

Supporting Information

Mechanism of Manganese-Catalyzed Oxygen Evolution from Experimental and Theoretical Analyses of ^{18}O Kinetic Isotope Effects

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Complete Computational Methods

Density functional theory. All geometries in the main paper were fully optimized at the B3LYP level^{1,2} of density functional theory with Grimme's D2 version of dispersion correction³ using the LanL2DZ pseudopotential basis set⁴ on Mn, the 3-21G basis set on C and H atoms,⁵ the 6-31G basis set on N atoms, the 6-31G(d) basis set on S atoms,^{6,7} and the 6-31+G(d) basis set on O atoms,^{8,9} along with the PCM aqueous continuum solvation model.¹⁰ Additionally, calculations were done at the M06-L level of density functional theory¹¹⁻¹³ using the Stuttgart [8s7p6d2f[6s5p3d1f] ECP10MDF contracted pseudopotential basis set¹⁴ on Mn and the 6-31G(d) basis set⁷ on all other atoms along with the SMD aqueous continuum solvation model.¹⁵ Non-analytical integral evaluations made use of a pruned grid having 99 radial shells and 590 angular points per shell with the Gaussian 09 software package.¹⁶ The nature of all stationary points was verified by analytic computation of vibrational frequencies, which were also used for the computation of zero-point vibrational energies, molecular partition functions, and for determining the reactants and products associated with each transition-state structure (by following the normal modes associated with imaginary frequencies). Partition functions were used in the computation of 298 K thermal contributions to the free energy employing the usual ideal-gas, rigid-rotator, harmonic oscillator approximation.¹⁷ Free energy contributions were added to single-point electronic energies computed with the LanL2DZ basis set on manganese and the 6-311+G(2df,p) basis set on all other atoms to arrive at final, composite free energies. The single point electronic energies were calculated with B3LYP with 15% Hartree-Fock exchange as suggested by a recent benchmark study.¹⁸ Dispersion was considered with Grimme's D2 version of dispersion correction.³

Solvation and standard state corrections. For the B3LYP calculations, solvation effects associated with water as solvent were accounted for using the PCM continuum solvation model.

The following atomic Coulomb radii were used for solute molecules: H (1.443 Å), C (1.9225 Å), N (1.83 Å), O (1.75 Å), S (2.0175 Å), and Mn (2.0 Å). A 1 M standard state was used for all species in aqueous solution except for water itself, for which a 55.6 M standard state was employed. Thus, for all molecules but water, the free energy in aqueous solution is computed as the 1 atm gas-phase free energy, plus an adjustment for the 1 atm to 1 M standard-state concentration change of $RT \ln (24.5)$, or 1.89 kcal/mol, plus the 1 M to 1 M transfer (solvation) free energy.¹⁷ In the case of water, the 1 atm gas-phase free energy is adjusted by the sum of a 1 atm to 55.6 M standard-state concentration change, or 4.27 kcal/mol, and the experimental 1 M to 1 M solvation free energy, -6.3 kcal/mol.¹⁹

Non-single-determinant state energies. Several possible intermediates in the oxygen-evolution mechanism have electronic structures that are not well described by a single determinant. In such instances, standard Kohn-Sham DFT is not directly applicable,^{17,20-22} and we adopt the Yamaguchi broken-spin-symmetry (BS) procedure^{23,24} to compute the energy of the spin-purified low-spin (LS) state as

$${}^{\text{LS}}E = \frac{{}^{\text{BS}}E \left({}^{\text{HS}}\langle S^2 \rangle - {}^{\text{LS}}\langle S^2 \rangle \right) - {}^{\text{HS}}E \left({}^{\text{BS}}\langle S^2 \rangle - {}^{\text{LS}}\langle S^2 \rangle \right)}{{}^{\text{HS}}\langle S^2 \rangle - {}^{\text{BS}}\langle S^2 \rangle} \quad (\text{S1})$$

where HS refers to the single-determinant high-spin coupled state that is related to the low-spin state by spin flip(s) and $\langle S^2 \rangle$ is the expectation value of the total spin operator applied to the appropriate determinant. This broken-symmetry DFT approach has routinely proven effective for the prediction of state-energy splitting in metal coordination compounds.^{21,25-28}

Calculation of O-18 kinetic isotope effects (¹⁸O-KIEs). The ¹⁸O equilibrium and kinetic isotope effects were calculated by employing the Transition State Theory as formulated by Bigeleisen

and Wolfsberg.²⁹ For each step of the catalytic mechanism, the vibrational frequencies of reactants and products were analyzed following the Bigeleisen and Goeppert-Mayer approach.³⁰ The Redlich-Teller product rule³¹ was employed to isotope exchange equations (Eqn. S2) for the initial (A) and final (B) states using the full set of vibrational frequencies obtained for both light (¹⁶O) and heavy (¹⁸O) isotopologues via DFT calculations.



¹⁸O-EIEs for the exchange reactions were obtained using the $3N - 6$ vibrational frequencies as

$$^{18}\text{O-EIE} = \text{ZPE} \times \text{EXC} \times \text{MMI} \quad (\text{S3})$$

with

$$\text{ZPE} = \frac{\prod_j^{3N-6} \frac{\exp(h\nu_j^{B(^{18}\text{O})})/2kT}{\exp(h\nu_j^{B(^{16}\text{O})})/2kT}}{\prod_i^{3N-6} \frac{\exp(h\nu_i^{A(^{18}\text{O})})/2kT}{\exp(h\nu_i^{A(^{16}\text{O})})/2kT}} \quad (\text{S4})$$

$$\text{EXC} = \frac{\prod_j^{3N-6} \frac{1 - \exp(-h\nu_j^{B(^{18}\text{O})})/kT}{1 - \exp(-h\nu_j^{B(^{16}\text{O})})/kT}}{\prod_i^{3N-6} \frac{1 - \exp(-h\nu_i^{A(^{18}\text{O})})/kT}{1 - \exp(-h\nu_i^{A(^{16}\text{O})})/kT}} \quad (\text{S5})$$

$$\text{MMI} = VP = \frac{\prod_j^{3N-6} (v_j^{B(^{16}\text{O})})/v_j^{B(^{18}\text{O})})}{\prod_i^{3N-6} (v_i^{A(^{16}\text{O})})/v_i^{A(^{18}\text{O})})} \quad (\text{S6})$$

where v is the associated vibrational frequency, h is the Planck's constant, k is the Boltzmann constant and T is the temperature in Kelvin units.

The ¹⁸O-KIEs associated with located transition state structures were calculated in a similar way,

$$^{18}\text{O-KIE} = v_{RC}^{18} \times \text{ZPE} \times \text{EXC} \times \text{VP} \quad (\text{S7})$$

$$^{18}\text{O-KIE} = v_{RC}^{18} \times ^{18}\text{K}_{\text{TS}} \quad (\text{S8})$$

where v_{RC}^{18} ^{31,32} is the ratio of the imaginary frequencies of the TSs associated with light (e.g. ¹⁶O) and heavy (e.g. ¹⁸O) isotopologues and $^{18}\text{K}_{\text{TS}}$ is the product of $\text{ZPE} \times \text{EXC} \times \text{VP}$ with $3N - 6$ vibrational frequencies for the reactant and $3N - 7$ vibrational frequencies for the TS (S9-S11).

$$\text{ZPE} = \frac{\prod_j^{3N-7} \frac{\exp(hv_j^{B(^{18}\text{O})})/2kT}{\exp(hv_j^{B(^{16}\text{O})})/2kT}}{\prod_i^{3N-6} \frac{\exp(hv_i^{A(^{18}\text{O})})/2kT}{\exp(hv_i^{A(^{16}\text{O})})/2kT}} \quad (\text{S9})$$

$$\text{EXC} = \frac{\prod_j^{3N-7} \frac{1 - \exp(-hv_j^{B(^{18}\text{O})})/kT}{1 - \exp(-hv_j^{B(^{16}\text{O})})/kT}}{\prod_i^{3N-6} \frac{1 - \exp(-hv_i^{A(^{18}\text{O})})/kT}{1 - \exp(-hv_i^{A(^{16}\text{O})})/kT}} \quad (\text{S10})$$

$$\text{MMI} = \text{VP} = \frac{\prod_j^{3N-7} (v_j^{B(^{16}\text{O})})/v_j^{B(^{18}\text{O})})}{\prod_i^{3N-6} (v_i^{A(^{16}\text{O})})/v_i^{A(^{18}\text{O})})} \quad (\text{S11})$$

The calculated ¹⁸O-EIEs and ¹⁸O-KIEs along with the reduced partition functions are tabulated in Table S1 and a full set of vibrations for the structures in Scheme 2 is available in the final part of the SI.

Table S1. Reduced partition function analysis for calculating the ^{18}O EIEs and ^{18}O KIEs with B3LYP-D2. Harmonic means are presented in the cases where more than one position is possible for ^{16}O : ^{18}O isotopic exchange.

	$^{18}\text{v}_{\text{RC}}$	ZPE	EXC	VP/ MMI	$^{18}\text{K}_{\text{TS}}$
KIE₁₋₀	1.0112	0.9706	0.9683	1.0576	0.9940
KIE₁	1.0116	0.9718	0.9691	1.0572	0.9956
EIE₁	-	0.9725	0.9731	1.0696	-
KIE₂	1.0326	1.0073	1.0495	0.9684	1.0237
EIE₂	-	0.9820	1.0528	0.9977	-
KIE₃₋₁	1.0277	1.0016	0.9971	1.0074	1.0069
EIE₃₋₂	1.0276	1.0124	1.0029	0.9741	0.9891
EIE₃	-	0.9940	0.9579	1.0345	-
KIE₄	1.0101	0.9999	1.0110	0.9898	1.0080
EIE₄	-	0.9940	0.9579	1.0345	-

Effect of density functional/basis set choice on calculated ^{18}O -KIEs. We have performed DFT calculations at three different level of theories for the O–O bond scission step starting with $[(\text{SO}_5)\text{Mn}^{\text{IV}}(\mu\text{-O})_2\text{Mn}^{\text{III}}(\text{AcO})(\text{terpy})_2]$ in order to test the dependence of calculated ^{18}O -KIEs on the level of theory employed. The geometries were optimized using:

- (1) M06-L level of density functional theory¹¹⁻¹³ using the Stuttgart [8s7p6d2f|6s5p3d1f] ECP10MDF contracted pseudopotential basis set¹⁴ on Mn and the 6-31G(d) basis set⁷ on all other atoms along with SMD aqueous continuum solvation model.¹⁵
- (2) mPWPW91^{33,34} level of density functional theory using the LanL2DZ pseudopotential basis set⁴ on Mn and the 6-311G(d) basis set⁷ on S, O, N and 6-31G on C, H atoms along with SMD aqueous continuum solvation model.¹⁵
- (3) B3LYP level of density functional theory^{1,2} using the LanL2DZ pseudopotential basis set⁴ on Mn and the 6-31G(d) basis set on S, O, 6-31G on N and 3-21G on C, H atoms along with IEFPCM solvation model.³⁵⁻³⁷

The results are summarized in Table S2 and reflect that the calculated ^{18}O -KIEs do not vary significantly (~ 0.0010) with changes in level of theories employed.

Table S2. Reduced partition function analysis for calculating the ^{18}O KIEs at three different levels of theory for the O–O bond scission step starting with $[(\text{SO}_5)\text{Mn}^{\text{IV}}(\mu\text{-O})_2\text{Mn}^{\text{III}}(\text{AcO})(\text{terpy})_2]$.

Method	$^{18}\text{v}_{\text{RC}}$	ZPE	VP	EXC	$^{18}K_{\text{TS}}$	$^{18}\text{O-KIE}$
M06-L^a	1.0256	1.0492	0.9745	1.0012	1.0237	1.0499
mPW^a	1.0284	1.0446	0.9720	1.0052	1.0206	1.0496
B3LYP^a	1.0292	1.0450	0.9711	1.0062	1.0211	1.0510

^a see text for further details

Effect of density functional/basis set choice on calculated barrier for O–O bond cleavage. We have performed DFT calculations for the O–O bond scission step starting with $[(\text{SO}_5)\text{Mn}^{\text{IV}}(\mu\text{-O})_2\text{Mn}^{\text{III}}(\text{AcO})(\text{terpy})_2]$ and $[(\text{SO}_5)\text{Mn}^{\text{III}}(\mu\text{-O})_2\text{Mn}^{\text{IV}}(\text{AcO})(\text{terpy})_2]$ with two different density functionals, including M06-L and B3LYP-D2 with 15% of Hartree-Fock exact exchange to test the dependence of calculated barriers on the level of theory employed. The methods are described below:

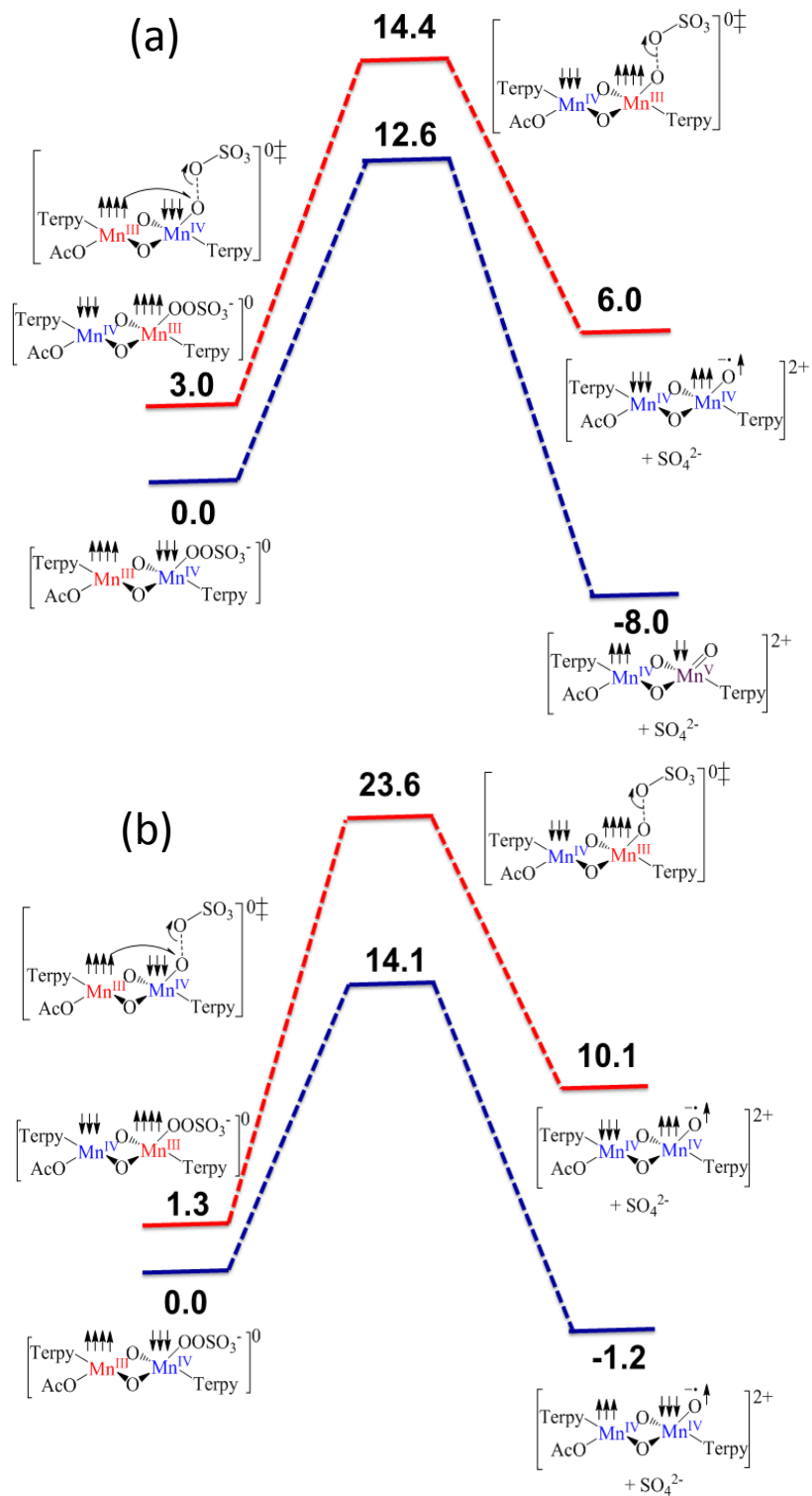
(1) Geometry optimizations were performed by using the M06-L level of density functional theory¹¹⁻¹³ using the Stuttgart [8s7p6d2f|6s5p3d1f] ECP10MDF contracted pseudopotential basis set¹⁴ on Mn and the 6-31G(d) basis set⁷ on all other atoms along with the SMD aqueous continuum solvation model.¹⁵ Single point energies were evaluated with M06-L using the Stuttgart [8s7p6d2f|6s5p3d1f] ECP10MDF contracted pseudopotential basis set¹⁴ and 6-311+G(2df,p) basis set on all other atoms.

(2) Geometry optimizations were performed with B3LYP and Grimme's D2 version of dispersion correction³ using the LanL2DZ pseudopotential basis set⁴ on Mn, the 3-21G basis set on C and H atoms,⁵ the 6-31G basis set on N atom, the 6-31G(d) basis set on S atom,^{6,7} and the 6-31+G(d) basis set on O atoms,^{8,9} along with PCM aqueous continuum solvation model.¹⁰ Single point energies were evaluated using B3LYP with 15% Hartree-Fock exchange (B3LYP15-D2), as suggested by a recent benchmark study,¹⁸ with the LanL2DZ pseudopotential basis set on manganese and the 6-311+G(2df,p) basis set on all other atoms.

