybrid-GGA UB3LYP[10] with dispersion correction (D3).[11] A relativistic effective core potential basis set SDD[12] was used for Mn, and a split-valence double-ζ basis set with one set of polarization functions 6-31G(d)[13] was used for the remaining atoms. This combination of functional and basis sets has been shown to give good results on transition metal complexes.[14] The resolution of identity (RIJ) and the chain-of-sphere (COSX) approximations on the correlation and the exchange interaction, respectively, with auxiliary basis sets of Karlsruhe double-ζ quality (def2-SVP/J and def2-SVP/C, respectively),[15] were used to improve the wall clock time with neglectable error being introduced.[16] Single point energy calculations followed by TD-DFT were performed using the optimized geometry according to the literature.[17] For the TD-DFT, the unrestricted hybrid-meta-GGA UTPSSh[18] functional with the scalar-relativistically recontracted (SARC)[19] version of the Karlsruhe basis set def2-TZVP(-f)[20] ("def2" version of the triplet-ζ basis set with one set of the angular momentum deleted) was applied to all atoms. Zero-order regular approximation was applied to recontract the basis set to account for relativistic effects and the integration grid was increased to 4. The RIJCOSX approximation with the decontracted auxiliary basis set def2-TZVP/J[15] was applied to Coulomb and exchange correlations of the electrons. Solvent effect was modeled using the conductor-like screening model (COSMO)[21] with a dielectric constant of 26.0 and refractive index of 1.528 for benzonitrile. For TD-DFT, the donor core orbital (Mn 1s) was localized and 100 excitations from the donor into the lowest unoccupied orbitals were performed to cover as many transitions as possible that could gave rise to the pre-edge feature in the XAS experiment. Transitions through quadruple moments were included in the calculation. The TammDancoff approximation[22] for TD-DFT was applied by default in Orca. The result of the TD-DFT calculations was plotted using orca_mapspc application using 3 eV Gaussian broadening to facilitate visual comparison to the experiment. An up-shift of 36.3 eV for the calculated spectrum was applied according to the literature[17] in order to fit the transition energy of the pre-edge.

Gaussian Calculations on Spin-state Ordering and Reactivity. The oxygen-atom transfer reactivity with dimethylsulfide (DMS) as a model substrate and $[(H_8Cz)Mn^V(O)(L)]$ with L = no ligand or CN^- was investigated by DFT calculations. We followed procedures as previously applied to manganese corrolazine complexes[7][23] that have been well tested and generally reproduce experimental free energies of activation to within 3 – 4 kcal mol^{-1}.[24] Geometries were optimized in Gaussian-09 using the unrestricted B3LYP[25] density functional method in combination with an LACVP basis set on manganese and 6-31G on the rest of the atoms, basis set BS1. An analytical frequency at the same level confirmed the structures as local minima (with real frequencies only) or first-order saddle points with a single imaginary frequency for the correct mode. To improve the quality of the energy calculations, we ran single point calculations on the optimized structures using an LACV3P+ basis set on manganese and 6-311+G* on the rest of the atoms, basis set BS2. Subsequently, we also did single points at UB3LYP/BS2 using the conductor polarized continuum model in Gaussian with a dielectric constant mimicking toluene to match the experimental kinetics. In addition, we investigated the effects of dispersion on the reaction energies by doing a single point UB3LYP-D3/BS2 calculation using the model of Grimme as implemented in Gaussian.[11]

As computational chemistry methods can be sensitive to the choice of the density functional method,[26] we did geometry optimizations and calculated spin-state orderings using UB3LYP,[25] UBP86[27] and M06[28] for a selection of structures, see details below. As follows, only minor differences in optimized geometries are observed, although some variation in the spin-state ordering is observed. Because of this variation, it was judged necessary to do a series of supporting *ab initio* multireference calculations, vide infra. We also tested the effect of the peripheral substituents on the spin-state ordering, geometries and relative energies by extending our model from $[(H_8Cz)Mn^V(O)(L)]$ to $[(Me_8Cz)Mn^V(O)(L)]$ and $[(MP_8Cz)Mn^V(O)(L)]$ for L = no ligand and $CN^–$, Me = methyl, and MP = *p*-methylphenyl. To test the effect of the basis set on the optimized geometries we ran calculations at UB3LYP/BS2 and UB3LYP/BS1. In agreement with previous studies, only minor differences were obtained.[29]

Orca calculations on *ab initio* multiconfiguration (MC) studies of $^1[(H_8Cz)Mn(O)(CN)]^-$ and $^3[(H_8Cz)Mn(O)(CN)]^-$: To study the energy ordering of the singlet and triplet spin states of $[(H_8Cz)Mn(O)(CN)]^-$ complete active space self-consistent field (CASSCF) calculations with different sizes of active space were performed to recover the static correlation of the system. Dynamic correlation of $[(H_8Cz)Mn(O)(CN)]^-$ was recovered using the *N*-electron valence second-order perturbation theory (NEVPT2) upon the converged MC wavefunctions from CASSCF (CASCI). The geometries of the singlet and triplet spin states were obtained from B3LYP/BS1. The resolution of identity approximation and the chain-of-sphere approximation (RIJCOSX) were applied to the Coulomb and exchange correlation, respectively, with auxiliary basis set corresponding to each atomic basis set throughout the calculations below. The initial guess of the MOs was obtained from DFT calculations using the BP86 density functional and a cc-pVTZ basis set on Mn and cc-pVDZ on the rest of the atoms, and integral grid of “4” and

COSX grid of “4” (notation in Orca) with molecular orbitals and unrestricted Hartree-Fock natural orbitals (UNO) for the singlet and triplet states, respectively. Choices of the active space followed literature precedent with slight modifications.[30] CASSCF calculations were performed utilizing the same basis set and grids as for DFT. Two different sizes of active space were obtained: the smaller active space of 10 electrons in 9 orbitals (10,9), which included all five Mn orbitals and four ligand orbitals giving rise to 9 LCAO-MOs, d_{xz}, d_{yz}, d_{xz}*, and d_{yz}* from combination of 2 Mn d_{π} orbitals with 2 O p_{π} orbitals, d_{z2} and d_{z2}* from Mn d_{z2} orbital and one of the two e_g-like LCAO of the first coordination sphere, d_{x2-y2} and d_{x2-y2}* from Mn d_{x2-y2} orbital and the other e_g-like LCAO of the first coordination sphere, the d_{xy} orbital does not have the right symmetry to interact with any ligand-based orbitals of close energy to form any significant MOs so it stayed AO-like; the larger active space of 12 electrons in 11 orbitals (12,11) includes all the orbitals in the smaller set and the HOMO and LUMO of the corrolazine π orbitals, which are of the a'' symmetry. Multireference perturbation theory of the *N*-electron valence type (NEVPT2) was applied on top of the converged CASSCF wavefunctions. For NEVPT2 calculations, integral transformation was performed using auxiliary basis set RI. CI vectors were truncated with a thresh of 1×10^{-10} before entering the third order density matrix and 1×10^{-14} before the fourth order density matrix, and each state was canonicalized before entering the perturbation treatment.

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Table S1. EXAFS fit results.

$(TBP_8Cz)Mn^V(O)$			$[(TBP_8Cz)Mn^V(O)(CN)]^-$		
	R / Å	σ^2 / Å^2		R / Å	σ^2 / Å^2
1 Mn-O	1.54	0.0032	1 Mn-O	1.53	0.0027
4 Mn-N	1.87	0.0027	4 Mn-N	1.87	0.0074
			1Mn-C/N	2.21	0.0014
8 MnC/N	2.88	0.0105	8 MnC/N	2.86	0.0043
16 MnC/N	3.00	0.0084	16 MnC/N	3.07	0.0049
6 MnC/N	3.29	0.0012	6 MnC/N	3.27	0.0014
ΔE_0 (eV)	-3.7		ΔE_0 (eV)	-3.6	
Error[a]	0.314		Error[a]	0.287	

[a] EXAFS error is defined as: $\boldsymbol{F} = [\, \sum k^6 (\chi_{exptl} - \chi_{calcd})^2 / \sum k^6 \chi_{exptl}^2 \,]^{1/2}$

EXAFS Fitting Results. Table S1 summarizes the best fits for the $(TBP_8Cz)Mn^V(O)$ and $[(TBP_8Cz)Mn^V(O)(CN)]^-$ complexes. For $(TBP_8Cz)Mn^V(O)$ the error value increases from 0.31 with inclusion of a short Mn-O vector to 0.49 when this vector is not included. Similarly for the $[(TBP_8Cz)Mn^V(O)(CN)]^-$, exclusion of the short Mn-O increases the fit error from 0.29 to 0.40, providing clear evidence for the presence of a short Mn-O bond in both complexes. Fits were also attempted in which the long 2.21 Å Mn-C/N vector was excluded from the $[(TBP_8Cz)Mn^V(O)(CN)]^-$ fits. These fits resulted in a modest increase in the error from 0.29 to 0.33. We also note that the increase in coordination number is further supported by the increase in outershell scattering (due to coordinated CN) and the decrease in pre-edge intensity (consistent with a more centrosymmetric 6-coordinate environment).

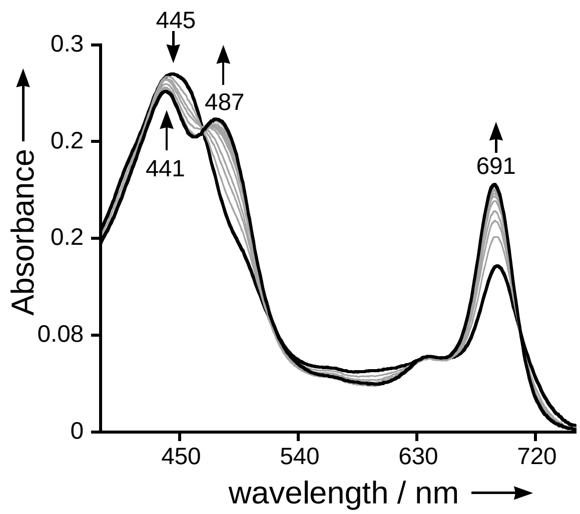


Figure S1. UV-vis spectral changes for the reaction of (TBP$_8$Cz)Mn^{III} (4.0 μM) + Bu$_4$N$^+$CN$^-$ (0.1-1.0 equiv) to give [(TBP$_8$Cz)Mn^{III}(CN)]$^-$ (441, 487, 691 nm) in toluene at 25 °C.

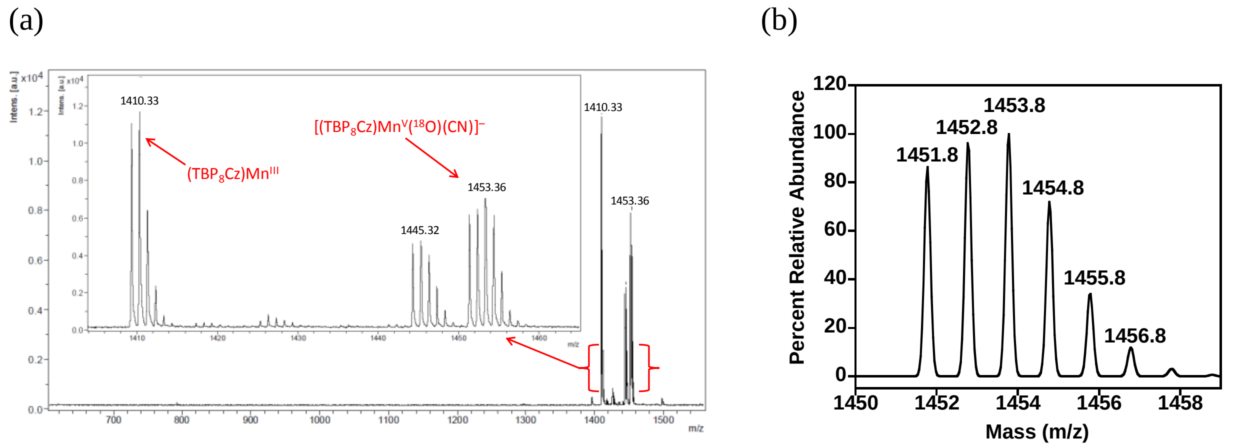


Figure S2. (a) LDI-Mass spectrum of $[(TBP_8Cz)Mn^V(^{18}O)(CN)]^-$. (b) Isotopic distribution for $[(TBP_8Cz)Mn^V(O)(CN)]^-$ showing ^{18}O incorporation of 35%.

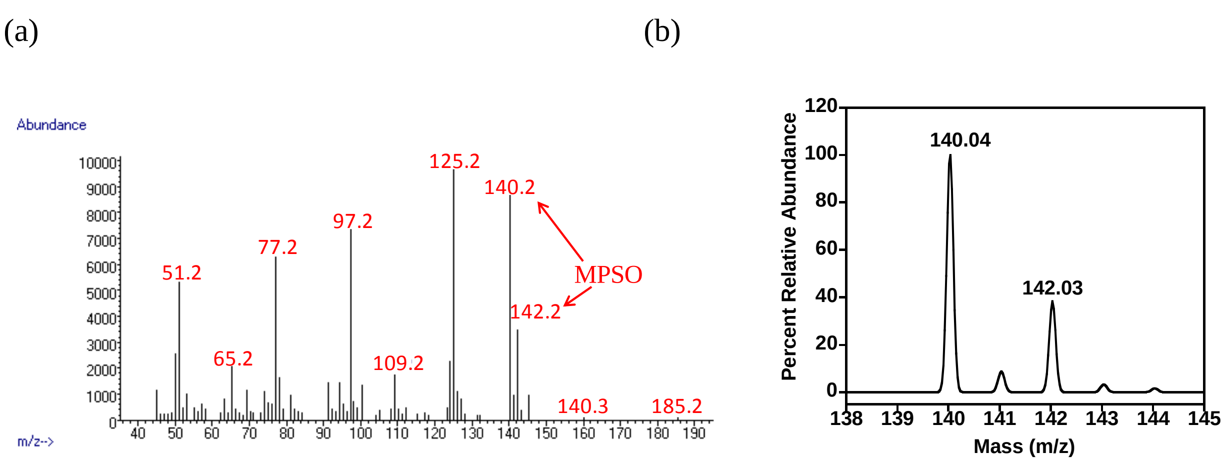


Figure S3. (a) GC-MS for the methyl phenyl sulfoxide product from the OAT reaction of $[(TBP_8Cz)Mn^V(O)(CN)]^-$ (^{18}O 35%) with thioanisole as the substrate. (b) Isotopic distribution of methyl phenyl sulfoxide showing ^{18}O incorporation of 25%.

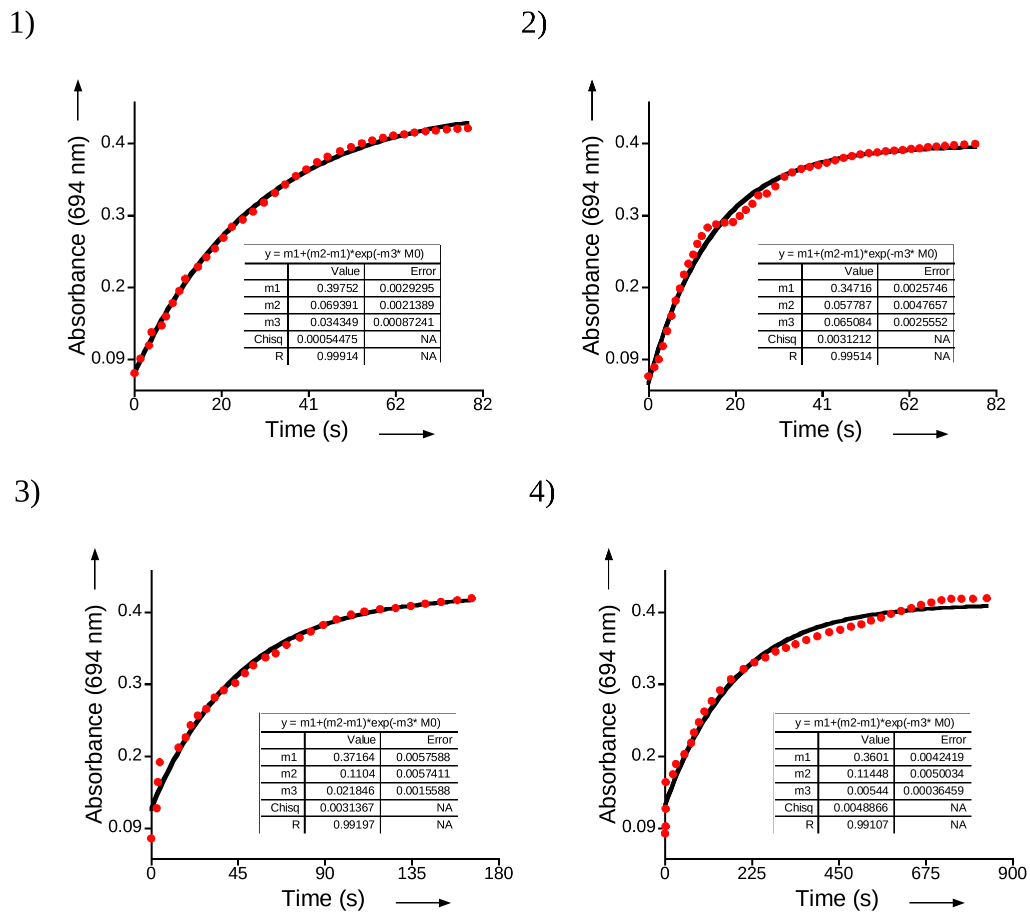


Figure S4. Changes in absorbance versus time for the growth of $[(TBP_8Cz)Mn^{III}(CN)]^-$ (694 nm) during the reaction of $[(TBP_8Cz)Mn^{V}(O)(CN)]^-$ with [DBS] = 1) 5.7 mM, 2) 8.6 mM, 3) 3.4 mM, and 4) 2.0 mM. Red circles = experimental data, solid black line = best fit.

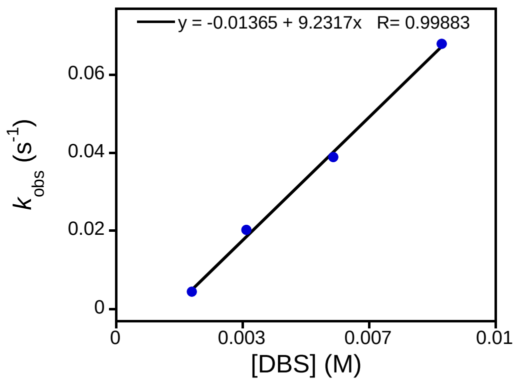


Figure S5. Plot of k_{obs} versus concentration of DBS with best fit line.

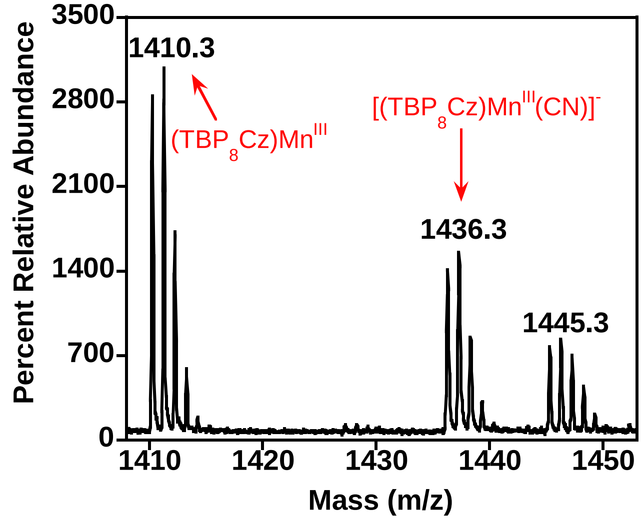


Figure S6. LDI-Mass spectrum of the completed reaction mixture for the reaction of $[(TBP_8Cz)Mn^{V}(O)(CN)]^{-}$ with DBS (5.7 mM).

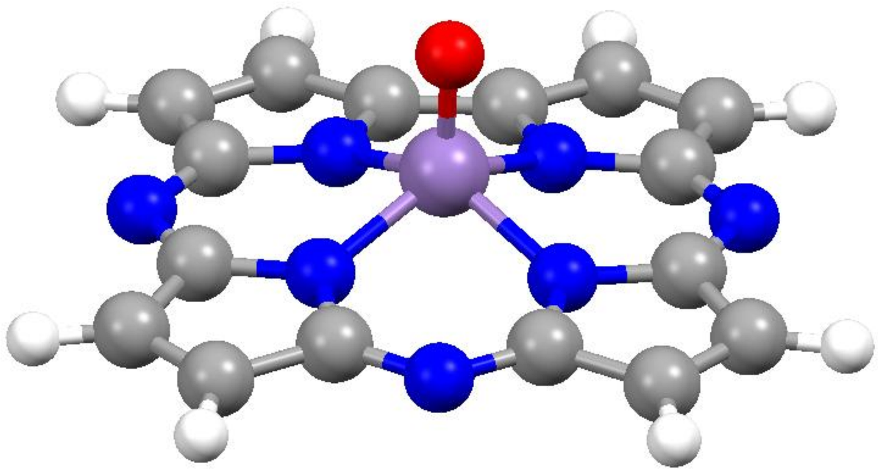


Fig S7. Optimized geometry for $^{1}[(H_8Cz)Mn^{V}(O)]$ using RIJCOSX-B3LYP-D3/SDD/6-31G(d).

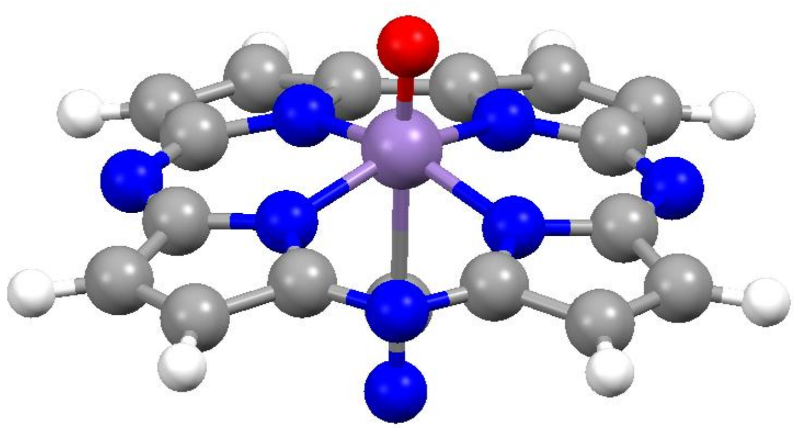


Fig S8. Optimized geometry for $^{1}[(H_8Cz)Mn^{V}(O)(CN)]^{-}$ using RIJCOSX-B3LYP-D3/SDD/6-31G(d).

Table S2. Selected molecular parameters from optimized geometries of singlet $(H_8Cz)Mn^V(O)$ and $[(H_8Cz)Mn^V(O)(CN)]^-$ using Orca with RIJCOSX-B3LYP-D3/SDD/6-31G(d). Distances shown in Å.

	Mn-O	Mn-L	$Mn\text{-}N_{av}$	Δ_{Mn}
$[(H_8Cz)Mn^V(O)]$	1.519		1.884	0.659
$[(H_8Cz)Mn^V(O)(CN)]^-$	1.548	2.192	1.896	0.525

Table S3. Spin densities from optimized geometries of singlet $(H_8Cz)Mn^V(O)$ and $[(H_8Cz)Mn^V(O)(CN)]^-$ using Orca with RIJCOSX-B3LYP-D3/SDD/6-31G(d).

Singlet spin states:	ρ(Mn)	ρ(O)	ρ(Cz)	ρ(L)
$[(H_8Cz)Mn^V(O)]$	0.00	0.00	0.00	
$[(H_8Cz)Mn^V(O)(CN)]^-$	0.00	0.00	0.00	0.00

Table S4. Fragment charges from optimized geometries of singlet $(H_8Cz)Mn^V(O)$ and $[(H_8Cz)Mn^V(O)(CN)]^-$ using Orca with RIJCOSX-B3LYP-D3/SDD/6-31G(d).

Singlet spin states:	*Q*(Mn)	*Q*(O)	*Q*(Cz)	*Q*(L)
$[(H_8Cz)Mn^V(O)]$	1.14	-0.37	-0.77	
$[(H_8Cz)Mn^V(O)(CN)]^-$	0.42	-0.39	-0.89	-0.13

Table S5. Comparison between selected molecular parameters from EXAFS of $(TBP_8Cz)Mn^V(O)$ and $[(TBP_8Cz)Mn^V(O)(CN)]^-$ versus those from optimized geometries of singlet $(H_8Cz)Mn^V(O)$ and $[(H_8Cz)Mn^V(O)(CN)]^-$ using Orca with RIJCOSX-B3LYP-D3/SDD/6-31G(d).

	$(Cz)Mn^V(O)$		$[(Cz)Mn^V(O)(CN)]^-$	
	EXAFS	DFT	EXAFS	DFT
Mn-O (Å)	1.54	1.519	1.53	1.548
Mn-N (Å)	1.87	1.884	1.87	1.896
Mn-C/N (Å)			2.21	2.192

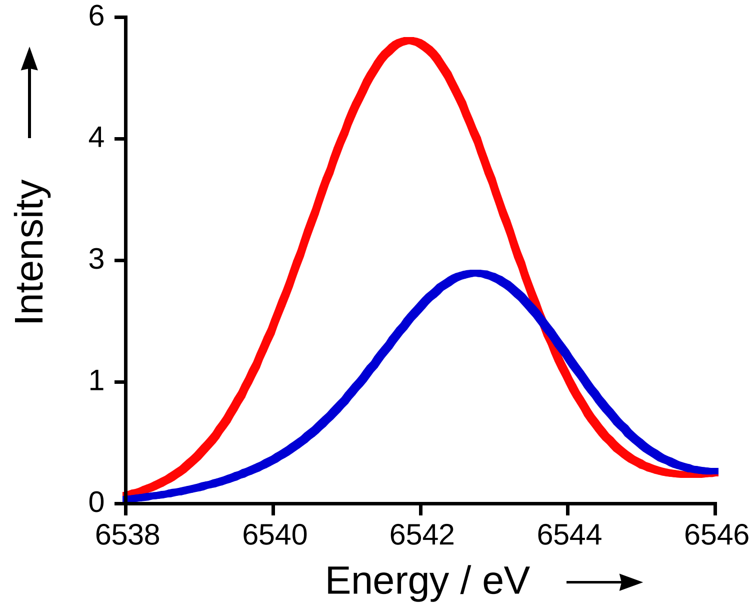


Fig S9. Calculated pre-edge absorption bands (TD-DFT) for $^1[(H_8Cz)Mn^V(O)]$ (blue) and $^1[(H_8Cz)Mn^V(O)(CN)]^-$ (red). The intensity does not reflect the normalized intensity from the experiment. The excitation energies are shifted to higher energy by 36.3 eV according to literature.[17]

Table S6. Optimized geometries of peripherally substituted manganese(V)-oxo corrolazines with MePh = *p*-methylphenyl, Me = methyl or H for systems without axial ligand or with CN^{-} as axial ligand. Data obtained through a full geometry optimization in Gaussian-09 with either B3LYP, BP86 or M06 methods in combination with basis set BS1.