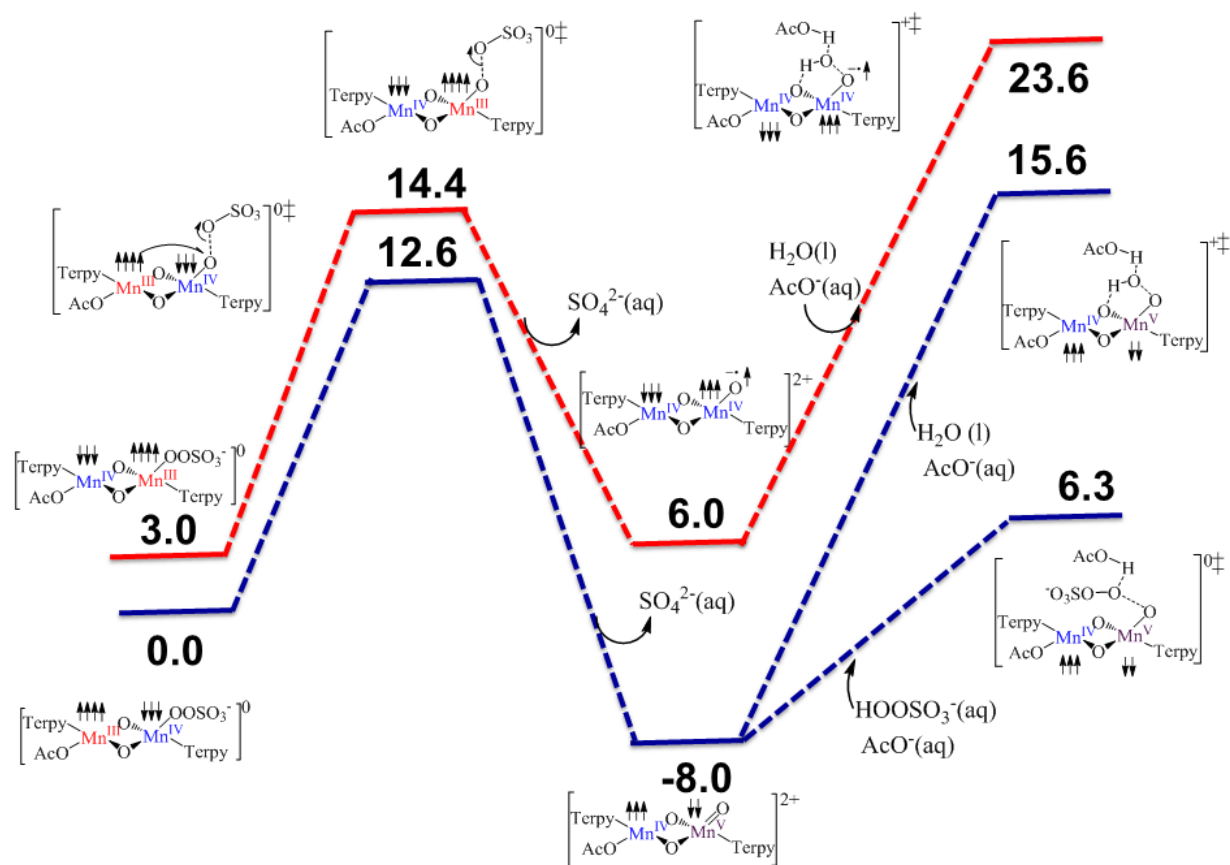
The complete mechanism of $[(\text{AcO})\text{Mn}^{\text{III}}(\mu\text{-O})_2\text{Mn}^{\text{IV}}(\text{AcO})(\text{terpy})_2]^+$ was explored with both B3LYP15-D2 and M06-L. As shown in Scheme S1, the B3LYP15-D2 free energy profile predicts that only the O–O bond cleavage of SO_5^{2-} bound to Mn(IV) is accessible since O–O bond cleavage of SO_5^{2-} bound to Mn(III) has a much higher energy barrier, inaccessible under

typical experimental conditions. In contrast, the M06-L functional predicts that both pathways have small energy barriers of 12.6 and 14.4 kcal/mol. Unlike the calculated ^{18}O -KIEs, the calculated free energies depend strongly on the chosen functional. However, both methods predict the O–O bond cleavage of SO_5^{2-} bound to Mn(IV) has a smaller barrier than O–O bond cleavage of SO_5^{2-} bound to Mn(III). Another difference is that the oxidized intermediate generated upon O–O bond cleavage of SO_5^{2-} is predicted to be the $\text{Mn}^{\text{V}}=\text{O}$ species (Mulliken atomic spin densities of -1.81 and -0.05 on Mn and O centers), according to M06-L, while a $\text{Mn}^{\text{IV}}-\text{O}^\bullet$ oxyl-radical species is predicted by B3LYP15-D2. High oxidation states are stabilized by M06-L causing the Mn center, rather than the terminal O atom to be preferentially oxidized. The most significant difference between the two functionals concerns the barriers for O–O bond formation through the nucleophilic attack of HSO_5^- and H_2O which are calculated to be 12.2 and 18.4 kcal/mol with B3LYP15-D2 (Scheme 2) consistent with experimental observation of O_2 evolution from the reaction of two peroxymonosulfate molecules as the prevalent pathway under high concentration of HSO_5^- , while oxygen atoms from water are incorporated into O_2 under low HSO_5^- concentration.³⁸ In contrast, the M06-L functional predicts that the barriers for O–O bond formation through the nucleophilic attack of HSO_5^- and H_2O are 14.3 and 23.6 kcal/mol (Scheme S2). The high water-nucleophilic attack barrier is inconsistent with experimental measurements of the kinetics associated with O_2 evolution. M06-L tends to over-stabilize the oxidized intermediate, as previously reported by Truhlar and co-workers “*predictions from M06-L were found to be somewhat sensitive to basis set, with the largest basis sets leading to underestimations of reduction potentials on the order of 300 mV*”,³⁹ and also consistent with the conclusions of a recent study by Siegbahn and co-workers.¹⁸ Thus, we only presented energy profiles obtained at the B3LYP15-D2 level in the main text. An additional mechanism of oxygen

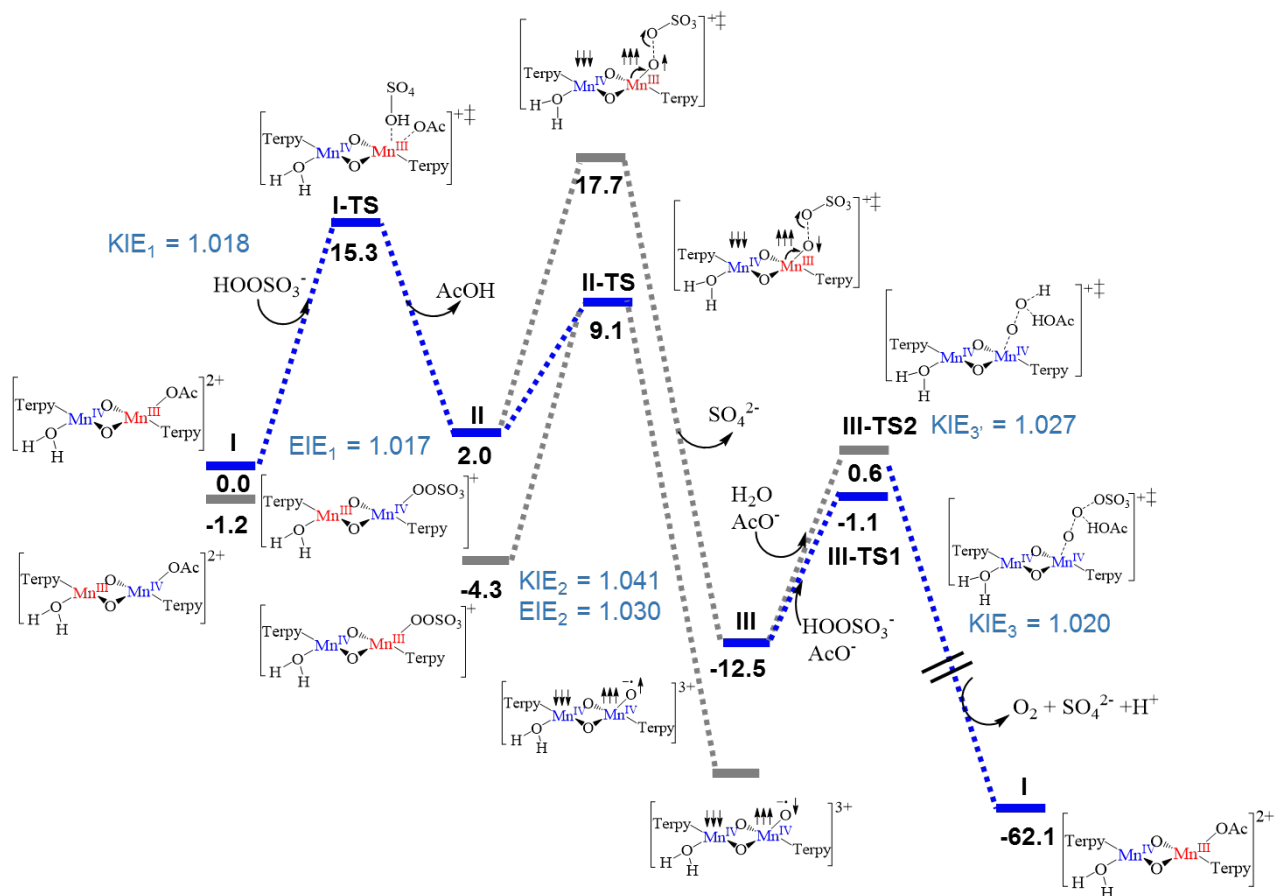
evolution from $[(\text{AcO})\text{Mn}^{\text{III}}(\mu\text{-O})_2\text{Mn}^{\text{IV}}(\text{H}_2\text{O})(\text{terpy})_2]^{2+}$ calculated using M06-L level is included in Scheme S3 for completeness. All the complete mechanisms calculated in the study show that the ligand substitution step of either H_2O or AcO^- substitution with HSO_5^- is the experimentally measured oxygen isotope sensitive step, hence indicating that it is rate-limiting during turnover.



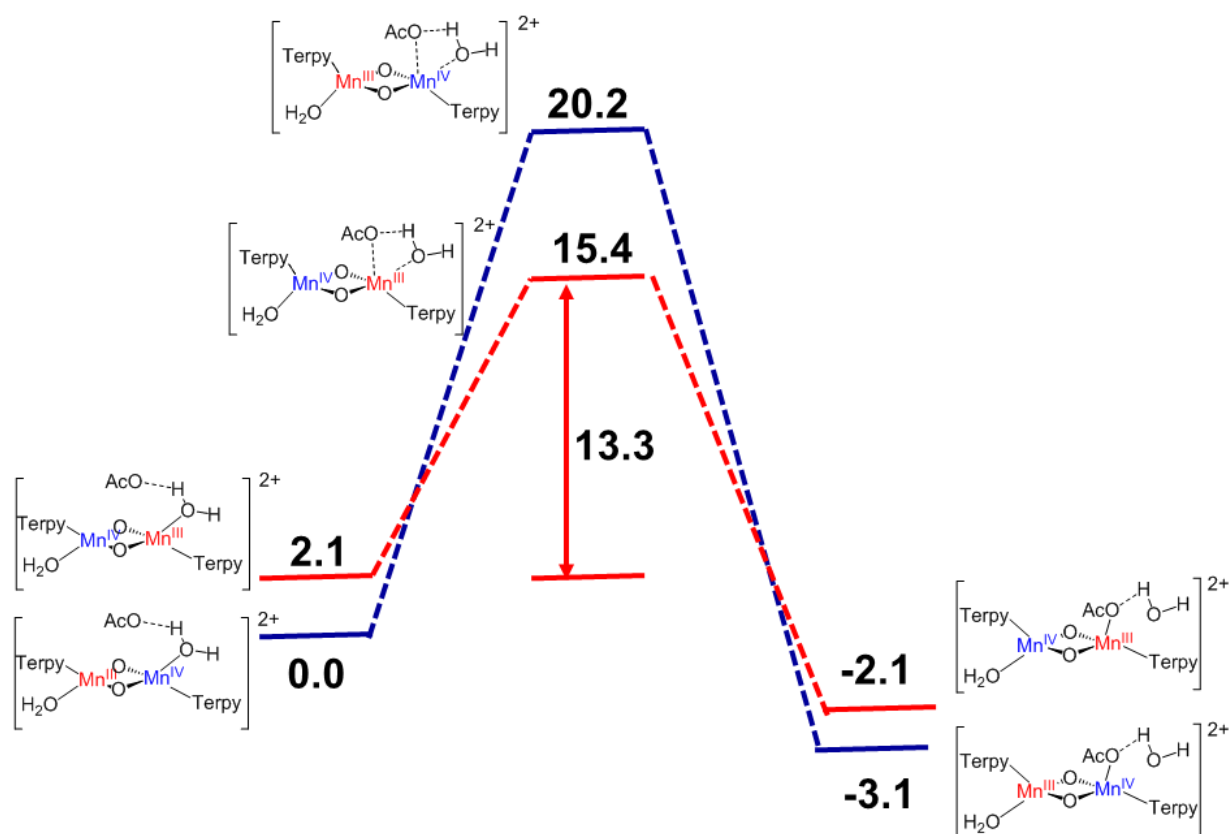
Scheme S1. O–O bond cleavage of SO_5^{2-} bound to either Mn(III) or Mn(IV) explored with (a) M06-L and (b) B3LYP15-D2.



Scheme S2. Free energy profile of O–O bond cleavage and O–O bond formation calculated at the M06-L level.



Scheme S3. Reaction mechanism of oxygen evolution catalyzed by $[(\text{AcO})\text{Mn}^{\text{III}}(\mu\text{-O})_2\text{Mn}^{\text{IV}}(\text{H}_2\text{O})(\text{terpy})_2]^{2+}$ activated with peroxymonosulfate explored at the M06-L level of theory. ^{18}O kinetic isotope effect (KIE) and equilibrium isotope effect (EIE) factors obtained at the M06-L level are indicated in blue. The activation energy and ^{18}O KIE of AcO^- replacement by HSO_5^- both agree with the experimental barrier and KIE.



Scheme S4. Free energy profile of H_2O replaced by AcO^- obtained at the B3LYP15-D2 level of theory. The activation barrier of replacing the water on Mn(IV) is much higher than the barrier to replace the water on Mn(III) with acetate. M06-L calculations give the same trend with the barrier of water displacement by acetate on Mn(IV) higher (18.0 kcal/mol) than water substitution on Mn(III) (10.7 kcal/mol). This difference is due to steric factors stemming from the Jahn-Teller distortions at the Mn(III) center that allow AcO^- binding to Mn(III) to proceed via a lower activation free energy. However, Coulombics cause AcO^- bound to Mn(IV) to be thermodynamically lower in energy.

References

- (1) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652.
- (2) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623-11627.
- (3) Grimme, S. *J. Comp. Chem.* **2006**, *27*, 1787-1799.
- (4) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299-310.
- (5) Binkley, J. S.; Pople, J. A.; Hehre, W. J. *J. Am. Chem. Soc.* **1980**, *102*, 939-947.
- (6) Francel, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. *J. Chem. Phys.* **1982**, *77*, 3654-3665.
- (7) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.
- (8) Hariharan, P. C.; Pople, J. A. *Theoret. Chim. Acta.* **1973**, *28*, 213-222.
- (9) Clark, T.; Chandrasekhar, J.; Spitznager, G. W.; Schleyer, P. V. R. *J. Comp. Chem.* **1983**, *4*, 294-301.
- (10) Tomasi, J. M., B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999-3093.
- (11) Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101-194118.
- (12) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157-167.
- (13) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241.
- (14) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866-872.
- (15) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378-6396.
- (16) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision A.02*; Gaussian, Inc.: Wallingford, CT, 2010.
- (17) Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*; 2nd ed.; John Wiley & Sons: Chichester, 2004.
- (18) Siegbahn, P. E. M.; Blomberg, M. R. A. *J. Chem. Theory Comput.* **2014**, *10*, 268-272.

- (19) Camaioni, D. M.; Schwerdtfeger, C. A. *J. Phys. Chem. A* **2005**, *109*, 10795-10797.
- (20) Ziegler, T.; Rauk, A.; Baerends, E. J. *Theoret. Chim. Acta.* **1977**, *43*, 261-271.
- (21) Noodleman, L. *J. Chem. Phys.* **1981**, *74*, 5737-5743.
- (22) Cramer, C. J.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2009**, *11*, 10757-10816.
- (23) Yamaguchi, K.; Jensen, F.; Dorigo, A.; Houk, K. N. *Chem. Phys. Lett.* **1988**, *149*, 537-542.
- (24) Soda, T.; Kitagawa, Y.; Onishi, T.; Takano, Y.; Shigeta, Y.; Nagao, H.; Yoshioka, Y.; Yamaguchi, K. *Chem. Phys. Lett.* **2000**, *319*, 223-230.
- (25) Noodleman, L.; Peng, C. Y.; Case, D. A.; Mouesca, J. M. *Coord. Chem. Rev.* **1995**, *144*, 199-244.
- (26) Ciofini, I.; Daul, C. A. *Coord. Chem. Rev.* **2003**, *238*, 187-209.
- (27) Harvey, J. N. *Struct. Bond.* **2004**, *112*, 151-183.
- (28) Neese, F. *Coord. Chem. Rev.* **2009**, *253*, 526-563.
- (29) Bigeleisen, J.; Wolfsberg, M. *Adv. Chem. Phys.* **1958**, *1*, 15-76.
- (30) Bigeleisen, J.; Mayer, M. G. *J. Chem. Phys.* **1947**, *15*, 261-267.
- (31) Wolfsberg, M.; Hook, W. A. V.; Paneth, P.; Rebelo, L. P. N. *Isotope Effects in the Chemical, Geochemical and Biosciences*; Springer: New York, 2010.
- (32) Roth, J. P.; Klinman, J. P. In *Isotope Effects in Chemistry and Biology*; A., K., Limbach, H.-H., Eds.; CRC Press: Boca Raton, FL, 2006, p 645.
- (33) Perdew, J. P. In *Electronic Structure of Solids '91*; Ziesche P., E. H., Ed.; Akademie Verlag: Berlin, 1991, p 11.
- (34) Adamo, C.; Barone, V. *J. Chem. Phys.* **1998**, *108*, 664-675.
- (35) Cancès, E.; Mennucci, B.; Tomasi, J. *J. Chem. Phys.* **1997**, *107*, 3032-3041.
- (36) Mennucci, B.; Tomasi, J. *J. Chem. Phys.* **1997**, *106*, 5151-5158.
- (37) Tomasi, J.; Mennucci, B.; Cancès, E. *J. Mol. Struct-Theochem.* **1999**, *464*, 211-226.
- (38) Limburg, J.; Vrettos, J. S.; Chen, H.; de Paula, J. C.; Crabtree, R. H.; Brudvig, G. W. *J. Am. Chem. Soc.* **2001**, *123*, 423-430.
- (39) Marenich, A. V.; Ho, J.; Coote, M. L.; Cramer, C. J.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2014**, *16*, 15068-15106.

Cartesian Coordinates and Energies of Optimized Structures

$\text{O}_{2(g)}$

E = -150.325484080 a.u.

O	0.00000000	0.00000000	0.60866400
O	0.00000000	0.00000000	-0.60866400

$\text{H}_2\text{O}_{(g)}$

E = -76.4169590041 a.u.

O	0.00000000	0.00000000	0.11701800
H	0.00000000	0.77578100	-0.46807100
H	0.00000000	-0.77578100	-0.46807100

$\text{CH}_3\text{COO}^- (\text{AcO}^-)$

E = -228.216162160 a.u.

C	0.18414900	-0.00083400	0.00003300
O	0.81910900	-1.10337900	-0.00001200
O	0.71725200	1.15580300	-0.00000100
C	-1.36411900	-0.04810200	-0.00000900
H	-1.74121000	0.47637000	0.88686300
H	-1.74118200	0.47665000	-0.88672500
H	-1.72867200	-1.07880300	-0.00017200

$\text{CH}_3\text{COOH} (\text{AcOH})$

E = -228.671224962 a.u.

C	-1.40232300	-0.11430200	0.00000000
H	-1.67905600	-0.69509900	-0.88758400
H	-1.92527700	0.84313600	0.00000700
H	-1.67905300	-0.69511200	0.88757400
C	0.09024600	0.12324100	0.00000100
O	0.64595200	1.21325300	0.00000000
O	0.78074600	-1.04544100	0.00000100
H	1.74225500	-0.84905600	-0.00000600



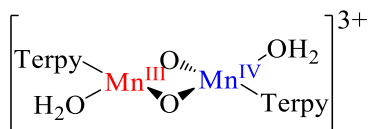
E = -699.370922467 a.u.

S	-0.00002700	0.00012200	0.00025800
O	-1.27442500	-0.36892000	0.74833000
O	-0.03655200	1.47783100	-0.36712500
O	1.20773100	-0.27305200	0.88706600
O	0.10330000	-0.83610300	-1.26878700



E = -774.950910602 a.u.

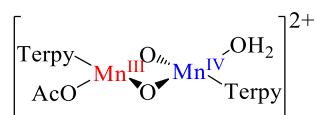
S	0.49404500	-0.06631200	-0.00481400
O	0.32622100	-0.95856300	-1.17736400
O	0.55758500	-0.77159500	1.29597000
O	1.45739600	1.04579500	-0.17380800
O	-0.95622600	0.87037200	0.03456800
O	-2.09195000	-0.02210500	0.13150400
H	-2.24892700	-0.25024000	-0.80993600



E = -1989.59305971 a.u.

Mn	-1.13670400	0.02674900	0.61606600
Mn	1.26002000	0.02948700	-0.58295800
O	-0.40276600	0.04477800	-1.11936800
O	0.63882800	0.03394600	1.05641000
O	-1.76894700	0.03334300	2.68152100
O	1.95461800	0.00802200	-2.58457300
N	-1.66663000	-2.09566000	0.76923700
N	-3.06100300	-0.03064600	-0.05614000
N	-1.77270500	2.12775900	0.70453000
N	1.61572200	-1.94681700	-0.65116800
N	3.14622200	-0.01513700	0.02161200
N	1.69810200	1.99295800	-0.59204000
C	-2.84528100	-2.40252600	0.16304300
C	-3.63641500	-1.23459000	-0.28381200
C	-4.90620600	-1.30260400	-0.86237500
C	-5.56232000	-0.11128000	-1.18285600
C	-4.96382100	1.12086000	-0.90723700
C	-3.69161400	1.13514500	-0.32945200
C	-2.95595700	2.35505700	0.07193500
C	2.83788100	-2.33491800	-0.16581300
C	3.70238100	-1.21939100	0.25622700
C	4.97561400	-1.28717500	0.82462800
C	5.62568100	-0.08570800	1.13567200
C	5.02029400	1.15187100	0.87904300
C	3.74702600	1.15647500	0.30728100
C	2.92464900	2.31961900	-0.07043600
C	0.75699400	-2.84541300	-1.16203600
C	3.19597600	-3.67768500	-0.15166900
C	1.07483400	-4.20447900	-1.18656100
C	2.29901000	-4.62342100	-0.66513100
C	0.87107300	2.94288300	-1.06295500
C	3.32236200	3.64834000	0.01542300
C	1.22864800	4.29114100	-1.01159300
C	2.45891400	4.64536900	-0.45702100
C	-0.88320700	-3.06418600	1.27426000
C	-3.25439600	-3.72890900	0.02531400
C	-2.43921000	-4.74158400	0.54386400
C	-1.24380200	-4.40997900	1.18523600
C	-3.42286600	3.65416100	-0.12895100
C	-1.04424500	3.15277700	1.17939200
C	-1.46464100	4.47573400	1.02806500

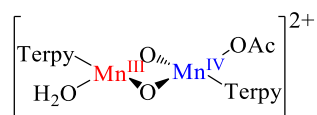
C	-2.66300700	4.72471000	0.35582500
H	-5.37587400	-2.25740900	-1.04909400
H	-5.47928100	2.04437000	-1.12732700
H	5.44477000	-2.24075300	1.02067300
H	5.52416800	2.07726100	1.11917300
H	2.41903800	0.82390300	-2.85610900
H	1.18330800	-0.07308000	-3.18136900
H	-1.53521100	-0.78436700	3.16125300
H	-1.41840800	0.77576500	3.20994000
H	-6.54575400	-0.14295600	-1.63260600
H	6.61110100	-0.11359900	1.58114500
H	0.36287300	-4.90888900	-1.59213000
H	2.56283500	-5.67263600	-0.66275400
H	4.15895900	-3.97812500	0.23788400
H	-0.18154200	-2.45546400	-1.52965900
H	0.54264600	5.03704700	-1.38674800
H	2.75341500	5.68474600	-0.39814500
H	4.28986600	3.89936000	0.42794900
H	-0.07305300	2.60048400	-1.46263600
H	-2.73946400	-5.77669200	0.44670900
H	-0.59357400	-5.17091100	1.59359100
H	-0.85766000	5.28237100	1.41485800
H	-3.00847200	5.73976800	0.20977900
H	-4.18442000	-3.97262700	-0.46864900
H	0.04547400	-2.74310900	1.72919200
H	-4.35437100	3.83372200	-0.64711800
H	-0.11220100	2.89621200	1.66652600



E = -2141.40635588 a.u.

Mn	1.08334400	-0.04780200	0.49101600
Mn	-1.33594400	-0.22447400	-0.69658400
O	0.33289700	-0.11720000	-1.22550700
O	-0.75521300	-0.19133500	0.93067000
O	-1.97663400	-0.29558200	-2.73810300
N	0.99857400	2.17954700	0.77814800
N	2.88322600	0.73409900	-0.36354500
N	2.35602400	-1.83119200	0.02614400
N	-1.81683200	1.72316600	-0.82660200
N	-3.24412400	-0.27934200	-0.14331800
N	-1.66432700	-2.21264900	-0.67005100
C	2.00317700	2.88763000	0.21226700
C	3.02807500	2.07296100	-0.48047000
C	4.09359900	2.60764700	-1.21128400
C	5.00152100	1.73216500	-1.81075400
C	4.84117500	0.35237600	-1.67102500
C	3.75400500	-0.12644100	-0.93084600
C	3.47090700	-1.56281300	-0.69978400
C	-3.06022700	2.05163700	-0.35651000
C	-3.87025400	0.89483500	0.06571700
C	-5.15687000	0.89871000	0.60791000
C	-5.74663800	-0.33340600	0.92042500
C	-5.06809000	-1.53823700	0.69328900
C	-3.78433000	-1.47816700	0.14817800
C	-2.88343300	-2.59907900	-0.17744300
C	-1.00735300	2.65777300	-1.35371100
C	-3.48656600	3.37531400	-0.35549000
C	-1.39200000	3.99812000	-1.39226600
C	-2.63629400	4.35991200	-0.87323300
C	-0.76007400	-3.12241300	-1.07118900
C	-3.19931000	-3.94758700	-0.05534000
C	-1.02585100	-4.48898900	-0.97004500
C	-2.25407400	-4.90266400	-0.45069500
C	0.03015700	2.79628400	1.47509300
C	2.04177800	4.28151400	0.30958000
C	1.02907200	4.93216400	1.02118800
C	0.01188100	4.18378000	1.62121400
C	4.29072400	-2.59347200	-1.16765100
C	2.03462000	-3.10288300	0.32869600
C	2.80886700	-4.17873300	-0.10992800
C	3.94915300	-3.91612900	-0.87242900

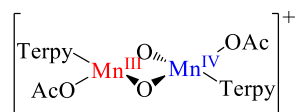
H	4.21060600	3.67665900	-1.31490300
H	5.54287300	-0.32816500	-2.13057200
H	-5.68194400	1.82672700	0.78401100
H	-5.52338800	-2.48771400	0.93738600
H	-2.39789500	-1.13846900	-2.99506600
H	-1.17671000	-0.21552700	-3.29564300
H	5.83127500	2.12383900	-2.38426900
H	-6.74126100	-0.35482400	1.34548600
H	-0.71770200	4.73397200	-1.80621900
H	-2.95108200	5.39505000	-0.87748800
H	-4.46554100	3.62998500	0.02678400
H	-0.04940300	2.31062500	-1.71227300
H	-0.27750300	-5.20174300	-1.28745400
H	-2.48261700	-5.95623400	-0.35929200
H	-4.16417300	-4.24518500	0.33166200
H	0.16980800	-2.73115100	-1.45764900
H	1.03824900	6.01108200	1.10621900
H	-0.78395300	4.66075000	2.17646500
H	2.51931900	-5.18993800	0.14205400
H	4.57033100	-4.72710600	-1.23006400
H	2.84075500	4.84834800	-0.14741600
H	-0.74104300	2.15592400	1.88242800
H	5.17716600	-2.37650900	-1.74618600
H	1.14839300	-3.23875500	0.93118000
C	1.56498400	-1.05218800	3.16938800
O	1.75992400	-0.07939500	2.31481800
O	0.84831600	-2.04625200	2.95868700
C	2.31767900	-0.86006500	4.48670500
H	2.03590000	0.10182000	4.93145400
H	2.08658500	-1.67418800	5.17724300
H	3.39576400	-0.83697600	4.28403100



E = -2141.40850342 a.u.

Mn	-1.28233800	-0.02151800	-0.73863300
Mn	1.18200600	0.06892800	0.33154200
O	-0.45558800	-0.05409400	0.94239600
O	0.42784400	0.08773700	-1.30389900
O	-2.09369200	-0.00389600	-2.76578600
N	-1.98147400	2.07128300	-0.77741900
N	-3.18039200	-0.11611100	0.05288600
N	-1.81604600	-2.15916500	-0.88616400
N	1.39319200	2.07374200	0.37609800
N	2.96624500	0.27178100	-0.52975100
N	1.72497600	-1.85728100	0.16290700
C	-3.12408300	2.27246800	-0.06664500
C	-3.81451100	1.03643700	0.36803800
C	-5.05304800	0.99882700	1.01482700
C	-5.61428900	-0.24457800	1.31756200
C	-4.95586500	-1.42289500	0.95643900
C	-3.72142200	-1.32912000	0.30741500
C	-2.94004200	-2.48339500	-0.19248400
C	2.51785800	2.55736800	-0.23629300
C	3.40865400	1.51669200	-0.78123800
C	4.61632800	1.69030100	-1.46138900
C	5.32371300	0.54564200	-1.85301300
C	4.83771900	-0.73708600	-1.56830800
C	3.62069800	-0.84582800	-0.88965200
C	2.92153100	-2.07390100	-0.47018600
C	0.54023900	2.89577000	1.00723800
C	2.77660400	3.92369400	-0.25636700
C	0.76201200	4.27399700	1.03367600
C	1.88372400	4.79146700	0.38474700
C	1.00600300	-2.88076700	0.65064300
C	3.40531200	-3.36608900	-0.64104600
C	1.45188500	-4.19748400	0.51404400
C	2.65809500	-4.44062100	-0.14187200
C	-1.30142400	3.11250400	-1.28661300
C	-3.59533900	3.56227800	0.18072200
C	-2.88702000	4.64969400	-0.34322800
C	-1.73281400	4.42677100	-1.09685000
C	-3.31635400	-3.81597800	-0.02034600
C	-1.06062800	-3.11748400	-1.44895200
C	-1.39070800	-4.46922600	-1.32947000
C	-2.52698300	-4.81786300	-0.59611100

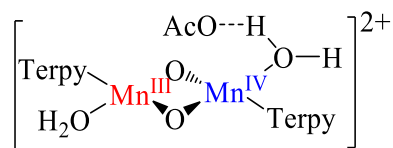
H	-5.57225400	1.91224300	1.26648600
H	-5.39802100	-2.38641900	1.16478800
H	4.99459500	2.67967500	-1.67780500
H	5.38931600	-1.61754300	-1.86633500
H	-1.75040100	-0.73294800	-3.31654200
H	-1.88999800	0.82238000	-3.24371300
H	-6.57112900	-0.29482200	1.82005800
H	6.26164900	0.65420500	-2.38124100
H	0.05539000	4.91716200	1.53841500
H	2.07156300	5.85693500	0.38127400
H	3.66400100	4.29980600	-0.74652400
H	-0.31986700	2.42917100	1.46658800
H	0.84990600	-5.00500300	0.90601200
H	3.02130700	-5.45248800	-0.26462800
H	4.34803300	-3.53037300	-1.14432000
H	0.08239200	-2.62159700	1.14348700
H	-3.23723600	5.65763200	-0.16272400
H	-1.16452400	5.24703400	-1.51270700
H	-0.76272200	-5.22100700	-1.78698500
H	-2.80199700	-5.85731200	-0.47330000
H	-4.49169500	3.72255500	0.76322800
H	-0.39304200	2.87589100	-1.82642400
H	-4.20207200	-4.07258000	0.54354400
H	-0.17797500	-2.78385200	-1.97990000
C	1.97280900	-0.60944100	3.10405600
O	2.16107600	0.11849000	2.03209900
O	1.07436300	-1.45255500	3.25652300
C	3.00748800	-0.32033700	4.19676000
H	2.98648400	0.74748200	4.44516000
H	2.79390000	-0.91640900	5.08704000
H	4.00833000	-0.56114700	3.81714400



E = -2293.21773521 a.u.