Singlet spin states:	B3LYP:				BP86:				M06:			
	Mn-O	Mn-L	Mn-N_{av}	Δ_{Mn}	Mn-O	Mn-L	Mn-N_{av}	Δ_{Mn}	Mn-O	Mn-L	Mn-N_{av}	Δ_{Mn}
$[((MePh)_8Cz)Mn^V(O)(CN)]^{-}$	1.579	2.158	1.894	0.316	1.605	2.150	1.897	0.319	1.571	2.149	1.882	0.323
$[((MePh)_8Cz)Mn^V(O)]$	1.554		1.884	0.544	1.577		1.888	0.526	1.544		1.869	0.529
$[(Me_8Cz)Mn^V(O)(CN)]^{-}$	1.577	2.176	1.890	0.327	1.601	2.166	1.892	0.327	1.569	2.160	1.880	0.332
$[(Me_8Cz)Mn^V(O)]$	1.553		1.882	0.570	1.575		1.885	0.563	1.554		1.881	0.564
$[(H_8Cz)Mn^V(O)(CN)]^{-}$	1.576	2.168	1.889	0.328	1.598	2.173	1.891	0.332	1.570	2.106	1.886	0.333
$[(H_8Cz)Mn^V(O)]$	1.550		1.883	0.569	1.570		1.887	0.566	1.539		1.871	0.561

Triplet spin states:	B3LYP:				BP86:				M06:			
	Mn-O	Mn-L	Mn-N_{av}	Δ_{Mn}	Mn-O	Mn-L	Mn-N_{av}	Δ_{Mn}	Mn-O	Mn-L	Mn-N_{av}	Δ_{Mn}
$[((MePh)_8Cz)Mn^V(O)(CN)]^{-}$	1.813	2.049	1.893	0.035	1.668	2.088	1.906	0.265	1.819	2.043	1.885	0.158
$[((MePh)_8Cz)Mn^V(O)]$	1.623		1.896	0.257	1.621		1.900	0.493	1.634		1.886	0.490
$[(Me_8Cz)Mn^V(O)(CN)]^{-}$	1.821	2.057	1.886	0.011	1.670	2.090	1.900	0.251	1.818	2.052	1.881	0.167
$[(Me_8Cz)Mn^V(O)]$	1.621		1.891	0.320	1.622		1.893	0.501	1.643		1.880	0.491
$[(H_8Cz)Mn^V(O)(CN)]^{-}$	1.824	2.051	1.885	0.023	1.670	2.080	1.898	0.243	1.815	2.048	1.881	0.163
$[(H_8Cz)Mn^V(O)]$	1.633		1.889	0.483	1.620		1.892	0.497	1.646		1.880	0.483

Table S7. Group spin densities and charges of peripherally substituted manganese(V)-oxo corrolazines with MePh = *p*-methylphenyl, Me = methyl or H for systems without axial ligand or with CN^- as axial ligand. Data obtained with B3LYP.

(a) *Spin densities*

triplet	ρ(Mn)	ρ(O)	ρ(Cz)	ρ(L)
$[(MePh_8Cz)Mn^V(O)(CN)]^-$	2.83	-0.86	0.06	-0.03
$[(MePh_8Cz)Mn^V(O)]$	2.21	-0.19	-0.02	-
$[(Me_8Cz)Mn^V(O)(CN)]^-$	2.84	-0.88	0.07	-0.03
$[(Me_8Cz)Mn^V(O)]$	2.19	-0.20	0.01	-
$[(H_8Cz)Mn^V(O)(CN)]^-$	2.86	-0.88	0.06	-0.03
$[(H_8Cz)Mn^V(O)]$	2.30	-0.32	0.02	-

(b) *Charges*

triplet	*Q*(Mn)	*Q*(O)	*Q*(Cz)	*Q*(L)
$[(MePh_8Cz)Mn^V(O)(CN)]^-$	0.73	-0.28	-1.15	-0.31
$[(MePh_8Cz)Mn^V(O)]$	1.07	-0.32	-0.75	-
$[(Me_8Cz)Mn^V(O)(CN)]^-$	0.71	-0.29	-1.10	-0.32
$[(Me_8Cz)Mn^V(O)]$	1.07	-0.32	-0.75	-
$[(H_8Cz)Mn^V(O)(CN)]^-$	0.71	-0.28	-1.11	-0.32
$[(H_8Cz)Mn^V(O)]$	1.07	-0.30	1.23	-

Table S8. Absolute (in au) and relative (in kcal mol^{-1}) energies of manganese(V)-oxo complexes in the singlet and triplet spin states with different corrolazine description.

B3LYP Results.

	BS1 E [au]	BS1 ZPE [au]	BS2 E [au]
Singlet:			
[(MePh$_8$Cz)Mn^V(O)(CN)]	-3431.991984	1.107094	-3433.555524
[(MePh$_8$Cz)Mn^V(O)]	-3339.144932	1.100991	-3340.645461
[(Me$_8$Cz)Mn^V(O)(CN)]	-1583.959692	0.456008	-1584.739108
[(Me$_8$Cz)Mn^V(O)]	-1491.125212	0.450230	-1491.840698
[(H$_8$Cz)Mn^V(O)(CN)]	-1269.478113	0.233621	-1270.127637
[(H$_8$Cz)Mn^V(O)]	-1176.635009	0.227895	-1177.220228
Triplet:			
[(MePh$_8$Cz)Mn^V(O)(CN)]	-3431.978888	1.104349	-3433.550095
[(MePh$_8$Cz)Mn^V(O)]	-3339.133523	1.099398	-3340.637066
[(Me$_8$Cz)Mn^V(O)(CN)]	-1583.946834	0.453118	-1584.732102
[(Me$_8$Cz)Mn^V(O)]	-1491.111615	0.448233	-1491.830838
[(H$_8$Cz)Mn^V(O)(CN)]	-1269.489329	0.231695	-1270.088264
[(H$_8$Cz)Mn^V(O)]	-1176.616592	0.225426	-1177.194338

	ΔE	ΔE+ZPE	ΔE	ΔE+ZPE
Singlet:	BS1	BS1	BS2	BS2
[(MePh$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(MePh$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
[(Me$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(Me$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
[(H$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(H$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
Triplet:				
[(MePh$_8$Cz)Mn^V(O)(CN)]	8.22	6.50	3.41	1.68
[(MePh$_8$Cz)Mn^V(O)]	7.16	6.16	5.27	4.27
[(Me$_8$Cz)Mn^V(O)(CN)]	8.07	6.26	4.40	2.58
[(Me$_8$Cz)Mn^V(O)]	8.53	7.28	6.19	4.93
[(H$_8$Cz)Mn^V(O)(CN)]	-7.04	-8.25	24.71	23.50
[(H$_8$Cz)Mn^V(O)]	11.56	10.01	16.25	14.70

Table S9. Absolute (in au) and relative (in kcal mol^{-1}) energies of manganese(V)-oxo complexes in the singlet and triplet spin states with different corrolazine description.

BP86 Results.

	BS1 E [au]	BS1 ZPE [au]	BS2 E [au]
Singlet:			
[(MePh$_8$Cz)Mn^V(O)(CN)]	-3432.205535	1.073675	-3433.674967
[(MePh$_8$Cz)Mn^V(O)]	-3339.349251	1.068811	-3340.757608
[(Me$_8$Cz)Mn^V(O)(CN)]	-1584.162377	0.455067	-1584.899341
[(Me$_8$Cz)Mn^V(O)]	-1491.121155	0.449191	-1491.995081
[(H$_8$Cz)Mn^V(O)(CN)]	-1269.690348	0.226027	-1270.306915
[(H$_8$Cz)Mn^V(O)]	-1176.837502	0.225441	-1177.393190
Triplet:			
[(MePh$_8$Cz)Mn^V(O)(CN)]	-3432.191417	1.072777	-3433.667770
[(MePh$_8$Cz)Mn^V(O)]	-3339.326321	1.067101	-3340.740549
[(Me$_8$Cz)Mn^V(O)(CN)]	-1584.150247	0.441479	-1584.889769
[(Me$_8$Cz)Mn^V(O)]	-1491.125080	0.434974	-1491.972654
[(H$_8$Cz)Mn^V(O)(CN)]	-1269.679262	0.225026	-1270.297099
[(H$_8$Cz)Mn^V(O)]	-1176.795971	0.218743	-1177.382711

	ΔE	ΔE+ZPE	ΔE	ΔE+ZPE
Singlet:	BS1	BS1	BS2	BS2
[(MePh$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(MePh$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
[(Me$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(Me$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
[(H$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(H$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
Triplet:				
[(MePh$_8$Cz)Mn^V(O)(CN)]	8.86	8.30	4.52	3.95
[(MePh$_8$Cz)Mn^V(O)]	14.39	13.32	10.71	9.63
[(Me$_8$Cz)Mn^V(O)(CN)]	7.61	-0.91	6.01	-2.52
[(Me$_8$Cz)Mn^V(O)]	-2.46	-11.38	14.07	5.15
[(H$_8$Cz)Mn^V(O)(CN)]	6.96	6.33	6.16	5.53
[(H$_8$Cz)Mn^V(O)]	26.06	21.86	6.58	2.37

Table S10. Absolute (in au) and relative (in kcal mol^{-1}) energies of manganese(V)-oxo complexes in the singlet and triplet spin states with different corrolazine description.

M06 Results.

	BS1 E [au]	BS1 ZPE [au]	BS2 E [au]
Singlet:			
[(MePh$_8$Cz)Mn^V(O)(CN)]	-3429.624538	1.105786	-3431.079827
[(MePh$_8$Cz)Mn^V(O)]	-3336.829484	1.099020	-3338.223232
[(Me$_8$Cz)Mn^V(O)(CN)]	-1583.957214	0.458342	-1583.696190
[(Me$_8$Cz)Mn^V(O)]	-1491.125181	0.450416	-1490.850984
[(H$_8$Cz)Mn^V(O)(CN)]	-1268.728049	0.234077	-1269.338981
[(H$_8$Cz)Mn^V(O)]	-1175.935321	0.228259	-1176.484848
Triplet:			
[(MePh$_8$Cz)Mn^V(O)(CN)]	-3429.657681	1.101811	-3431.094108
[(MePh$_8$Cz)Mn^V(O)]	-3336.815024	1.095606	-3338.205183
[(Me$_8$Cz)Mn^V(O)(CN)]	-1582.948193	0.453414	-1583.709349
[(Me$_8$Cz)Mn^V(O)]	-1490.162898	0.446456	-1490.836738
[(H$_8$Cz)Mn^V(O)(CN)]	-1268.748190	0.231534	-1269.350973
[(H$_8$Cz)Mn^V(O)]	-1175.911628	0.224969	-1176.470582

	ΔE	ΔE+ZPE	ΔE	ΔE+ZPE
Singlet:	BS1	BS1	BS2	BS2
[(MePh$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(MePh$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
[(Me$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(Me$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
[(H$_8$Cz)Mn^V(O)(CN)]	0.00	0.00	0.00	0.00
[(H$_8$Cz)Mn^V(O)]	0.00	0.00	0.00	0.00
Triplet:				
[(MePh$_8$Cz)Mn^V(O)(CN)]	-8.14	-10.64	-8.96	-11.46
[(MePh$_8$Cz)Mn^V(O)]	9.07	6.93	11.33	9.18
[(Me$_8$Cz)Mn^V(O)(CN)]	15.18	12.08	-8.26	-11.35
[(Me$_8$Cz)Mn^V(O)]	16.79	14.31	8.94	6.45
[(H$_8$Cz)Mn^V(O)(CN)]	-12.64	-14.23	-7.53	-9.12
[(H$_8$Cz)Mn^V(O)]	14.87	12.80	8.95	6.89

Table S11. Absolute energies along the reaction mechanism of DMS sulfoxidation by $[(H_8Cz)Mn(O)CN]^-$ as obtained with Gaussian-09.

	From UB3LYP/BS1 freq:		BS2//BS1
	E [au]	ZPE [au]	E [au]
$^1[Mn^V(O)(Cz)CN]^-$	-1269.478148	0.233601	-1270.131529
$^1RC_{CN}$	-1747.455612	0.311231	-1748.193316
$^1TS_{SO,CN}$	-1747.423017	0.309701	-1748.167815
$^1P_{CN}$	-1747.431900	0.310220	-1748.199134

Table S12. Relative energies along the reaction mechanism of DMS sulfoxidation by $[(H_8Cz)Mn(O)CN]^-$ as obtained with Gaussian-09 in the gas-phase.

	ΔE	ΔE+ZPE	ΔE	ΔE+ZPE
	[BS1]	[BS1]	[BS2]	[BS2]
$^1\mathbf{RC}_{CN}$	-5.72	-5.07	-4.05	-3.39
$^1\mathbf{TS}_{SO,CN}$	14.73	14.43	11.95	11.65
$^1\mathbf{P}_{CN}$	9.16	9.18	-7.70	-7.68

Table S13. Group spin densities and charges of optimized geometries (UB3LYP/BS1) along the sulfoxidation mechanism of DMS by $[(H_8Cz)Mn(O)(CN)]^-$.

Spin densities:	ρ_{Mn}	ρ_O	ρ_{Cz}	ρ_L	ρ_{DMS}
$^1[Mn^V(O)(Cz)CN]^-$	0.00	0.00	0.00	0.00	
$^1\mathbf{RC}_{CN}$	0.00	0.00	0.00	0.00	0.00
$^1\mathbf{TS}_{SO,CN}$	0.04	-0.01	-0.01	-0.01	-0.01
$^1\mathbf{P}_{CN}$	0.00	-0.01	0.00	0.00	0.00

Charges:	Q_{Mn}	Q_O	Q_{Cz}	Q_L	Q_{DMS}
$^1[Mn^V(O)(Cz)CN]^-$	0.47	-0.27	-0.98	-0.21	
$^1\mathbf{RC}_{CN}$	0.48	-0.30	-0.96	-0.20	-0.02
$^1\mathbf{TS}_{SO,CN}$	0.58	-0.47	-1.36	-0.28	0.53
$^1\mathbf{P}_{CN}$	0.67	-0.60	-1.48	-0.36	0.78

Table S14. Group spin densities and charges of single point UB3LYP/BS2 on UB3LYP/BS1 optimized geometries along the mechanism of DMS sulfoxidation by $^{1}[(H_8Cz)Mn(O)(CN)]^{-}$.

Spin densities:	ρ_{Mn}	ρ_{O}	ρ_{Cz}	ρ_{L}	ρ_{DMS}
$^{1}[Mn^{V}(O)(Cz)CN]^{-}$	0.00	0.00	0.00	0.00	
^{1}**RC**$_{CN}$	0.00	0.00	0.00	0.00	0.00
^{1}**TS**$_{SO,CN}$	0.00	0.00	-0.02	0.01	0.01
^{1}**P**$_{CN}$	0.00	-0.01	0.01	0.00	0.00

Charges:	Q_{Mn}	Q_{O}	Q_{Cz}	Q_{L}	Q_{DMS}
$^{1}[Mn^{V}(O)(Cz)CN]^{-}$	-2.33	0.02	3.45	-2.14	
^{1}**RC**$_{CN}$	-3.20	0.10	4.37	-2.20	-0.07
^{1}**TS**$_{SO,CN}$	-1.10	0.03	0.09	-0.41	0.39
^{1}**P**$_{CN}$	-0.31	-0.01	-0.56	-0.60	0.48

Table S15. Absolute energies along the reaction mechanism of DMS sulfoxidation by $[(H_8Cz)Mn(O)]$ as obtained with Gaussian-09 as obtained with B3LYP.

	E [au]	ZPE [au]	E [au]
$^1[Mn^V(O)(Cz)]$	-1176.635104	0.227955	-1177.224190
^{1}**RC**$_{NL}$	-1654.604826	0.304846	-1655.281048
^{1}**TS**$_{SO,NL}$	-1654.562834	0.302900	-1655.250474
^{1}**P**$_{NL}$	-1654.562751	0.303678	-1655.259882

Table S16. Relative energies along the reaction mechanism of DMS sulfoxidation by $[(H_8Cz)Mn(O)]$ as obtained with Gaussian-09 as obtained with B3LYP in the gas phase.

	ΔE	ΔE+ZPE	ΔE	ΔE+ZPE
	[BS1]	[BS1]	[BS2]	[BS2]
^{1}**RC**$_{NL}$	-0.87	-0.67	-0.96	-0.76
^{1}**TS**$_{SO,NL}$	25.48	24.46	18.23	17.20
^{1}**P**$_{NL}$	25.54	25.00	12.33	11.79

Table S17. Relative energies (in kcal mol^{-1}) along the reaction mechanism of DMS sulfoxidation by either $[(H_8Cz)Mn(O)]$ or $[(H_8Cz)Mn(O)(CN)]^-$ as obtained in Gaussian after a single point in solvent with a toluene dielectric constant.

	ΔE_s+ZPE
	[BS2]
^{1}**RC**$_{CN}$	-0.3
^{1}**TS**$_{SO,CN}$	10.1
^{1}**P**$_{CN}$	-9.7
^{1}**RC**$_{NL}$	-0.7
^{1}**TS**$_{SO,NL}$	21.1
^{1}**P**$_{NL}$	15.3

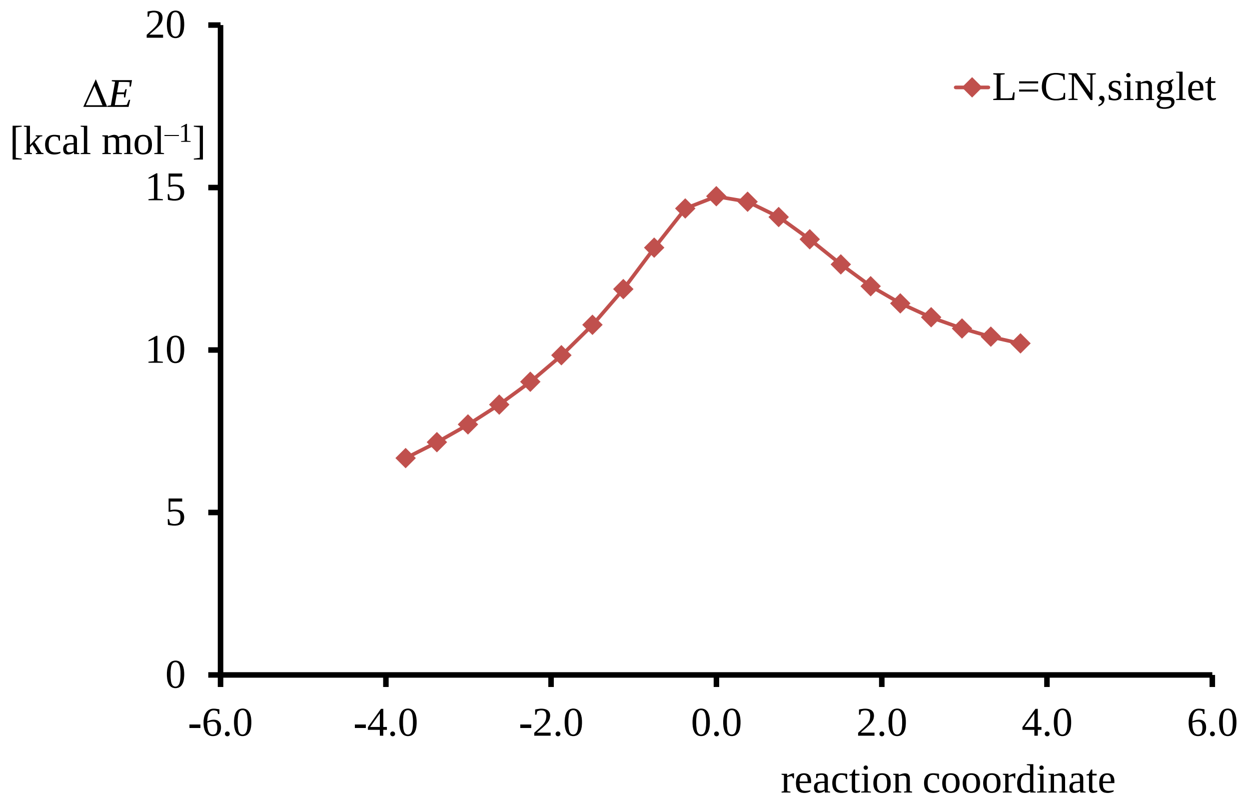


Figure S10. IRC scan starting from $^{1}\mathbf{TS}_{SO,CN}$ as calculated at UB3LYP/BS1 in Gaussian. The reaction starts on the left-hand-side with reactants and proceeds via the TS to a radical intermediate. Energies are calculated in kcal/mol.

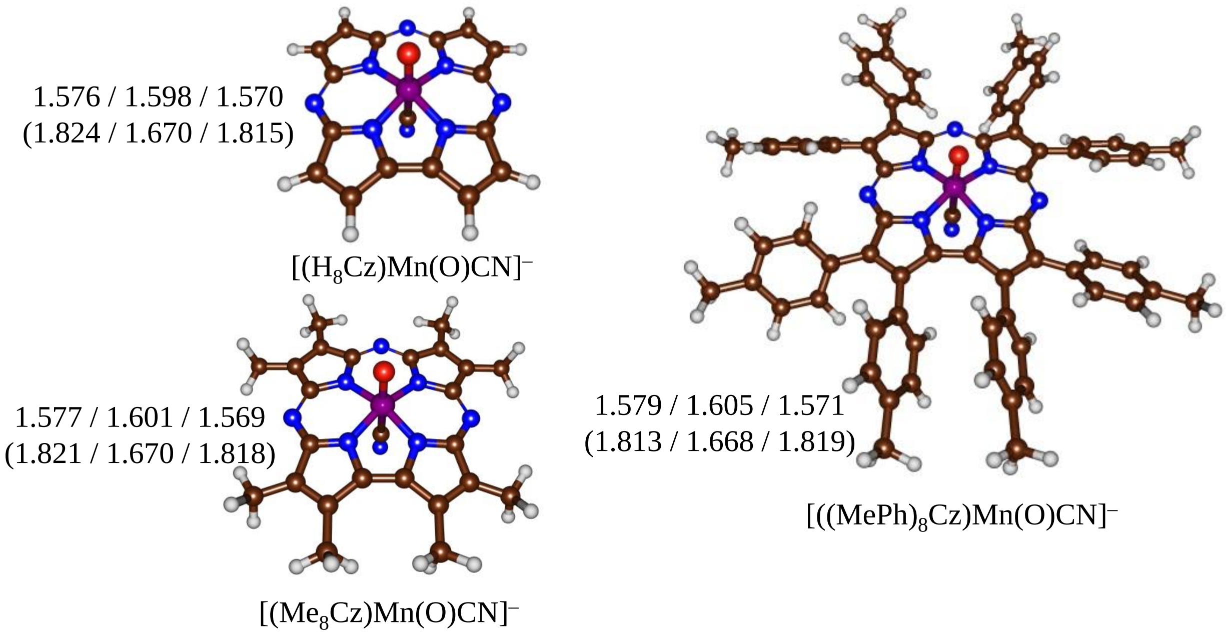
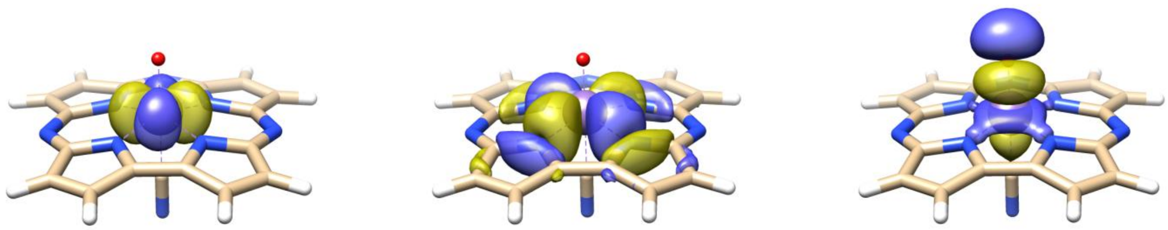
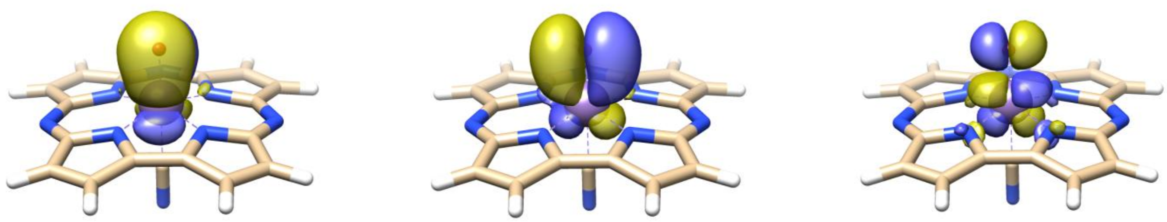


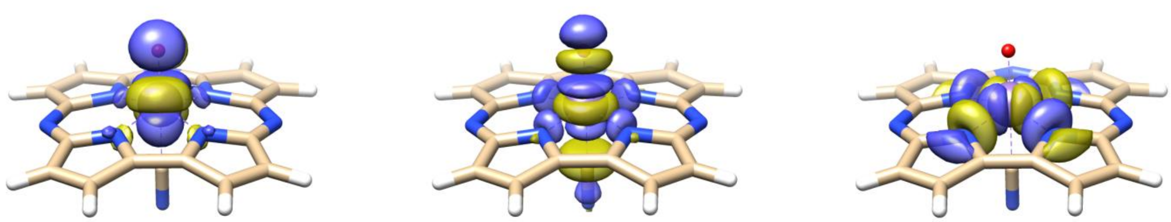
Figure S11. Optimized geometries of $^{1,3}[(R_8Cz)Mn^{V}(O)CN]^{-}$ with R = H, Me or MePh with bond lengths in angstroms ($^{3}[(R_8Cz)Mn^{V}(O)CN]^{-}$ lengths in parentheses). The three sets of data represent B3LYP, BP86 and M06 optimized geometries.



Mn 3d$_{xy}$ [1.975001] Mn 3d$_{x2-y2}$ [1.972651] Mn 3d$_{z2}$ [1.924957]

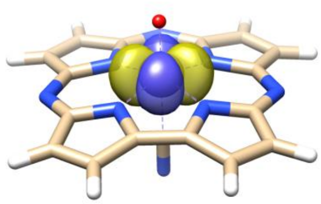


Mn 3d$_{yz}$ [1.861523] Mn 3d$_{xz}$ [1.858944] Mn 3d$_{xz}$* [0.151159]

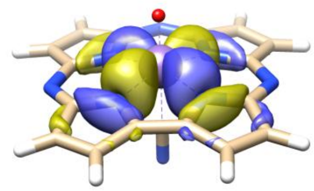


Mn 3d$_{yz}$* [0.146417] Mn 3d$_{z2}$* [0.078829] Mn 3d$_{x2-y2}$* [0.030519]

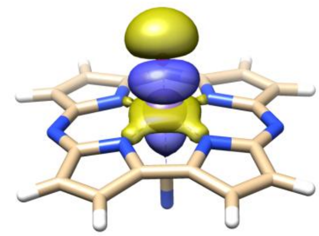
Figure S12. Active natural orbitals of $^{1}[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(10,9)/cc-pVTZ/cc-pVDZ. The opposite phases are shown in either blue or yellow.



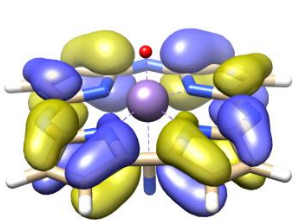
Mn 3d_{xy} [1.974953]



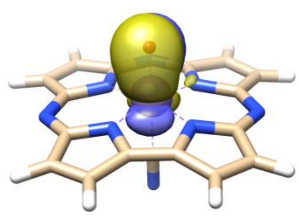
Mn 3d_{x2-y2} [1.971932]



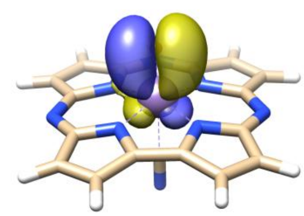
Mn 3d_{z2} [1.924922]



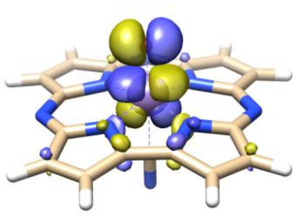
Cz a'' [1.887589]



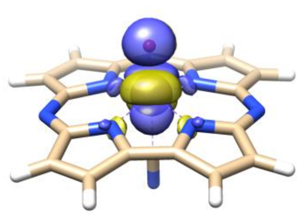
Mn 3d_{yz} [1.861443]



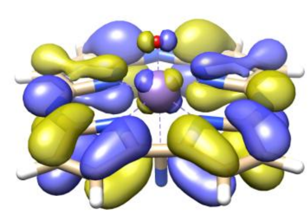
Mn 3d_{xz} [1.859111]



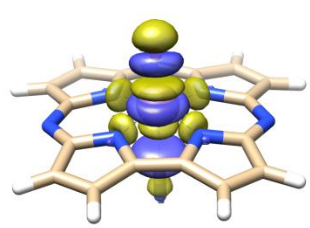
Mn 3d_{xz}* [0.154040]



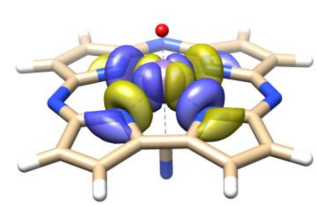
Mn 3d_{yz}* [0.146413]



Cz a'' [0.109659]



Mn 3d_{z2}* [0.078859]



Mn 3d_{x2-y2}* [0.031079]

Figure S13. Active natural orbitals of $^{1}[(H_8Cz)Mn(O)(CN)]^{-}$ from RIJCOSX-CASSCF(12,11)/cc-pVTZ/cc-pVDZ. The opposite phases are shown in either blue or yellow.