Mn	-1.22189100	-0.04578800	0.60080900
Mn	1.28241600	-0.09446600	-0.42357000
O	-0.35782100	-0.16905600	-1.05072300
O	0.54383200	0.00204700	1.17881200
N	-2.33326700	-1.96848000	0.16780900
N	-3.01839700	0.51804600	-0.44325900
N	-1.37368800	2.19654100	0.75152800
N	1.78277100	-2.01897600	-0.11812500
N	3.08484800	0.12004200	0.40867500
N	1.55456000	1.89578200	-0.60906000
C	-3.37914200	-1.83881400	-0.68635700
C	-3.75700400	-0.44717800	-1.03004400
C	-4.80847600	-0.11056400	-1.89102300
C	-5.07518500	1.23870300	-2.12934900
C	-4.30472600	2.22445100	-1.50941700
C	-3.26717800	1.82948100	-0.65914100
C	-2.37987400	2.77463800	0.05744800
C	2.97527500	-2.22165300	0.52318900
C	3.71221800	-0.98569000	0.84510400
C	4.92837900	-0.86139800	1.52286100
C	5.44461000	0.42539000	1.72335100
C	4.76517500	1.55772900	1.25403400
C	3.55508200	1.36799700	0.58245700
C	2.68527600	2.39295100	-0.02385100
C	1.01246400	-3.05398800	-0.48679000
C	3.41131400	-3.51057900	0.81329900
C	1.39747000	-4.36802800	-0.21226400
C	2.60819400	-4.59622700	0.44309600
C	0.72059200	2.69520200	-1.29415800
C	2.96782900	3.75477700	-0.07784800
C	0.96332300	4.06534700	-1.39403100
C	2.09084100	4.59991000	-0.76711300
C	-1.94286800	-3.18924400	0.57797800
C	-4.05212000	-2.96127600	-1.17784900
C	-3.63448800	-4.23154300	-0.77146300
C	-2.56927400	-4.35175100	0.12389500
C	-2.54192800	4.16333300	0.05033000
C	-0.52047400	2.93976700	1.47451400
C	-0.62879300	4.33005300	1.52124600
C	-1.65131800	4.94526300	0.79202400
H	-5.40361000	-0.87669000	-2.36607700

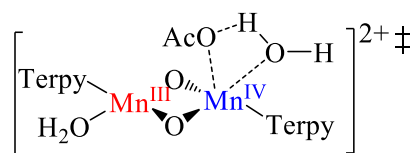
H	-4.50320900	3.27122100	-1.68863700
H	5.45387500	-1.73325100	1.88630600
H	5.16537600	2.55022100	1.40761300
H	-5.88014900	1.52040500	-2.79534800
H	6.38258700	0.54699900	2.24874000
H	0.75178600	-5.18386000	-0.50677800
H	2.92969400	-5.60528200	0.66556100
H	4.35592300	-3.66352100	1.31697800
H	0.09564400	-2.80663600	-0.99702500
H	0.27109500	4.69197900	-1.93797600
H	2.29372800	5.66147800	-0.81781000
H	3.85922500	4.14274100	0.39553800
H	-0.14390800	2.21601100	-1.73015900
H	-4.13993900	-5.11205200	-1.14669900
H	-2.22548900	-5.31908200	0.46473800
H	0.07569300	4.91092200	2.10056800
H	-1.75667200	6.02245500	0.79885200
H	-4.88284100	-2.85464600	-1.86065400
H	-1.12142000	-3.21334500	1.27903700
H	-3.34224800	4.62666800	-0.50945800
H	0.26472600	2.39545500	1.98236300
C	2.12585000	-1.03277900	-3.13698900
O	2.26431600	-0.18273500	-2.15696300
O	1.25000000	-1.91346300	-3.21774000
C	3.18565600	-0.85506100	-4.23203200
H	4.17754200	-1.05186100	-3.80559100
H	2.99586800	-1.54132000	-5.06068300
H	3.17058600	0.18088900	-4.59107700
O	-2.06286200	-0.03995200	2.38860300
C	-1.88204900	-0.93795300	3.31715200
O	-1.07427400	-1.88481500	3.24837700
C	-2.77736600	-0.73845600	4.54392000
H	-2.63134600	0.27211800	4.94371500
H	-3.82754500	-0.83383400	4.23982400
H	-2.54511400	-1.48157200	5.31018500



E = -2217.84929917 a.u.

Mn	-0.86456800	0.17004700	-1.15302400
Mn	1.27930400	-0.19668100	0.42289900
O	-0.45481700	-0.07808300	0.62661500
O	0.92843500	-0.02267200	-1.34552000
O	-1.12115100	0.24558900	-3.29010900
O	1.54990000	-0.39839600	2.32978200
N	-1.03469700	2.36256100	-1.23473500
N	-2.82110700	0.55843100	-0.56053200
N	-1.93379800	-1.79203100	-1.34901800
N	1.78243500	1.73871400	0.64805900
N	3.22881300	-0.28113200	0.04034500
N	1.53632900	-2.18294900	0.24395400
C	-2.16028900	2.85494300	-0.65587000
C	-3.14363000	1.83111200	-0.23571800
C	-4.32454500	2.10041700	0.46096000
C	-5.15543600	1.03157300	0.80826000
C	-4.80812100	-0.27478400	0.45553200
C	-3.61304500	-0.48727300	-0.23899800
C	-3.11050300	-1.81319800	-0.66843300
C	3.08548500	2.04191600	0.36277400
C	3.90695800	0.88043900	-0.02444800
C	5.24632000	0.86991300	-0.42052900
C	5.83048900	-0.36132000	-0.74649600
C	5.09349900	-1.55137500	-0.68102400
C	3.75824900	-1.47776300	-0.27801100
C	2.79038500	-2.58133000	-0.13562200
C	0.93687900	2.67551800	1.10539500
C	3.55062000	3.34660500	0.49559100
C	1.35464700	3.99643800	1.27203900
C	2.67044700	4.33521000	0.95195300
C	0.56501900	-3.07881100	0.48217200
C	3.07597300	-3.92983000	-0.31793900
C	0.80097700	-4.44574400	0.31999200
C	2.06427200	-4.87183200	-0.09214800
C	-0.07748200	3.18927900	-1.68677000
C	-2.34001000	4.22948200	-0.49377300
C	-1.34521400	5.09590700	-0.96001200
C	-0.20183900	4.57493900	-1.57131200
C	-3.77289200	-3.01601300	-0.41708900
C	-1.39743100	-2.93265000	-1.81704300

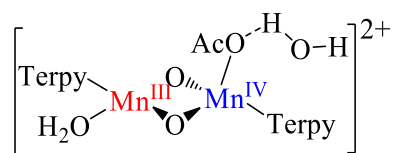
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H	-5.44656100	-1.10401700	0.72337400
H	5.81458200	1.78743300	-0.47920000
H	5.54361600	-2.49962500	-0.93929900
H	2.33902100	-0.93218100	2.53412500
H	0.28496000	-1.09660300	2.84662800
H	-0.24921000	0.28818400	-3.72969400
H	-1.54896700	-0.56948500	-3.61675200
H	-6.07110500	1.21662200	1.35406600
H	6.86603400	-0.39320700	-1.05839200
H	0.65200000	4.73596500	1.62846000
H	3.01539400	5.35484400	1.06198500
H	4.58019600	3.58193100	0.26282400
H	-0.07110500	2.34769900	1.31390500
H	0.00139700	-5.14853400	0.50702600
H	2.26895600	-5.92539400	-0.22921800
H	4.06726700	-4.23806700	-0.62062700
H	-0.38217700	-2.67820200	0.81245100
H	-1.46511000	6.16518200	-0.84457800
H	0.58464200	5.22117700	-1.93559100
H	-1.55839400	-5.07146400	-1.99325700
H	-3.70915000	-5.14907600	-0.70616400
H	-3.23266700	4.61921500	-0.02459400
H	0.79997900	2.71926400	-2.11290400
H	-4.70383000	-3.03079700	0.13220000
H	-0.45513500	-2.84231600	-2.34341200
C	-1.67489800	-0.90814900	3.11432800
O	-0.56201300	-1.64318400	3.08429100
O	-2.77685100	-1.46204600	3.11865000
C	-1.53688200	0.60633000	3.20936200
H	-0.50667100	0.92432800	3.04997400
H	-2.18768100	1.06740000	2.46045200
H	-1.87345300	0.91708900	4.20737700



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Mn	-1.18500500	0.05995400	-0.96795600
Mn	1.21763400	-0.05625800	0.22317300
O	-0.44840000	-0.05828900	0.73474200
O	0.60604000	0.04907300	-1.40531100
O	-1.81279800	0.11618600	-3.00965000
O	3.04838500	0.53617700	2.45098300
N	-1.64451000	2.20377600	-1.03590500
N	-3.08994700	0.15749400	-0.24149700
N	-1.89566500	-2.02818900	-1.09146700
N	1.56642900	1.90689300	0.41387200
N	3.09843300	0.02680700	-0.38601800
N	1.65657400	-2.00233300	0.12240300
C	-2.80033100	2.52789600	-0.39661200
C	-3.61893700	1.37230700	0.03394200
C	-4.86721200	1.46499300	0.65460000
C	-5.54894300	0.28676900	0.96964500
C	-4.99520500	-0.95605700	0.65196800
C	-3.74272600	-0.99487500	0.03341000
C	-3.05175900	-2.22955100	-0.40272200
C	2.77781000	2.32877300	-0.06793800
C	3.64289600	1.24590100	-0.56341500
C	4.91354300	1.35065300	-1.13089600
C	5.57340000	0.16958600	-1.49874100
C	4.97923700	-1.08398600	-1.29931700
C	3.70598900	-1.12530000	-0.72796700
C	2.88882600	-2.30617700	-0.39685900
C	0.71260100	2.76811100	0.99095700
C	3.13087300	3.67072600	-0.00597800
C	1.02776600	4.12400600	1.09816500
C	2.24163100	4.57931900	0.58394600
C	0.82853900	-2.96664900	0.55802000
C	3.29621600	-3.62883300	-0.51700500
C	1.19073000	-4.31152800	0.46091100
C	2.42943400	-4.64344100	-0.08812800
C	-0.83479300	3.16251400	-1.51700600
C	-3.16041600	3.86178400	-0.20297500
C	-2.31863800	4.86421300	-0.69799400
C	-1.14561100	4.51563200	-1.37130300
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C	-1.21075100	-3.07000600	-1.59417300

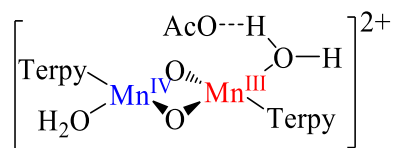
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H	-5.29987200	2.42895500	0.87985400
H	-5.52972000	-1.86867600	0.87193400
H	5.37486200	2.31647100	-1.28165100
H	5.48933600	-1.99361300	-1.58325500
H	3.82790200	0.02161900	2.17883100
H	2.37114100	-0.14237300	2.75867300
H	-1.44448700	0.84613500	-3.54322500
H	-1.64535400	-0.70771000	-3.50612100
H	-6.51649800	0.33712200	1.45101100
H	6.55822100	0.22673500	-1.94299200
H	0.32085800	4.79857000	1.55969000
H	2.50335800	5.62740900	0.64367000
H	4.08590400	3.99833800	-0.39312100
H	-0.21842100	2.35204500	1.34702700
H	0.50376400	-5.07157900	0.80506600
H	2.72938600	-5.67947300	-0.17517800
H	4.27198900	-3.86183200	-0.92091600
H	-0.10471600	-2.63848400	0.99062500
H	-2.57992800	5.90475900	-0.55641600
H	-0.47441400	5.26860000	-1.76009200
H	-1.07654500	-5.20410700	-1.82588300
H	-3.17378500	-5.61361400	-0.51372300
H	-4.07215100	4.11866300	0.31775000
H	0.07650200	2.82657600	-1.99565600
H	-4.43996400	-3.67768500	0.39489700
H	-0.29690400	-2.83629300	-2.12577100
C	0.03860500	-0.93024500	3.31282700
O	1.20058500	-1.25163000	2.86290300
O	-0.90060100	-1.75280100	3.48254000
C	-0.19478000	0.54307100	3.69275500
H	0.60414100	1.18071000	3.30678100
H	-1.15883100	0.87647300	3.29506600
H	-0.22251500	0.62568200	4.78797500



E = -2217.85268429 a.u.

Mn	-1.42272600	0.02672000	-0.78360100
Mn	1.05952200	-0.14146400	0.22642100
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O	0.28250300	-0.02266200	-1.38574300
O	-2.19707800	0.07529700	-2.81815600
O	4.44651300	1.13455500	1.90453600
N	-1.77226500	2.18952100	-0.86891200
N	-3.28053900	0.26339000	0.08065400
N	-2.31482900	-2.01561800	-0.81425300
N	1.40790800	1.83974700	0.34705400
N	2.83710900	-0.01802800	-0.65921700
N	1.47463000	-2.08884500	-0.01984200
C	-2.84372000	2.60449100	-0.14286500
C	-3.69413400	1.51508100	0.38731700
C	-4.86593600	1.70458200	1.12460100
C	-5.59391500	0.58176900	1.52671200
C	-5.16275600	-0.70054700	1.17776400
C	-3.98481100	-0.83433200	0.43709600
C	-3.42800200	-2.12110200	-0.04004500
C	2.52912500	2.27928700	-0.30112600
C	3.33782300	1.20584200	-0.90450500
C	4.53201400	1.32797900	-1.61727600
C	5.16976600	0.15514700	-2.04213000
C	4.62500500	-1.10591800	-1.76378000
C	3.42050100	-1.16246300	-1.05808000
C	2.65454800	-2.35843800	-0.66274100
C	0.63505600	2.68594900	1.04802600
C	2.86572200	3.62865800	-0.29163100
C	0.93935100	4.04614300	1.10961500
C	2.05721400	4.52179300	0.42108000
C	0.68761500	-3.08015000	0.42817600
C	3.05524100	-3.67253900	-0.87855100
C	1.04359300	-4.41700400	0.23677000
C	2.23603400	-4.71348500	-0.42369200
C	-0.95822100	3.07934900	-1.46040200
C	-3.10305300	3.96393700	0.03605300
C	-2.25339900	4.89559200	-0.57068600
C	-1.17329400	4.45307800	-1.33808800
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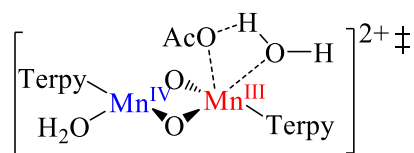
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C	-3.40043500	-4.51194600	-0.30196200
H	-5.20474200	2.69941200	1.37508600
H	-5.73199300	-1.57037500	1.47154000
H	4.95563300	2.30023000	-1.82682000
H	5.12029500	-2.00879400	-2.09205500
H	5.05479100	0.54381400	1.42757300
H	3.59050900	0.64018600	1.94944700
H	-1.55710200	0.47601300	-3.43755000
H	-2.36992100	-0.82489200	-3.15413200
H	-6.50173300	0.70640700	2.10200800
H	6.09889800	0.22325100	-2.59234200
H	0.29711000	4.71084900	1.66949900
H	2.30555600	5.57469800	0.44218900
H	3.74977300	3.96977700	-0.81256800
H	-0.23036500	2.25327500	1.53004000
H	0.38758200	-5.19782400	0.59522400
H	2.53273700	-5.74163800	-0.58421300
H	3.98722300	-3.87984000	-1.38615000
H	-0.21312600	-2.77818800	0.93870200
H	-2.43701800	5.95444800	-0.44348600
H	-0.49954000	5.15017600	-1.81630100
H	-1.79181000	-5.25537400	-1.54882000
H	-3.82233100	-5.48654800	-0.09386200
H	-3.94654400	4.29405900	0.62611000
H	-0.11724700	2.67033300	-2.00591300
H	-4.87355400	-3.44698100	0.86148800
H	-0.86826200	-2.95698000	-1.95449200
C	1.76778600	-0.96459900	2.99548500
O	2.05813300	-0.24544100	1.93123300
O	0.80753800	-1.73930600	3.08719100
C	2.76114200	-0.75049000	4.13882200
H	3.76934800	-1.01766700	3.80065200
H	2.77099500	0.30991100	4.41836700
H	2.48021000	-1.36180500	4.99916900



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Mn	1.18453900	-0.25207300	0.60666800
Mn	-0.97820200	0.10618300	-0.97334600
O	0.74118600	-0.13500000	-1.22390600
O	-0.67955900	0.02507200	0.71402800
O	1.24360900	-0.59911200	2.49846800
O	-1.29820000	0.16899900	-3.07938100
N	1.55665300	1.92103000	0.96848400
N	3.23392000	0.09695300	0.08338500
N	2.09661900	-2.26741500	0.32040500
N	-1.02436200	2.11134500	-1.07250500
N	-2.91474000	0.44096400	-0.66051500
N	-1.70401100	-1.77452400	-1.03519700
C	2.75863500	2.39392200	0.56484500
C	3.67463400	1.37183400	0.00620100
C	4.91534100	1.65629200	-0.57320500
C	5.68095100	0.59888800	-1.07007200
C	5.20806100	-0.71269900	-0.98225300
C	3.95943300	-0.93640800	-0.39286600
C	3.33454700	-2.27154100	-0.23312700
C	-2.21986600	2.68411300	-0.73154600
C	-3.29576600	1.71599400	-0.44971400
C	-4.59241600	1.97967600	-0.00550000
C	-5.44886200	0.89249400	0.21727600
C	-5.01742800	-0.42298900	0.00390900
C	-3.70906700	-0.62304000	-0.44142300
C	-3.02567100	-1.90281100	-0.70125600
C	0.02634700	2.86463700	-1.43940300
C	-2.35652300	4.06794700	-0.70833400
C	-0.06247800	4.25672600	-1.45208000
C	-1.26137800	4.86155400	-1.06996000
C	-0.95641000	-2.85325300	-1.32849400
C	-3.62046200	-3.15816500	-0.64332800
C	-1.50123300	-4.13661500	-1.27857600
C	-2.84505800	-4.28792700	-0.92853600
C	0.64975700	2.73461000	1.53393400
C	3.07628700	3.74867700	0.69489400
C	2.13331500	4.60501800	1.27235700
C	0.90581300	4.09531300	1.70705700
C	3.95714700	-3.47070900	-0.58896100
C	1.45691500	-3.42319000	0.57452600

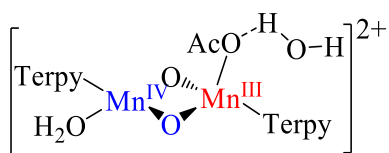
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C	3.28481100	-4.67416300	-0.35455500
H	5.27200200	2.67382200	-0.64256500
H	5.79429000	-1.53432300	-1.36726400
H	-4.92381500	2.99384300	0.16812200
H	-5.67380600	-1.26091300	0.19132900
H	-1.85421000	-0.55824000	-3.41943800
H	-0.42758500	0.06689100	-3.51389200
H	-0.06260300	-1.45162200	2.70522700
H	1.99288900	-1.18520700	2.71245000
H	6.64154200	0.79637700	-1.52737500
H	-6.45642800	1.07207200	0.56811400
H	0.79877000	4.84341200	-1.73762100
H	-1.35037300	5.93972700	-1.05672500
H	-3.29943500	4.51594400	-0.42657500
H	0.93077700	2.32938500	-1.69047600
H	-0.87611800	-4.98976900	-1.50314500
H	-3.29019000	-5.27290200	-0.88082400
H	-4.66472200	-3.25193500	-0.37875700
H	0.07568300	-2.66283600	-1.58693700
H	2.35773500	5.65815600	1.38122200
H	0.15865500	4.73592900	2.15491700
H	1.48149100	-5.57091300	0.44760500
H	3.74883500	-5.61311500	-0.62750200
H	4.03304400	4.12895100	0.36507900
H	-0.28870300	2.27416400	1.81448500
H	4.94322100	-3.47269300	-1.03181100
H	0.48451100	-3.34215000	1.04347700
C	-2.04134400	-1.40862400	2.73542100
O	-0.88251800	-2.07450700	2.68244600
O	-3.09177700	-1.98478800	2.45099300
C	-2.01886700	0.03518900	3.22145900
H	-1.00521300	0.43718400	3.23528000
H	-2.64774300	0.63732300	2.55890700
H	-2.44411500	0.06068000	4.23384100



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Mn	1.09388400	-0.29453200	0.60265800
Mn	-1.18530400	-0.06550800	-0.87119200
O	0.52070000	-0.34329000	-1.17518200
O	-0.77730600	-0.01623800	0.79962500
O	2.53833000	-0.18356700	2.59478700
O	-1.61351200	-0.14573400	-2.94633900
N	1.19141200	1.91039000	1.03998200
N	3.00100500	0.40511500	-0.16187300
N	2.34436100	-2.13260400	0.09322800
N	-1.23366400	1.92570800	-1.10265500
N	-3.10665000	0.28353700	-0.53888900
N	-1.88741600	-1.94702000	-0.75011500
C	2.28998600	2.56506500	0.59115800
C	3.27946400	1.72663900	-0.11668300
C	4.43214700	2.22973800	-0.73038000
C	5.28764500	1.34222800	-1.38499000
C	4.99039400	-0.02096500	-1.41163800
C	3.82372700	-0.46647600	-0.78048100
C	3.41568100	-1.88543000	-0.70051100
C	-2.43126200	2.51715600	-0.80304100
C	-3.50809300	1.56758600	-0.47107900
C	-4.82621000	1.85586900	-0.11323700
C	-5.68385400	0.78449000	0.16946700
C	-5.23335700	-0.54056000	0.09867800
C	-3.90463300	-0.76654200	-0.26437800
C	-3.20453000	-2.05793000	-0.38997200
C	-0.17433700	2.65969300	-1.48499000
C	-2.56435800	3.90048300	-0.84513700
C	-0.25512500	4.05065100	-1.54955900
C	-1.45840000	4.67482200	-1.21464600
C	-1.12351800	-3.03869800	-0.92903000
C	-3.77569200	-3.30840100	-0.18138900
C	-1.64669700	-4.31763500	-0.73391300
C	-2.98334700	-4.45090100	-0.35166600
C	0.21283500	2.58209300	1.67260000
C	2.43113000	3.94379000	0.77362900
C	1.41728800	4.64486600	1.43089600
C	0.28997400	3.95789900	1.88872400
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C	1.91813100	-3.39758700	0.27237700

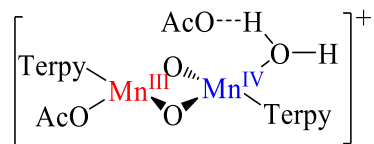
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C	3.62815200	-4.22992200	-1.19724300
H	4.65644200	3.28606400	-0.70359800
H	5.65397600	-0.71749200	-1.90285300
H	-5.17295000	2.87781300	-0.05319000
H	-5.89518600	-1.36504700	0.32270900
H	-2.05042200	-0.97601700	-3.21950300
H	-0.77441500	-0.10911400	-3.44812600
H	1.93350500	-0.92689600	2.86284100
H	3.36306600	-0.60062900	2.28834600
H	6.18325800	1.71090700	-1.86739500
H	-6.70921000	0.98337300	0.45143200
H	0.61324000	4.62208000	-1.84412800
H	-1.54209200	5.75300900	-1.24485300
H	-3.51026900	4.36248000	-0.59849000
H	0.72770900	2.11203100	-1.71538600
H	-1.01044500	-5.18027500	-0.87518500
H	-3.41098900	-5.43138200	-0.18949000
H	-4.81486600	-3.38988700	0.10604000
H	-0.09668300	-2.86373100	-1.21535100
H	1.50589900	5.71369700	1.57536300
H	-0.51696300	4.47219500	2.39243700
H	2.16421000	-5.48067100	-0.20309400
H	4.12531700	-5.04374700	-1.70920200
H	3.30589200	4.46391400	0.41054500
H	-0.64376300	1.99699500	1.97515900
H	4.93009800	-2.71125000	-2.00135500
H	1.07315600	-3.51370600	0.93564100
C	-0.56455300	-1.65995300	2.94685900
O	0.54743000	-1.78564800	2.28698300
O	-1.53447800	-2.44028700	2.82559100
C	-0.62188100	-0.49664800	3.94619700
H	-0.21522300	0.40989900	3.48840900
H	-1.64804700	-0.32015000	4.27956300
H	0.00287100	-0.74763100	4.81511500



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Mn	0.97283700	-0.15481600	0.34324600
Mn	-1.51539800	-0.14075000	-0.69090100
O	0.12374400	-0.17833600	-1.31887200
O	-0.83202200	-0.13671600	0.89791900
O	4.02876700	1.40130100	2.28468300
O	-2.28442400	-0.17159300	-2.68488300
N	1.13081400	2.06488200	0.58279600
N	2.79035300	0.40931800	-0.61185900
N	2.03675200	-2.07587300	-0.09724900
N	-1.84827100	1.83708300	-0.81640600
N	-3.38492400	-0.04344900	-0.02898400
N	-1.99300600	-2.09610500	-0.62213200
C	2.15454100	2.65538400	-0.07514900
C	3.05277800	1.72357000	-0.79385100
C	4.12980000	2.12502600	-1.58893500
C	4.92537900	1.14343300	-2.18470700
C	4.64667300	-0.20854000	-1.97498200
C	3.55446900	-0.55286100	-1.17026100
C	3.15868600	-1.94435700	-0.84960600
C	-3.03706700	2.26387300	-0.28725800
C	-3.90793200	1.17738000	0.19509400
C	-5.16008300	1.28655100	0.80305000
C	-5.82592300	0.10707000	1.16169200
C	-5.25539000	-1.14892800	0.91457800
C	-4.00094600	-1.19425700	0.30365600
C	-3.20940900	-2.38399700	-0.05950100
C	-0.99868500	2.70306900	-1.39490500
C	-3.36344200	3.61543800	-0.28512100
C	-1.28360000	4.06821100	-1.43281600
C	-2.46991400	4.52810000	-0.85891600
C	-1.18450700	-3.07546000	-1.06278900
C	-3.62041900	-3.70339200	0.09306500
C	-1.54902100	-4.41663200	-0.93431000
C	-2.77474200	-4.73078500	-0.34437300
C	0.28463100	2.78944100	1.33223200
C	2.33700100	4.03948000	-0.02468000
C	1.45369300	4.80345800	0.74467800
C	0.41826300	4.17418600	1.44264700
C	3.88804500	-3.06464400	-1.25673600
C	1.61916800	-3.29552500	0.28928200

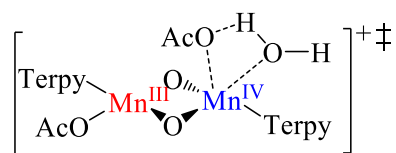
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C	3.44596200	-4.33424700	-0.87435400
H	4.34301100	3.17327700	-1.74049300
H	5.26250100	-0.97102500	-2.42936700
H	-5.60101700	2.25501800	0.99234600
H	-5.76975600	-2.05752100	1.19383100
H	-2.72887700	-1.00840600	-2.92216400
H	-1.52333100	-0.09181100	-3.29451600
H	3.21729200	0.83533300	2.25985000
H	4.56437400	1.10842200	1.52762300
H	5.76167400	1.43106000	-2.80815900
H	-6.79553700	0.16652400	1.63778700
H	-0.57775000	4.74659400	-1.89003100
H	-2.70687500	5.58372300	-0.86310500
H	-4.29977400	3.94645200	0.14282400
H	-0.08880900	2.28196500	-1.79675700
H	-0.87614700	-5.18689700	-1.28452600
H	-3.07826100	-5.76295900	-0.22979900
H	-4.58201000	-3.92463200	0.53545300
H	-0.24912200	-2.75924400	-1.50174200
H	1.57689200	5.87730900	0.79928200
H	-0.27827500	4.74040200	2.04557400
H	1.93334900	-5.42243800	0.23185600
H	3.99623900	-5.21344200	-1.18362400
H	3.15062400	4.51192900	-0.55692900
H	-0.51329000	2.23897100	1.81358400
H	4.78309400	-2.95554600	-1.85240900
H	0.73464800	-3.32292700	0.90874800
C	1.55995700	-1.11447000	3.04922700
O	1.78724900	-0.20491000	2.12721600
O	0.71364400	-2.01435200	2.94668700
C	2.45517500	-0.96427700	4.27712700
H	2.36485800	0.05285000	4.67605400
H	2.17580100	-1.69430000	5.03977200
H	3.50004600	-1.11741600	3.97928300



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Mn	-0.86231600	-0.07315000	0.97235900
Mn	1.34199300	-0.23096000	-0.58924300
O	-0.39662900	-0.19069100	-0.81395900
O	0.99050100	-0.16428300	1.15095100
O	1.66207300	-0.37717900	-2.52785900
N	-2.20402500	-1.87549900	0.64441200
N	-2.76251600	0.69287600	0.27527600
N	-0.79565600	2.16742600	1.22261300
N	1.75187600	-2.20038600	-0.48107600
N	3.29904700	-0.18085800	-0.20162900
N	1.71752700	1.73795900	-0.76569100
C	-3.30762100	-1.60981100	-0.09823500
C	-3.65155200	-0.17629100	-0.24675400
C	-4.80626700	0.28675100	-0.88840000
C	-5.00810100	1.66392700	-0.99441900
C	-4.06646600	2.55068500	-0.46784300
C	-2.93686700	2.02898600	0.17176600
C	-1.85792100	2.86032700	0.75352500
C	3.03731300	-2.51449300	-0.13627500
C	3.91378300	-1.34638200	0.07084400
C	5.23795400	-1.33607600	0.51606600
C	5.87232500	-0.09686700	0.67509200
C	5.19923400	1.10060800	0.39750700
C	3.87815700	1.02522100	-0.04908600
C	2.97706300	2.13542500	-0.41216200
C	0.85151100	-3.15930300	-0.74415400
C	3.43289200	-3.84416400	-0.02509700
C	1.19196900	-4.50967200	-0.64546500
C	2.49467700	-4.85256100	-0.27742900
C	0.81276600	2.62002500	-1.22225100
C	3.33382400	3.47959900	-0.46590800
C	1.12168500	3.97757000	-1.30829300
C	2.38888800	4.41060600	-0.91223400
C	-1.82536400	-3.14915600	0.85798900
C	-4.04767300	-2.63971900	-0.68659100
C	-3.64077600	-3.96221700	-0.48889800
C	-2.51980100	-4.22572700	0.30139200
C	-1.89249600	4.25630500	0.82426200
C	0.24399300	2.80145400	1.78849800
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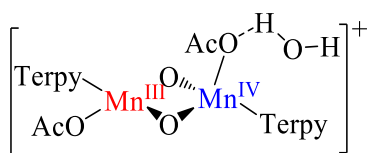
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H	-5.52841800	-0.40512600	-1.29660500
H	-4.20717000	3.61825700	-0.55746800
H	5.75451700	-2.25856400	0.74148000
H	5.68670900	2.05615600	0.53031800
H	2.47186900	0.09274600	-2.79595900
H	0.47367900	0.24264400	-3.17806600
H	-5.89193200	2.04452500	-1.48944500
H	6.89585700	-0.06352500	1.02443200
H	0.44419200	-5.26403100	-0.84805100
H	2.78427400	-5.89168200	-0.19232300
H	4.45155000	-4.08638500	0.24559900
H	-0.13559100	-2.82096200	-1.02079300
H	0.37557600	4.67272100	-1.66595800
H	2.64712500	5.46037500	-0.95825900
H	4.32984800	3.78925300	-0.18005400
H	-0.14444400	2.21013600	-1.50821200
H	-4.19506100	-4.77226000	-0.94519200
H	-2.18057500	-5.23729900	0.47981800
H	1.12415200	4.68375900	2.35061700
H	-0.81602000	6.00494200	1.46903000
H	-4.91637000	-2.42157300	-1.29142800
H	-0.95058900	-3.28288200	1.47827700
H	-2.73705600	4.81182100	0.44145400
H	1.06004200	2.16985800	2.11384700
C	-1.48490900	0.02753100	-3.46322800
O	-0.36636900	0.74246700	-3.55814400
O	-2.58381500	0.57291300	-3.60639700
C	-1.36231700	-1.47638100	-3.24534900
H	-2.02484000	-1.77291200	-2.42783800
H	-1.69045700	-1.98117500	-4.16380000
H	-0.33693700	-1.76236000	-3.01276500
O	-1.30406000	-0.09968500	2.89775900
C	-1.03160700	-1.08300700	3.70988800
O	-0.37528800	-2.09833600	3.40395400
C	-1.60115500	-0.89284800	5.11861000
H	-1.31260900	-1.72622400	5.76318900
H	-1.23124100	0.05079200	5.53765600
H	-2.69500100	-0.83005300	5.05776800



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Mn	-1.14156600	-0.09682900	0.89297300
Mn	1.27358700	-0.15439100	-0.32490500
O	-0.39824700	-0.16286100	-0.80758400
O	0.73082400	-0.13077200	1.30584800
O	3.05486200	-1.05130900	-2.61757700
N	-2.31944800	-1.92665500	0.40129300
N	-2.92544900	0.60447400	-0.07516600
N	-1.14278400	2.13656000	1.11448500
N	1.65659300	-2.12150400	-0.31675700
N	3.19120600	-0.14582100	0.18406700
N	1.69511100	1.79224100	-0.49313000
C	-3.35005400	-1.71863400	-0.45802300
C	-3.68336200	-0.29995300	-0.72748000
C	-4.69640700	0.12152600	-1.59634100
C	-4.89742900	1.49200100	-1.77627000
C	-4.09423900	2.41361800	-1.10043200
C	-3.09679500	1.93265900	-0.24631700
C	-2.14917300	2.79571200	0.49493300
C	2.90064400	-2.47273900	0.13529500
C	3.76951700	-1.32898200	0.46402600
C	5.06226800	-1.34991800	0.99016500
C	5.70653200	-0.12440700	1.21111400
C	5.07510900	1.09052100	0.91159700
C	3.78151100	1.04727700	0.38832500
C	2.92642800	2.17355300	-0.03095200
C	0.77979200	-3.05232900	-0.72515700
C	3.27148600	-3.81004200	0.20892100
C	1.10250100	-4.41013800	-0.67827600
C	2.35708700	-4.79031000	-0.20006200
C	0.84483300	2.68618900	-1.02589700
C	3.30179200	3.51173900	-0.04514700
C	1.17460700	4.04105200	-1.07108000
C	2.40626100	4.45678400	-0.56265200
C	-1.95912500	-3.17948600	0.73770000
C	-4.03696600	-2.79238000	-1.03018400
C	-3.65246100	-4.09504400	-0.69963500
C	-2.60452300	-4.29565100	0.20144100
C	-2.24569700	4.18804400	0.56388000
C	-0.22138100	2.80351000	1.82887900
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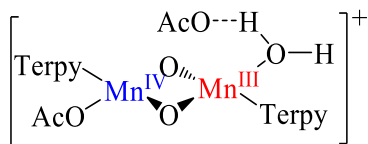
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H	-5.30915400	-0.59440700	-2.12434200
H	-4.23198700	3.47543100	-1.24541400
H	5.55169400	-2.28472700	1.22453700
H	5.57384200	2.03424800	1.08171700
H	3.81964700	-0.48627700	-2.41242000
H	2.33736100	-0.42239400	-2.93659700
H	-5.67175900	1.84011200	-2.44715500
H	6.70804700	-0.11660300	1.62051700
H	0.37546100	-5.14118500	-1.00368100
H	2.63037500	-5.83607400	-0.14964600
H	4.25626100	-4.08130100	0.56418600
H	-0.17113200	-2.68514900	-1.08024700
H	0.46990200	4.74630200	-1.48788000
H	2.67853600	5.50399300	-0.57737000
H	4.27390600	3.80761800	0.32522300
H	-0.08389600	2.29179100	-1.40885400
H	-4.16959900	-4.93848300	-1.13853000
H	-2.28479700	-5.28996400	0.48243100
H	0.49681900	4.71155800	2.51797400
H	-1.34098000	5.96918000	1.36571500
H	-4.85353000	-2.62315800	-1.71738900
H	-1.14201100	-3.26493800	1.43960300
H	-3.04772200	4.71301300	0.06397200
H	0.56046100	2.20188300	2.27354600
C	-0.02588400	0.36302600	-3.46657100
O	1.17586400	0.69620000	-3.15509500
O	-0.95151400	1.19139600	-3.68764900
C	-0.34012800	-1.13839300	-3.60198700
H	-1.24130400	-1.37124000	-3.02529300
H	-0.52791800	-1.37114500	-4.65884300
H	0.49218200	-1.74717800	-3.23939100
O	-1.78663100	-0.12533900	2.71649800
C	-1.53188900	-1.07280900	3.58570100
O	-0.77989300	-2.03967500	3.37383400
C	-2.25710500	-0.88274300	4.91736400
H	-1.99103100	-1.68322900	5.61112500
H	-1.98528200	0.09028300	5.34414300
H	-3.33989900	-0.88456500	4.74085000