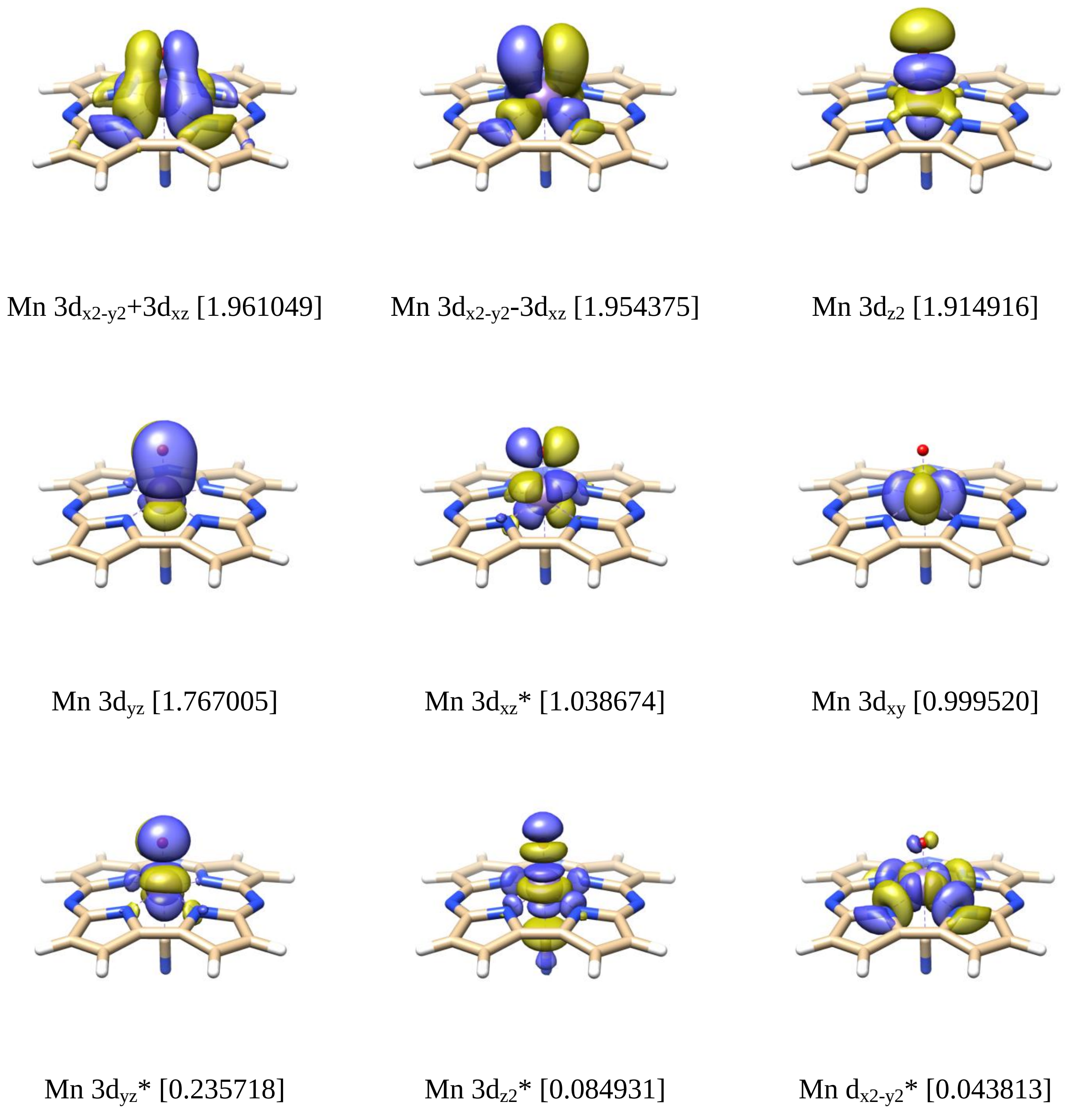
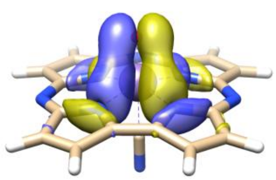
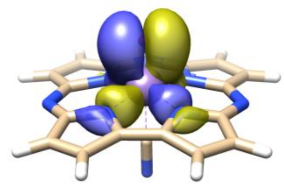


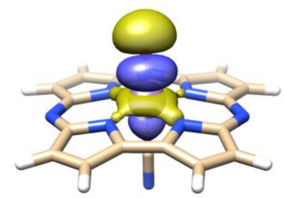
Figure S14. Active natural orbitals of $^{3}[(H_8Cz)Mn(O)(CN)]^{-}$ from RIJCOSX-CASSCF(10,9)/cc-pVTZ/cc-pVDZ using the optimized geometry of $^{1}[(H_8Cz)Mn(O)(CN)]^{-}$. The opposite phases are shown in either blue or yellow.



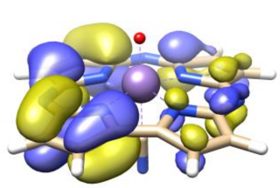
Mn $3d_{x2-y2}+3d_{xz}$ [1.960308]



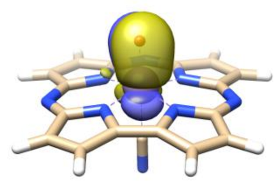
Mn $3d_{x2-y2}-d_{xz}$ [1.954265]



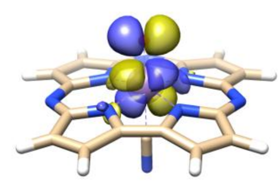
Mn $3d_{z2}$ [1.914919]



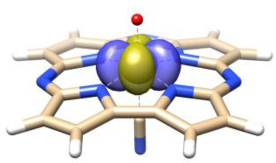
Cz a'' [1.885676]



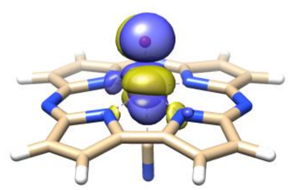
Mn $3d_{yz}$ [1.766834]



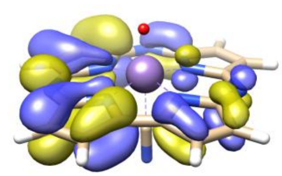
Mn $3d_{xz}$* [1.038569]



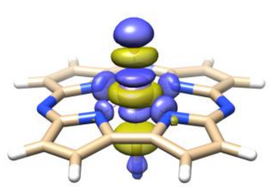
Mn $3d_{xy}$ [0.999511]



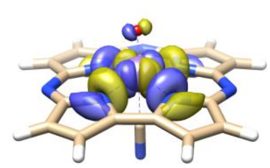
Mn $3d_{yz}$* [0.236022]



Cz a'' [0.114514]

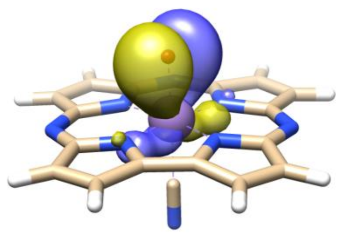
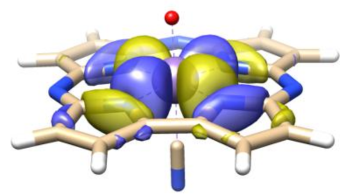
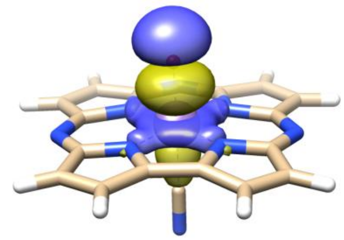


Mn $3d_{z2}$* [0.084989]

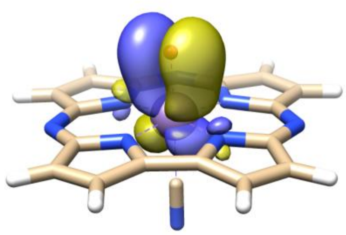
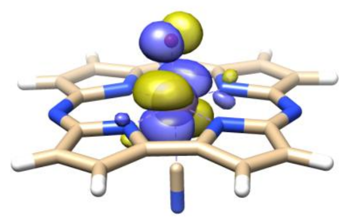
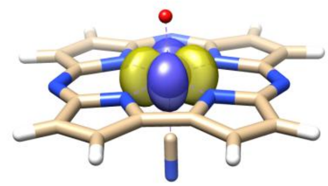


Mn $3d_{x2-y2}$* [0.044393]

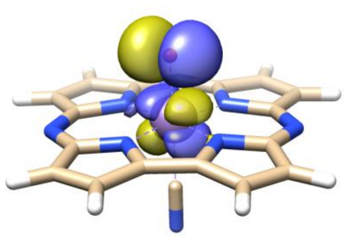
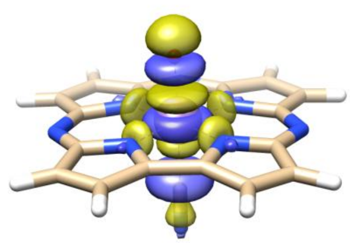
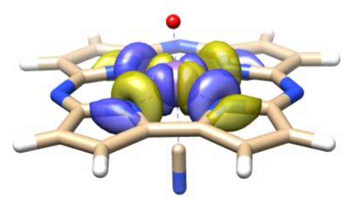
Figure S15. Active natural orbitals of $^{3}[(H_8Cz)Mn(O)(CN)]^{-}$ from RIJCOSX-CASSCF(12,11)/cc-pVTZ/cc-pVDZ using the optimized geometry of $^{1}[(H_8Cz)Mn(O)(CN)]^{-}$. The opposite phases are shown in either blue or yellow.

Mn $3d_{xz}$ [1.977523] Mn $3d_{x2-y2}$ [1.955870] Mn $3d_{z2}$ [1.886001]

Mn $3d_{yz}$ [1.404638] Mn $3d_{xz}^{*}$ [1.020547] Mn $3d_{xy}$ [0.999852]

Mn $3d_{yz}^{*}$ [0.596532] Mn $3d_{z2}^{*}$ [0.114226] Mn $3d_{x2-y2}^{*}$ [0.044812]

Figure S16. Active natural orbitals of $^3[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(10,9)/cc-pVTZ/cc-pVDZ using the optimized geometry of $^3[(H_8Cz)Mn(O)(CN)]^-$. The opposite phases are shown in either blue or yellow.

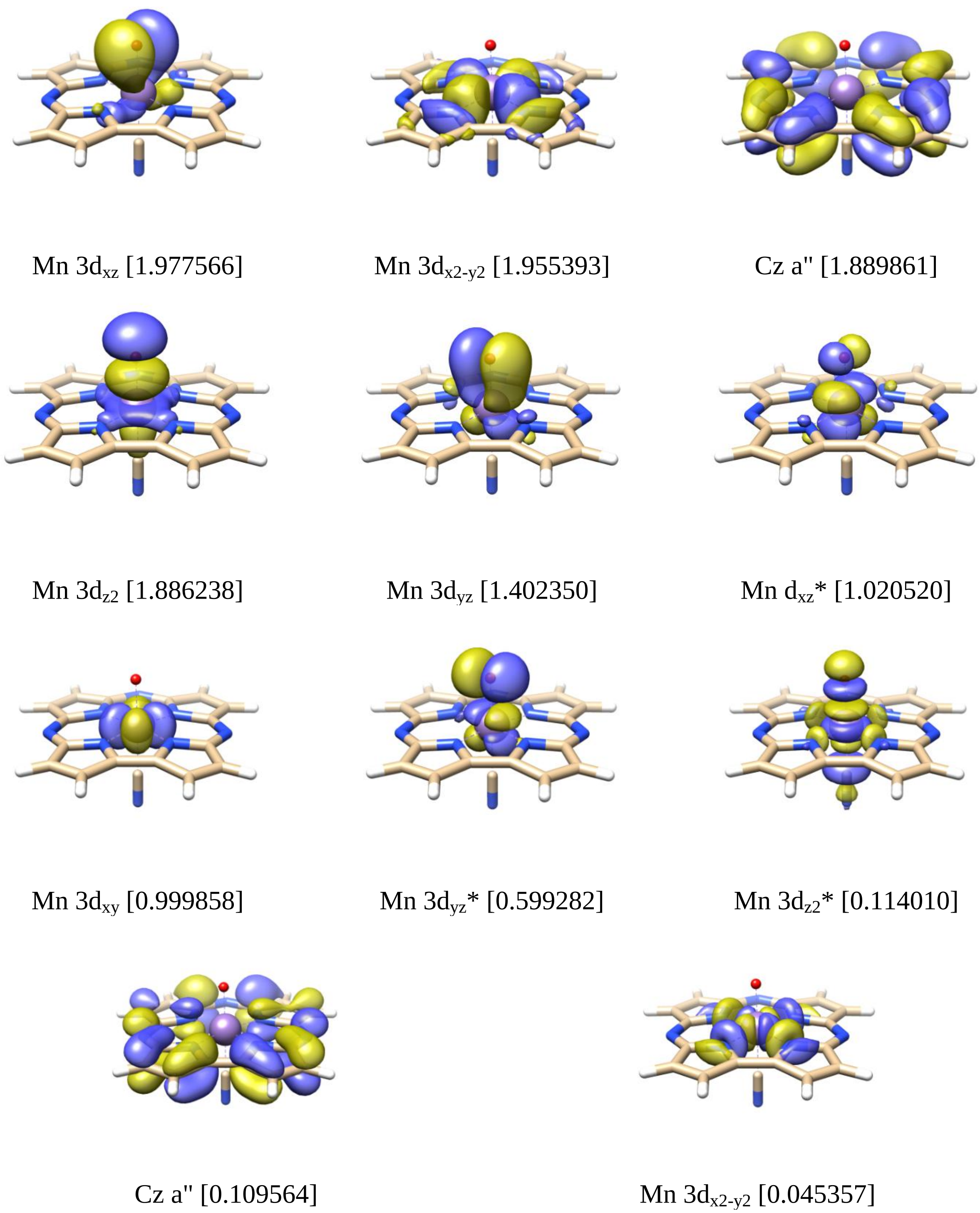


Figure S17. Active natural orbitals of $^3[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(12,11)/cc-pVTZ/cc-pVDZ using the optimized geometry of $^3[(H_8Cz)Mn(O)(CN)]^-$. The opposite phases are shown in either blue or yellow.

Table S18. Configuration state functions with weight larger than 1.00% for $^{1}[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(10,9)/cc-pVTZ/cc-VDZ

Configuration	CSF	Weight (%)
1	222220000	81.75
2	222111100	3.14
3	222202000	2.63
4	222020200	2.53
5	221211010	1.80
6	221120110	1.75

Table S19. Configuration state functions with weight larger than 1.00% for $^{1}[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(12,11)/cc-pVTZ/cc-VDZ

Configuration	CSF	Weight (%)
1	22222200000	77.12
2	22202200200	3.87
3	22221111000	2.82
4	22220202000	2.37
5	22222020000	2.28
6	22121201010	1.65
7	22122110010	1.61

Table S20. Configuration state functions with weight larger than 1.00% for $^{3}[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(10,9)/cc-pVTZ/cc-VDZ using the optimized geometry of $^{1}[(H_8Cz)Mn(O)(CN)]^-$.

Configuration	CSF	Weight (%)
1	222211000	78.71
2	222011200	5.68
3	222111100	4.08
4	221111110	2.42
5	212121100	1.39

Table S21. Configuration state functions with weight larger than 1.00% for $^{3}[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(12,11)/cc-pVTZ/cc-VDZ using the optimized geometry of $^{1}[(H_8Cz)Mn(O)(CN)]^-$.

Configuration	CSF	Weight (%)
1	22222110000	74.14
2	22220112000	5.65
3	22202110200	4.42
4	22221111000	3.84
5	22121111010	2.27
6	21221211000	1.28

Table S22. Configuration state functions with weight larger than 1.00% for $^3[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(10,9)/cc-pVTZ/cc-VDZ using the optimized geometry of $^3[(H_8Cz)Mn(O)(CN)]^-$.

Configuration	CSF	Weight (%)
1	222211000	54.20
2	222111100	18.36
3	222011200	15.88
4	221111110	2.18
5	220211020	1.14
6	221211010	1.04

Table S23. Configuration state functions with weight larger than 1.00% for $^3[(H_8Cz)Mn(O)(CN)]^-$ from RIJCOSX-CASSCF(12,11)/cc-pVTZ/cc-VDZ using the optimized geometry of $^3[(H_8Cz)Mn(O)(CN)]^-$.

Configuration	CSF	Weight (%)
1	22222110000	51.02
2	22221111000	17.42
3	22220112000	15.04
4	22022110020	2.83
5	22211111100	2.04
6	22202110200	1.06

Table S24. Group spin densities of $^1[(H_8Cz)Mn(O)(CN)]^-$, $^3[(H_8Cz)Mn(O)(CN)]^-$ with singlet optimized geometry, and $^3[(H_8Cz)Mn(O)(CN)]^-$ with triplet optimized geometry from RIJCOSX-CASSCF/cc-pVTZ/cc-VDZ with active space of (10,9) or (12,11)

Spin state	Geometry	Active Space	ρ_{Mn}	ρ_{O}	ρ_{Cz}	ρ_{CN}
0	Singlet	(10,9)	0.00	0.00	0.00	0.00
0	Singlet	(12,11)	0.00	0.00	0.00	0.00
1	Singlet	(10,9)	2.11	-0.09	-0.02	0.00
1	Singlet	(12,11)	2.11	-0.09	-0.02	0.00
1	Triplet	(10,9)	2.52	-0.47	-0.05	0.00
1	Triplet	(12,11)	2.52	-0.47	-0.04	0.00

Table S25. Absolute energies (in au) and relative energies (in kcal mol^{-1} with respect to the singlet spin state of the same size of active space) of $^{1}[(H_8Cz)Mn(O)(CN)]^{-}$, $^{3}[(H_8Cz)Mn(O)(CN)]^{-}$ with singlet optimized geometry, and $^{3}[(H_8Cz)Mn(O)(CN)]^{-}$ with triplet optimized geometry from RIJCOSX-CASSCF/cc-pVTZ/cc-VDZ with active space of (10,9) or (12,11)

Spin state	Geometry	Active Space	E	ΔE
0	Singlet	(10,9)	-2321.09	0.00
1	Singlet	(10,9)	-2321.08	5.55
1	Triplet	(10,9)	-2321.08	1.38
0	Singlet	(12,11)	-2321.10	0.00
1	Singlet	(12,11)	-2321.09	4.66
1	Triplet	(12,11)	-2321.09	1.30

Table S26. Absolute energies (in au) and relative energies (in kcal mol^{-1} with respect to the singlet spin state of the same size of active space) of $^{1}[(H_8Cz)Mn(O)(CN)]^{-}$, $^{3}[(H_8Cz)Mn(O)(CN)]^{-}$ with singlet optimized geometry, and $^{3}[(H_8Cz)Mn(O)(CN)]^{-}$ with triplet optimized geometry from RIJCOSX-RI-NEVPT2/cc-pVTZ/cc-VDZ with active space of (10,9) or (12,11)

Spin state	Geometry	Active Space	E	ΔE
0	Singlet	(10,9)	-2325.47	0.00
1	Singlet	(10,9)	-2325.45	12.82
1	Triplet	(10,9)	-2325.45	13.44
0	Singlet	(12,11)	-2325.46	0.00
1	Singlet	(12,11)	-2325.43	16.21
1	Triplet	(12,11)	-2325.44	12.51

Cartesian coordinates of all optimized geometries reported here:

Pre-edge calculation Cartesians:

$^{1}[(H_8Cz)Mn(O)]$: B3LPY/SDD/6-31G(d):

25	-0.118208	0.013148	-0.044082
7	0.607793	-1.349666	-1.136944
6	0.238935	-2.698577	-1.104624
7	-0.328362	-3.354888	-0.099196
6	-0.577519	-2.703614	1.032588
7	-0.353634	-1.357899	1.209212
6	-0.638693	-1.001538	2.512653
6	-0.341357	0.353213	2.727290
7	0.137983	0.933665	1.568959
6	0.534659	2.225613	1.825411
7	1.133426	3.010700	0.935690
6	1.434195	2.510461	-0.257720
7	1.179296	1.217970	-0.726589
6	1.748807	1.110142	-1.992819
7	1.762051	0.032203	-2.763407
6	1.240428	-1.114463	-2.353752
6	1.260727	-2.342335	-3.103408
6	0.644337	-3.301613	-2.348828
1	0.487399	-4.345167	-2.584108
1	1.707212	-2.436602	-4.083194
6	2.360423	2.368414	-2.328172
6	2.166385	3.219564	-1.275209
1	2.511604	4.237346	-1.158138
1	2.880995	2.551624	-3.257678
6	0.243849	2.486736	3.207216
6	-0.287826	1.333230	3.761398
1	-0.593026	1.179206	4.787547
1	0.447494	3.425846	3.703025
6	-1.088231	-2.171219	3.194064
6	-1.056715	-3.216285	2.286482
1	-1.327502	-4.247751	2.464664
1	-1.388221	-2.223442	4.231702
8	-1.471037	0.369291	-0.636488

$^{1}[(H_8Cz)Mn(O)(CN)]^{-}$: B3LPY/SDD/6-31G(d):

25	-0.038668	0.004014	0.088996
7	1.882593	0.005792	-0.033297
6	2.685756	1.123697	-0.027104
7	2.315080	2.400659	-0.120332
6	1.016966	2.729682	-0.254498
7	-0.025423	1.857833	-0.179813
6	-1.208414	2.453717	-0.558502
6	-2.243500	1.500303	-0.735769
7	-1.813274	0.215669	-0.459725
6	-2.716350	-0.707830	-0.898628
7	-2.506911	-2.035855	-0.948231
6	-1.299765	-2.539425	-0.696281
7	-0.151712	-1.858180	-0.350177
6	0.921467	-2.702609	-0.349177
7	2.212178	-2.390396	-0.186036
6	2.638013	-1.127257	-0.066073
6	4.033345	-0.715813	-0.015320
6	4.061513	0.651909	0.010007
1	4.918858	1.311952	0.019469
1	4.863253	-1.410199	-0.021417
6	0.417590	-4.036898	-0.633199
6	-0.931221	-3.936491	-0.843970
1	-1.633099	-4.713305	-1.116962
1	1.046893	-4.915626	-0.686604
6	-3.852931	0.032275	-1.373837
6	-3.555218	1.389412	-1.283984
1	-4.180267	2.213174	-1.602854
1	-4.753712	-0.418417	-1.769581
6	-0.919398	3.832943	-0.792714
6	0.445253	4.008088	-0.591038
1	1.012871	4.923460	-0.697187
1	-1.633167	4.587588	-1.095832
8	-0.049423	-0.169509	1.627267
6	0.236695	0.067451	-2.084985
7	0.386143	0.080074	-3.246184

Equatorial ligand effect Cartesians:

$^{1}[((MePh)_8Cz)Mn(O)CN]^{-}$: B3LYP:

25	6.693673000	8.805011000	10.496169000
7	7.126991000	7.455824000	9.187447000
7	7.832368000	10.127779000	9.638544000
7	6.700687000	9.801556000	12.066214000
7	6.094982000	7.500898000	11.669653000
7	8.384911000	8.853462000	7.654929000
7	7.799323000	11.825729000	11.364694000
7	6.181153000	5.518669000	10.305573000
6	6.761100000	6.127857000	9.264660000
6	7.198789000	5.475002000	8.026666000
6	7.834476000	6.444506000	7.250698000
6	7.811753000	7.697175000	8.023620000
6	8.407344000	9.963717000	8.410364000
6	9.066755000	11.226425000	8.053953000
6	8.868532000	12.112580000	9.111781000
6	8.100686000	11.381090000	10.137138000
6	7.177589000	11.062319000	12.288691000
6	6.877691000	11.383219000	13.673430000
6	6.272951000	10.236915000	14.252147000
6	6.195331000	9.225045000	13.225590000
6	5.880890000	7.845103000	13.003584000
6	5.458371000	6.641517000	13.675505000
6	5.444469000	5.598460000	12.712713000
6	5.898510000	6.162317000	11.457429000
6	7.058049000	4.030382000	7.771434000
6	5.850511000	3.355198000	8.036251000
1	5.011390000	3.915516000	8.429062000
6	5.728857000	1.982784000	7.805133000
1	4.783678000	1.488668000	8.015944000
6	6.805052000	1.228761000	7.309733000
6	8.012126000	1.901241000	7.048302000
1	8.863913000	1.341903000	6.668560000
6	8.139492000	3.271891000	7.275979000
1	9.084135000	3.765879000	7.077235000
6	6.683345000	-0.265344000	7.096794000
6	8.349833000	6.321759000	5.875966000
6	7.681818000	5.527649000	4.920300000
1	6.777685000	5.002502000	5.205112000
6	8.161176000	5.413735000	3.614062000
1	7.622952000	4.794617000	2.900343000
6	9.319806000	6.092927000	3.202715000
6	9.979997000	6.893955000	4.150312000
1	10.872758000	7.441567000	3.858159000
6	9.508600000	7.010201000	5.458614000
1	10.016580000	7.652568000	6.164086000
6	9.826442000	5.991500000	1.779888000
6	9.746005000	11.441324000	6.760814000
6	10.767678000	10.572078000	6.335033000
1	11.060005000	9.750870000	6.979207000
6	11.403549000	10.759129000	5.103601000
1	12.193050000	10.075665000	4.801078000
6	11.039802000	11.811829000	4.249546000
6	10.016884000	12.679484000	4.674349000
1	9.709417000	13.499335000	4.029104000
6	9.382426000	12.500531000	5.904352000
1	8.590567000	13.176752000	6.208013000

6	11.719783000	12.012159000	2.911126000
1	12.250741000	12.972879000	2.866648000
1	12.449692000	11.220048000	2.713575000
1	10.993260000	12.008378000	2.088022000
6	9.345265000	13.498208000	9.260093000
6	10.568486000	13.924818000	8.702051000
1	11.190211000	13.211987000	8.174271000
6	10.996360000	15.249105000	8.825220000
1	11.944404000	15.545096000	8.382387000
6	10.229914000	16.202733000	9.514809000
6	9.018926000	15.775328000	10.089074000
1	8.406755000	16.487078000	10.638243000
6	8.582582000	14.455236000	9.968092000
1	7.655819000	14.146623000	10.434185000
6	10.689368000	17.639807000	9.644012000
1	10.842087000	17.921712000	10.694646000
1	11.634558000	17.804382000	9.115227000
1	9.949396000	18.337680000	9.229469000
6	7.102184000	12.707558000	14.277107000
6	8.241043000	13.469746000	13.931671000
1	8.943533000	13.067586000	13.213752000
6	8.448798000	14.737318000	14.476845000
1	9.332357000	15.300297000	14.185935000
6	7.537548000	15.300845000	15.386642000
6	6.397958000	14.550071000	15.721181000
1	5.665336000	14.968321000	16.407544000
6	6.180701000	13.281607000	15.179462000
1	5.281702000	12.737304000	15.444096000
6	7.786328000	16.664178000	15.995349000
1	6.857795000	17.110575000	16.368740000
1	8.223814000	17.355269000	15.264720000
1	8.485176000	16.605761000	16.842420000
6	5.807907000	10.126759000	15.651342000
6	6.682023000	10.396875000	16.723343000
1	7.716630000	10.643273000	16.509485000
6	6.232155000	10.355028000	18.043349000
1	6.928050000	10.565162000	18.852082000
6	4.894253000	10.044946000	18.345642000
6	4.026467000	9.762640000	17.278380000
1	2.991669000	9.503280000	17.485007000
6	4.472930000	9.800982000	15.954466000
1	3.783961000	9.583147000	15.144759000
6	4.405102000	10.037194000	19.778469000
1	5.162848000	9.628540000	20.457735000
1	3.495484000	9.436385000	19.886408000
1	4.171291000	11.052378000	20.130065000
6	5.121430000	6.481307000	15.108866000
6	6.088507000	6.703080000	16.110127000
1	7.077105000	7.045799000	15.822709000
6	5.794096000	6.471450000	17.455118000
1	6.559549000	6.649682000	18.205996000
6	4.524813000	6.015151000	17.854891000
6	3.557995000	5.807143000	16.857898000
1	2.567592000	5.457968000	17.139585000
6	3.849136000	6.033983000	15.508951000
1	3.091633000	5.851968000	14.753312000
6	4.218399000	5.757638000	19.315332000
1	4.866417000	4.973845000	19.730295000
1	3.180119000	5.437589000	19.454276000
1	4.375041000	6.658812000	19.922385000
6	5.094878000	4.178980000	12.891992000
6	5.440442000	3.455473000	14.054577000
1	5.986390000	3.950302000	14.848386000
6	5.109924000	2.106535000	14.187011000
1	5.399055000	1.574680000	15.090656000
6	4.422660000	1.419292000	13.170033000
6	4.081567000	2.136081000	12.012610000
1	3.556595000	1.629044000	11.206839000
6	4.410096000	3.486120000	11.872185000
6	4.077679000	-0.047333000	13.318197000
1	4.980564000	-0.663190000	13.427103000
1	3.455441000	-0.229917000	14.204738000
1	3.529710000	-0.414825000	12.444181000
8	5.456986000	9.343058000	9.673901000
6	8.600351000	8.212186000	11.203445000
1	7.294748000	-0.601216000	6.250578000
1	7.018859000	-0.824864000	7.982076000
1	5.645166000	-0.558467000	6.901596000
1	9.629426000	6.914922000	1.217134000
1	10.910382000	5.821913000	1.749355000
1	9.342458000	5.168653000	1.242233000
1	4.152870000	4.013310000	10.962519000
7	9.676774000	7.894354000	11.574704000