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Mn	-1.33157500	0.02441700	0.65643300
Mn	1.17331600	-0.26363900	-0.32674600
O	-0.45269700	-0.16297400	-0.97885600
O	0.43105100	-0.12985400	1.25882400
O	4.61212900	0.82334500	-2.10340100
N	-2.62274700	-1.75540800	0.14402300
N	-3.01962000	0.80111700	-0.42544700
N	-1.24304100	2.26294700	0.85737600
N	1.47333100	-2.24129100	-0.07547200
N	2.97657600	-0.25429300	0.52262100
N	1.64571600	1.68957100	-0.45343600
C	-3.59751200	-1.49944300	-0.76432700
C	-3.82987600	-0.06692600	-1.06650100
C	-4.81799000	0.40018000	-1.94116200
C	-4.94242200	1.77639500	-2.13997000
C	-4.09348600	2.66000700	-1.47046500
C	-3.12634100	2.13647100	-0.60684700
C	-2.16483700	2.96310300	0.15821500
C	2.64620800	-2.57937000	0.54446400
C	3.49114300	-1.43116000	0.92120900
C	4.69542100	-1.44751800	1.62959200
C	5.31463200	-0.22182000	1.90852700
C	4.74563500	0.98812700	1.48828300
C	3.54469400	0.93877800	0.77735600
C	2.79354800	2.06145900	0.18735100
C	0.60364000	-3.18641300	-0.46545200
C	2.96145200	-3.91423700	0.77979200
C	0.86574000	-4.54014500	-0.24930900
C	2.05821600	-4.90552700	0.37773000
C	0.91804100	2.58098300	-1.14676000
C	3.20269900	3.39127100	0.18848900
C	1.29299200	3.92337700	-1.19725700
C	2.43758800	4.33265700	-0.50880900
C	-2.37079200	-3.02060200	0.52773200
C	-4.33089400	-2.53744900	-1.34618500
C	-4.05297100	-3.85467900	-0.97044100
C	-3.06587500	-4.10381200	-0.01406800
C	-2.17935000	4.36069700	0.18826600
C	-0.33632900	2.89144900	1.62291500
C	-0.29839100	4.28356500	1.70753900

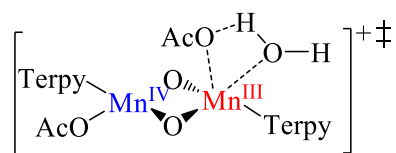
C	-1.23030500	5.02324300	0.97240400
H	-5.47350700	-0.28699700	-2.45576300
H	-4.17890400	3.72634100	-1.62168900
H	5.13349400	-2.37855200	1.96049700
H	5.22443500	1.93289900	1.70369700
H	5.10469900	0.39424400	-1.38333100
H	3.73005200	0.36990400	-2.13209000
H	-5.69689500	2.15844500	-2.81505200
H	6.24607900	-0.20937700	2.45878700
H	0.14202500	-5.27905300	-0.56464800
H	2.28708600	-5.94795200	0.55576700
H	3.89153900	-4.17363400	1.26682200
H	-0.29789900	-2.83586200	-0.94320900
H	0.68647900	4.62664800	-1.74991700
H	2.73996000	5.37152000	-0.51935700
H	4.10663800	3.68094800	0.70646400
H	0.03094500	2.19680800	-1.62947100
H	-4.60603700	-4.67160100	-1.41583200
H	-2.83271200	-5.11023500	0.30657700
H	0.44781100	4.77067800	2.31996300
H	-1.22070900	6.10494800	1.00772400
H	-5.10142800	-2.33075000	-2.07506900
H	-1.60119600	-3.14343400	1.27625300
H	-2.91095000	4.92088600	-0.37708500
H	0.37228200	2.25393100	2.13510800
C	1.78332400	-0.79511100	-3.29308400
O	2.14496800	-0.42129000	-2.08981700
O	2.41175300	-0.42154600	-4.30158700
C	0.59435300	-1.74258500	-3.40996600
H	-0.22690400	-1.38221400	-2.78541100
H	0.28425300	-1.82305500	-4.45435500
H	0.89533100	-2.73264600	-3.04377100
O	-2.18523300	0.08100800	2.42676100
C	-2.07988800	-0.84929400	3.33696000
O	-1.36579300	-1.86509400	3.23704600
C	-2.93511300	-0.58737200	4.57928300
H	-2.78573800	-1.37821100	5.31782400
H	-2.66484700	0.38433300	5.01011600
H	-3.99156200	-0.54547700	4.28583700



E = -2369.65738463 a.u.

Mn	1.31213100	0.13764700	-0.62148500
Mn	-0.99408800	-0.19455800	0.72474100
O	0.71138800	-0.10483600	1.13592700
O	-0.46122600	0.04006800	-0.95027000
O	1.60747700	0.48853800	-2.68488000
N	1.99367700	-1.92550900	-1.03762400
N	3.29957900	0.09167700	0.02521400
N	1.90695800	2.27715500	-0.40334200
N	-1.25021000	-2.17051900	0.45166100
N	-2.87727300	-0.22996400	0.06892400
N	-1.50308100	1.74654500	0.93020500
C	3.19806000	-2.24110400	-0.49812400
C	3.91565600	-1.10788300	0.13064000
C	5.14843700	-1.21103300	0.78142200
C	5.72321200	-0.05455200	1.31479600
C	5.07758500	1.17758200	1.18421200
C	3.84653300	1.22376100	0.52310500
C	3.06380400	2.45870900	0.28359900
C	-2.44784000	-2.53067600	-0.10845900
C	-3.37458800	-1.40965900	-0.34253000
C	-4.65199700	-1.45566300	-0.90563600
C	-5.36750200	-0.25549100	-1.01912800
C	-4.81860800	0.95643700	-0.58157400
C	-3.53383600	0.93756100	-0.03234500
C	-2.75745000	2.07367800	0.49292900
C	-0.33409200	-3.09623900	0.77602600
C	-2.72793600	-3.86490000	-0.38027500
C	-0.57203600	-4.45226500	0.53923000
C	-1.77523800	-4.83737100	-0.05126300
C	-0.70450500	2.66659400	1.49415400
C	-3.22349700	3.37973700	0.59842000
C	-1.12480900	3.99088100	1.63153800
C	-2.39275000	4.35016800	1.17123800
C	1.27381000	-2.84802800	-1.69564700
C	3.70210200	-3.54033000	-0.58035700
C	2.95154000	-4.50975800	-1.25486000
C	1.72727100	-4.16199700	-1.83124800
C	3.47074000	3.73338700	0.68083000
C	1.14615000	3.32726400	-0.75691500
C	1.50257000	4.63096700	-0.40150100

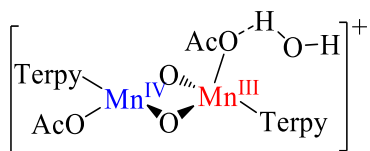
C	2.67124200	4.82975600	0.33719000
H	5.64524600	-2.16625200	0.87267800
H	5.52160000	2.07703300	1.58571900
H	-5.07686600	-2.39052800	-1.24367400
H	-5.36861500	1.88242600	-0.67284800
H	0.81559800	1.07558100	-3.00976300
H	2.41385600	1.01733100	-2.83043800
H	6.67462400	-0.11266100	1.82692400
H	-6.35825100	-0.26592800	-1.45374800
H	0.18621300	-5.17717500	0.79904700
H	-1.97741900	-5.88085900	-0.25406300
H	-3.67249700	-4.13869200	-0.82990700
H	0.58019900	-2.72922000	1.21463500
H	-0.45963600	4.71698800	2.07702300
H	-2.73819200	5.37182900	1.25995900
H	-4.21482000	3.63105200	0.24676800
H	0.26828500	2.32084300	1.81466500
H	3.32433500	-5.52304100	-1.33072800
H	1.12644800	-4.89017300	-2.35835900
H	0.87188000	5.46065500	-0.69024600
H	2.96715600	5.82674900	0.63727100
H	4.65710100	-3.79195000	-0.14052000
H	0.31975900	-2.52064500	-2.09013000
H	4.38763600	3.87475600	1.23597200
H	0.26006200	3.10005200	-1.33726900
C	-1.52406400	1.63343000	-3.16430900
O	-0.31842800	2.04577600	-3.36392600
O	-2.45715000	2.37119600	-2.75121900
C	-1.84189900	0.16815300	-3.51368300
H	-0.92954000	-0.43257100	-3.51889600
H	-2.54822900	-0.24393700	-2.78803800
H	-2.30319700	0.14000600	-4.51136000
O	-1.75520400	-0.39493400	2.53815500
C	-1.39477800	-1.19046000	3.50998300
O	-0.40549900	-1.94365200	3.50265900
C	-2.34223500	-1.11694600	4.71330600
H	-1.98442100	-1.76235000	5.51883100
H	-2.40660900	-0.07982900	5.06368400
H	-3.34552300	-1.43195300	4.39999200



E = -2369.64076156 a.u.

Mn	1.25516100	-0.01546200	-0.24359700
Mn	-1.26010600	0.01545200	0.74971700
O	0.30382200	-0.11251400	1.47595100
O	-0.40068300	0.08627600	-0.85987300
O	3.44579800	-0.53252800	-2.52830300
N	1.66279700	-2.04522400	-0.54698100
N	3.10108000	-0.17685400	0.51407600
N	1.90291600	1.97585200	-0.21959300
N	-1.74286100	-1.91291400	0.46217700
N	-2.92838500	0.21599700	-0.33547400
N	-1.48834300	2.01947400	0.77807300
C	2.79939000	-2.48319800	0.07139200
C	3.61404200	-1.41483100	0.68355000
C	4.83809800	-1.57046800	1.33695300
C	5.50367400	-0.42349900	1.78633600
C	4.96793800	0.85061100	1.56275600
C	3.74015100	0.94814200	0.90462600
C	3.04864400	2.18799600	0.49343800
C	-2.82252200	-2.12822300	-0.35417200
C	-3.46896700	-0.89974700	-0.85232200
C	-4.51390900	-0.79079400	-1.77418700
C	-4.94695300	0.49305800	-2.13187200
C	-4.34940100	1.63695800	-1.58469900
C	-3.31157600	1.46061000	-0.66598800
C	-2.52035000	2.50060900	0.01856700
C	-1.07573000	-2.93955500	1.01324200
C	-3.23980400	-3.42262300	-0.64410300
C	-1.46158800	-4.25848800	0.76408300
C	-2.54882300	-4.50024700	-0.07570200
C	-0.71823600	2.84522200	1.50420100
C	-2.77140600	3.86741800	-0.04405300
C	-0.93755500	4.22397300	1.49151300
C	-1.96726900	4.73807300	0.70184900
C	0.86693600	-2.90424700	-1.20417800
C	3.14691400	-3.83092100	0.05386400
C	2.32086100	-4.73106900	-0.63134800
C	1.17332500	-4.26489000	-1.27476400
C	3.51458400	3.47833200	0.72837700
C	1.21685900	3.00536400	-0.74187500
C	1.64124400	4.32212100	-0.55049100

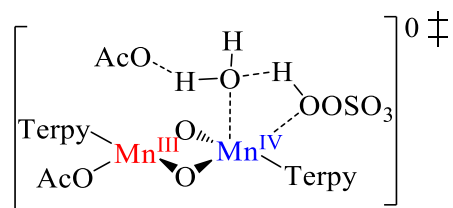
C	2.79427000	4.55772600	0.20032900
H	5.26483300	-2.55246300	1.48398600
H	5.49662000	1.73755600	1.88207600
H	-4.96805300	-1.67069000	-2.20768300
H	-4.67517100	2.62665500	-1.87281000
H	2.69284700	0.07878100	-2.79075000
H	4.03210200	0.00362000	-1.96814500
H	6.45291600	-0.52192300	2.29621000
H	-5.74939600	0.60326500	-2.84922800
H	-0.90310000	-5.06936000	1.21003500
H	-2.86115900	-5.51387900	-0.28996900
H	-4.08959300	-3.58537200	-1.29280300
H	-0.23715400	-2.67923100	1.64015700
H	-0.29828600	4.87112000	2.07511800
H	-2.14998900	5.80390900	0.66649600
H	-3.58502900	4.24158200	-0.65039500
H	0.08047800	2.38072900	2.06623100
H	2.57623600	-5.78227300	-0.65975000
H	0.51393400	-4.93543800	-1.80781400
H	1.06842600	5.13624700	-0.97197100
H	3.13859100	5.56930200	0.37180900
H	4.04374700	-4.17152900	0.55285700
H	-0.01836400	-2.48160200	-1.65779300
H	4.41826100	3.64160500	1.29925500
H	0.33526700	2.74884900	-1.31208300
C	0.32883400	0.83728600	-3.51689400
O	1.48439500	1.17021200	-3.07579300
O	-0.60151200	1.65688000	-3.76607900
C	0.06996600	-0.65741900	-3.78592900
H	0.89127500	-1.26898300	-3.40435500
H	-0.86551100	-0.95452300	-3.30047900
H	-0.03018200	-0.81555300	-4.86809600
O	-2.40504000	0.02320200	2.33031000
C	-2.34981400	-0.72928700	3.40085100
O	-1.50811600	-1.61465600	3.62118300
C	-3.46909400	-0.40812500	4.39683800
H	-3.38524100	-1.04743000	5.27867100
H	-3.40138800	0.64646200	4.69045400
H	-4.44042700	-0.56373200	3.91151100



E = -2369.66201340 a.u.

Mn	1.13679000	0.12576600	-0.42092000
Mn	-1.43077400	0.18604500	0.41227700
O	0.15617900	0.12360800	1.16679300
O	-0.56578700	0.20352100	-1.13278100
O	4.40133500	-1.33798200	-2.13684200
N	1.30321000	-2.09012100	-0.70906700
N	2.86376800	-0.49018300	0.67869600
N	2.21683400	2.02206000	0.14594600
N	-1.88360100	-1.76809700	0.31457500
N	-3.16248700	0.25967300	-0.57560800
N	-1.73729800	2.17979900	0.33331100
C	2.23996000	-2.71517100	0.04068400
C	3.08554500	-1.81362100	0.85762900
C	4.08289400	-2.25155200	1.73377100
C	4.83854200	-1.29749700	2.42011200
C	4.60058800	0.06287400	2.21793200
C	3.59106700	0.44468000	1.32607300
C	3.25538400	1.85139400	1.00172200
C	-3.01344800	-2.07498400	-0.39637900
C	-3.73254200	-0.90453400	-0.93096200
C	-4.89425100	-0.88987000	-1.70799800
C	-5.41899800	0.35227600	-2.08792000
C	-4.80105900	1.54783700	-1.69697500
C	-3.64254900	1.46715800	-0.92069900
C	-2.83576800	2.57661800	-0.37921700
C	-1.16737900	-2.72822100	0.92041500
C	-3.42558000	-3.39617500	-0.53255900
C	-1.54181600	-4.06971400	0.82373400
C	-2.67596800	-4.40535800	0.08459800
C	-0.94939200	3.07575700	0.94753200
C	-3.13835900	3.92789600	-0.51482100
C	-1.20992200	4.44445800	0.85007300
C	-2.30997500	4.87206200	0.10436200
C	0.51919700	-2.78297200	-1.54943300
C	2.39182600	-4.10319300	-0.01092600
C	1.57328500	-4.83396800	-0.87852600
C	0.63068400	-4.16942500	-1.66846500
C	3.96388600	2.94687100	1.50311200
C	1.86719700	3.25638700	-0.25784300
C	2.53117100	4.39433300	0.20552900

C	3.58939200	4.23286500	1.10277600
H	4.26685500	-3.30637900	1.87818900
H	5.18563100	0.80458800	2.74192300
H	-5.37451300	-1.81118800	-2.00620400
H	-5.20800700	2.50630100	-1.98739000
H	3.58056500	-0.78156200	-2.15844700
H	4.66242000	-1.37515000	-1.20104100
H	5.61240800	-1.61385600	3.10708900
H	-6.31636200	0.38913100	-2.69128500
H	-0.94046300	-4.82544400	1.30854500
H	-2.98156000	-5.43894300	-0.01191300
H	-4.31598100	-3.63152700	-1.09929400
H	-0.29688500	-2.39963400	1.46481500
H	-0.55313400	5.14819600	1.34218700
H	-2.52966700	5.92721700	0.00863300
H	-4.00545600	4.23475200	-1.08371300
H	-0.10993100	2.67340400	1.49649900
H	1.67483000	-5.90996900	-0.93621700
H	-0.01528600	-4.70990400	-2.34665200
H	2.22126700	5.37484300	-0.12991900
H	4.12379700	5.09377200	1.48328800
H	3.13214300	-4.60435700	0.59681700
H	-0.21507000	-2.20613100	-2.09703200
H	4.79132400	2.80729800	2.18427100
H	1.04947400	3.31268500	-0.96167600
C	2.00484200	1.13178200	-3.07072100
O	2.13713900	0.21764600	-2.14104000
O	1.17491800	2.05492800	-3.03661300
C	2.98845700	0.96259600	-4.22964300
H	2.85650600	-0.03021200	-4.67703100
H	2.82629700	1.73655300	-4.98297300
H	4.01382300	1.02343800	-3.84443300
O	-2.54932500	0.29144100	2.05580500
C	-2.53573200	-0.44004600	3.13647300
O	-1.68560600	-1.30275900	3.42169700
C	-3.71516800	-0.13839400	4.06983200
H	-3.62811000	-0.71662900	4.99268800
H	-3.73581600	0.93378200	4.29816200
H	-4.65136200	-0.39438100	3.55746800



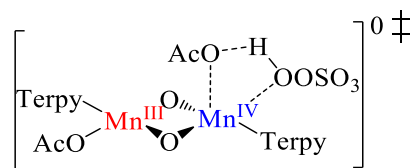
Transition state of HOOSO_3^- replacing H_2O bound to Mn^{IV} with acetate H-bonded (**I₀-TS** in Scheme 2)

E = -3144.60675372 a.u.

Mn	-2.03802600	-0.26958300	0.76449800
Mn	0.62632600	-0.29907000	0.31139500
O	-0.82339100	-0.17941500	-0.64924100
O	-0.37081900	-0.42856200	1.70086100
O	1.50288100	-1.13399800	-2.45396700
N	-3.06192500	-1.96977700	-0.27312400
N	-3.53683900	0.62799000	-0.47536100
N	-2.08923800	1.91500000	1.30986100
N	1.08001500	-2.25334900	0.24027800
N	2.34785800	-0.32000300	1.30119500
N	1.03356400	1.66139300	0.38350200
C	-3.86528300	-1.59505900	-1.30105200
C	-4.15904200	-0.14610800	-1.38863900
C	-5.02209100	0.42449800	-2.33075800
C	-5.22429700	1.80556300	-2.30484100
C	-4.57031300	2.59113100	-1.35407600
C	-3.71617200	1.96692700	-0.44012200
C	-2.93292700	2.68819100	0.58779200
C	2.19235100	-2.62995500	0.94409100
C	2.92691500	-1.50766100	1.55101300
C	4.14226900	-1.55451300	2.23437500
C	4.72423100	-0.34325700	2.62660700
C	4.11354400	0.88099700	2.32392800
C	2.89683000	0.86056300	1.64189500
C	2.13775400	2.00832200	1.11928400
C	0.36024900	-3.15516900	-0.44753800
C	2.58223600	-3.96419800	0.98867700
C	0.70349600	-4.50705400	-0.43528900
C	1.82144500	-4.91440500	0.29624700
C	0.31641800	2.59350000	-0.26617500
C	2.50553400	3.34069400	1.25115300
C	0.64831100	3.94612100	-0.17522400
C	1.74411800	4.32194000	0.59999500
C	-2.77865700	-3.27140500	-0.07724100
C	-4.38122300	-2.53830500	-2.19346000
C	-4.06753200	-3.88762000	-2.00822800
C	-3.26267900	-4.26449400	-0.93088000

C	-3.02283200	4.06362100	0.81833700
C	-1.33732500	2.44777000	2.28756200
C	-1.38429400	3.81174900	2.57891100
C	-2.23476500	4.62730200	1.82630200
H	-5.52458700	-0.18862000	-3.06430800
H	-4.71223100	3.66182300	-1.33353900
H	4.62797700	-2.49859000	2.43762000
H	4.57967300	1.81698300	2.59816100
H	-5.88480300	2.26813200	-3.02623600
H	5.67103100	-0.35100700	3.15052400
H	0.10035900	-5.21443100	-0.98758300
H	2.10768200	-5.95764700	0.32340900
H	3.46342800	-4.25319600	1.54509200
H	-0.48279300	-2.77041700	-1.00025800
H	0.04752900	4.67550000	-0.69981200
H	2.01750300	5.36473500	0.69449100
H	3.37464500	3.60947300	1.83587100
H	-0.51978700	2.23571100	-0.84110200
H	-4.45262300	-4.63092900	-2.69421400
H	-3.00783900	-5.30030600	-0.75188600
H	-0.76235900	4.22077300	3.36333900
H	-2.28607400	5.69100800	2.01932800
H	-5.01153600	-2.23364900	-3.01670700
H	-2.15530800	-3.49763600	0.77582500
H	-3.69002200	4.68191600	0.23432100
H	-0.67827300	1.76323900	2.80474700
O	3.13243200	0.51165100	-1.30600500
H	2.60352800	-0.11009900	-1.90556700
H	1.86178800	-1.95069600	-2.84084900
H	0.89000400	-0.69580800	-3.13187100
O	4.15080300	-0.39703500	-0.81244700
S	5.67746100	0.19199900	-1.27327200
O	6.51040100	-0.84030500	-0.60906100
O	5.70188500	0.16553800	-2.75673800
O	5.77768400	1.55175000	-0.69100000
O	-3.17194600	-0.51265900	2.31410900
C	-3.16670000	-1.59800100	3.05015500
O	-2.37503400	-2.54451600	2.90159700
C	-4.24453900	-1.59963100	4.13317400
H	-5.23114700	-1.53017400	3.65844100
H	-4.18054300	-2.51284800	4.72881700
H	-4.11580400	-0.72127100	4.77712100
O	-0.25418400	0.13867900	-3.94328600
C	-0.20824000	1.32762400	-3.45394800
O	0.85341900	1.94272900	-3.16153600
C	-1.56704300	1.99496000	-3.17643000

H	-2.21549200	1.91824700	-4.05656700
H	-2.04156800	1.44386900	-2.35869400
H	-1.44481900	3.04277900	-2.88722900

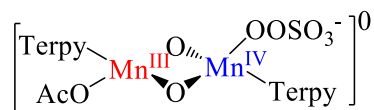


Transition state of HOOSO₃⁻ replacing AcO⁻ bound to Mn^{IV} (**I-TS** in Scheme 2)

E = -3068.16977499 a.u.

Mn	-2.07094100	-0.16960300	0.72077400
Mn	0.59242600	0.00785800	0.30215800
O	-0.83631100	-0.17832600	-0.67450200
O	-0.42182800	-0.00032800	1.68701900
O	3.06816900	-0.69187700	-1.29887700
N	-2.84837500	-2.14193800	0.01784500
N	-3.53912100	0.28601200	-0.77436300
N	-2.37709000	2.04927600	0.80022500
N	1.17487100	-1.90285000	0.46798000
N	2.29230200	0.23619300	1.29706300
N	0.86054800	1.98115800	0.12836500
C	-3.58897100	-2.08132100	-1.11842000
C	-3.97038200	-0.71989300	-1.56212000
C	-4.71765300	-0.44555800	-2.71324900
C	-4.99663700	0.88589500	-3.02959900
C	-4.53099600	1.91478100	-2.20754800
C	-3.78944100	1.57948900	-1.07031400
C	-3.20196700	2.56909100	-0.13840900
C	2.31327400	-2.10702900	1.20299400
C	2.95940900	-0.86988700	1.67347800
C	4.17566800	-0.74283100	2.34404800
C	4.65863600	0.54767200	2.59962200
C	3.95343200	1.67941500	2.17263200
C	2.74574700	1.48595900	1.50079400
C	1.90930600	2.50239000	0.83789100
C	0.53597500	-2.92891800	-0.11780300
C	2.81077100	-3.39145000	1.38620700
C	0.99553200	-4.23877300	0.02996600
C	2.13864200	-4.47044600	0.79601600
C	0.10698100	2.75914500	-0.66706200
C	2.17177400	3.86718100	0.80782000
C	0.33131500	4.13357000	-0.74014200
C	1.36132100	4.69294000	0.01807500
C	-2.48466600	-3.33392700	0.52777700
C	-3.95998200	-3.24452400	-1.79769100
C	-3.56567700	-4.48317100	-1.28380400
C	-2.82470200	-4.53338100	-0.10096000
C	-3.44432700	3.94384400	-0.19939500
C	-1.78580200	2.84055500	1.71042900

C	-1.99082000	4.22104600	1.71416900
C	-2.82839100	4.77525400	0.74127600
H	-5.06949900	-1.24414800	-3.34987500
H	-4.72912900	2.94843100	-2.45219600
H	4.73855200	-1.61516300	2.64521000
H	4.34126600	2.67446900	2.34107200
H	2.45124800	-0.10655600	-1.89213300
H	-5.56823600	1.12089700	-3.91774500
H	5.60248000	0.67063300	3.11445400
H	0.45752100	-5.04792600	-0.44415000
H	2.51408100	-5.47641900	0.92996600
H	3.70918500	-3.54778600	1.96710500
H	-0.33618500	-2.67427100	-0.69996500
H	-0.29763700	4.74218700	-1.37397100
H	1.54821400	5.75831300	-0.01389800
H	2.99984000	4.27305900	1.37253000
H	-0.66239000	2.25782800	-1.23357600
H	-3.83934000	-5.39395400	-1.80055400
H	-2.50890700	-5.47516700	0.32688900
H	-1.49722200	4.84130300	2.44970900
H	-3.00078200	5.84328700	0.71122200
H	-4.54306600	-3.19189200	-2.70608500
H	-1.91281000	-3.30217100	1.44420500
H	-4.09881900	4.35772900	-0.95387400
H	-1.12474400	2.34640600	2.41042700
C	0.42020900	0.30709100	-3.14697600
O	1.41124100	0.80017000	-2.48418700
O	-0.46174700	1.00928800	-3.70492100
C	0.32821000	-1.22428900	-3.26720200
H	0.43320600	-1.51007100	-4.32168100
H	1.10630200	-1.71676600	-2.67774400
H	-0.65534100	-1.54796000	-2.91104900
O	-3.23266900	-0.23896300	2.26333300
C	-3.12659300	-1.11392600	3.23432100
O	-2.23242800	-1.97328200	3.31322100
C	-4.22569200	-0.98250600	4.28792600
H	-4.08232300	-1.72210700	5.07863400
H	-4.20421400	0.02900400	4.71144600
H	-5.20234200	-1.12897800	3.81023300
O	4.04260600	0.28919700	-0.85642800
S	5.59027800	-0.23647000	-1.30766500
O	5.60302100	-0.27476600	-2.79163700
O	6.37648100	0.86552600	-0.69945500
O	5.77178600	-1.56300600	-0.66901400

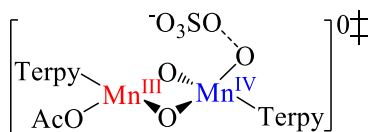


Complex with SO_5^{2-} binding to Mn^{IV} (**II** in Scheme 2)

E = -2839.49935038 a.u.

Mn	0.93642300	0.55075300	0.11014400
Mn	-1.62987400	-0.04724500	-0.52037900
O	-0.08312700	0.53600400	-1.35532700
O	-0.51453100	0.03161200	0.97077100
O	2.00427300	0.83063000	1.73595200
N	0.86661600	2.56642000	0.19896900
N	2.51505400	1.03450800	-1.01302800
N	1.73914500	-1.25574300	-0.21361500
N	-3.08430800	1.36228500	0.49674500
N	-2.98581200	-1.28645800	0.60916600
N	-1.23240300	-2.17541000	-1.14845400
C	1.80329500	3.22324000	-0.55041800
C	2.74438100	2.33599900	-1.26007500
C	3.79055300	2.69951600	-2.11155600
C	4.55917000	1.67813800	-2.68668300
C	4.28936100	0.33086700	-2.41320800
C	3.23376400	0.03281400	-1.54788700
C	2.79612300	-1.29154400	-1.07612800
C	-3.89581900	0.78057300	1.41453200
C	-3.83046100	-0.69894300	1.48253500
C	-4.57919400	-1.47397200	2.37642700
C	-4.43067000	-2.86153900	2.34912400
C	-3.55586900	-3.45355600	1.43592800
C	-2.83783800	-2.62996600	0.56280100
C	-1.89109200	-3.13430800	-0.45936100
C	-3.09267200	2.69817400	0.33707100
C	-4.73956000	1.54987600	2.22179300
C	-3.90654200	3.52599900	1.11331400
C	-4.73772500	2.93914800	2.07042400
C	-0.37932300	-2.49880600	-2.13347400
C	-1.67971000	-4.48892100	-0.73417000
C	-0.12847400	-3.82971900	-2.46927400
C	-0.78502600	-4.83433800	-1.75143200
C	-0.03219200	3.24059000	0.93320100
C	1.82615100	4.61434600	-0.58842600
C	0.88053700	5.32703500	0.15893600
C	-0.05581400	4.63656800	0.93190600
C	3.41592200	-2.49702900	-1.38829600
C	1.30890000	-2.37115500	0.39855400
C	1.90823800	-3.60364000	0.14324400

C	2.96335100	-3.66697800	-0.77032300
H	3.99909400	3.73882800	-2.32294500
H	4.88220300	-0.45720800	-2.85623100
H	-5.25625400	-1.01125100	3.07932800
H	-3.43387100	-4.52680000	1.40865700
H	5.37296900	1.93448800	-3.35207600
H	-4.99380000	-3.47894000	3.03666200
H	-3.88388800	4.59751500	0.96701200
H	-5.38042500	3.55104300	2.69023400
H	-5.38576900	1.08367300	2.95180300
H	-2.43813200	3.08812500	-0.42860000
H	0.57034700	-4.06896100	-3.25897200
H	-0.60463300	-5.87697700	-1.97927600
H	-2.20096200	-5.25677500	-0.17986800
H	0.11626300	-1.66814700	-2.61836400
H	0.88184400	6.40891100	0.13806700
H	-0.79760800	5.15886700	1.52021500
H	1.53762700	-4.49028300	0.63780600
H	3.43503100	-4.61442600	-0.99622600
H	2.56661200	5.12904900	-1.18550100
H	-0.73022400	2.64005800	1.49896600
H	4.24716100	-2.51495000	-2.08011500
H	0.47070200	-2.25056600	1.06843900
O	2.24588900	-0.40875400	2.45094500
S	3.90809700	-0.66897300	2.57415800
O	3.88645500	-2.00849700	3.22165400
O	4.45999900	-0.65174700	1.19751200
O	4.43599000	0.42328400	3.43772600
O	-2.80947300	0.00961800	-2.11616300
C	-3.09980400	1.07760000	-2.80401300
O	-2.56989600	2.19576300	-2.64760400
C	-4.19020200	0.85342600	-3.85711300
H	-5.12574800	0.58386300	-3.35026000
H	-4.33924600	1.75848800	-4.45060300
H	-3.90581500	0.01876200	-4.50875500

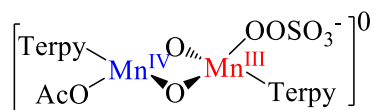


Transition state of O–O bond cleavage of SO_5^{2-} upon binding to Mn^{IV} (**II-TS** in Scheme 2)

E = -2839.47271159 a.u.

Mn	0.97800000	0.47304300	0.26089500
Mn	-1.59079800	-0.28363900	-0.33602600
O	-0.32786700	0.41352100	-1.27767000
O	-0.47718100	-0.22233600	1.07667700
O	1.98508500	0.71272500	1.66406900
N	0.64764800	2.46582000	0.43667400
N	2.24566900	1.18863900	-1.09547000
N	1.86994900	-1.21727800	-0.34575300
N	-2.64454200	1.32652800	0.28064400
N	-2.93006000	-1.15143400	0.88800500
N	-1.24825500	-2.24217800	-0.70459300
C	1.34367100	3.25555300	-0.43496700
C	2.22338400	2.50957500	-1.35190200
C	2.98023500	3.02029300	-2.41022100
C	3.72853700	2.12335900	-3.18250700
C	3.71287100	0.74991200	-2.90541500
C	2.94026400	0.30151900	-1.83198800
C	2.76840300	-1.08406900	-1.36299800
C	-3.60482800	1.06995300	1.22511200
C	-3.72563100	-0.34891300	1.61210800
C	-4.55676000	-0.90652600	2.58866800
C	-4.51929400	-2.29529300	2.77084300
C	-3.68058600	-3.10499900	1.99216600
C	-2.87506900	-2.48560500	1.03304700
C	-1.94606800	-3.12134000	0.07809500
C	-2.48559800	2.56284100	-0.21750500
C	-4.41437800	2.09236800	1.70803600
C	-3.28037900	3.62383200	0.22339700
C	-4.24683100	3.38696600	1.20011700
C	-0.45966200	-2.67967500	-1.69888000
C	-1.80568900	-4.49392000	-0.10423000
C	-0.29912700	-4.04473900	-1.94064600
C	-0.96739700	-4.95894000	-1.12456200
C	-0.13561400	3.01290800	1.38120800
C	1.22432900	4.64266300	-0.39045200
C	0.39558800	5.21846200	0.57899400
C	-0.28408300	4.39704200	1.48121700
C	3.47707400	-2.18256900	-1.83946200
C	1.69042600	-2.40251800	0.25737900
C	2.39230200	-3.53440100	-0.15642400

C	3.28538300	-3.42421500	-1.22477500
H	2.97766600	4.07838500	-2.63219600
H	4.27675700	0.05352100	-3.51036900
H	-5.20570200	-0.28429700	3.18895700
H	-3.65649900	-4.17671900	2.13167900
H	4.31871200	2.49471200	-4.00997300
H	-5.14876900	-2.75062600	3.52398100
H	-3.12426700	4.61133600	-0.18760500
H	-4.87031600	4.19379300	1.56252400
H	-5.16947900	1.87932000	2.45235000
H	-1.71544000	2.67931600	-0.96315000
H	0.35102800	-4.37210900	-2.73950200
H	-0.84893400	-6.02291200	-1.28179400
H	-2.35421500	-5.18360500	0.52280600
H	0.05271900	-1.91656600	-2.26753500
H	0.29148500	6.29422300	0.63148900
H	-0.93049500	4.81106600	2.24239800
H	2.22168200	-4.48006000	0.33891100
H	3.83277000	-4.29048300	-1.57298600
H	1.77708200	5.25789300	-1.08736600
H	-0.64954500	2.32019000	2.03356400
H	4.18052900	-2.06467000	-2.65263800
H	0.96244700	-2.42445100	1.05509300
O	2.71733900	-0.69812400	2.37383500
S	4.31624200	-0.54678400	2.22208600
O	4.79589400	-1.85444700	2.78184200
O	4.64626200	-0.37622800	0.77742900
O	4.74829700	0.62765100	3.04607100
O	-2.98713100	-0.50520700	-1.74974200
C	-3.36921500	0.30605300	-2.69504600
O	-2.87715400	1.42269100	-2.94378600
C	-4.54104700	-0.24976600	-3.51643600
H	-5.40784800	-0.38924200	-2.85807700
H	-4.79766200	0.43674300	-4.32682800
H	-4.26610500	-1.22882000	-3.92702200

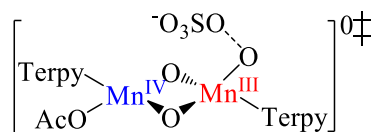


Complex with SO_5^{2-} binding to Mn^{III}

E = -2839.49699546 a.u.