[1][((MePh)$_8$Cz)Mn(O)] B3LYP:

25	6.735128000	8.785631000	10.492848000
7	7.361005000	7.415399000	9.340381000
7	8.023686000	9.976740000	9.769132000
7	6.972679000	9.693925000	12.106938000
7	6.390758000	7.430928000	11.732378000
7	8.597616000	8.763306000	7.747939000
7	7.930074000	11.772490000	11.411461000
7	6.315831000	5.465553000	10.367976000
6	6.910040000	6.087340000	9.348422000
6	7.262817000	5.463518000	8.083744000
6	7.963791000	6.409320000	7.333566000
6	8.029413000	7.623227000	8.131646000
6	8.611355000	9.855640000	8.508670000
6	9.188015000	11.129789000	8.126508000
6	8.943968000	12.027134000	9.168032000
6	8.243515000	11.288930000	10.208957000
6	7.357285000	10.998109000	12.335503000
6	6.991038000	11.337056000	13.694149000
6	6.417014000	10.181125000	14.273416000
6	6.438147000	9.142799000	13.272500000
6	6.138697000	7.773209000	13.061978000
6	5.652767000	6.591237000	13.730417000
6	5.609147000	5.552964000	12.771425000
6	6.100960000	6.098070000	11.525107000
6	6.940808000	4.066965000	7.741939000
6	5.654478000	3.543824000	7.981215000
1	4.901512000	4.177078000	8.434392000
6	5.339717000	2.229732000	7.630620000
1	4.336371000	1.854428000	7.813215000
6	6.294533000	1.385358000	7.039475000
6	7.580576000	1.905543000	6.809968000
1	8.338328000	1.273051000	6.355633000
6	7.900739000	3.219759000	7.152675000
1	8.899462000	3.597033000	6.962828000
6	5.956030000	-0.045185000	6.681536000
6	8.459251000	6.309384000	5.948908000
6	7.682063000	5.684509000	4.950731000
1	6.716126000	5.267034000	5.210348000
6	8.134603000	5.606157000	3.633982000
1	7.513400000	5.122818000	2.884665000
6	9.376605000	6.147856000	3.257385000
6	10.149506000	6.770464000	4.251437000
1	11.112260000	7.199455000	3.987392000
6	9.701824000	6.855467000	5.571428000
1	10.308089000	7.356162000	6.314883000
6	9.846767000	6.089165000	1.820498000
6	9.820636000	11.374546000	6.815921000
6	10.865146000	10.555588000	6.350304000
1	11.213719000	9.737252000	6.970087000
6	11.458879000	10.791196000	5.106845000
1	12.270192000	10.150487000	4.772022000
6	11.025627000	11.841103000	4.281490000
6	9.976788000	12.655923000	4.746931000
1	9.618900000	13.472994000	4.125873000
6	9.385500000	12.430911000	5.989684000

1	8.576949000	13.070684000	6.326226000
6	11.650394000	12.085756000	2.925186000
1	11.923768000	13.140001000	2.793090000
1	12.554643000	11.484487000	2.787476000
1	10.955078000	11.829427000	2.114443000
6	9.319855000	13.447020000	9.271792000
6	10.536680000	13.924373000	8.743115000
1	11.223957000	13.231179000	8.273040000
6	10.873690000	15.277273000	8.822790000
1	11.819775000	15.615213000	8.408827000
6	10.014163000	16.208716000	9.429355000
6	8.805422000	15.730766000	9.967996000
1	8.122723000	16.426139000	10.449352000
6	8.462050000	14.380567000	9.895190000
1	7.530898000	14.038705000	10.328145000
6	10.367479000	17.678247000	9.498277000
1	10.292996000	18.060874000	10.523725000
1	11.387088000	17.861445000	9.145028000
1	9.688804000	18.281537000	8.880565000
6	7.110012000	12.695393000	14.251382000
6	8.225541000	13.505256000	13.946822000
1	9.008162000	13.113408000	13.310352000
6	8.314850000	14.811778000	14.429859000
1	9.182024000	15.414018000	14.173012000
6	7.301316000	15.365676000	15.230450000
6	6.187119000	14.561243000	15.528455000
1	5.379565000	14.969575000	16.130337000
6	6.090067000	13.253811000	15.052518000
1	5.208623000	12.668355000	15.283460000
6	7.409236000	16.776562000	15.764990000
1	6.420798000	17.228222000	15.904156000
1	7.983420000	17.418297000	15.087674000
1	7.916188000	16.796580000	16.739631000
6	5.857662000	10.092946000	15.639508000
6	6.630333000	10.444299000	16.762496000
1	7.667587000	10.731891000	16.625361000
6	6.073671000	10.435254000	18.043210000
1	6.690071000	10.708400000	18.895458000
6	4.728065000	10.083610000	18.248802000
6	3.961127000	9.724294000	17.126857000
1	2.921992000	9.436944000	17.259351000
6	4.513674000	9.725964000	15.844670000
1	3.899620000	9.453204000	14.992397000
6	4.114950000	10.112256000	19.632189000
1	4.876818000	9.994451000	20.409924000
1	3.374161000	9.314661000	19.758032000
1	3.600663000	11.064693000	19.821637000
6	5.288440000	6.455053000	15.158341000
6	6.228097000	6.714380000	16.174726000
1	7.219345000	7.066486000	15.907122000
6	5.902880000	6.511295000	17.517329000
1	6.645676000	6.718748000	18.282489000
6	4.630024000	6.047545000	17.896091000
6	3.689381000	5.803887000	16.880544000
1	2.695583000	5.453157000	17.146240000
6	4.011009000	5.999358000	15.535159000
1	3.272539000	5.792374000	14.767520000
6	4.295461000	5.801151000	19.351166000
1	4.727445000	4.855669000	19.705862000
1	3.213868000	5.745182000	19.508991000
1	4.690874000	6.596450000	19.992473000
6	5.197429000	4.149046000	12.946119000
6	5.543893000	3.409953000	14.097036000
1	6.131237000	3.878310000	14.877628000
6	5.150791000	2.079100000	14.238755000
1	5.436401000	1.532962000	15.133906000
6	4.396366000	1.429970000	13.244548000
6	4.052312000	2.166315000	12.098686000
1	3.468824000	1.691269000	11.314716000
6	4.446608000	3.496834000	11.946434000
6	3.995982000	-0.020760000	13.395713000
1	4.822045000	-0.691782000	13.121924000
1	3.719194000	-0.255071000	14.430109000
1	3.145497000	-0.270052000	12.752642000
8	5.372495000	9.231901000	9.892495000
1	6.543680000	-0.393902000	5.825322000
1	6.164757000	-0.725633000	7.518428000
1	4.895246000	-0.154473000	6.431301000
1	9.465593000	6.942349000	1.242586000
1	10.939731000	6.114536000	1.754722000
1	9.497550000	5.178602000	1.321065000
1	4.177407000	4.038595000	11.048327000

[1][((MePh)$_8$Cz)Mn(O)CN]$^-$: BP86:

25	6.680663321	8.790661957	10.489595775
7	7.135656125	7.428097328	9.191064850
7	7.821242427	10.122179331	9.637121162
7	6.651975518	9.804561463	12.050547662
7	6.074995456	7.487120498	11.664743394
7	8.416462788	8.830449926	7.651950632
7	7.762783996	11.848941764	11.359767217
7	6.179765563	5.473497525	10.310427226
6	6.757440003	6.094230163	9.258020497
6	7.175486430	5.444453044	8.003634708
6	7.820569877	6.422537065	7.221407232
6	7.821706594	7.672316489	8.014755236
6	8.432907746	9.946569051	8.414741345
6	9.114753036	11.206566638	8.066090927
6	8.883450138	12.112786848	9.116529813
6	8.083646148	11.387681867	10.130243083
6	7.129995929	11.077619411	12.279896138
6	6.823756583	11.402855061	13.670708186
6	6.218207586	10.244507752	14.254041425
6	6.148024997	9.226183879	13.224851960
6	5.855369142	7.835307169	13.009828903
6	5.457632538	6.625819660	13.696632159
6	5.463269881	5.563737456	12.736966403
6	5.899718835	6.130086980	11.464923895
6	6.998472378	4.005626236	7.723675299
6	5.767274060	3.351592760	7.985100737
1	4.940745528	3.932157730	8.401568887
6	5.602368740	1.983141635	7.710516704
1	4.635860661	1.505863197	7.913533947
6	6.656937738	1.208852515	7.174686498
6	7.889052009	1.858966576	6.923381935
1	8.727284974	1.281948909	6.513874033
6	8.060199354	3.225417040	7.193552939
1	9.023884244	3.704240443	6.996964428
6	6.485739330	-0.275802920	6.906804618
6	8.294919978	6.317230163	5.827900305
6	7.637953014	5.475032004	4.890034725
1	6.770222122	4.892631064	5.209634100
6	8.075869863	5.388491237	3.559100623
1	7.545245768	4.730092286	2.860308594
6	9.178171313	6.144470948	3.097359425
6	9.823729362	6.995248772	4.025255588
1	10.671298358	7.608193164	3.695570729
6	9.396314808	7.084295093	5.359100545
1	9.882553872	7.776254747	6.047845806
6	9.633557095	6.072088228	1.651196677
6	9.857893257	11.401566187	6.803072971
6	10.888789878	10.502075500	6.433182706
1	11.128530918	9.670635967	7.101851814
6	11.604427667	10.677526392	5.235211735
1	12.404204094	9.972959912	4.976915791
6	11.314898968	11.747016129	4.358866712
6	10.279993015	12.641582757	4.725902110
1	10.028066642	13.475660633	4.059181577
6	9.565707697	12.475434310	5.922472837
1	8.766055126	13.174502359	6.184738062

6	12.083640851	11.936499538	3.062768945
1	12.617674371	12.906431496	3.042850349
1	12.833354112	11.138472853	2.920976388
1	11.408229792	11.922340818	2.186107457
6	9.358920152	13.500182303	9.265192206
6	10.594947115	13.930322603	8.713293608
1	11.229112010	13.208747763	8.192761196
6	11.019780712	15.263716827	8.835104017
1	11.980096888	15.563362682	8.397755148
6	10.239613794	16.225957742	9.516298554
6	9.017519549	15.794606162	10.086080393
1	8.393556667	16.513829577	10.630768481
6	8.583103512	14.465138640	9.967329285
1	7.646147505	14.150089564	10.431370412
6	10.694544946	17.669833105	9.637643820
1	10.792331250	17.978930561	10.696437611
1	11.674292759	17.823758532	9.151604839
1	9.973020731	18.364835819	9.165237660
6	7.043073309	12.729542351	14.274988527
6	8.167595801	13.515411476	13.896715428
1	8.855200835	13.122398668	13.145440494
6	8.375017450	14.789424917	14.446856347
1	9.248926292	15.371621947	14.130978641
6	7.478938395	15.338485956	15.393935177
6	6.352657486	14.565015544	15.759260206
1	5.628942058	14.974259248	16.474858500
6	6.134901961	13.289827404	15.213935555
1	5.243754309	12.726766606	15.501649996
6	7.728145272	16.704627416	16.007174362
1	6.796305100	17.143601088	16.406638212
1	8.147672104	17.409995236	15.266344895
1	8.451061669	16.647849907	16.845848234
6	5.751236782	10.134240896	15.654490041
6	6.613924860	10.455984790	16.733757122
1	7.647828236	10.742229612	16.518563648
6	6.155522949	10.413518514	18.059339109
1	6.843075996	10.664390147	18.876321750
6	4.820668101	10.053510105	18.361301341
6	3.966242442	9.716912201	17.286899217
1	2.933083751	9.415917823	17.494762123
6	4.420535577	9.753696502	15.957621879
1	3.741398169	9.494243704	15.139488811
6	4.318692958	10.057284182	19.794405017
1	5.109830052	9.744380402	20.500494788
1	3.457853183	9.377032079	19.921943463
1	3.988142812	11.068675829	20.106081882
6	5.135570966	6.479635479	15.136808736
6	6.100416479	6.787121788	16.130244277
1	7.072416188	7.184125804	15.821819674
6	5.828153091	6.568722949	17.489945626
1	6.592551571	6.812649524	18.236666426
6	4.583736640	6.043164431	17.912775663
6	3.616052899	5.755798622	16.923092033
1	2.641076620	5.354593192	17.225733343
6	3.884917944	5.966603009	15.559369696
1	3.128609464	5.722564240	14.806676501
6	4.309407249	5.783281559	19.383050738
1	4.912276557	4.935649474	19.763904486
1	3.246732747	5.539050452	19.557156314
1	4.562380924	6.663385118	20.002841344
6	5.169046993	4.134820064	12.947959988
6	5.506111529	3.462214994	14.154437761
1	6.008013503	4.011667229	14.953981378
6	5.225000456	2.098586942	14.324580320
1	5.505106450	1.606365169	15.264034289
6	4.598527880	1.343757936	13.304382025
6	4.270594542	2.008942271	12.101590271
1	3.793043853	1.446068478	11.290608232
6	4.550915092	3.372699044	11.921083672
6	4.322036062	-0.137417678	13.488131688
1	5.253668075	-0.733462788	13.421972557
1	3.873395295	-0.348539400	14.476908805
1	3.632060615	-0.516430637	12.713983112
8	5.452691461	9.314698090	9.600820068
6	8.577586767	8.225409802	11.203126840
1	7.110235526	-0.608189080	6.057544527
1	6.780533852	-0.882963171	7.785891434
1	5.434323545	-0.525741805	6.675903367
1	9.349571436	6.984970670	1.090796617
1	10.733126920	5.977014550	1.575544936
1	9.181803383	5.209545588	1.129904838
1	4.312720289	3.862054128	10.974617849
7	9.666242288	7.916268489	11.589635328

^{1}[((MePh)$_8$Cz)Mn(O)]: BP86:

25	6.665290000	8.825846000	10.444392000
7	7.284749000	7.454754000	9.282860000
7	7.955590000	10.023940000	9.725669000
7	6.875240000	9.741108000	12.066309000
7	6.277993000	7.468648000	11.677922000
7	8.555133000	8.806315000	7.688857000
7	7.903097000	11.819615000	11.402938000
7	6.265977000	5.469896000	10.325406000
6	6.863175000	6.104452000	9.302673000
6	7.254607000	5.466213000	8.050950000
6	7.936581000	6.430342000	7.282087000
6	7.974027000	7.660169000	8.072781000
6	8.568111000	9.899842000	8.466521000
6	9.176539000	11.173736000	8.099925000
6	8.925743000	12.078087000	9.151110000
6	8.201907000	11.337802000	10.185033000
6	7.312090000	11.033118000	12.321460000
6	6.984561000	11.353675000	13.703628000
6	6.378365000	10.192775000	14.272305000
6	6.346442000	9.176942000	13.244226000
6	6.033946000	7.805218000	13.024483000
6	5.568455000	6.613745000	13.699118000
6	5.540761000	5.562246000	12.734980000
6	6.023515000	6.117985000	11.479669000
6	7.027012000	4.038069000	7.755344000
6	5.780648000	3.420505000	8.029857000
1	4.971512000	4.020622000	8.452544000
6	5.577933000	2.057141000	7.758812000
1	4.602359000	1.605473000	7.971014000
6	6.608183000	1.254554000	7.217386000
6	7.852805000	1.872667000	6.944748000
1	8.669739000	1.273615000	6.526204000
6	8.061093000	3.235177000	7.205231000
1	9.033657000	3.688036000	6.992056000
6	6.400263000	-0.226880000	6.964191000
6	8.419570000	6.310200000	5.894103000
6	7.675755000	5.566583000	4.939355000
1	6.743509000	5.083878000	5.243659000
6	8.114183000	5.454573000	3.611830000
1	7.517755000	4.879575000	2.894293000
6	9.307470000	6.078444000	3.179292000
6	10.043259000	6.826755000	4.128939000
1	10.967274000	7.327685000	3.818395000
6	9.610628000	6.947274000	5.458027000
1	10.180586000	7.549242000	6.167547000
6	9.773328000	5.969991000	1.739869000
6	9.819175000	11.413506000	6.791369000
6	10.833882000	10.550057000	6.311263000
1	11.160326000	9.714389000	6.936108000
6	11.423698000	10.762869000	5.053421000
1	12.212470000	10.086160000	4.705383000
6	11.016783000	11.832871000	4.225508000
6	10.001968000	12.695927000	4.707945000
1	9.662176000	13.529404000	4.082204000
6	9.415952000	12.496073000	5.966181000

1	8.627241000	13.169009000	6.314802000
6	11.640167000	12.057010000	2.860149000
1	12.177221000	13.023766000	2.813334000
1	12.361865000	11.260398000	2.610725000
1	10.870768000	12.076513000	2.065369000
6	9.312780000	13.496710000	9.263460000
6	10.525441000	13.979583000	8.705149000
1	11.203412000	13.282078000	8.206859000
6	10.868162000	15.338603000	8.790188000
1	11.811784000	15.683117000	8.351895000
6	10.021083000	16.272394000	9.431300000
6	8.818308000	15.788193000	10.000297000
1	8.142560000	16.487252000	10.506638000
6	8.468709000	14.431739000	9.924407000
1	7.540606000	14.081545000	10.380381000
6	10.383288000	17.743832000	9.509959000
1	10.499315000	18.076933000	10.559090000
1	11.330156000	17.954935000	8.984052000
1	9.597125000	18.377043000	9.056591000
6	7.170307000	12.685443000	14.305342000
6	8.305495000	13.476768000	13.976290000
1	9.040006000	13.085363000	13.269460000
6	8.472153000	14.756655000	14.525638000
1	9.355873000	15.345118000	14.253818000
6	7.519334000	15.305421000	15.416784000
6	6.383739000	14.522798000	15.732879000
1	5.620027000	14.931568000	16.404469000
6	6.209017000	13.239912000	15.193109000
1	5.311593000	12.668726000	15.441927000
6	7.718213000	16.681091000	16.023575000
1	6.768673000	17.095367000	16.404569000
1	8.131047000	17.392965000	15.286097000
1	8.428109000	16.646974000	16.873478000
6	5.852145000	10.082627000	15.651944000
6	6.665091000	10.412376000	16.766481000
1	7.708386000	10.698030000	16.600779000
6	6.143017000	10.383390000	18.068261000
1	6.790340000	10.641101000	18.914647000
6	4.791679000	10.034591000	18.307848000
6	3.987848000	9.693125000	17.196532000
1	2.942554000	9.407393000	17.356373000
6	4.506055000	9.712302000	15.890566000
1	3.862063000	9.455171000	15.043880000
6	4.223296000	10.055815000	19.714800000
1	4.931433000	9.622717000	20.444651000
1	3.278249000	9.489459000	19.777270000
1	4.010837000	11.090938000	20.046919000
6	5.182353000	6.476643000	15.123479000
6	6.107429000	6.737657000	16.165648000
1	7.109765000	7.098882000	15.915426000
6	5.756163000	6.518378000	17.506997000
1	6.489695000	6.721977000	18.295007000
6	4.470428000	6.041561000	17.859394000
6	3.544626000	5.800280000	16.818685000
1	2.540983000	5.436350000	17.066647000
6	3.892231000	6.008531000	15.473666000
1	3.166473000	5.799691000	14.681805000
6	4.106264000	5.789534000	19.310978000
1	4.725961000	4.983445000	19.748367000
1	3.048777000	5.492102000	19.415731000
1	4.267697000	6.691629000	19.929943000
6	5.139654000	4.155377000	12.914844000
6	5.428832000	3.436456000	14.106907000
1	5.972348000	3.930052000	14.916069000
6	5.044440000	2.095649000	14.248845000
1	5.290515000	1.562196000	15.174414000
6	4.351068000	1.415102000	13.217703000
6	4.066468000	2.129977000	12.032707000
1	3.533615000	1.626483000	11.218265000
6	4.454229000	3.470217000	11.877772000
6	3.938100000	-0.035351000	13.384292000
1	4.817985000	-0.690380000	13.531561000
1	3.284009000	-0.171472000	14.266523000
1	3.390670000	-0.402629000	12.499390000
8	5.293686000	9.290282000	9.819289000
1	6.946286000	-0.565309000	6.065365000
1	6.766576000	-0.833955000	7.815655000
1	5.331557000	-0.467235000	6.826072000
1	9.670193000	6.936865000	1.210139000
1	10.839048000	5.681256000	1.679525000
1	9.186479000	5.220238000	1.181908000
1	4.233734000	3.998788000	10.948209000

^{1}[((MePh)$_8$Cz)Mn(O)CN]$^{-}$: M06:

25	6.828024918	8.758478945	10.505840311
7	7.244207515	7.434129555	9.225411332
7	7.969647553	10.035164122	9.678681443
7	6.859283313	9.738064005	12.099097708
7	6.226171201	7.448040820	11.689538026
7	8.491766875	8.804927943	7.672151542
7	7.920904562	11.752223830	11.392912170
7	6.261506707	5.495342139	10.318386260
6	6.838656322	6.110220948	9.291493945
6	7.231922851	5.470447335	8.044935966
6	7.886515385	6.425256556	7.277656223
6	7.918521988	7.659490166	8.055318304
6	8.516533196	9.903331991	8.436253857
6	9.122463740	11.181069644	8.074186563
6	8.941954163	12.044792113	9.150547625
6	8.220549599	11.299598144	10.178786627
6	7.297960973	10.998289159	12.317951331
6	6.955626097	11.331502530	13.685854390
6	6.352158379	10.189091109	14.252775030
6	6.321328393	9.170693420	13.235016608
6	5.999568188	7.800412954	13.008982767
6	5.545125806	6.613435008	13.679107506
6	5.532681561	5.571312268	12.728282198
6	5.997321404	6.127993886	11.477209988
6	6.988908211	4.055499268	7.752459872
6	5.758900354	3.455306070	8.064832746
1	4.980647694	4.063451190	8.515439000
6	5.538090586	2.104277767	7.808861669
1	4.575017620	1.659690974	8.057539802
6	6.534213443	1.303830011	7.237681897
6	7.759935190	1.904633436	6.919918805
1	8.549390117	1.300262787	6.475311911
6	7.987031855	3.253192520	7.174145835
1	8.949837232	3.698280455	6.935077702
6	6.311960601	-0.164288576	6.997524456
6	8.399810434	6.302346446	5.911218060
6	7.657885080	5.638810992	4.921150839
1	6.693340850	5.209312321	5.181712383
6	8.135604939	5.538028084	3.617240431
1	7.539960260	5.025767601	2.863312713
6	9.366506971	6.096518236	3.254679487
6	10.107773593	6.757684248	4.243350833
1	11.070125622	7.197261069	3.981949567
6	9.635231885	6.863904069	5.546793189
1	10.212048998	7.386922464	6.302775597
6	9.879799284	6.010485470	1.843609054
6	9.690422073	11.446906031	6.748809842
6	10.533125156	10.516174283	6.123750084
1	10.776758108	9.598573446	6.649102885
6	11.040025730	10.755640586	4.847799478
1	11.689971465	10.017440497	4.380346992
6	10.721885932	11.925124819	4.150731642
6	9.879018697	12.856547039	4.774909631
1	9.610147315	13.769804340	4.245392777
6	9.371183864	12.623439144	6.047348752
1	8.706829932	13.348877496	6.510026179

6	11.256849193	12.186771615	2.769072474
1	11.921468065	13.061514068	2.752903999
1	11.825151376	11.328584416	2.392509796
1	10.443430500	12.387741385	2.058965338
6	9.425486420	13.416750390	9.331264631
6	10.632207206	13.844361614	8.749987785
1	11.211349235	13.144712926	8.153863190
6	11.098524333	15.143100523	8.933593037
1	12.038953470	15.446819984	8.474670282
6	10.387704186	16.062889588	9.712899287
6	9.189274683	15.636464078	10.302382889
1	8.619950767	16.331942662	10.918584349
6	8.713830970	14.341970560	10.119950015
1	7.794556668	14.025344926	10.602774693
6	10.888224104	17.466383465	9.920358616
1	11.088268850	17.667204352	10.982055183
1	11.817920161	17.644830968	9.366169833
1	10.150565042	18.208969704	9.585724146
6	7.124387388	12.669715943	14.256476868
6	8.208801653	13.479641572	13.865892601
1	8.921992184	13.090543107	13.146799684
6	8.347315542	14.773218431	14.358053260
1	9.191113702	15.380447097	14.033048417
6	7.418952548	15.312787866	15.257092020
6	6.336548197	14.512437601	15.640592954
1	5.591524202	14.916407061	16.324170684
6	6.187299290	13.218296626	15.150188565
1	5.323877634	12.629607598	15.447144698
6	7.590337625	16.705669725	15.797716329
1	6.656026609	17.084612715	16.227653908
1	7.909056028	17.402465303	15.012491357
1	8.353686764	16.739192009	16.587564689
6	5.798604578	10.078638420	15.609136305
6	6.562142115	10.431957731	16.733403998
1	7.597138991	10.732811262	16.592240109
6	6.006196456	10.405644458	18.006929583
1	6.610975919	10.691611168	18.866642640
6	4.670373051	10.027777233	18.203280357
6	3.921100500	9.640270211	17.087477501
1	2.892521991	9.309595478	17.222718960
6	4.471346527	9.673042748	15.808504270
1	3.874671602	9.377447052	14.947782531
6	4.069309845	10.039934605	19.581078094
1	4.749526784	9.592195133	20.317465971
1	3.125755025	9.482125898	19.607945608
1	3.858269654	11.063541171	19.917867438
6	5.170459772	6.505643139	15.097486552
6	6.079226604	6.859685479	16.108702057
1	7.054175689	7.251533120	15.827478220
6	5.740373920	6.715259700	17.451026563
1	6.452893406	7.005927504	18.222594980
6	4.488223004	6.212283460	17.830226093
6	3.579708898	5.869116494	16.822030968
1	2.599202367	5.484441580	17.097787153
6	3.914890299	6.009231090	15.475582843
1	3.203485102	5.733214371	14.700283348
6	4.134238020	6.078783358	19.286949438
1	4.796000358	5.367722932	19.800964303
1	3.103039337	5.729951506	19.418239090
1	4.232781363	7.042578380	19.805754519
6	5.204386998	4.157854279	12.919090310
6	5.503147341	3.483062153	14.117012152
1	5.976499979	4.025364229	14.930582446
6	5.225291678	2.129199647	14.261664524
1	5.479019149	1.625162290	15.193013272
6	4.637790878	1.393181518	13.223124306
6	4.341989602	2.061403114	12.032037429
1	3.896919473	1.507608656	11.207109976
6	4.620216275	3.416813791	11.878439738
6	4.356822990	-0.074883984	13.390883213
1	5.280243133	-0.637773476	13.580896388
1	3.686491692	-0.261805530	14.240150284
1	3.888476122	-0.496213010	12.494333681
8	5.473777722	9.294837361	9.917402473
6	8.719697964	8.117510414	11.298242088
1	6.818984298	-0.501601860	6.084967373
1	6.703055434	-0.768406491	7.828460840
1	5.244992246	-0.396467751	6.899666667
1	9.939776105	7.003909883	1.378612559
1	10.889910707	5.580046164	1.811664894
1	9.227587707	5.387648981	1.218315202
1	4.406940697	3.914700926	10.938773238
7	9.781759508	7.781666310	11.696793224

^{1}[((MePh)$_8$Cz)Mn(O)]: M06:

25	6.837906791	8.770257329	10.513557945
7	7.448535876	7.413848828	9.358717819
7	8.110460640	9.959583715	9.796839220
7	7.064883477	9.671404611	12.118665891
7	6.485473792	7.420377578	11.736851898
7	8.615044814	8.782309380	7.747009886
7	8.019401072	11.742933866	11.439403115
7	6.416630016	5.462568329	10.379120686
6	7.009448120	6.087964505	9.368749778
6	7.338857583	5.476586030	8.101401292
6	7.980296379	6.436546384	7.326307279
6	8.067221212	7.638395098	8.131431362
6	8.661771199	9.855506194	8.525438480
6	9.233026464	11.126723431	8.149117746
6	9.020042932	12.008131984	9.204235013
6	8.335731724	11.263442813	10.242501117
6	7.438760873	10.972182141	12.354028699
6	7.042156757	11.311494223	13.699238628
6	6.459604780	10.158581043	14.260570300
6	6.499079706	9.127289586	13.268108929
6	6.191830901	7.768952677	13.052449669
6	5.661282209	6.606891923	13.699752873
6	5.641910001	5.566567698	12.752630207
6	6.185291071	6.095339907	11.526765363
6	7.072604716	4.067068783	7.801817738
6	5.831800316	3.485884008	8.102655169
1	5.055345238	4.100746153	8.546964496
6	5.590571965	2.142639824	7.828589120
1	4.618723537	1.711776261	8.061940256
6	6.577128920	1.334413481	7.252216646
6	7.815253436	1.917756123	6.948419587
1	8.594548138	1.306057734	6.497715188
6	8.062017898	3.258783028	7.217939343
1	9.029696684	3.693337458	6.979687768
6	6.329843300	-0.123992103	6.986411362
6	8.372964050	6.358862732	5.916192624
6	7.601112159	5.611416290	5.009395249
1	6.723392224	5.080037673	5.366357061
6	7.934555019	5.558325756	3.660631331
1	7.317298839	4.978855715	2.976848220
6	9.044053721	6.252153741	3.162987614
6	9.811446699	7.000072623	4.065383949
1	10.673452588	7.554835780	3.698241348
6	9.485803182	7.056497085	5.415922538
1	10.076595487	7.663404647	6.092570604
6	9.389530924	6.223568922	1.700970220
6	9.810343146	11.366581212	6.822280632
6	10.767294065	10.493682538	6.287719621
1	11.109134976	9.654241063	6.887270095
6	11.277277192	10.694168196	5.006574409
1	12.022459168	10.006853743	4.609743250
6	10.846243361	11.766483932	4.218860000
6	9.893075275	12.643082430	4.758570293
1	9.540323630	13.479729060	4.157865401
6	9.383441452	12.450473828	6.036818130

1	8.635105337	13.131495370	6.434319243
6	11.378081696	11.984375470	2.829775852
1	11.944183417	12.922637887	2.759868311
1	12.042690062	11.169651095	2.522606779
1	10.561721956	12.046329667	2.098639724
6	9.416926557	13.412616460	9.333836068
6	10.581818577	13.896550726	8.714695960
1	11.208875004	13.213437455	8.147905543
6	10.945996014	15.235612171	8.823831779
1	11.852781437	15.586546075	8.335219319
6	10.167916446	16.141216852	9.555313145
6	9.012135780	15.656692235	10.183160446
1	8.391195966	16.341268841	10.759081413
6	8.638744273	14.321682307	10.077285172
1	7.744445925	13.968411656	10.579628883
6	10.549563548	17.590442989	9.670046216
1	10.754925410	17.868501660	10.712223770
1	11.444475480	17.817675456	9.080704645
1	9.740250881	18.243179152	9.317642866
6	7.129385296	12.663932034	14.254939240
6	8.166429876	13.535188567	13.869239951
1	8.913859765	13.190058521	13.162587632
6	8.220444369	14.836578419	14.355907896
1	9.028809665	15.492713475	14.037718409
6	7.251246092	15.321770554	15.243410514
6	6.214462522	14.458868146	15.620222759
1	5.438778628	14.820099166	16.292788359
6	6.150325219	13.156413013	15.137874237
1	5.320275039	12.520259961	15.430937915
6	7.330348175	16.722337434	15.781311255
1	6.356406953	17.065629659	16.147739012
1	7.672420074	17.426449233	15.013367625
1	8.038414811	16.787924816	16.618751935
6	5.867792541	10.043531165	15.599886570
6	6.605640847	10.374735357	16.746853639
1	7.642154271	10.685962336	16.638362680
6	6.017856512	10.317077304	18.005666442
1	6.602601151	10.573427354	18.887489646
6	4.677721511	9.933497077	18.159988110
6	3.947043087	9.598653180	17.015072816
1	2.910887133	9.281462488	17.116771848
6	4.531830111	9.648221760	15.752351245
1	3.950355288	9.386039929	14.870580214
6	4.045098243	9.898330771	19.523075034
1	4.722883183	9.459449970	20.266711481
1	3.118896486	9.311895848	19.517763624
1	3.794358811	10.908453707	19.874384679
6	5.222089883	6.510952167	15.098806073
6	6.104758134	6.807566622	16.148103222
1	7.111113216	7.149897327	15.914686575
6	5.702632959	6.662505015	17.471417245
1	6.394561343	6.906613724	18.276038327
6	4.409564686	6.225066365	17.788570937
6	3.528809084	5.938023289	16.738965250
1	2.519619805	5.600679697	16.967485723
6	3.927126934	6.075694452	15.411978816
1	3.237760686	5.838028420	14.605103359
6	3.990836204	6.067987908	19.223555174
1	4.496132292	5.215521945	19.696909772
1	2.911074670	5.904536651	19.311494574
1	4.248472835	6.959283556	19.810599760
6	5.205100259	4.179910864	12.921943991
6	5.387471275	3.487136452	14.133519366
1	5.869301777	3.985375217	14.970175582
6	4.972895373	2.167687621	14.266971306
1	5.130566717	1.647688373	15.210346323
6	4.360167997	1.486903652	13.204397019
6	4.183270884	2.173864100	11.999295838
1	3.714238825	1.664704009	11.159631189
6	4.598516978	3.494256974	11.856293324
6	3.919393657	0.059124366	13.364977802
1	4.774481765	-0.602101401	13.557754919
1	3.229161350	-0.053172107	14.211167796
1	3.411005364	-0.306132243	12.466097232
8	5.486422490	9.217479708	9.916626428
1	6.837811563	-0.455921032	6.073127006
1	6.704257266	-0.746276729	7.810782195
1	5.260161602	-0.335261987	6.876436946
1	9.164808210	7.186231280	1.222292440
1	10.457815625	6.028191450	1.545355038
1	8.823284897	5.450052724	1.170752008
1	4.465120206	4.005500669	10.909266914

$[(Me_8Cz)Mn(O)CN]^-$: B3LYP:

6	-2.149723000	-1.937721000	0.203386000
6	-3.602813000	-1.942665000	0.052366000
6	-4.025581000	-0.626663000	0.088040000
6	-2.837827000	0.208615000	0.264459000
6	-1.702208000	2.288637000	0.295250000
6	-1.640397000	3.743567000	0.152292000
6	-0.304903000	4.100878000	0.145298000
6	0.475670000	2.872602000	0.279635000
6	2.446015000	1.595980000	0.226676000
6	3.841232000	1.319783000	-0.023684000
6	4.010372000	-0.076171000	-0.037152000
6	2.721385000	-0.664904000	0.214835000
6	2.040242000	-1.911508000	0.192168000
6	2.245080000	-3.304492000	-0.107636000
6	0.980360000	-3.918750000	-0.121883000
6	-0.009479000	-2.903020000	0.152107000
25	0.043298000	-0.020809000	0.708791000
7	-0.416550000	1.825413000	0.407306000
7	1.833206000	0.387312000	0.424327000
7	0.672758000	-1.740437000	0.393779000
7	-2.826140000	1.552948000	0.249123000
7	1.812003000	2.788528000	0.203088000
7	-1.354476000	-3.013499000	0.106922000
8	-0.208490000	0.093485000	2.262791000
7	-1.753951000	-0.624331000	0.369755000
6	4.875164000	2.378528000	-0.253665000
6	5.298156000	-0.800149000	-0.305474000
6	3.557819000	-3.982677000	-0.372108000
6	0.645866000	-5.353551000	-0.391822000
6	0.302309000	5.460904000	0.003471000
6	-2.847582000	4.618738000	0.029823000
6	-5.414553000	-0.084486000	-0.033420000
6	-4.416186000	-3.185157000	-0.130635000
1	-3.717669000	4.011631000	-0.236437000
1	-2.710637000	5.394975000	-0.734612000
1	-3.078771000	5.133763000	0.973990000
1	1.341724000	5.370865000	-0.325616000
1	0.304927000	6.010472000	0.956602000
1	-0.246538000	6.076368000	-0.720802000
1	5.729317000	2.279696000	0.431549000
1	4.426490000	3.364697000	-0.103365000
1	5.277457000	2.344732000	-1.275962000
1	6.160043000	-0.157951000	-0.090503000
1	5.382648000	-1.112954000	-1.356690000
1	5.392897000	-1.701908000	0.309396000
1	3.402595000	-4.999254000	-0.748521000
1	4.172481000	-4.061398000	0.536398000
1	4.151850000	-3.439825000	-1.116976000
1	1.104152000	-5.715969000	-1.321909000
1	-0.439213000	-5.461039000	-0.481479000
1	0.985079000	-6.018242000	0.415795000
1	-5.167032000	-3.066903000	-0.923109000
1	-4.957800000	-3.459904000	0.786627000
1	-3.760018000	-4.020818000	-0.390982000
1	-5.975583000	-0.580810000	-0.836370000
1	-5.374663000	0.988266000	-0.243186000

1	-5.990774000	-0.221649000	0.893566000
6	0.011215000	0.028285000	-1.438267000
7	-0.029498000	0.065843000	-2.620108000

^{1}[(Me$_8$Cz)Mn(O)] B3LYP:

6	-2.130425000	-1.919177000	0.139200000
6	-3.572932000	-1.927492000	0.044973000
6	-3.999945000	-0.610069000	0.048611000
6	-2.825793000	0.224196000	0.153728000
6	-1.709327000	2.271170000	0.183890000
6	-1.642233000	3.711583000	0.113490000
6	-0.303468000	4.065830000	0.141836000
6	0.469486000	2.847482000	0.221350000
6	2.419450000	1.608881000	0.171847000
6	3.822649000	1.328622000	-0.020620000
6	3.976602000	-0.062196000	-0.056526000
6	2.668011000	-0.639936000	0.121088000
6	1.996469000	-1.872894000	0.094104000
6	2.219720000	-3.277009000	-0.130769000
6	0.966540000	-3.900905000	-0.130213000
6	-0.030834000	-2.882162000	0.084546000
25	0.012822000	-0.007104000	0.824299000
7	-0.410944000	1.753306000	0.271854000
7	1.759949000	0.402393000	0.292784000
7	0.624251000	-1.678509000	0.253017000
7	-2.831163000	1.555263000	0.147995000
7	1.805084000	2.792975000	0.177321000
7	-1.359323000	-3.008537000	0.069911000
8	-0.043265000	-0.005296000	2.376639000
7	-1.688494000	-0.588731000	0.232426000
6	4.861742000	2.394990000	-0.162478000
6	5.251294000	-0.824224000	-0.266440000
6	3.542960000	-3.952337000	-0.334951000
6	0.646297000	-5.350486000	-0.317910000
6	0.298722000	5.432693000	0.083432000
6	-2.839517000	4.603111000	0.033063000
6	-5.395824000	-0.080882000	-0.028307000
6	-4.393281000	-3.173361000	-0.051495000
1	-3.733880000	4.016356000	-0.188503000
1	-2.719395000	5.368351000	-0.743441000
1	-3.012036000	5.131067000	0.980675000
1	1.366271000	5.366197000	-0.138600000
1	0.189607000	5.959693000	1.041150000
1	-0.183940000	6.053013000	-0.680973000
1	5.863485000	1.975056000	-0.284248000
1	4.872501000	3.052605000	0.714667000
1	4.653609000	3.033076000	-1.029548000
1	6.121786000	-0.169027000	-0.179813000
1	5.289425000	-1.287272000	-1.261018000
1	5.366993000	-1.625771000	0.471042000
1	3.405146000	-5.004662000	-0.597294000
1	4.159244000	-3.919223000	0.572703000
1	4.121988000	-3.482850000	-1.137844000
1	1.150727000	-5.770752000	-1.196128000
1	-0.431303000	-5.478269000	-0.446758000
1	0.952134000	-5.949655000	0.549907000
1	-5.238377000	-3.046948000	-0.737643000
1	-4.809277000	-3.455354000	0.925741000
1	-3.777822000	-4.007588000	-0.396922000
1	-5.999284000	-0.641397000	-0.751694000
1	-5.386840000	0.972633000	-0.317417000
1	-5.906013000	-0.152433000	0.941833000

^{1}[(Me$_8$Cz)Mn(O)CN]$^{-}$: BP86:

6	-2.160402000	-1.949628000	0.185235000
6	-3.622371000	-1.957298000	0.049616000
6	-4.049203000	-0.630993000	0.092705000
6	-2.852879000	0.207718000	0.255299000
6	-1.709668000	2.297022000	0.281354000
6	-1.649319000	3.758444000	0.139242000
6	-0.302744000	4.118913000	0.126275000
6	0.480307000	2.884976000	0.260191000
6	2.458984000	1.603448000	0.217547000
6	3.863597000	1.327072000	-0.020705000
6	4.035288000	-0.079765000	-0.035924000
6	2.739763000	-0.672626000	0.207211000
6	2.055859000	-1.924937000	0.183000000
6	2.260566000	-3.323761000	-0.121765000
6	0.984860000	-3.940585000	-0.140800000
6	-0.009961000	-2.918102000	0.132329000
25	0.045648000	-0.023166000	0.693547000
7	-0.412556000	1.827669000	0.389311000
7	1.836576000	0.384662000	0.416019000
7	0.676579000	-1.745314000	0.385156000
7	-2.845184000	1.561445000	0.238921000
7	1.829594000	2.807029000	0.187579000
7	-1.362073000	-3.038301000	0.084350000
8	-0.263852000	0.101943000	2.260261000
7	-1.757103000	-0.629962000	0.345664000
6	4.900606000	2.391255000	-0.233907000
6	5.330491000	-0.800386000	-0.299163000
6	3.574175000	-4.006781000	-0.390021000
6	0.644679000	-5.376939000	-0.415184000
6	0.308029000	5.481217000	-0.020784000
6	-2.861461000	4.634470000	0.024264000
6	-5.442886000	-0.084590000	-0.003498000
6	-4.436625000	-3.205883000	-0.120309000
1	-3.749423000	4.009248000	-0.169598000
1	-2.758949000	5.372323000	-0.795013000
1	-3.049148000	5.208959000	0.954115000
1	1.380683000	5.380665000	-0.258464000
1	0.224250000	6.077155000	0.910761000
1	-0.181389000	6.066733000	-0.822936000
1	5.740187000	2.307640000	0.485075000
1	4.434621000	3.383699000	-0.108951000
1	5.339292000	2.346620000	-1.250460000
1	6.196014000	-0.171677000	-0.021027000
1	5.449858000	-1.059832000	-1.370915000
1	5.399575000	-1.741525000	0.273835000
1	3.413270000	-5.029754000	-0.773494000
1	4.195112000	-4.092758000	0.524519000
1	4.174516000	-3.458078000	-1.139153000
1	1.124672000	-5.749734000	-1.340876000
1	-0.448595000	-5.472912000	-0.529162000
1	0.960901000	-6.048825000	0.408124000
1	-5.191272000	-3.099578000	-0.923509000
1	-4.986261000	-3.472284000	0.805498000
1	-3.770372000	-4.049491000	-0.368519000
1	-6.010380000	-0.547703000	-0.834020000
1	-5.399622000	1.005516000	-0.167271000
1	-6.024267000	-0.264281000	0.923785000
6	0.003978000	0.028618000	-1.436056000
7	-0.040888000	0.067107000	-2.631364000

^{1}[(Me$_8$Cz)Mn(O)] BP86:

6	-2.142431000	-1.931685000	0.139665000
6	-3.592672000	-1.940744000	0.058316000
6	-4.024052000	-0.612309000	0.066044000
6	-2.843121000	0.226768000	0.159062000
6	-1.722264000	2.283823000	0.183606000
6	-1.656236000	3.731933000	0.116431000
6	-0.305725000	4.089245000	0.135829000
6	0.471566000	2.864644000	0.209217000
6	2.431200000	1.619696000	0.159228000
6	3.844440000	1.338626000	-0.012667000
6	4.000947000	-0.064641000	-0.051608000
6	2.684503000	-0.644507000	0.102892000
6	2.009416000	-1.886069000	0.081358000
6	2.233389000	-3.297330000	-0.134084000
6	0.968307000	-3.925532000	-0.130955000

6	-0.032898000	-2.898980000	0.076929000
25	0.014598000	-0.004946000	0.798783000
7	-0.414991000	1.760903000	0.266550000
7	1.764049000	0.404734000	0.266704000
7	0.625677000	-1.686026000	0.243066000
7	-2.856075000	1.567613000	0.154548000
7	1.816987000	2.816123000	0.166938000
7	-1.371418000	-3.032646000	0.067853000
8	-0.030903000	0.004969000	2.373026000
7	-1.695279000	-0.590327000	0.232806000
6	4.891061000	2.406044000	-0.127952000
6	5.284791000	-0.824292000	-0.240472000
6	3.558020000	-3.980237000	-0.330690000
6	0.644479000	-5.379590000	-0.309086000
6	0.300318000	5.458613000	0.080476000
6	-2.859979000	4.622399000	0.054696000
6	-5.424216000	-0.081812000	0.009013000
6	-4.414375000	-3.190867000	-0.028176000
1	-3.767201000	4.020355000	-0.114558000
1	-2.772293000	5.369543000	-0.756254000
1	-2.996773000	5.185184000	0.998622000
1	1.385621000	5.384079000	-0.094464000
1	0.146995000	6.006642000	1.030538000
1	-0.150293000	6.071813000	-0.721991000
1	5.905985000	1.981187000	-0.197208000
1	4.860447000	3.086323000	0.742805000
1	4.721399000	3.033512000	-1.022851000
1	6.159465000	-0.164630000	-0.115499000
1	5.353022000	-1.270587000	-1.251345000
1	5.380902000	-1.647636000	0.489306000
1	3.415267000	-5.031410000	-0.631701000
1	4.159442000	-3.982340000	0.598737000
1	4.164394000	-3.486405000	-1.110813000
1	1.079589000	-5.788510000	-1.240483000
1	-0.448819000	-5.513425000	-0.351702000
1	1.030514000	-5.992680000	0.527526000
1	-5.195549000	-3.112484000	-0.806933000
1	-4.931619000	-3.401183000	0.928635000
1	-3.767487000	-4.053368000	-0.256219000
1	-6.015001000	-0.576943000	-0.784070000
1	-5.410276000	1.003340000	-0.181878000
1	-5.959991000	-0.250003000	0.963629000

$^{1}[(Me_8Cz)Mn(O)CN]^{-}$: M06:

6	-2.135694000	-1.935684000	0.182279000
6	-3.581128000	-1.937444000	0.022630000
6	-4.001526000	-0.626863000	0.065427000
6	-2.820310000	0.203433000	0.250392000
6	-1.691220000	2.276068000	0.279777000
6	-1.629888000	3.721408000	0.120214000
6	-0.299522000	4.077792000	0.111236000
6	0.478230000	2.858545000	0.264750000
6	2.435668000	1.586131000	0.238683000
6	3.825130000	1.306773000	-0.019414000
6	3.991001000	-0.081552000	-0.027731000
6	2.707543000	-0.663818000	0.243862000
6	2.032737000	-1.902352000	0.218247000
6	2.240018000	-3.281933000	-0.106598000
6	0.983445000	-3.895388000	-0.135706000
6	-0.006611000	-2.891693000	0.149983000
25	0.037573000	-0.021516000	0.724836000
7	-0.409185000	1.817148000	0.403612000
7	1.824264000	0.383881000	0.457744000
7	0.668151000	-1.734515000	0.422735000
7	-2.809700000	1.541520000	0.232821000
7	1.811464000	2.775234000	0.193832000
7	-1.344461000	-3.008190000	0.085009000
8	-0.267611000	0.135658000	2.258796000
7	-1.740817000	-0.629862000	0.359745000
6	4.837158000	2.367786000	-0.270494000
6	5.249977000	-0.831286000	-0.310801000
6	3.547156000	-3.943739000	-0.386256000
6	0.657010000	-5.315238000	-0.442244000
6	0.295211000	5.430698000	-0.056837000
6	-2.823903000	4.596669000	-0.022247000
6	-5.382511000	-0.089986000	-0.055559000
6	-4.392262000	-3.168086000	-0.174041000
1	-3.723541000	3.978641000	-0.115109000
1	-2.749239000	5.240745000	-0.909912000
1	-2.951949000	5.259114000	0.846400000
1	1.379456000	5.342848000	-0.186041000
1	0.106446000	6.071785000	0.816851000
1	-0.120784000	5.949300000	-0.932177000
1	5.852332000	1.960115000	-0.341787000
1	4.820364000	3.120294000	0.528452000
1	4.618544000	2.901856000	-1.205164000
1	6.132629000	-0.196817000	-0.162407000
1	5.282448000	-1.196318000	-1.348027000
1	5.353334000	-1.704742000	0.346221000
1	3.394778000	-4.958354000	-0.773031000
1	4.169649000	-4.025346000	0.516511000
1	4.129506000	-3.386773000	-1.132030000
1	1.052921000	-5.625372000	-1.419345000
1	-0.431405000	-5.438053000	-0.462154000
1	1.066251000	-6.005644000	0.309080000
1	-5.134164000	-3.041102000	-0.974435000
1	-4.943289000	-3.444019000	0.736878000
1	-3.734808000	-4.005227000	-0.432981000
1	-5.944549000	-0.595748000	-0.852279000
1	-5.343356000	0.982348000	-0.275571000
1	-5.953565000	-0.219405000	0.875358000
6	0.029963000	0.025294000	-1.395897000
7	0.003389000	0.065277000	-2.577823000

$^{1}[(Me_8Cz)Mn(O)]$: M06:

6	-2.131033000	-1.918979000	0.133514000
6	-3.574747000	-1.927570000	0.050935000
6	-4.002288000	-0.610548000	0.062829000
6	-2.827046000	0.224463000	0.156644000
6	-1.710352000	2.271975000	0.183216000
6	-1.643900000	3.712781000	0.116273000
6	-0.304869000	4.067156000	0.137760000
6	0.468793000	2.848503000	0.212768000
6	2.419540000	1.609493000	0.164152000
6	3.825385000	1.328900000	-0.011154000
6	3.979897000	-0.062370000	-0.046206000
6	2.668694000	-0.639866000	0.112239000
6	1.996810000	-1.873549000	0.084028000
6	2.220485000	-3.279600000	-0.129517000
6	0.966579000	-3.902639000	-0.131429000
6	-0.031169000	-2.882058000	0.074168000
25	0.013864000	-0.006481000	0.805485000
7	-0.411788000	1.754931000	0.264229000
7	1.759134000	0.402662000	0.274710000
7	0.624122000	-1.678130000	0.236397000
7	-2.831901000	1.555151000	0.154579000
7	1.804346000	2.793104000	0.171719000
7	-1.359859000	-3.007701000	0.063273000
8	-0.041171000	-0.003905000	2.358311000
7	-1.689729000	-0.588608000	0.225903000
6	4.866813000	2.395741000	-0.136293000
6	5.257462000	-0.825032000	-0.237443000
6	3.544377000	-3.957704000	-0.320574000
6	0.645889000	-5.353372000	-0.312385000
6	0.296751000	5.434855000	0.083527000
6	-2.842420000	4.604229000	0.049111000
6	-5.399623000	-0.081984000	0.008660000
6	-4.395710000	-3.173915000	-0.037653000
1	-3.741409000	4.014806000	-0.147229000
1	-2.738219000	5.359927000	-0.739532000

1	-2.994578000	5.144303000	0.993641000
1	1.366596000	5.368750000	-0.129161000
1	0.178114000	5.962262000	1.040224000
1	-0.179427000	6.054671000	-0.686076000
1	5.871708000	1.976702000	-0.235899000
1	4.858437000	3.056826000	0.738609000
1	4.675800000	3.030399000	-1.010304000
1	6.127747000	-0.172736000	-0.126219000
1	5.314788000	-1.277998000	-1.236095000
1	5.355816000	-1.634708000	0.493931000
1	3.407189000	-5.008870000	-0.589299000
1	4.149774000	-3.929973000	0.594945000
1	4.134008000	-3.485491000	-1.114425000
1	1.131267000	-5.772020000	-1.202703000
1	-0.434399000	-5.483644000	-0.417576000
1	0.973570000	-5.952244000	0.547810000
1	-5.238137000	-3.053402000	-0.728782000
1	-4.816231000	-3.446033000	0.940502000
1	-3.779075000	-4.011720000	-0.373124000
1	-6.009294000	-0.630250000	-0.719215000
1	-5.394689000	0.977016000	-0.261167000
1	-5.900351000	-0.173321000	0.982369000

$^{1}[(H_8Cz)Mn(O)CN]^{-}$: B3LYP:

6	-2.143712000	-1.946860000	0.158639000
6	-3.594645000	-1.941718000	0.023155000
6	-4.015348000	-0.635151000	0.060781000
6	-2.836207000	0.207814000	0.221568000
6	-1.699074000	2.288148000	0.257659000
6	-1.627319000	3.738817000	0.134494000
6	-0.301050000	4.095061000	0.126647000
6	0.488384000	2.876763000	0.244168000
6	2.459910000	1.603600000	0.205238000
6	3.849959000	1.305967000	-0.028445000
6	4.005914000	-0.081750000	-0.040217000
6	2.719976000	-0.661898000	0.201142000
6	2.041049000	-1.906713000	0.178166000
6	2.254028000	-3.295467000	-0.099904000
6	1.003217000	-3.914747000	-0.125602000
6	-0.003740000	-2.912857000	0.120871000
25	0.044338000	-0.017439000	0.662538000
7	-0.408146000	1.828073000	0.355603000
7	1.836029000	0.393597000	0.394216000
7	0.673474000	-1.740718000	0.352959000
7	-2.825476000	1.553447000	0.217295000
7	1.826775000	2.797691000	0.180413000
7	-1.349795000	-3.026415000	0.074543000
8	-0.253508000	0.089583000	2.207228000
7	-1.752074000	-0.628838000	0.308852000
1	4.615568000	2.049983000	-0.191697000
1	4.922723000	-0.623539000	-0.222381000
1	3.208902000	-3.767758000	-0.279960000
1	0.794663000	-4.956399000	-0.320168000
1	0.129439000	5.080102000	0.025950000
1	-2.494537000	4.376488000	0.050414000
1	-5.020497000	-0.250483000	-0.025524000
1	-4.186771000	-2.834836000	-0.109335000
6	0.016667000	0.029373000	-1.469006000
7	-0.023156000	0.066691000	-2.650386000

$^{1}[(H_8Cz)Mn(O)]$: B3LYP:

6	-2.127594000	-1.925470000	0.137040000
6	-3.565111000	-1.919901000	0.033653000
6	-3.988908000	-0.614379000	0.043579000
6	-2.825805000	0.226538000	0.159578000
6	-1.710766000	2.271558000	0.195364000
6	-1.632438000	3.707338000	0.118995000
6	-0.305525000	4.058091000	0.138895000
6	0.476319000	2.850216000	0.221981000
6	2.425948000	1.615250000	0.168201000

6	3.817709000	1.313833000	-0.029449000
6	3.959193000	-0.067780000	-0.065587000
6	2.659815000	-0.637891000	0.116312000
6	1.988569000	-1.869308000	0.094347000
6	2.216009000	-3.264678000	-0.124722000
6	0.977693000	-3.894510000	-0.124701000
6	-0.032516000	-2.893629000	0.086639000
25	0.012058000	-0.005938000	0.824361000
7	-0.409941000	1.756535000	0.279209000
7	1.758528000	0.407554000	0.286765000
7	0.619176000	-1.682584000	0.249803000
7	-2.834388000	1.557938000	0.162482000
7	1.810058000	2.800346000	0.177088000
7	-1.362260000	-3.017910000	0.072619000
8	-0.044665000	-0.002826000	2.373069000
7	-1.689397000	-0.590332000	0.237236000
1	4.590508000	2.058512000	-0.141265000
1	4.873436000	-0.620016000	-0.221898000
1	3.177944000	-3.729444000	-0.279360000
1	0.771827000	-4.943823000	-0.269027000
1	0.132641000	5.042148000	0.079603000
1	-2.498585000	4.346843000	0.052701000
1	-4.994694000	-0.230889000	-0.026434000
1	-4.154003000	-2.819114000	-0.058454000

$^{1}[(H_8Cz)Mn(O)CN]^{-}$: BP86:

6	-2.153688000	-1.958807000	0.145158000
6	-3.612333000	-1.955241000	0.019208000
6	-4.036397000	-0.638927000	0.059602000
6	-2.850266000	0.207611000	0.212456000
6	-1.706232000	2.298612000	0.248161000
6	-1.635316000	3.756385000	0.133583000
6	-0.298723000	4.116038000	0.123038000
6	0.494345000	2.891755000	0.231104000
6	2.474869000	1.613787000	0.192873000
6	3.874240000	1.314686000	-0.030968000
6	4.032048000	-0.082564000	-0.045874000
6	2.739646000	-0.667441000	0.188100000
6	2.057786000	-1.917729000	0.164505000
6	2.269880000	-3.315657000	-0.103553000
6	1.009903000	-3.937300000	-0.126582000
6	-0.003174000	-2.926940000	0.107599000
25	0.048305000	-0.017597000	0.644867000
7	-0.403196000	1.832132000	0.338167000
7	1.840822000	0.393571000	0.381319000
7	0.678748000	-1.741775000	0.337401000
7	-2.843512000	1.562891000	0.207838000
7	1.846289000	2.819317000	0.168212000
7	-1.355910000	-3.051699000	0.060961000
8	-0.302082000	0.094495000	2.201763000
7	-1.754865000	-0.634698000	0.289766000
1	4.647282000	2.065595000	-0.186924000
1	4.958081000	-0.627736000	-0.224340000
1	3.232308000	-3.795173000	-0.277581000
1	0.798618000	-4.989413000	-0.310957000
1	0.134766000	5.110192000	0.027738000
1	-2.510273000	4.400016000	0.059183000
1	-5.050784000	-0.251208000	-0.017942000
1	-4.210181000	-2.856046000	-0.108321000
6	-0.001089000	0.034364000	-1.469401000
7	-0.050062000	0.075242000	-2.664017000

$^{1}[(H_8Cz)Mn(O)]$: BP86:

6	-2.138585000	-1.938263000	0.138015000
6	-3.582733000	-1.932161000	0.037892000
6	-4.009692000	-0.617011000	0.045346000
6	-2.841629000	0.229300000	0.156507000
6	-1.721629000	2.283375000	0.190384000
6	-1.641257000	3.725965000	0.118154000
6	-0.304424000	4.079028000	0.141915000

6	0.481039000	2.866041000	0.223011000
6	2.437529000	1.624068000	0.169633000
6	3.837784000	1.321122000	-0.026625000
6	3.982182000	-0.069526000	-0.064702000
6	2.677354000	-0.642769000	0.116097000
6	2.002991000	-1.880787000	0.092853000
6	2.230212000	-3.281538000	-0.127717000
6	0.982344000	-3.914091000	-0.125925000
6	-0.033524000	-2.907580000	0.085447000
25	0.010947000	-0.005696000	0.820252000
7	-0.410801000	1.761501000	0.275899000
7	1.764512000	0.408286000	0.289628000
7	0.622030000	-1.687507000	0.251458000
7	-2.857057000	1.570319000	0.156946000
7	1.825846000	2.822344000	0.178927000
7	-1.372245000	-3.042906000	0.071856000
8	-0.048416000	-0.002705000	2.389242000
7	-1.694274000	-0.592495000	0.234414000
1	4.613741000	2.075632000	-0.133903000
1	4.903956000	-0.626121000	-0.220496000
1	3.198607000	-3.753806000	-0.278976000
1	0.771929000	-4.972049000	-0.264900000
1	0.135939000	5.071954000	0.090376000
1	-2.513065000	4.372845000	0.056727000
1	-5.024605000	-0.231910000	-0.017720000
1	-4.178194000	-2.838210000	-0.045439000

^{1}[(H$_8$Cz)Mn(O)CN]$^{-}$: M06:

6	-2.131834000	-1.941527000	0.154925000
6	-3.577054000	-1.934757000	0.016180000
6	-3.995107000	-0.632258000	0.058409000
6	-2.819396000	0.204482000	0.225279000
6	-1.686837000	2.275531000	0.261642000
6	-1.618705000	3.720201000	0.133749000
6	-0.297412000	4.076925000	0.120000000
6	0.490558000	2.864427000	0.239581000
6	2.450490000	1.596399000	0.203171000
6	3.834027000	1.300167000	-0.030861000
6	3.990269000	-0.081878000	-0.040678000
6	2.709919000	-0.659808000	0.203184000
6	2.034644000	-1.899192000	0.181433000
6	2.245706000	-3.281907000	-0.100810000
6	0.999302000	-3.897408000	-0.127510000
6	-0.002279000	-2.900105000	0.121442000
25	0.043735000	-0.016644000	0.669577000
7	-0.399675000	1.818650000	0.359121000
7	1.827337000	0.390767000	0.398869000
7	0.672530000	-1.731756000	0.360936000
7	-2.808889000	1.544542000	0.222193000
7	1.822599000	2.786675000	0.173523000
7	-1.342068000	-3.016075000	0.069502000
8	-0.286103000	0.105213000	2.199578000
7	-1.740088000	-0.630519000	0.313437000
1	4.595373000	2.048755000	-0.199671000
1	4.906104000	-0.626109000	-0.226009000
1	3.201702000	-3.751966000	-0.286202000
1	0.783748000	-4.937400000	-0.329042000
1	0.137476000	5.060666000	0.013923000
1	-2.491929000	4.351709000	0.050197000
1	-4.998191000	-0.239311000	-0.029163000
1	-4.165325000	-2.830901000	-0.122116000
6	0.010747000	0.028246000	-1.439742000
7	-0.038670000	0.069208000	-2.620949000

^{1}[(H$_8$Cz)Mn(O)]: M06:

6	-2.119153000	-1.916365000	0.142101000
6	-3.552543000	-1.911822000	0.053012000
6	-3.974745000	-0.610622000	0.062526000
6	-2.814018000	0.226520000	0.164487000
6	-1.704520000	2.261282000	0.201209000
6	-1.628423000	3.692661000	0.139808000
6	-0.306083000	4.042581000	0.158751000
6	0.473247000	2.838178000	0.226219000
6	2.413386000	1.609828000	0.169946000
6	3.802425000	1.312789000	-0.004221000
6	3.946873000	-0.064104000	-0.049177000
6	2.651560000	-0.636188000	0.104705000
6	1.982486000	-1.863129000	0.082807000
6	2.205825000	-3.257194000	-0.106282000
6	0.969787000	-3.882272000	-0.096982000
6	-0.034840000	-2.880450000	0.090253000
25	0.014423000	-0.006517000	0.798945000
7	-0.408837000	1.747207000	0.271493000
7	1.747316000	0.404904000	0.262557000
7	0.615485000	-1.671090000	0.225964000
7	-2.825985000	1.553054000	0.174784000
7	1.801261000	2.792117000	0.189805000
7	-1.360227000	-3.006242000	0.087366000
8	-0.032637000	-0.007879000	2.337108000
7	-1.680977000	-0.585896000	0.229947000
1	4.573790000	2.063289000	-0.095170000
1	4.865618000	-0.614257000	-0.191131000
1	3.167756000	-3.727527000	-0.248906000
1	0.757885000	-4.934035000	-0.221422000
1	0.137372000	5.025974000	0.108301000
1	-2.499705000	4.327945000	0.082677000
1	-4.979872000	-0.221027000	-0.000022000
1	-4.137688000	-2.815589000	-0.031432000

^{3}[((MePh)$_8$Cz)Mn(O)CN]$^{-}$: B3LYP:

25	6.585963000	8.836694000	10.416549000
7	7.023053000	7.484571000	9.136826000
7	7.695175000	10.155959000	9.547924000
7	6.595525000	9.822415000	12.027640000
7	5.884603000	7.525450000	11.611384000
7	8.309819000	8.859048000	7.608251000
7	7.701211000	11.823305000	11.313397000
7	6.063807000	5.556499000	10.266678000
6	6.652253000	6.179315000	9.212608000
6	7.107191000	5.499429000	7.980726000
6	7.757026000	6.449659000	7.200302000
6	7.734549000	7.717701000	7.964269000
6	8.328296000	9.992561000	8.370104000
6	9.057814000	11.228380000	8.048322000
6	8.844030000	12.116259000	9.101338000
6	8.002397000	11.407220000	10.085857000
6	7.066310000	11.074046000	12.254627000
6	6.797805000	11.388299000	13.650035000
6	6.184381000	10.245731000	14.220153000
6	6.082477000	9.245380000	13.172506000
6	5.739127000	7.861275000	12.929431000
6	5.410247000	6.619285000	13.654879000
6	5.401506000	5.582417000	12.716210000
6	5.758376000	6.184952000	11.409141000
6	6.964961000	4.050032000	7.758100000
6	5.749154000	3.386813000	8.014919000
1	4.901211000	3.960610000	8.367661000
6	5.629620000	2.007780000	7.825920000
1	4.678115000	1.522673000	8.028408000
6	6.716882000	1.235640000	7.385752000
6	7.931527000	1.896913000	7.130786000
1	8.791391000	1.323293000	6.793315000
6	8.056348000	3.274276000	7.313830000
1	9.006814000	3.759989000	7.122668000
6	6.598793000	-0.265305000	7.226623000
6	8.302588000	6.309781000	5.839666000
6	7.672290000	5.481713000	4.886221000
1	6.777003000	4.937925000	5.163671000
6	8.176773000	5.360163000	3.590710000
1	7.667358000	4.715279000	2.878610000

6	9.323426000	6.065083000	3.187044000
6	9.946455000	6.897580000	4.132209000
1	10.828739000	7.465048000	3.846626000
6	9.450377000	7.021812000	5.430698000
1	9.929453000	7.690575000	6.131899000
6	9.850161000	5.961288000	1.771869000
6	9.826217000	11.414163000	6.801516000
6	10.841962000	10.507007000	6.445353000
1	11.061251000	9.676666000	7.107434000
6	11.568687000	10.670020000	5.261684000
1	12.352861000	9.958589000	5.014489000
6	11.304372000	11.735766000	4.387327000
6	10.286833000	12.640689000	4.742004000
1	10.056586000	13.472328000	4.079933000
6	9.561842000	12.485668000	5.924389000
1	8.777154000	13.191518000	6.175053000
6	12.080809000	11.908826000	3.098598000
1	12.584995000	12.883706000	3.058632000
1	12.846256000	11.133284000	2.988367000
1	11.421278000	11.851870000	2.222237000
6	9.364746000	13.480767000	9.287502000
6	10.631873000	13.867716000	8.804268000
1	11.255880000	13.138475000	8.302235000
6	11.100678000	15.173140000	8.972093000
1	12.082820000	15.438832000	8.588545000
6	10.332360000	16.145586000	9.632657000
6	9.075310000	15.757489000	10.130537000
1	8.459822000	16.484407000	10.655321000
6	8.598493000	14.456715000	9.964987000
1	7.634365000	14.179192000	10.370947000
6	10.836567000	17.562110000	9.811043000
1	10.923610000	17.828045000	10.873124000
1	11.822869000	17.694266000	9.353216000
1	10.155641000	18.292190000	9.353014000
6	7.068283000	12.697798000	14.269108000
6	8.230085000	13.425948000	13.928330000
1	8.916734000	13.011246000	13.202011000
6	8.485382000	14.677128000	14.491985000
1	9.386215000	15.213578000	14.203954000
6	7.601028000	15.256685000	15.417930000
6	6.438409000	14.540124000	15.747997000
1	5.725339000	14.971326000	16.446875000
6	6.173847000	13.289403000	15.186361000
1	5.259702000	12.770772000	15.448673000
6	7.901674000	16.599157000	16.049858000
1	6.989033000	17.079881000	16.420044000
1	8.376695000	17.281425000	15.334711000
1	8.587328000	16.498447000	16.903746000
6	5.728413000	10.125334000	15.621658000
6	6.603557000	10.400810000	16.691921000
1	7.634764000	10.658529000	16.474952000
6	6.160259000	10.349840000	18.014202000
1	6.857515000	10.565632000	18.820459000
6	4.828051000	10.021543000	18.322327000
6	3.959258000	9.731722000	17.257454000
1	2.928368000	9.459099000	17.467989000
6	4.398590000	9.782443000	15.931374000
1	3.707158000	9.562281000	15.124161000
6	4.344493000	10.002846000	19.757389000
1	5.128545000	9.652073000	20.439212000
1	3.474333000	9.347864000	19.877293000
1	4.047836000	11.005918000	20.096547000
6	5.168504000	6.466870000	15.108556000
6	6.185108000	6.746401000	16.044052000
1	7.135603000	7.134924000	15.693182000
6	5.988900000	6.509903000	17.405913000
1	6.791031000	6.730740000	18.105171000
6	4.772300000	5.993382000	17.888165000
6	3.754541000	5.731999000	16.956758000
1	2.802609000	5.337025000	17.303171000
6	3.946886000	5.963672000	15.591102000
1	3.152561000	5.739196000	14.886428000
6	4.573184000	5.734051000	19.366772000
1	5.335726000	5.049214000	19.760787000
1	3.591948000	5.289431000	19.565137000
1	4.643293000	6.662459000	19.948864000
6	5.175125000	4.143334000	12.915088000
6	5.603596000	3.465234000	14.077829000
1	6.130040000	4.010931000	14.850650000
6	5.375761000	2.099138000	14.237717000
1	5.723710000	1.604189000	15.141416000
6	4.714212000	1.348368000	13.248913000
6	4.295582000	2.018658000	12.088705000
1	3.789748000	1.461500000	11.304183000
6	4.523439000	3.385901000	11.919013000
6	4.490144000	-0.138028000	13.424734000
1	5.427591000	-0.700211000	13.311542000
1	4.094427000	-0.370358000	14.421563000
1	3.783132000	-0.525198000	12.683259000
8	5.185612000	9.372232000	9.786942000
6	8.543772000	8.214163000	11.245615000
1	7.229148000	-0.633413000	6.408519000
1	6.913774000	-0.789986000	8.140037000
1	5.565432000	-0.565926000	7.019514000
1	9.548345000	6.828544000	1.167600000
1	10.946065000	5.921944000	1.752916000
1	9.471400000	5.064446000	1.269240000
1	4.209817000	3.877358000	11.007087000
7	9.590177000	7.862050000	11.673301000

^{3}[((MePh)$_8$Cz)Mn(O)]: B3LYP:

25	6.482969000	8.866316000	10.366306000
7	7.182858000	7.481458000	9.263483000
7	7.727358000	10.124099000	9.583374000
7	6.720364000	9.760539000	12.005939000
7	6.008231000	7.490680000	11.635662000
7	8.401136000	8.834617000	7.662677000
7	7.738743000	11.818717000	11.310870000
7	6.141850000	5.529779000	10.301235000
6	6.734098000	6.153624000	9.290052000
6	7.087955000	5.517355000	8.005243000
6	7.736490000	6.468473000	7.232971000
6	7.811625000	7.702414000	8.048923000
6	8.419540000	9.947568000	8.414279000
6	9.184848000	11.166460000	8.105531000
6	8.939068000	12.068273000	9.129609000
6	8.048577000	11.372990000	10.099247000
6	7.116045000	11.039459000	12.230302000
6	6.778006000	11.385943000	13.610313000
6	6.203515000	10.241750000	14.194242000
6	6.181626000	9.201764000	13.177992000
6	5.854225000	7.840587000	12.981668000
6	5.536058000	6.613282000	13.710771000
6	5.538632000	5.565313000	12.778381000
6	5.876313000	6.165702000	11.472677000
6	6.838620000	4.094227000	7.716228000
6	5.583811000	3.507028000	7.970532000
1	4.786626000	4.116339000	8.378416000
6	5.356870000	2.156823000	7.693251000
1	4.375887000	1.730515000	7.885458000
6	6.372434000	1.340384000	7.168358000
6	7.627049000	1.927049000	6.920463000
1	8.430482000	1.317371000	6.515832000
6	7.858289000	3.276275000	7.186533000
1	8.834461000	3.705081000	6.987248000
6	6.136754000	-0.130189000	6.901873000
6	8.184091000	6.379704000	5.833154000
6	7.448475000	5.626463000	4.891410000
1	6.554094000	5.102839000	5.206935000
6	7.845793000	5.560199000	3.556866000

1	7.255724000	4.978293000	2.853987000
6	8.988778000	6.242128000	3.101753000
6	9.719973000	6.992739000	4.037684000
1	10.602934000	7.537345000	3.714459000
6	9.328588000	7.066490000	5.375013000
1	9.891899000	7.677903000	6.065100000
6	9.395045000	6.200261000	1.645559000
6	9.995944000	11.318294000	6.881562000
6	11.010502000	10.393828000	6.571731000
1	11.203343000	9.569689000	7.249829000
6	11.775497000	10.531933000	5.409479000
1	12.560349000	9.810725000	5.197554000
6	11.548680000	11.587683000	4.512620000
6	10.529915000	12.508410000	4.822128000
1	10.329454000	13.331701000	4.141659000
6	9.768065000	12.380032000	5.983347000
1	8.984635000	13.098909000	6.198215000
6	12.361374000	11.731769000	3.244454000
1	12.799477000	12.734281000	3.160597000
1	13.178825000	11.004617000	3.208447000
1	11.739199000	11.577194000	2.352976000
6	9.458415000	13.426829000	9.328909000
6	10.742161000	13.802331000	8.878799000
1	11.374791000	13.069648000	8.393040000
6	11.214494000	15.102693000	9.060822000
1	12.208985000	15.361782000	8.708193000
6	10.430206000	16.082202000	9.694351000
6	9.153895000	15.705785000	10.152425000
1	8.526103000	16.439926000	10.650250000
6	8.674987000	14.407945000	9.979733000
1	7.695476000	14.141701000	10.354547000
6	10.935771000	17.495244000	9.881521000
1	10.957351000	17.775164000	10.942756000
1	11.948612000	17.613926000	9.483547000
1	10.288754000	18.220893000	9.371636000
6	6.930122000	12.736082000	14.177002000
6	8.061072000	13.525264000	13.877397000
1	8.826511000	13.129620000	13.222785000
6	8.187961000	14.817134000	14.391146000
1	9.068103000	15.403168000	14.140864000
6	7.197041000	15.375920000	15.215955000
6	6.063524000	14.594166000	15.502784000
1	5.271640000	15.008668000	16.120917000
6	5.929625000	13.301562000	14.997399000
1	5.035897000	12.731517000	15.222036000
6	7.348270000	16.767235000	15.789576000
1	6.374162000	17.243629000	15.944460000
1	7.940063000	17.411009000	15.129619000
1	7.857419000	16.743930000	16.763075000
6	5.687388000	10.139076000	15.575506000
6	6.483737000	10.517794000	16.674136000
1	7.503128000	10.847223000	16.502722000
6	5.974652000	10.478220000	17.972900000
1	6.609603000	10.771197000	18.804823000
6	4.653470000	10.065924000	18.224264000
6	3.864429000	9.678186000	17.128230000
1	2.845161000	9.342217000	17.295708000
6	4.369927000	9.711269000	15.826453000
1	3.738430000	9.413358000	14.996174000
6	4.093668000	10.060218000	19.630381000
1	4.875246000	9.858511000	20.371569000
1	3.311540000	9.302102000	19.746361000
1	3.647299000	11.031303000	19.886750000
6	5.309801000	6.467928000	15.166789000
6	6.316821000	6.797498000	16.094650000
1	7.252201000	7.218051000	15.739548000
6	6.131086000	6.574680000	17.460112000
1	6.924224000	6.835653000	18.155212000
6	4.935435000	6.019051000	17.950671000
6	3.926716000	5.706659000	17.024153000
1	2.990687000	5.283410000	17.377577000
6	4.108219000	5.924575000	15.655944000
1	3.320483000	5.662227000	14.957239000
6	4.753184000	5.757025000	19.429387000
1	5.382494000	4.923048000	19.768061000
1	3.715008000	5.502627000	19.665041000
1	5.030221000	6.633212000	20.027574000
6	5.346049000	4.122458000	12.982464000
6	5.779638000	3.461816000	14.153937000
1	6.279432000	4.023427000	14.933004000
6	5.588007000	2.090936000	14.315561000
1	5.938177000	1.608676000	15.224422000
6	4.956195000	1.318583000	13.322770000
6	4.529777000	1.973042000	12.155831000
1	4.043673000	1.400601000	11.370578000
6	4.723716000	3.344126000	11.981968000
6	4.771055000	-0.171714000	13.500746000
1	5.717264000	-0.710322000	13.353770000
1	4.415992000	-0.414501000	14.509309000
1	4.049034000	-0.573495000	12.782635000
8	5.061983000	9.291293000	9.772251000
1	6.690604000	-0.471899000	6.020148000
1	6.466594000	-0.745856000	7.750366000
1	5.074914000	-0.342399000	6.738086000
1	9.001570000	7.068965000	1.099222000
1	10.484999000	6.213990000	1.532652000
1	9.013129000	5.302070000	1.148204000
1	4.403639000	3.819462000	11.064136000

^{3}[((MePh)$_8$Cz)Mn(O)CN]$^{-}$: BP86:

25	6.576332000	8.804410000	10.368585000
7	6.906085000	7.502358000	9.078413000
7	7.636624000	10.164685000	9.512344000
7	6.575924000	9.809681000	12.012382000
7	5.862979000	7.504612000	11.572592000
7	8.264212000	8.869330000	7.553356000
7	7.644779000	11.851358000	11.290609000
7	5.985912000	5.518077000	10.212355000
6	6.554135000	6.139352000	9.162659000
6	7.020652000	5.489766000	7.937914000
6	7.675425000	6.464150000	7.150569000
6	7.650635000	7.724012000	7.905473000
6	8.297627000	9.988228000	8.313414000
6	9.028561000	11.227579000	8.009948000
6	8.794801000	12.121668000	9.072125000
6	7.938578000	11.414572000	10.046493000
6	7.023406000	11.087669000	12.222021000
6	6.747161000	11.399429000	13.633715000
6	6.144572000	10.246357000	14.207609000
6	6.062906000	9.229636000	13.153839000
6	5.722030000	7.842579000	12.918862000
6	5.383164000	6.618784000	13.631638000
6	5.351001000	5.563825000	12.674895000
6	5.701501000	6.152335000	11.378503000
6	6.914071000	4.035111000	7.707800000
6	5.711941000	3.333083000	7.975151000
1	4.843542000	3.890476000	8.333385000
6	5.631989000	1.942206000	7.791126000
1	4.688833000	1.425098000	8.003279000
6	6.745804000	1.194447000	7.346237000
6	7.946181000	1.895878000	7.079081000
1	8.828639000	1.341173000	6.737925000
6	8.032346000	3.284890000	7.256304000
1	8.974798000	3.803141000	7.057925000
6	6.672960000	-0.314382000	7.197101000
6	8.208754000	6.320118000	5.781737000
6	7.610005000	5.422681000	4.856001000
1	6.745596000	4.830528000	5.166481000
6	8.100374000	5.294147000	3.546789000
1	7.612501000	4.594861000	2.856720000

6	9.200477000	6.058844000	3.095293000
6	9.786680000	6.965710000	4.010142000
1	10.629096000	7.589018000	3.687284000
6	9.306588000	7.097906000	5.322042000
1	9.747949000	7.831858000	5.997747000
6	9.723325000	5.928254000	1.675984000
6	9.837743000	11.420390000	6.788175000
6	10.847641000	10.487556000	6.442910000
1	11.017968000	9.627654000	7.096954000
6	11.635287000	10.668974000	5.291773000
1	12.418056000	9.938732000	5.053336000
6	11.443084000	11.779985000	4.440695000
6	10.428877000	12.707943000	4.782643000
1	10.253096000	13.575620000	4.134779000
6	9.641400000	12.534837000	5.931657000
1	8.861509000	13.262300000	6.176883000
6	12.294769000	11.980176000	3.199008000
1	12.874906000	12.921956000	3.250446000
1	13.012719000	11.151702000	3.067146000
1	11.672317000	12.034405000	2.285256000
6	9.326193000	13.481576000	9.276777000
6	10.606655000	13.867027000	8.798555000
1	11.230776000	13.131902000	8.284945000
6	11.087476000	15.173547000	8.985016000
1	12.080964000	15.439646000	8.603825000
6	10.321354000	16.150362000	9.661608000
6	9.051915000	15.763499000	10.153655000
1	8.435227000	16.496014000	10.688545000
6	8.561733000	14.461338000	9.969774000
1	7.587083000	14.180756000	10.373994000
6	10.845914000	17.559355000	9.871907000
1	11.134947000	17.732661000	10.927534000
1	11.736106000	17.754605000	9.248097000
1	10.081517000	18.318184000	9.619123000
6	7.011467000	12.712618000	14.251040000
6	8.159763000	13.463999000	13.875557000
1	8.827247000	13.060470000	13.111708000
6	8.422374000	14.717901000	14.449487000
1	9.315055000	15.272328000	14.136113000
6	7.559928000	15.279738000	15.419561000
6	6.407126000	14.542971000	15.779062000
1	5.707495000	14.963968000	16.511652000
6	6.133845000	13.289394000	15.208583000
1	5.225007000	12.754391000	15.494245000
6	7.871832000	16.618019000	16.065527000
1	6.958391000	17.099158000	16.459486000
1	8.341786000	17.314216000	15.346896000
1	8.575402000	16.505230000	16.915168000
6	5.683682000	10.126683000	15.610097000
6	6.547647000	10.449812000	16.687996000
1	7.581948000	10.732182000	16.471318000
6	6.089890000	10.420447000	18.014454000
1	6.778124000	10.677546000	18.829034000
6	4.754206000	10.067384000	18.319952000
6	3.899919000	9.720385000	17.247993000
1	2.865911000	9.423753000	17.458755000
6	4.352976000	9.748059000	15.917858000
1	3.671989000	9.485694000	15.102155000
6	4.248881000	10.092249000	19.752098000
1	5.055478000	9.853327000	20.469211000
1	3.429770000	9.366982000	19.904876000
1	3.856788000	11.092744000	20.026056000
6	5.182756000	6.470769000	15.094076000
6	6.214895000	6.823659000	16.001282000
1	7.143846000	7.248339000	15.608769000
6	6.063766000	6.618148000	17.381696000
1	6.876961000	6.902426000	18.059314000
6	4.878823000	6.055854000	17.913085000
6	3.845713000	5.717530000	17.009537000
1	2.913919000	5.288431000	17.396930000
6	3.991622000	5.919606000	15.625712000
1	3.183219000	5.641160000	14.942459000
6	4.733892000	5.817471000	19.405169000
1	5.385088000	4.990148000	19.749831000
1	3.694996000	5.555256000	19.672206000
1	5.018007000	6.715078000	19.985066000
6	5.118479000	4.123698000	12.892240000
6	5.547634000	3.455980000	14.072653000
1	6.076720000	4.018387000	14.845187000
6	5.327655000	2.081745000	14.248242000
1	5.682817000	1.595463000	15.165362000
6	4.673839000	1.307520000	13.259250000
6	4.256615000	1.967391000	12.081443000
1	3.759156000	1.391173000	11.292054000
6	4.472656000	3.343241000	11.897055000
6	4.439212000	-0.179000000	13.460282000
1	5.377032000	-0.704409000	13.724013000
1	3.719513000	-0.372632000	14.280118000
1	4.037056000	-0.648553000	12.545372000
8	5.172202000	9.627789000	10.002326000
6	8.427679000	8.237959000	11.149429000
1	7.290711000	-0.669023000	6.351754000
1	7.041288000	-0.826923000	8.108289000
1	5.635147000	-0.653738000	7.028077000
1	9.616363000	6.877427000	1.115591000
1	10.798564000	5.665628000	1.661074000
1	9.178523000	5.146590000	1.117346000
1	4.160848000	3.827089000	10.968826000
7	9.501444000	7.925898000	11.572549000

^{3}[((MePh)$_8$Cz)Mn(O)]: BP86:

25	6.479377000	8.854603000	10.345450000
7	7.150572000	7.470225000	9.266698000
7	7.667463000	10.137354000	9.560921000
7	6.698208000	9.751471000	11.974209000
7	5.952571000	7.488943000	11.604223000
7	8.386204000	8.829905000	7.647716000
7	7.665093000	11.862086000	11.283252000
7	6.089751000	5.492213000	10.287116000
6	6.677412000	6.127904000	9.263701000
6	7.009156000	5.515952000	7.979488000
6	7.680944000	6.480849000	7.203757000
6	7.780584000	7.696399000	8.017624000
6	8.407738000	9.947816000	8.389036000
6	9.187666000	11.152846000	8.105131000
6	8.904672000	12.078220000	9.124536000
6	7.990649000	11.406261000	10.063017000
6	7.059917000	11.078134000	12.196174000
6	6.712500000	11.410034000	13.571767000
6	6.161780000	10.236238000	14.165025000
6	6.166185000	9.197776000	13.156174000
6	5.833914000	7.822162000	12.954824000
6	5.549546000	6.598738000	13.697827000
6	5.523665000	5.536093000	12.756883000
6	5.824081000	6.124796000	11.448327000
6	6.758418000	4.090514000	7.682256000
6	5.505217000	3.491497000	7.964795000
1	4.705711000	4.104361000	8.387842000
6	5.282534000	2.129926000	7.699326000
1	4.300901000	1.693019000	7.915561000
6	6.300444000	1.311385000	7.157909000
6	7.552258000	1.911698000	6.878087000
1	8.359659000	1.299849000	6.459691000
6	7.780006000	3.272238000	7.132068000
1	8.757532000	3.711506000	6.912578000
6	6.073003000	-0.168237000	6.912256000
6	8.138854000	6.384582000	5.805383000
6	7.419783000	5.602172000	4.860466000
1	6.526860000	5.059152000	5.179908000
6	7.827229000	5.534414000	3.520270000

1	7.247375000	4.930360000	2.812994000
6	8.964409000	6.241216000	3.059736000
6	9.679071000	7.019822000	3.999988000
1	10.559987000	7.584207000	3.673708000
6	9.279119000	7.095547000	5.342770000
1	9.831446000	7.728234000	6.038751000
6	9.380995000	6.196083000	1.602321000
6	10.068856000	11.289784000	6.926205000
6	11.066995000	10.320770000	6.658837000
1	11.182414000	9.472009000	7.339433000
6	11.917678000	10.450719000	5.546780000
1	12.691597000	9.695407000	5.368274000
6	11.798755000	11.543464000	4.659320000
6	10.793655000	12.506415000	4.924220000
1	10.674533000	13.359364000	4.246116000
6	9.945338000	12.386674000	6.034941000
1	9.174328000	13.140821000	6.219010000
6	12.714576000	11.687883000	3.457794000
1	13.279600000	12.638780000	3.491972000
1	13.446759000	10.863692000	3.407630000
1	12.140990000	11.687417000	2.511405000
6	9.425309000	13.441068000	9.324353000
6	10.736667000	13.805627000	8.920165000
1	11.390455000	13.054189000	8.471000000
6	11.209048000	15.115067000	9.100802000
1	12.227242000	15.366903000	8.783192000
6	10.399875000	16.115848000	9.688265000
6	9.096563000	15.749267000	10.102552000
1	8.446023000	16.501836000	10.562932000
6	8.616029000	14.442984000	9.929671000
1	7.609637000	14.184493000	10.265046000
6	10.907396000	17.533191000	9.874387000
1	10.966407000	17.804657000	10.945825000
1	11.913505000	17.661458000	9.440278000
1	10.235533000	18.268558000	9.393336000
6	6.858589000	12.755346000	14.157536000
6	7.977150000	13.571764000	13.835880000
1	8.726988000	13.196794000	13.136758000
6	8.112268000	14.855800000	14.386639000
1	8.985902000	15.462235000	14.121949000
6	7.143311000	15.383295000	15.271951000
6	6.019097000	14.578186000	15.574801000
1	5.240056000	14.971116000	16.238227000
6	5.876401000	13.292051000	15.033895000
1	4.988635000	12.702278000	15.274197000
6	7.310555000	16.758117000	15.890870000
1	6.333926000	17.212880000	16.134979000
1	7.848980000	17.444568000	15.213077000
1	7.892653000	16.706593000	16.832888000
6	5.654830000	10.128648000	15.551698000
6	6.442230000	10.564231000	16.647923000
1	7.455823000	10.933313000	16.465023000
6	5.933186000	10.532980000	17.955161000
1	6.560965000	10.873652000	18.786614000
6	4.620854000	10.072907000	18.219780000
6	3.844458000	9.621780000	17.127459000
1	2.831342000	9.245773000	17.306628000
6	4.349481000	9.646034000	15.816650000
1	3.725901000	9.301944000	14.986067000
6	4.057577000	10.089519000	19.628855000
1	4.847732000	9.922710000	20.382767000
1	3.284567000	9.313107000	19.764286000
1	3.587183000	11.065287000	19.861950000
6	5.398610000	6.460564000	15.165734000
6	6.423439000	6.895498000	16.044196000
1	7.311073000	7.385077000	15.631317000
6	6.320852000	6.686986000	17.428854000
1	7.128260000	7.029968000	18.085312000
6	5.193559000	6.041687000	17.990898000
6	4.164222000	5.626073000	17.113962000
1	3.275876000	5.133319000	17.525002000
6	4.262224000	5.827654000	15.727025000
1	3.459346000	5.486362000	15.066453000
6	5.107977000	5.786903000	19.484193000
1	5.760293000	4.944120000	19.786324000
1	4.078666000	5.534392000	19.792531000
1	5.431810000	6.670312000	20.064027000
6	5.338283000	4.091267000	12.983196000
6	5.837208000	3.437163000	14.142709000
1	6.383093000	4.012647000	14.893769000
6	5.655391000	2.059145000	14.327024000
1	6.058861000	1.581249000	15.227341000
6	4.969670000	1.271248000	13.369897000
6	4.480748000	1.920566000	12.213966000
1	3.951470000	1.335044000	11.453800000
6	4.662138000	3.299153000	12.018153000
6	4.785533000	-0.220106000	13.576631000
1	5.753727000	-0.755533000	13.530805000
1	4.341580000	-0.440429000	14.565807000
1	4.126908000	-0.655294000	12.805352000
8	5.060423000	9.333339000	9.724029000
1	6.626562000	-0.521445000	6.023956000
1	6.418043000	-0.774194000	7.773264000
1	5.002846000	-0.393338000	6.760856000
1	8.996248000	7.075975000	1.049390000
1	10.480875000	6.201543000	1.494859000
1	8.991473000	5.294750000	1.097704000
1	4.287620000	3.773729000	11.108629000

^{3}[((MePh)$_8$Cz)Mn(O)CN]$^{-}$: M06:

25	0.104324028	-0.046683680	15.301953545
7	1.138965445	-0.020580392	13.727325875
7	0.656488272	1.658585993	15.895538473
7	-0.846418724	-0.358932051	16.895110704
7	-0.398820929	-1.843673712	15.023413104
7	2.140272287	2.152562742	14.052253452
7	-0.472302188	1.705942791	18.038211105
7	0.725325050	-2.292949563	12.964499442
6	1.273058455	-1.084210997	12.850984050
6	2.209481505	-0.662719615	11.817696700
6	2.625533600	0.630958503	12.122453988
6	1.963203724	1.014599749	13.368929594
6	1.551984194	2.441393415	15.220773139
6	1.745879633	3.654369970	16.006755918
6	0.958589524	3.547491407	17.149725702
6	0.284665849	2.249231493	17.086087188
6	-0.980348037	0.458626071	17.971012642
6	-1.710779035	-0.292865873	18.972601376
6	-1.934673175	-1.583424865	18.441609830
6	-1.361947305	-1.617709909	17.122550687
6	-1.068302285	-2.502923256	16.028068351
6	-1.192908983	-3.873182853	15.596859771
6	-0.571504788	-3.979256617	14.334897616
6	-0.051738830	-2.666183629	14.001409382
6	2.660009173	-1.557062148	10.747710968
6	1.746173131	-2.361778754	10.050942514
1	0.691535585	-2.291206615	10.299724566
6	2.179916214	-3.241520784	9.061445936
1	1.453916498	-3.856942643	8.531897899
6	3.536117995	-3.352257174	8.737280199
6	4.448880183	-2.546235809	9.432009758
1	5.510020458	-2.621279975	9.198413889
6	4.022511328	-1.667669507	10.421165069
1	4.745562390	-1.062476265	10.962153943
6	4.014262099	-4.328323619	7.697714416
6	3.492186077	1.517595634	11.342692463
6	3.480775922	1.485774746	9.937225681
1	2.818004743	0.792284047	9.426564387
6	4.294417807	2.335461217	9.194075723
1	4.265676230	2.292254432	8.106267495

6	5.141281228	3.256853600	9.821508123
6	5.143438791	3.299381136	11.221547710
1	5.784395216	4.016980413	11.732600010
6	4.336854044	2.449981976	11.970934794
1	4.328918486	2.513745482	13.053414948
6	6.002644341	4.196146936	9.022789238
6	2.622605878	4.746779716	15.570447969
6	3.943164873	4.478316767	15.182690150
1	4.301968159	3.453664357	15.225562512
6	4.786538429	5.504483621	14.760191794
1	5.810759023	5.274144797	14.470015166
6	4.340606243	6.828960800	14.708157782
6	3.019280565	7.096651425	15.094712186
1	2.651367904	8.121270245	15.055699392
6	2.173681058	6.076617600	15.516578639
1	1.149955766	6.299194463	15.806888126
6	5.240791573	7.942734428	14.246863366
1	5.317641501	8.735761010	15.002796714
1	6.253176648	7.577295266	14.040297259
1	4.860664683	8.409247398	13.327982552
6	0.827734136	4.478019198	18.274388547
6	1.889532143	5.310222507	18.667535650
1	2.837693644	5.247751512	18.141584602
6	1.746103543	6.205696999	19.723784466
1	2.583943655	6.841302090	20.006271585
6	0.545195286	6.299239687	20.435697979
6	-0.508298890	5.455299159	20.059746515
1	-1.450932338	5.503435088	20.603870372
6	-0.375911588	4.562772601	19.001380450
1	-1.198038630	3.906741303	18.733972583
6	0.383845437	7.265105793	21.577513128
1	0.287788259	6.739904151	22.537748978
1	1.243180772	7.941517096	21.652991838
1	-0.518373669	7.879122649	21.455841819
6	-2.184770763	0.270601897	20.239241409
6	-1.479451754	1.317750030	20.865168748
1	-0.572391037	1.690331983	20.399284206
6	-1.951822622	1.894341685	22.038951265
1	-1.391427563	2.709403531	22.495536244
6	-3.135664174	1.450911567	22.643057256
6	-3.837497850	0.411327878	22.023143671
1	-4.768593907	0.059379265	22.465202593
6	-3.376364258	-0.168441434	20.844685206
1	-3.959064688	-0.954581926	20.374008101
6	-3.627616660	2.072207062	23.920924984
1	-4.666660909	1.789899522	24.127792554
1	-3.576975811	3.167764460	23.877641956
1	-3.021036715	1.755697850	24.780888427
6	-2.629031427	-2.694138002	19.107604505
6	-2.221232585	-3.140703956	20.374215625
1	-1.365700986	-2.665363845	20.848448774
6	-2.898345214	-4.172306493	21.014644957
1	-2.563990217	-4.512349847	21.993979038
6	-4.002672679	-4.792162614	20.414052084
6	-4.405200087	-4.349813111	19.150085567
1	-5.244502169	-4.837118708	18.656365073
6	-3.729522512	-3.317985172	18.503665168
1	-4.046995475	-2.987782494	17.516480165
6	-4.731348865	-5.905081122	21.114819344
1	-4.034359816	-6.553886067	21.661573258
1	-5.285836226	-6.527204317	20.401457299
1	-5.453627346	-5.518108598	21.846965414
6	-1.802936067	-4.978273619	16.351489142
6	-1.306123355	-5.327381701	17.616341499
1	-0.504178535	-4.733609393	18.049649328
6	-1.821872872	-6.420249772	18.305120579
1	-1.432409142	-6.668463833	19.291621960
6	-2.850841367	-7.196735147	17.757897051
6	-3.356707631	-6.838190749	16.502229312
1	-4.162395777	-7.426584121	16.065322792
6	-2.841841540	-5.746374642	15.806607869
1	-3.230338349	-5.485846070	14.824771462
6	-3.382064909	-8.392377339	18.500112881
1	-2.749300841	-9.277229715	18.342602649
1	-4.395961715	-8.650395339	18.171148147
1	-3.412536906	-8.205862532	19.581518523
6	-0.376666515	-5.173904739	13.511530470
6	-0.211305275	-6.452206962	14.079007374
1	-0.221882080	-6.565307019	15.158974180
6	-0.005027153	-7.567914305	13.276285099
1	0.131460370	-8.544490354	13.739609110
6	0.047165425	-7.459158187	11.879282502
6	-0.110471135	-6.189827545	11.314214813
1	-0.062729640	-6.078401610	10.232033366
6	-0.317449196	-5.067197563	12.111244482
6	0.287241760	-8.674784599	11.026831099
1	1.289433656	-9.091022898	11.198634857
1	-0.434570752	-9.471647050	11.251281559
1	0.204826722	-8.436457435	9.960134025
8	-1.356637149	0.613898495	14.443019036
6	1.752622927	-0.776237758	16.262963261
1	4.799129217	-3.891012191	7.067507943
1	4.437499954	-5.229332748	8.163280519
1	3.194638490	-4.650047178	7.044696528
1	5.601515315	5.219009221	9.041136386
1	7.022948010	4.243401947	9.424842405
1	6.066861267	3.884918984	7.973670915
1	-0.414183992	-4.085618706	11.658581347
7	2.717756453	-1.169933016	16.818308039

^{3}[((MePh)$_8$Cz)Mn(O)]: M06:

25	0.028482725	0.011582636	15.115231298
7	1.369115068	-0.018435449	13.813091251
7	0.704026840	1.618345972	15.877785488
7	-0.483034791	-0.488232327	16.839244436
7	-0.052133220	-1.883853919	14.948137244
7	2.122710210	2.276615069	14.047849938
7	-0.360050952	1.577562083	18.040230250
7	1.151540805	-2.279842249	12.938152844
6	1.585784566	-1.027194643	12.866040805
6	2.444204340	-0.499845219	11.828201802
6	2.741919362	0.820155414	12.152479233
6	2.073371115	1.121397423	13.400593785
6	1.521973472	2.514717534	15.209098132
6	1.624840751	3.725060528	15.993382226
6	0.867730292	3.540416014	17.146573910
6	0.311179362	2.198591607	17.074308988
6	-0.707701897	0.296816394	17.952957462
6	-1.345138470	-0.533329273	18.947131450
6	-1.471545130	-1.823002706	18.395605520
6	-0.914457440	-1.787732528	17.075624608
6	-0.595053410	-2.627067672	15.980187548
6	-0.525540855	-4.012472772	15.597603284
6	0.093372672	-4.071599167	14.336749285
6	0.410050876	-2.711372838	13.958186664
6	2.958854249	-1.326005604	10.733358686
6	2.122251160	-2.217980096	10.045069164
1	1.070075980	-2.265172017	10.308757426
6	2.628348137	-3.033347672	9.036552864
1	1.962569645	-3.715118793	8.510256976
6	3.982584971	-2.991889711	8.685218673
6	4.815710946	-2.094936063	9.368674207
1	5.871725765	-2.047561875	9.109454670
6	4.316854965	-1.276662487	10.375140666
1	4.981413628	-0.596849403	10.902200904
6	4.540224295	-3.901795757	7.627129925
6	3.504166897	1.802509658	11.378341256
6	3.423224838	1.819406682	9.975455863
1	2.792245752	1.093944506	9.468658639
6	4.129225844	2.759530507	9.232853739

1	4.049106317	2.757940040	8.147566192
6	4.935002443	3.718725157	9.859701589
6	5.012110640	3.703073826	11.257923472
1	5.628906738	4.442832347	11.765529555
6	4.310232973	2.765763086	12.007403393
1	4.368258169	2.781604436	13.090240768
6	5.673326160	4.756223929	9.062130597
6	2.385077876	4.897852974	15.545164397
6	3.721251649	4.773426864	15.142062086
1	4.198774518	3.798117173	15.190378043
6	4.436155804	5.882530992	14.693568758
1	5.475481963	5.766660422	14.390833541
6	3.840672095	7.146557283	14.629435723
6	2.503619517	7.268611337	15.036384035
1	2.020305087	8.242844972	14.987537655
6	1.786459657	6.167027634	15.487544906
1	0.748206607	6.276903264	15.791118339
6	4.600597416	8.347700253	14.140544528
1	4.738225709	9.087409273	14.940251849
1	5.592861678	8.069560976	13.769106816
1	4.065022043	8.850849447	13.325365651
6	0.689817571	4.431997254	18.293963689
6	1.692267011	5.342612701	18.669279580
1	2.621628777	5.376369944	18.108088133
6	1.513617459	6.194403839	19.754721810
1	2.304205388	6.891179498	20.026074830
6	0.334825999	6.168131466	20.509258228
6	-0.659750602	5.250237243	20.144954557
1	-1.584082243	5.209343390	20.719088185
6	-0.491640858	4.397678560	19.060063473
1	-1.271641320	3.688675645	18.802697148
6	0.134136997	7.086666228	21.681583559
1	0.099747708	6.527249396	22.625980156
1	0.943070732	7.821165151	21.758868632
1	-0.812856973	7.635240847	21.598799776
6	-1.812902766	-0.037562463	20.243105043
6	-1.124358808	0.993993261	20.909226769
1	-0.242608776	1.428061624	20.448705000
6	-1.576386438	1.474518385	22.133563293
1	-1.028487116	2.274347215	22.628670740
6	-2.723333435	0.949371719	22.741868778
6	-3.417728584	-0.065752415	22.070814577
1	-4.324118147	-0.473705885	22.514106541
6	-2.975680539	-0.551247965	20.845448549
1	-3.544732161	-1.325933538	20.339590828
6	-3.183457921	1.448269934	24.082394627
1	-4.256831296	1.280075175	24.225666853
1	-2.987992423	2.520826471	24.198370674
1	-2.659355219	0.932926208	24.899165698
6	-2.060967650	-3.008968684	19.029387671
6	-1.646634996	-3.428689012	20.302934424
1	-0.875063143	-2.865425589	20.822715960
6	-2.208695207	-4.555498187	20.892571700
1	-1.867555459	-4.879045020	21.874349098
6	-3.200974560	-5.294673745	20.234095046
6	-3.618680613	-4.867726052	18.968562954
1	-4.375420481	-5.440760757	18.436208469
6	-3.055740999	-3.744623804	18.369237349
1	-3.382991313	-3.430403697	17.380045835
6	-3.797036588	-6.519302691	20.869481864
1	-3.069744242	-7.025847524	21.515973337
1	-4.133427879	-7.234494184	20.108957671
1	-4.666415327	-6.269407193	21.492439702
6	-0.940838423	-5.179961810	16.390384147
6	-0.358390155	-5.437727396	17.639257458
1	0.346702878	-4.721486040	18.055969782
6	-0.661957380	-6.603963768	18.334966129
1	-0.204302068	-6.787980772	19.305619779
6	-1.554325001	-7.546121388	17.808004630
6	-2.154567601	-7.272544747	16.571795554
1	-2.859564881	-7.988547286	16.153232176
6	-1.853073456	-6.108862258	15.869500348
1	-2.306626746	-5.919376040	14.899394366
6	-1.837858476	-8.827417296	18.542346826
1	-1.104147827	-9.604052938	18.285638592
1	-2.830036740	-9.222116735	18.293834538
1	-1.790298339	-8.683693311	19.628840006
6	0.484229840	-5.250214511	13.560226893
6	0.865457221	-6.455884762	14.180915392
1	0.878305827	-6.526426642	15.264851789
6	1.250250559	-7.553628225	13.421451820
1	1.549255689	-8.473656367	13.920976534
6	1.272195393	-7.497833033	12.020303565
6	0.900319095	-6.298370169	11.404590781
1	0.917120464	-6.229718897	10.318662818
6	0.515533176	-5.192834766	12.157119679
6	1.702793264	-8.692488891	11.216611632
1	2.767102996	-8.913628910	11.372846627
1	1.142442446	-9.591157270	11.504629514
1	1.550863312	-8.529849883	10.144123339
8	-1.306814785	0.579965692	14.365242524
1	5.335304021	-3.409863719	7.054331914
1	4.974407988	-4.807207880	8.073104693
1	3.763386340	-4.223293204	6.924366612
1	5.143719204	5.718521286	9.078171661
1	6.676838609	4.932970272	9.467794480
1	5.778568263	4.455887149	8.013753931
1	0.246758337	-4.265941489	11.661279448

$^{3}[(Me_8Cz)Mn(O)CN]^{-}$: B3LYP:

6	-2.164166000	-1.929183000	0.215503000
6	-3.619039000	-1.940663000	-0.030745000
6	-4.046357000	-0.632451000	-0.011072000
6	-2.858368000	0.207739000	0.253733000
6	-1.728473000	2.295399000	0.282313000
6	-1.652252000	3.764785000	0.124175000
6	-0.321647000	4.105166000	0.133464000
6	0.454600000	2.853027000	0.304430000
6	2.448273000	1.587607000	0.296394000
6	3.856507000	1.314387000	-0.064432000
6	4.021306000	-0.060829000	-0.065867000
6	2.720935000	-0.651407000	0.302343000
6	2.048886000	-1.900238000	0.256228000
6	2.259689000	-3.299843000	-0.077299000
6	1.000577000	-3.909829000	-0.105739000
6	0.011194000	-2.884896000	0.202289000
25	0.009180000	-0.001439000	0.742550000
7	-0.437828000	1.824877000	0.431001000
7	1.865786000	0.402099000	0.572041000
7	0.676007000	-1.744067000	0.446141000
7	-2.846851000	1.575011000	0.219775000
7	1.800088000	2.775484000	0.237083000
7	-1.356923000	-2.977138000	0.127370000
8	-0.089395000	-0.034498000	2.366618000
7	-1.794794000	-0.591093000	0.433183000
6	4.835550000	2.392140000	-0.403469000
6	5.258827000	-0.831762000	-0.414844000
6	3.574156000	-3.968291000	-0.358427000
6	0.653716000	-5.335752000	-0.407766000
6	0.319214000	5.447463000	-0.011585000
6	-2.859674000	4.632757000	-0.030032000
6	-5.414420000	-0.071656000	-0.230381000
6	-4.399478000	-3.193274000	-0.273762000
1	-3.634797000	4.102067000	-0.592203000
1	-2.624794000	5.571173000	-0.545096000
1	-3.296472000	4.891572000	0.945473000
1	1.246526000	5.361583000	-0.587247000
1	0.591219000	5.871255000	0.966073000
1	-0.345035000	6.163732000	-0.508152000
1	5.801445000	1.988308000	-0.723253000

1	5.009813000	3.054163000	0.455449000
1	4.444351000	3.025516000	-1.209312000
1	6.114127000	-0.165325000	-0.564949000
1	5.124893000	-1.409942000	-1.338799000
1	5.527843000	-1.545510000	0.374533000
1	3.437912000	-5.042556000	-0.521250000
1	4.281586000	-3.849093000	0.473403000
1	4.059068000	-3.559228000	-1.254812000
1	1.277877000	-5.753173000	-1.206994000
1	-0.393720000	-5.398629000	-0.719408000
1	0.770951000	-5.986053000	0.472070000
1	-5.333077000	-2.993508000	-0.811710000
1	-4.661624000	-3.695582000	0.668836000
1	-3.801940000	-3.903349000	-0.854959000
1	-6.087569000	-0.806297000	-0.685669000
1	-5.366365000	0.811454000	-0.877083000
1	-5.869735000	0.256947000	0.714922000
6	0.065544000	-0.029692000	-1.507794000
7	0.077110000	-0.000341000	-2.692841000

^{3}[(Me$_8$Cz)Mn(O)] B3LYP:

6	-2.107152000	-1.911548000	0.145849000
6	-3.577431000	-1.920163000	0.031235000
6	-4.001678000	-0.614761000	0.048912000
6	-2.804556000	0.231497000	0.172645000
6	-1.711531000	2.308171000	0.244731000
6	-1.648372000	3.766547000	0.029331000
6	-0.321435000	4.115904000	0.061084000
6	0.450305000	2.875434000	0.289123000
6	2.392585000	1.576816000	0.224752000
6	3.812599000	1.308567000	0.003611000
6	3.976924000	-0.073118000	-0.030622000
6	2.663703000	-0.668652000	0.180568000
6	2.019989000	-1.912290000	0.196622000
6	2.243072000	-3.311813000	-0.174012000
6	0.997881000	-3.926198000	-0.197463000
6	0.006494000	-2.903374000	0.158515000
25	-0.000469000	-0.003042000	0.905723000
7	-0.445480000	1.821768000	0.451376000
7	1.752315000	0.386282000	0.349643000
7	0.651958000	-1.761591000	0.444853000
7	-2.830107000	1.569573000	0.171359000
7	1.776511000	2.784859000	0.217656000
7	-1.350381000	-3.000589000	0.100021000
8	-0.041231000	-0.053983000	2.502421000
7	-1.682041000	-0.576666000	0.242245000
6	4.832815000	2.388625000	-0.163125000
6	5.252893000	-0.829701000	-0.247045000
6	3.561259000	-3.943281000	-0.506179000
6	0.642935000	-5.339617000	-0.535182000
6	0.323352000	5.450704000	-0.116476000
6	-2.859071000	4.612320000	-0.192139000
6	-5.383861000	-0.055522000	-0.037520000
6	-4.368933000	-3.180756000	-0.082999000
1	-3.519353000	4.159893000	-0.940479000
1	-2.593257000	5.620258000	-0.522770000
1	-3.448389000	4.704057000	0.729553000
1	1.199683000	5.371029000	-0.768450000
1	0.682382000	5.845067000	0.843618000
1	-0.368725000	6.183122000	-0.541356000
1	5.841624000	1.985213000	-0.284645000
1	4.835395000	3.061923000	0.702372000
1	4.606661000	3.008542000	-1.039764000
1	6.119953000	-0.165497000	-0.202432000
1	5.269843000	-1.325130000	-1.226565000
1	5.391190000	-1.607414000	0.512703000
1	3.432720000	-4.991442000	-0.790055000
1	4.249926000	-3.916163000	0.347770000
1	4.058543000	-3.432188000	-1.339741000
1	1.323006000	-5.770477000	-1.277229000
1	-0.376986000	-5.387479000	-0.928559000
1	0.674721000	-5.984914000	0.353810000
1	-5.405407000	-2.984611000	-0.369416000
1	-4.378624000	-3.724479000	0.870501000
1	-3.919635000	-3.854351000	-0.820134000
1	-6.112160000	-0.819739000	-0.323307000
1	-5.427193000	0.762541000	-0.765088000
1	-5.697521000	0.366662000	0.926617000

^{3}[(Me$_8$Cz)Mn(O)CN]$^-$: BP86:

6	-2.153462000	-1.945071000	0.164627000
6	-3.621350000	-1.952232000	0.068435000
6	-4.052701000	-0.627422000	0.116290000
6	-2.857227000	0.220460000	0.244497000
6	-1.707945000	2.318032000	0.332470000
6	-1.641376000	3.770907000	0.144024000
6	-0.293056000	4.132676000	0.130943000
6	0.491920000	2.909413000	0.306461000
6	2.472670000	1.617788000	0.280364000
6	3.868569000	1.329443000	0.024373000
6	4.031410000	-0.078998000	0.019080000
6	2.738009000	-0.668685000	0.278847000
6	2.055615000	-1.931065000	0.256200000
6	2.268067000	-3.325660000	-0.116297000
6	1.001744000	-3.942422000	-0.151549000
6	0.004308000	-2.927023000	0.183752000
25	0.033051000	0.013698000	0.648512000
7	-0.401880000	1.852823000	0.475769000
7	1.842184000	0.393478000	0.486352000
7	0.695566000	-1.770941000	0.481008000
7	-2.835626000	1.572401000	0.261895000
7	1.839869000	2.816141000	0.240975000
7	-1.346200000	-3.029847000	0.091853000
8	-0.461787000	-0.123811000	2.237452000
7	-1.757971000	-0.620675000	0.271578000
6	4.910008000	2.383456000	-0.219878000
6	5.321076000	-0.806964000	-0.250244000
6	3.583492000	-3.984047000	-0.431347000
6	0.656503000	-5.359928000	-0.510481000
6	0.314033000	5.490620000	-0.065344000
6	-2.848347000	4.642316000	-0.044820000
6	-5.451204000	-0.088404000	0.046053000
6	-4.436435000	-3.203958000	-0.073409000
1	-3.741513000	4.009075000	-0.178224000
1	-2.746996000	5.300728000	-0.929667000
1	-3.024689000	5.301179000	0.829270000
1	1.393537000	5.386592000	-0.267895000
1	0.198511000	6.132293000	0.831595000
1	-0.154805000	6.030885000	-0.910606000
1	5.769343000	2.291268000	0.473949000
1	4.459832000	3.381599000	-0.082553000
1	5.317449000	2.334851000	-1.248997000
1	6.191167000	-0.176026000	0.007386000
1	5.425920000	-1.081541000	-1.319725000
1	5.394952000	-1.740283000	0.334675000
1	3.427530000	-5.013098000	-0.800324000
1	4.242256000	-4.049082000	0.457901000
1	4.143218000	-3.431251000	-1.209256000
1	1.120093000	-5.674954000	-1.465367000
1	-0.438259000	-5.449966000	-0.614163000
1	0.984145000	-6.081471000	0.264778000
1	-5.273703000	-3.070938000	-0.784972000
1	-4.878571000	-3.522158000	0.892750000
1	-3.793883000	-4.028146000	-0.427567000
1	-6.052320000	-0.603794000	-0.727753000
1	-5.422144000	0.989716000	-0.186247000
1	-5.990347000	-0.207605000	1.007774000
6	0.056192000	0.014219000	-1.441135000
7	0.065639000	0.028588000	-2.637167000

^{3}[(Me$_8$Cz)Mn(O)]: BP86:

6	-2.183763000	-1.938132000	0.188973000
6	-3.626986000	-1.946901000	-0.054826000
6	-4.057114000	-0.622074000	-0.056799000
6	-2.884524000	0.211059000	0.196246000
6	-1.716472000	2.263042000	0.216041000
6	-1.640994000	3.714598000	0.208819000
6	-0.291950000	4.071775000	0.213275000
6	0.495692000	2.849957000	0.222136000
6	2.479966000	1.618606000	0.208782000
6	3.874622000	1.335834000	-0.112380000
6	4.024389000	-0.062568000	-0.121485000
6	2.719628000	-0.631607000	0.192740000
6	2.014613000	-1.861577000	0.118136000
6	2.232164000	-3.278674000	-0.065755000
6	0.966984000	-3.904917000	-0.052954000
6	-0.039317000	-2.874304000	0.124900000
25	-0.006175000	0.005946000	0.809537000
7	-0.396150000	1.736956000	0.224124000
7	1.839841000	0.419799000	0.447938000
7	0.626232000	-1.651833000	0.231466000
7	-2.851347000	1.551338000	0.173067000
7	1.836634000	2.803784000	0.186589000
7	-1.378745000	-3.012556000	0.104877000
8	-0.041567000	-0.014427000	2.431345000
7	-1.764604000	-0.612052000	0.390139000
6	4.895236000	2.392581000	-0.421686000
6	5.279841000	-0.819380000	-0.453897000
6	3.557074000	-3.966045000	-0.247373000
6	0.646588000	-5.362119000	-0.215948000
6	0.310423000	5.443809000	0.188008000
6	-2.842575000	4.609981000	0.184398000
6	-5.436054000	-0.075270000	-0.272210000
6	-4.418442000	-3.200401000	-0.274395000
1	-3.743017000	4.030234000	-0.074154000
1	-2.722956000	5.430946000	-0.546513000
1	-3.016367000	5.078314000	1.172620000
1	1.374788000	5.385027000	-0.091099000
1	0.251731000	5.928002000	1.182271000
1	-0.212948000	6.105537000	-0.526396000
1	5.851596000	2.206526000	0.100438000
1	4.518858000	3.381948000	-0.113944000
1	5.119243000	2.446438000	-1.505052000
1	6.132930000	-0.130073000	-0.568699000
1	5.181034000	-1.382052000	-1.402048000
1	5.542753000	-1.549626000	0.333018000
1	3.435244000	-5.061767000	-0.230215000
1	4.271223000	-3.695146000	0.551429000
1	4.029733000	-3.700650000	-1.212149000
1	0.963824000	-5.744369000	-1.205096000
1	-0.440664000	-5.517139000	-0.124278000
1	1.149351000	-5.982476000	0.549917000
1	-5.282882000	-3.025919000	-0.938927000
1	-4.812860000	-3.601535000	0.679937000
1	-3.779224000	-3.983845000	-0.714850000
1	-6.061514000	-0.774106000	-0.854159000
1	-5.393665000	0.891537000	-0.801765000
1	-5.952726000	0.106852000	0.690367000

^{3}[(Me$_8$Cz)Mn(O)CN]$^-$: M06:

6	-2.157076088	-1.948752244	0.152810117
6	-3.604890026	-1.943009093	0.042818320
6	-4.028012035	-0.629735605	0.108645926
6	-2.849989322	0.207675025	0.256330093
6	-1.712024965	2.292958153	0.282197397
6	-1.642607877	3.738633214	0.156757123
6	-0.308380259	4.094180611	0.117770719
6	0.478825334	2.878886955	0.221944208
6	2.451203040	1.599602576	0.182175229
6	3.848673850	1.311706115	-0.039064401
6	4.004923272	-0.078109579	-0.043776037
6	2.706301579	-0.656702941	0.178953672
6	2.023265500	-1.907195863	0.158536226
6	2.239460452	-3.299945762	-0.130584837
6	0.986438451	-3.921224307	-0.153932616
6	-0.012610277	-2.912475516	0.109035805
25	-0.000921733	0.003677513	0.448249170
7	-0.419611176	1.833915139	0.354694984
7	1.835119798	0.399959586	0.350041757
7	0.661988817	-1.752891324	0.334178977
7	-2.827768652	1.549130951	0.258794979
7	1.810279374	2.787970769	0.150256260
7	-1.357740010	-3.016103727	0.059113244
8	-0.055925229	0.022520009	2.265540468
7	-1.765528465	-0.631706407	0.315548981
6	4.893391522	2.351479383	-0.248725062
6	5.284525785	-0.811819896	-0.272161909
6	3.553559153	-3.960030545	-0.382052324
6	0.669812646	-5.349649767	-0.431933132
6	0.274005945	5.454799435	-0.029228585
6	-2.831470458	4.627175699	0.055801032
6	-5.417861041	-0.107667741	0.017193524
6	-4.433693069	-3.165414200	-0.134103123
1	-3.746000461	4.025759175	0.092037585
1	-2.831659354	5.198420214	-0.883635482
1	-2.863824345	5.358206303	0.876341848
1	1.361417603	5.381275110	-0.137039245
1	0.057413686	6.088058964	0.843388965
1	-0.129517586	5.973401336	-0.910308996
1	5.674502187	2.311635447	0.524201529
1	4.431910843	3.344499644	-0.215551383
1	5.393511359	2.240096405	-1.220926834
1	6.146337880	-0.193591157	0.010548620
1	5.416492014	-1.089409349	-1.328663350
1	5.329528504	-1.736819340	0.316157023
1	3.411516400	-4.975613636	-0.770919404
1	4.157518603	-4.040479345	0.533670852
1	4.150173464	-3.402587894	-1.116573475
1	1.097485937	-5.687115515	-1.386210690
1	-0.417192052	-5.475820597	-0.483210832
1	1.053129305	-6.018904174	0.351316825
1	-5.070345038	-3.095681699	-1.027516538
1	-5.101007353	-3.333582434	0.723469191
1	-3.783694689	-4.040547012	-0.239486719
1	-5.926155310	-0.466384734	-0.889037232
1	-5.399694999	0.987097507	-0.005670490
1	-6.029260303	-0.423378635	0.875024953
6	0.028921815	0.010354901	-1.603542177
7	0.043504996	0.014544470	-2.785042900

^{3}[(Me$_8$Cz)Mn(O)]: M06:

6	-2.152997000	-1.928974000	0.180907000
6	-3.591804000	-1.932621000	0.062836000
6	-4.018018000	-0.619555000	0.095860000
6	-2.848333000	0.211130000	0.237108000
6	-1.703635000	2.259819000	0.240947000
6	-1.626644000	3.694603000	0.175274000
6	-0.291710000	4.048109000	0.177296000
6	0.489903000	2.840853000	0.240916000
6	2.454312000	1.609273000	0.237954000
6	3.844267000	1.323470000	-0.012272000
6	3.989952000	-0.062148000	-0.048225000
6	2.690129000	-0.633253000	0.183469000
6	2.000537000	-1.859170000	0.119013000
6	2.216714000	-3.257450000	-0.106433000
6	0.967558000	-3.879932000	-0.110514000
6	-0.032837000	-2.869865000	0.102658000
25	-0.003519000	0.002554000	0.785985000
7	-0.394517000	1.753010000	0.281798000
7	1.809498000	0.409704000	0.397879000

7	0.631080000	-1.666334000	0.250661000
7	-2.819394000	1.540924000	0.229101000
7	1.820280000	2.782245000	0.211663000
7	-1.358287000	-2.997287000	0.096587000
8	-0.112964000	-0.024853000	2.424853000
7	-1.729749000	-0.610778000	0.308364000
6	4.883778000	2.363900000	-0.236238000
6	5.251456000	-0.802571000	-0.336001000
6	3.533891000	-3.925733000	-0.305586000
6	0.658729000	-5.321461000	-0.312003000
6	0.291012000	5.412770000	0.103477000
6	-2.807598000	4.594183000	0.106421000
6	-5.406809000	-0.103101000	-0.017049000
6	-4.414874000	-3.158997000	-0.100320000
1	-3.731390000	4.008331000	0.115997000
1	-2.794067000	5.204046000	-0.807102000
1	-2.829971000	5.288960000	0.956625000
1	1.378965000	5.354855000	0.004213000
1	0.061367000	5.994782000	1.006439000
1	-0.110062000	5.973553000	-0.750890000
1	5.681687000	2.308151000	0.516224000
1	4.432743000	3.359439000	-0.178400000
1	5.358150000	2.261544000	-1.220964000
1	6.125249000	-0.168824000	-0.147562000
1	5.304035000	-1.125406000	-1.385550000
1	5.348601000	-1.698442000	0.288244000
1	3.399668000	-4.967692000	-0.614776000
1	4.129118000	-3.930604000	0.617633000
1	4.131539000	-3.423843000	-1.076873000
1	1.047299000	-5.691124000	-1.270153000
1	-0.425151000	-5.473098000	-0.303510000
1	1.095600000	-5.944722000	0.479215000
1	-5.018684000	-3.119151000	-1.016979000
1	-5.112476000	-3.286118000	0.738361000
1	-3.771932000	-4.043074000	-0.148162000
1	-5.905596000	-0.485306000	-0.917403000
1	-5.402613000	0.990200000	-0.060645000
1	-6.017855000	-0.408007000	0.843176000

$^{3}[(H_8Cz)Mn(O)CN]^{-}$: B3LYP:

6	-2.157375000	-1.960193000	0.206553000
6	-3.608996000	-1.946856000	0.136133000
6	-4.033298000	-0.637092000	0.182756000
6	-2.860676000	0.217127000	0.282625000
6	-1.719241000	2.309444000	0.317053000
6	-1.638213000	3.762813000	0.279971000
6	-0.308288000	4.117020000	0.262440000
6	0.487534000	2.898734000	0.289359000
6	2.471328000	1.616640000	0.254409000
6	3.874691000	1.312967000	0.091306000
6	4.023050000	-0.075860000	0.070523000
6	2.717744000	-0.655640000	0.226275000
6	2.032712000	-1.912640000	0.192952000
6	2.260733000	-3.326546000	0.043560000
6	1.014917000	-3.954564000	0.030674000
6	-0.005492000	-2.935659000	0.165316000
25	0.002896000	0.010036000	0.400732000
7	-0.421554000	1.847032000	0.338939000
7	1.841655000	0.407015000	0.363198000
7	0.666167000	-1.753670000	0.277066000
7	-2.842938000	1.564743000	0.297614000
7	1.826507000	2.810848000	0.249206000
7	-1.359171000	-3.037377000	0.144179000
8	-0.079728000	-0.040785000	2.221755000
7	-1.768283000	-0.625441000	0.318070000
1	4.655118000	2.051778000	-0.016081000
1	4.948358000	-0.619248000	-0.056265000
1	3.223218000	-3.808536000	-0.048129000
1	0.819988000	-5.012072000	-0.071732000
1	0.116209000	5.109132000	0.224540000
1	-2.500983000	4.411631000	0.257579000
1	-5.045359000	-0.263547000	0.138426000
1	-4.211500000	-2.838638000	0.049030000
6	0.026307000	0.037561000	-1.648389000
7	0.023663000	0.058198000	-2.829641000

$^{3}[(H_8Cz)Mn(O)]$: B3LYP:

6	-2.116661000	-1.940680000	0.122000000
6	-3.554953000	-1.922050000	0.028492000
6	-3.978589000	-0.615010000	0.045896000
6	-2.821680000	0.235271000	0.156588000
6	-1.719376000	2.309475000	0.236428000
6	-1.639822000	3.746896000	0.122559000
6	-0.311102000	4.096779000	0.130048000
6	0.471326000	2.886894000	0.245939000
6	2.417669000	1.613309000	0.162433000
6	3.809245000	1.306017000	-0.030856000
6	3.954400000	-0.076665000	-0.060639000
6	2.659579000	-0.655535000	0.121035000
6	2.000461000	-1.903277000	0.136244000
6	2.232019000	-3.295718000	-0.133401000
6	0.997838000	-3.931451000	-0.129163000
6	-0.014105000	-2.935819000	0.134146000
25	-0.003596000	0.002985000	0.765678000
7	-0.420246000	1.811517000	0.338856000
7	1.754881000	0.394620000	0.260615000
7	0.641536000	-1.741912000	0.334843000
7	-2.827862000	1.566678000	0.179400000
7	1.804860000	2.801034000	0.181784000
7	-1.349312000	-3.032744000	0.081577000
8	-0.058464000	0.019256000	2.397441000
7	-1.682891000	-0.597155000	0.201445000
1	4.583253000	2.049558000	-0.142069000
1	4.872818000	-0.624376000	-0.207677000
1	3.190684000	-3.749513000	-0.334177000
1	0.794542000	-4.972988000	-0.324544000
1	0.124039000	5.079404000	0.035256000
1	-2.501869000	4.387603000	0.023913000
1	-4.986580000	-0.236284000	-0.016644000
1	-4.150014000	-2.817420000	-0.061154000

$^{3}[(H_8Cz)Mn(O)CN]^{-}$: BP86:

6	-2.148044000	-1.956149000	0.144102000
6	-3.612809000	-1.952122000	0.092295000
6	-4.041378000	-0.636624000	0.138201000
6	-2.855439000	0.220617000	0.220258000
6	-1.704880000	2.320078000	0.301680000
6	-1.630218000	3.772264000	0.153529000
6	-0.292952000	4.134525000	0.134987000
6	0.505275000	2.919434000	0.268002000
6	2.488141000	1.631417000	0.233606000
6	3.883238000	1.321782000	0.011908000
6	4.032405000	-0.077201000	0.004308000
6	2.737687000	-0.659647000	0.231525000
6	2.056457000	-1.921115000	0.213960000
6	2.279223000	-3.323442000	-0.084717000
6	1.027438000	-3.948699000	-0.110130000
6	0.010534000	-2.937801000	0.161210000
25	0.036491000	0.021046000	0.567905000
7	-0.391293000	1.857290000	0.412108000
7	1.844759000	0.405208000	0.409050000
7	0.695267000	-1.761387000	0.400101000
7	-2.833827000	1.574087000	0.247898000
7	1.855385000	2.831963000	0.207417000
7	-1.342395000	-3.045257000	0.090107000
8	-0.449717000	-0.136065000	2.157520000
7	-1.754957000	-0.624019000	0.214228000
1	4.661717000	2.066569000	-0.144883000
1	4.958479000	-0.626879000	-0.159647000
1	3.243988000	-3.791833000	-0.275748000

1	0.815792000	-4.994019000	-0.329588000
1	0.134110000	5.128820000	0.016408000
1	-2.503446000	4.412941000	0.044152000
1	-5.061455000	-0.257823000	0.108509000
1	-4.215577000	-2.855120000	0.012174000
6	0.030064000	0.017767000	-1.512313000
7	0.018225000	0.025149000	-2.708036000

^{3}[(H$_8$Cz)Mn(O)]: BP86:

6	-2.116545000	-1.947178000	0.107297000
6	-3.563537000	-1.929867000	0.074565000
6	-3.990213000	-0.614740000	0.106429000
6	-2.825091000	0.241396000	0.161700000
6	-1.728782000	2.330452000	0.226493000
6	-1.646385000	3.768649000	0.037627000
6	-0.309777000	4.118479000	0.061990000
6	0.469070000	2.906047000	0.259745000
6	2.419059000	1.617230000	0.191106000
6	3.822254000	1.309877000	0.023482000
6	3.967078000	-0.081117000	-0.028189000
6	2.662118000	-0.661338000	0.124754000
6	2.007244000	-1.918471000	0.144457000
6	2.245113000	-3.305547000	-0.190885000
6	1.004822000	-3.944687000	-0.213322000
6	-0.008985000	-2.952576000	0.106239000
25	-0.009817000	0.003848000	0.779290000
7	-0.426861000	1.825981000	0.401278000
7	1.741029000	0.391338000	0.254129000
7	0.644664000	-1.761065000	0.374540000
7	-2.838946000	1.579789000	0.170169000
7	1.810652000	2.816682000	0.200678000
7	-1.352823000	-3.049314000	0.055918000
8	-0.046856000	-0.009070000	2.399174000
7	-1.665887000	-0.589566000	0.159685000
1	4.604863000	2.060840000	-0.059020000
1	4.894920000	-0.633173000	-0.164051000
1	3.212035000	-3.749763000	-0.418978000
1	0.795964000	-4.983401000	-0.460047000
1	0.134973000	5.102171000	-0.069658000
1	-2.512310000	4.408383000	-0.115683000
1	-5.008310000	-0.233794000	0.077700000
1	-4.165728000	-2.833161000	0.009217000

^{3}[(H$_8$Cz)Mn(O)CN]$^{-}$: M06:

6	-2.145800000	-1.948252000	0.190729000
6	-3.590322000	-1.935745000	0.080632000
6	-4.014403000	-0.631644000	0.128580000
6	-2.847675000	0.217609000	0.267633000
6	-1.710464000	2.300356000	0.305081000
6	-1.630591000	3.747561000	0.228767000
6	-0.305665000	4.099836000	0.207186000
6	0.485820000	2.885963000	0.272128000
6	2.460131000	1.607913000	0.245812000
6	3.848999000	1.307512000	0.026518000
6	4.000175000	-0.076364000	0.015741000
6	2.710940000	-0.654116000	0.237455000
6	2.029263000	-1.906201000	0.206821000
6	2.251787000	-3.306578000	-0.008927000
6	1.008667000	-3.928539000	-0.031479000
6	-0.002358000	-2.919576000	0.162659000
25	0.004251000	0.010000000	0.462641000
7	-0.418959000	1.840078000	0.355805000
7	1.839895000	0.402356000	0.413215000
7	0.670573000	-1.748799000	0.331385000
7	-2.829541000	1.559475000	0.275122000
7	1.817074000	2.796325000	0.220244000
7	-1.349993000	-3.017812000	0.119763000
8	-0.150282000	-0.030368000	2.270987000
7	-1.761710000	-0.621221000	0.334541000
1	4.618450000	2.050721000	-0.130713000
1	4.918783000	-0.620934000	-0.154537000
1	3.212778000	-3.783920000	-0.143642000
1	0.805539000	-4.979421000	-0.184044000
1	0.124783000	5.089012000	0.139448000
1	-2.497530000	4.391200000	0.179843000
1	-5.023593000	-0.251523000	0.056511000
1	-4.185294000	-2.830551000	-0.036218000
6	0.045358000	0.024127000	-1.584535000
7	0.062144000	0.032507000	-2.765719000

^{3}[(H$_8$Cz)Mn(O)]: M06:

6	-2.114296000	-1.935785000	0.122306000
6	-3.548204000	-1.919468000	0.028456000
6	-3.970290000	-0.616537000	0.053117000
6	-2.815115000	0.228505000	0.166822000
6	-1.711105000	2.296678000	0.239971000
6	-1.633457000	3.730329000	0.142683000
6	-0.308882000	4.079857000	0.143641000
6	0.472590000	2.873499000	0.239601000
6	2.415333000	1.606984000	0.164332000
6	3.802691000	1.301879000	-0.028050000
6	3.947977000	-0.075709000	-0.055807000
6	2.656455000	-0.652609000	0.127371000
6	1.995559000	-1.895322000	0.137895000
6	2.224414000	-3.285753000	-0.115093000
6	0.992791000	-3.917333000	-0.114020000
6	-0.015803000	-2.922712000	0.131298000
25	-0.004769000	0.003502000	0.746750000
7	-0.413710000	1.800480000	0.319919000
7	1.756760000	0.393004000	0.266824000
7	0.638924000	-1.728940000	0.320922000
7	-2.814989000	1.555690000	0.191659000
7	1.801782000	2.789533000	0.179420000
7	-1.345692000	-3.021860000	0.082030000
8	-0.074320000	0.048507000	2.390781000
7	-1.682988000	-0.601384000	0.207386000
1	4.574478000	2.048719000	-0.142996000
1	4.866715000	-0.624737000	-0.202729000
1	3.184794000	-3.743724000	-0.303038000
1	0.786272000	-4.961546000	-0.297870000
1	0.129493000	5.063271000	0.060121000
1	-2.500512000	4.368778000	0.061349000
1	-4.977357000	-0.232046000	-0.008392000
1	-4.139533000	-2.818418000	-0.064353000

Sulfoxidation mechanism:

^{1}**TS**$_{SO,CN}$:

25	0.449706000	0.162783000	0.520927000
7	1.099132000	0.128932000	2.309770000
7	2.142992000	-0.213280000	-0.277830000
7	-0.337197000	0.434119000	-1.150428000
7	-1.252484000	0.681607000	1.101182000
6	0.344471000	0.389131000	3.439939000
6	1.231513000	0.183998000	4.580759000
6	2.470513000	-0.173616000	4.097859000
6	2.392114000	-0.203732000	2.641080000
6	3.281673000	-0.476488000	0.441639000
6	4.349457000	-0.706429000	-0.530674000
6	3.812236000	-0.552484000	-1.786906000
6	2.395662000	-0.220611000	-1.635440000
6	0.231414000	0.389726000	-2.394995000
6	-0.802797000	0.821422000	-3.314316000
6	-1.942120000	1.139802000	-2.572909000
6	-1.636862000	0.906362000	-1.184101000
6	-2.172399000	1.059835000	0.135218000
6	-3.321554000	1.554901000	0.847730000
6	-3.037994000	1.483689000	2.213540000
6	-1.699561000	0.950711000	2.369053000
7	-0.951401000	0.766912000	3.489850000
7	3.400547000	-0.485681000	1.787511000

7	1.524220000	0.049853000	-2.629328000
1	0.931741000	0.318095000	5.610126000
1	3.368631000	-0.385228000	4.659716000
1	5.371436000	-0.934206000	-0.265048000
1	4.313544000	-0.634118000	-2.740510000
1	-0.684685000	0.895498000	-4.385985000
1	-2.878428000	1.510595000	-2.965915000
1	-4.231369000	1.933733000	0.403278000
1	-3.677415000	1.797393000	3.026314000
8	0.241283000	-1.620850000	0.609332000
16	-1.548237000	-2.512784000	0.534909000
6	-1.644860000	-2.758196000	2.398419000
6	-0.730768000	-4.129150000	0.038479000
1	-0.594438000	-4.083277000	-1.041763000
1	-1.362904000	-4.974321000	0.317862000
1	0.240025000	-4.149118000	0.534582000
1	-0.629222000	-2.950382000	2.745530000
1	-2.328231000	-3.577353000	2.631123000
1	-2.000505000	-1.813833000	2.809973000
6	1.021347000	2.105461000	0.482958000
7	1.359016000	3.238413000	0.461618000

^{1}**RC**$_{\mathrm{CN}}$:

25	-0.338831000	0.166225000	-0.328936000
7	0.254893000	-0.060353000	1.490298000
7	1.355918000	-0.394637000	-1.063571000
7	-0.750104000	0.988424000	-1.944171000
7	-1.701546000	1.275353000	0.270797000
6	-0.422218000	0.357194000	2.623058000
6	0.333091000	-0.129855000	3.768972000
6	1.443828000	-0.784497000	3.293104000
6	1.408017000	-0.721930000	1.837208000
6	2.339276000	-1.006654000	-0.327011000
6	3.400762000	-1.378666000	-1.255274000
6	3.033055000	-0.948870000	-2.506405000
6	1.734545000	-0.297575000	-2.390377000
6	-0.081799000	0.986388000	-3.145038000
6	-0.829461000	1.854726000	-4.020182000
6	-1.886118000	2.406728000	-3.294382000
6	-1.819383000	1.876552000	-1.965706000
6	-2.374773000	2.044890000	-0.673314000
6	-3.321996000	2.841372000	0.045849000
6	-3.162176000	2.560999000	1.404098000
6	-2.100060000	1.597722000	1.547014000
7	-1.524121000	1.123019000	2.673285000
7	2.363228000	-1.183342000	1.007621000
7	1.079011000	0.334813000	-3.377217000
1	0.045394000	0.044981000	4.794757000
1	2.236253000	-1.256540000	3.854311000
1	4.306113000	-1.886901000	-0.959148000
1	3.582390000	-1.028663000	-3.432368000
1	-0.576739000	2.046350000	-5.052436000
1	-2.611258000	3.120531000	-3.657243000
1	-4.016560000	3.546562000	-0.386951000
1	-3.707510000	2.995812000	2.228508000
8	-0.896795000	-1.312331000	-0.398361000
16	-0.780347000	-5.221222000	1.636291000
6	-1.491525000	-3.601283000	2.308078000
6	0.539113000	-4.500351000	0.486398000
1	0.982306000	-5.344310000	-0.045569000
1	1.301653000	-3.977675000	1.065939000
1	0.069852000	-3.809373000	-0.215198000
1	-1.776576000	-2.957162000	1.475023000
1	-0.752761000	-3.096022000	2.932363000
1	-2.367330000	-3.867509000	2.902803000
6	0.814820000	1.929561000	-0.070302000
7	1.475253000	2.898840000	0.081038000

^{1}**P**$_{\mathrm{CN}}$:

25	0.279057000	0.557140000	-0.056590000
7	0.836890000	0.283738000	1.727790000
7	1.905535000	0.003750000	-0.832166000
7	-0.537744000	0.681438000	-1.743378000
7	-1.489091000	0.876422000	0.501715000
6	0.036499000	0.435634000	2.854580000
6	0.864619000	0.078235000	4.001235000
6	2.108757000	-0.282603000	3.532852000
6	2.090216000	-0.164526000	2.079004000
6	3.004387000	-0.399963000	-0.109778000
6	4.038534000	-0.763527000	-1.073015000
6	3.519258000	-0.584375000	-2.335190000
6	2.149685000	-0.100637000	-2.197515000
6	-0.002694000	0.511380000	-2.985817000
6	-1.078685000	0.769222000	-3.924785000
6	-2.226867000	1.074771000	-3.190795000
6	-1.876330000	1.016745000	-1.791946000
6	-2.433063000	1.153927000	-0.473563000
6	-3.650709000	1.470151000	0.225765000
6	-3.388534000	1.381568000	1.597684000
6	-1.999844000	1.006310000	1.763703000
7	-1.272752000	0.769725000	2.893815000
7	3.100173000	-0.472630000	1.236486000
7	1.286161000	0.136039000	-3.203990000
1	0.522744000	0.106760000	5.026111000
1	2.968770000	-0.600185000	4.104783000
1	5.025600000	-1.109160000	-0.801692000
1	4.002899000	-0.763703000	-3.284747000
1	-0.989219000	0.725028000	-5.001082000
1	-3.200983000	1.311827000	-3.596131000
1	-4.595893000	1.738248000	-0.226163000
1	-4.083397000	1.572704000	2.403398000
8	-0.036359000	-1.574258000	-0.118705000
16	-1.623461000	-2.204746000	0.107809000
6	-1.690108000	-2.606910000	1.961981000
6	-1.312822000	-3.950320000	-0.542700000
1	-1.165704000	-3.844885000	-1.616863000
1	-2.175152000	-4.581113000	-0.318941000
1	-0.399330000	-4.312098000	-0.069951000
1	-0.745186000	-3.083668000	2.225438000
1	-2.550399000	-3.255263000	2.140827000
1	-1.794680000	-1.652018000	2.478096000
6	0.719482000	2.468884000	-0.077519000
7	0.991349000	3.619335000	-0.090595000