Mn	-0.92294800	0.45721400	-0.23954700
Mn	1.65621000	-0.16347000	0.33099100
O	0.29239300	0.52059900	1.19918100
O	0.59388800	-0.25578000	-1.07353900
O	-1.97191800	0.62872800	-1.86654100
O	2.99206700	-0.17309300	1.83172500
N	-1.12993900	2.69893400	-0.33421100
N	-2.48177200	0.96066000	1.12485700
N	-1.86936700	-1.47546000	0.32773100
N	1.41547600	-2.10315000	0.84269100
N	3.11661500	-1.02143600	-0.73317300
N	2.59434300	1.46165700	-0.39671600
C	-0.46682600	3.48992200	-1.19450200
C	-0.55579400	4.88168700	-1.12571200
C	-1.35991700	5.45000100	-0.13386300
C	-2.06702000	4.62172100	0.74294100
C	-1.93937600	3.23589200	0.61105300
C	-2.68638900	2.25724600	1.43787300
C	-3.57392800	2.60603400	2.46178700
C	-4.23742600	1.58676400	3.14884900
C	-4.01995700	0.25123600	2.80341300
C	-3.12384000	-0.03776300	1.76861700
C	-2.82753500	-1.40335100	1.27836000
C	-3.50523100	-2.54800500	1.70523300
C	-3.19638100	-3.77201100	1.10407900
C	-2.22371100	-3.82522200	0.10131500
C	-1.57151900	-2.64479400	-0.25753500
C	0.56912600	-2.51712500	1.79866300
C	0.46829500	-3.86919600	2.13120100
C	1.26078300	-4.79405500	1.44962900
C	2.15731700	-4.35060900	0.46977800
C	2.22894700	-2.98926800	0.19054600
C	3.18785700	-2.36385200	-0.73980500
C	4.13050500	-2.99647500	-1.55430100
C	4.97265900	-2.19423000	-2.33601400
C	4.87640000	-0.79712500	-2.30031700
C	3.91076000	-0.22418700	-1.46766400
C	3.62824000	1.20811000	-1.25850400
C	4.33744300	2.25491200	-1.83853600
C	3.97840200	3.57176400	-1.52463100

C	2.92946800	3.80838100	-0.63570500
C	2.25337300	2.72001700	-0.07917900
H	0.14845400	2.99024300	-1.93181800
H	-0.00548900	5.49573600	-1.82556700
H	-1.44475800	6.52550600	-0.04652000
H	-2.70520400	5.04993100	1.50318200
H	-3.74534300	3.64143900	2.71788900
H	-4.92405300	1.83317900	3.94810400
H	-4.53291800	-0.54245400	3.32714200
H	-4.26565800	-2.49005500	2.47183200
H	-3.71332200	-4.67120600	1.41417000
H	-1.96346300	-4.75766800	-0.38100900
H	-0.78764500	-2.61729800	-1.00245600
H	-0.03309200	-1.75026100	2.26374100
H	-0.22990200	-4.17953200	2.89558900
H	1.19280400	-5.84916300	1.67984800
H	2.79766100	-5.04713200	-0.05400000
H	4.20906300	-4.07429500	-1.57931700
H	5.70975900	-2.66132800	-2.97568900
H	5.52924900	-0.17987100	-2.90134400
H	5.15431900	2.04800600	-2.51617900
H	4.51714900	4.39817200	-1.96946900
H	2.62508800	4.81273900	-0.37600600
H	1.43854900	2.82946800	0.61845800
C	3.40964500	0.79523200	2.59632400
O	2.89703900	1.92742300	2.68569900
C	4.64954900	0.41583200	3.41785100
H	4.91321100	1.22177000	4.10686300
H	5.48596900	0.22507200	2.73302600
H	4.45155100	-0.50672900	3.97609300
O	-2.22268100	-0.67268500	-2.47091500
S	-3.88406100	-0.93908300	-2.55947300
O	-3.86777600	-2.32620500	-3.09934600
O	-4.43014300	-0.81419700	-1.18624900
O	-4.41906400	0.08072300	-3.50461400

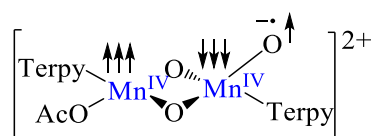


Transition state of O–O bond cleavage of SO_5^{2-} upon binding to Mn^{III}

E = -2839.45782336 a.u.

Mn	-0.88907200	0.45094500	-0.20719300
Mn	1.68308100	-0.29537800	0.34561700
O	0.39073900	0.33723000	1.30084600
O	0.54685700	-0.21093700	-1.06286900
O	-2.03324300	0.63006400	-1.65184400
O	3.07037600	-0.52362300	1.73892800
N	-0.68827600	2.48511800	-0.46195400
N	-2.22870800	1.15170800	1.12003000
N	-1.89469300	-1.29380000	0.37424300
N	1.37203600	-2.27100600	0.62987200
N	3.03513000	-1.08041100	-0.90875500
N	2.66616900	1.36600100	-0.23314400
C	0.09654900	3.04986600	-1.39441000
C	0.21771700	4.43703100	-1.48414000
C	-0.48675200	5.23614300	-0.58065700
C	-1.31140100	4.63823700	0.37933800
C	-1.40731200	3.24912600	0.41222700
C	-2.28093000	2.48319100	1.32187200
C	-3.12522400	3.00298000	2.30563300
C	-3.89406100	2.10762500	3.05976500
C	-3.82314900	0.73023800	2.82429300
C	-2.96387100	0.26900300	1.82261300
C	-2.78828800	-1.12857600	1.38687600
C	-3.50754200	-2.21049800	1.88879500
C	-3.33477500	-3.46438100	1.29328200
C	-2.45219600	-3.60475800	0.21942400
C	-1.73483400	-2.48810700	-0.21240400
C	0.56681300	-2.76323800	1.58416300
C	0.42108100	-4.14047000	1.75971100
C	1.12118100	-5.00710200	0.91925200
C	1.97431600	-4.48472000	-0.06070300
C	2.09753500	-3.10395600	-0.17844300
C	3.02656600	-2.41165700	-1.09157900
C	3.87120100	-2.97798700	-2.04972200
C	4.69861100	-2.12080700	-2.78814000
C	4.68578800	-0.73695800	-2.56905400
C	3.81771200	-0.23260900	-1.59620100
C	3.63795500	1.17096900	-1.18036300
C	4.39422000	2.24031800	-1.64729400
C	4.15802400	3.51757400	-1.12326400

C	3.17673600	3.69242900	-0.14816600
C	2.43859700	2.58608600	0.27863100
H	0.63294000	2.37146800	-2.04407600
H	0.86200000	4.87046400	-2.23602600
H	-0.40183300	6.31408100	-0.62215500
H	-1.87488800	5.23882100	1.08006300
H	-3.18178500	4.06824300	2.48048600
H	-4.55304000	2.48613200	3.83001800
H	-4.42079500	0.03747300	3.39988000
H	-4.20396300	-2.07392700	2.70505000
H	-3.89048800	-4.31766200	1.66008000
H	-2.30144600	-4.56019100	-0.26367300
H	-1.01004400	-2.53704900	-1.01333000
H	0.03413500	-2.03463000	2.17870800
H	-0.24233500	-4.51254500	2.52742200
H	1.01491500	-6.07855600	1.02585600
H	2.54410600	-5.13723400	-0.70793500
H	3.88408100	-4.04566300	-2.21882100
H	5.35844600	-2.53446600	-3.53927600
H	5.32555800	-0.07843200	-3.13953800
H	5.15904000	2.07855600	-2.39448100
H	4.73906300	4.36025600	-1.47422100
H	2.96646200	4.66566000	0.27233900
H	1.66154800	2.65263600	1.02356600
C	3.41339800	0.28398200	2.70661200
O	2.89194700	1.38527400	2.95430400
C	4.57475900	-0.26270500	3.54623900
H	4.80499900	0.42134100	4.36643200
H	5.45624500	-0.38628100	2.90466600
H	4.30388200	-1.24815100	3.94403300
O	-2.92064200	-0.80284900	-2.40250700
S	-4.48351200	-0.57686200	-2.16338200
O	-5.07990800	-1.83621700	-2.73489800
O	-4.74378000	-0.43911500	-0.69830400
O	-4.90772000	0.64509700	-2.92599400

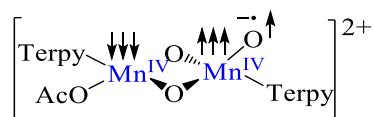


Antiparallel-spin $\text{Mn}^{\text{IV}}\text{-O}^\bullet$ oxyl-radical species generated from the O–O cleavage of SO_5^{2-} upon binding to Mn^{IV} (**III** in Scheme 2)

E = -2140.10168976 a.u.

Mn	1.32516200	-0.07233200	-1.09744900
Mn	-1.00254500	0.10864700	0.37583700
O	0.66390000	-0.08581000	0.77695800
O	-0.38968400	0.11713700	-1.38169500
O	1.97449600	-0.08858100	-2.63766900
O	-1.80306900	0.17645400	2.11643800
N	1.46372700	-2.07824700	-1.02464600
N	3.03911300	-0.27339300	-0.13423100
N	1.85595100	1.85767700	-0.90159300
N	-1.13501300	2.11642600	0.44031800
N	-2.81626200	0.39248600	-0.41357100
N	-1.64369200	-1.78797100	0.24194300
C	0.62335500	-2.90359100	-1.66826500
C	0.79595400	-4.28710100	-1.60278500
C	1.85009100	-4.80336000	-0.84687400
C	2.72941900	-3.93136900	-0.19354200
C	2.52708100	-2.56054200	-0.31383000
C	3.40136500	-1.51578100	0.24093200
C	4.49813900	-1.68000100	1.08897500
C	5.17228200	-0.53559800	1.53317200
C	4.75215000	0.74303300	1.14551900
C	3.65090100	0.84812000	0.29382500
C	3.01096700	2.07573900	-0.20374200
C	3.50052300	3.36739400	-0.03849100
C	2.80485100	4.43244900	-0.62287000
C	1.64404000	4.18282600	-1.35760900
C	1.18894600	2.86957600	-1.47936000
C	-0.24635300	2.89114800	1.08323900
C	-0.41674500	4.27419700	1.14383600
C	-1.52555300	4.84727000	0.51817800
C	-2.45954300	4.02813000	-0.12741200
C	-2.25348400	2.65260100	-0.13861400
C	-3.19814000	1.65521900	-0.67446500
C	-4.39475700	1.88119000	-1.35798200
C	-5.15193900	0.76740900	-1.74730300
C	-4.72447900	-0.53556100	-1.45942100
C	-3.51594100	-0.69587900	-0.77624200
C	-2.86720200	-1.95131600	-0.35703800
C	-3.42561700	-3.21779300	-0.48352800

C	-2.73413200	-4.31895100	0.03759600
C	-1.50684600	-4.12707800	0.67102000
C	-0.97835400	-2.83748400	0.75245600
H	-0.19228100	-2.43934700	-2.20527200
H	0.10164100	-4.93518900	-2.11815200
H	1.99463600	-5.87251100	-0.76858200
H	3.56403100	-4.30781200	0.38168800
H	4.80946700	-2.66702900	1.40097400
H	6.02108000	-0.64001100	2.19557900
H	5.25837200	1.62783100	1.50431000
H	4.41165700	3.53646900	0.51842900
H	3.17215200	5.44336700	-0.50708200
H	1.08549700	4.98497400	-1.81838100
H	0.28377500	2.60935100	-2.01018600
H	0.60231500	2.38301200	1.51935300
H	0.31755200	4.87957700	1.65574300
H	-1.67231500	5.91892500	0.53906900
H	-3.34065600	4.44666500	-0.59383700
H	-4.72659200	2.88549700	-1.58157500
H	-6.08185200	0.91666700	-2.27971800
H	-5.31141600	-1.39190400	-1.76015200
H	-4.38660000	-3.33954500	-0.96398500
H	-3.15770900	-5.31083700	-0.04838900
H	-0.94770800	-4.95580000	1.08150900
H	-0.02939400	-2.61913200	1.21694200
C	-1.47555100	-0.49151700	3.20317000
O	-0.58250300	-1.34442800	3.27875600
C	-2.34462900	-0.09948900	4.39892400
H	-2.04474900	-0.66770700	5.28230200
H	-3.39693800	-0.29904100	4.16286200
H	-2.23607000	0.97530500	4.58820800

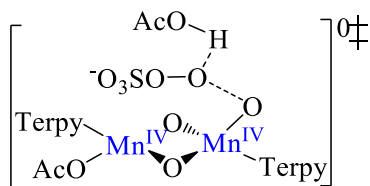


Parallel-spin $\text{Mn}^{\text{IV}}\text{-O}^\bullet$ oxyl-radical species generated from the O-O cleavage of SO_5^{2-} upon binding to Mn^{III}

E = -2140.09290087 a.u.

Mn	1.33107300	-0.03518100	-0.83991100
Mn	-1.09073400	0.06149800	0.36559300
O	0.59290200	-0.06775600	0.85885200
O	-0.38411500	0.07444600	-1.31746400
O	2.07715700	-0.02941600	-2.54550500
O	-1.95275500	0.10773000	2.09213900
N	1.66516300	-1.99814000	-0.93652600
N	3.10715100	-0.12697500	0.01826200
N	1.82470200	1.89378100	-0.84322200
N	-1.27297500	2.06239700	0.42327300
N	-2.88091000	0.28888800	-0.46328600
N	-1.65518400	-1.85580000	0.20216600
C	0.87408900	-2.85970700	-1.60143900
C	1.15581400	-4.22598500	-1.60221100
C	2.26607300	-4.69004000	-0.89413400
C	3.09375700	-3.78212300	-0.22078200
C	2.78429300	-2.42848300	-0.26785100
C	3.60120300	-1.34385800	0.30325800
C	4.79246700	-1.44289000	1.02591200
C	5.42670500	-0.25595300	1.41828700
C	4.89459500	0.99665600	1.08171400
C	3.69973300	1.03061800	0.35891100
C	2.97400800	2.20341200	-0.15931700
C	3.38768800	3.52565700	-0.05153800
C	2.63583000	4.52419700	-0.68438000
C	1.49494200	4.18092900	-1.41256200
C	1.10666300	2.84304800	-1.47080500
C	-0.40523500	2.86341600	1.06288900
C	-0.60396300	4.24361900	1.09980600
C	-1.72002100	4.78425200	0.45849500
C	-2.63158700	3.93700200	-0.18298800
C	-2.39559800	2.56658500	-0.17526000
C	-3.30447100	1.54112300	-0.71637200
C	-4.50810100	1.73149400	-1.39768300
C	-5.23051700	0.59669900	-1.79125800
C	-4.76150400	-0.69309300	-1.51008800
C	-3.54736700	-0.82013900	-0.83030000
C	-2.85919200	-2.05717000	-0.42264500
C	-3.35579400	-3.34392600	-0.59443500

C	-2.61611800	-4.42706400	-0.10266300
C	-1.40465400	-4.19835600	0.54896000
C	-0.94364100	-2.88758900	0.68596400
H	0.01380600	-2.43485200	-2.10023600
H	0.50235200	-4.90338900	-2.13311300
H	2.49539500	-5.74700900	-0.86980800
H	3.96966700	-4.11759700	0.31723700
H	5.21340900	-2.40793700	1.27089800
H	6.34908200	-0.30713200	1.98115600
H	5.39730800	1.90991400	1.36696300
H	4.28360300	3.76991700	0.50238600
H	2.94672700	5.55787000	-0.61192300
H	0.89880700	4.93048200	-1.91284800
H	0.21508800	2.50864900	-1.98275700
H	0.44910600	2.37998100	1.51600400
H	0.11422300	4.87151200	1.60742000
H	-1.88907100	5.85275000	0.46273300
H	-3.51646500	4.33091500	-0.66336300
H	-4.87150500	2.72619200	-1.61502100
H	-6.16594700	0.71882200	-2.32077800
H	-5.32273400	-1.56556800	-1.81325200
H	-4.30341200	-3.49718700	-1.09180900
H	-2.98976500	-5.43482900	-0.22695800
H	-0.80961000	-5.01290200	0.93685600
H	-0.01626500	-2.63995700	1.17818500
C	-1.67985600	-0.60089500	3.16648200
O	-0.77959500	-1.44631600	3.25492100
C	-2.61602300	-0.27068500	4.32973200
H	-2.34674700	-0.86144600	5.20815100
H	-3.64979900	-0.48746400	4.03386900
H	-2.54542700	0.79926100	4.55954600

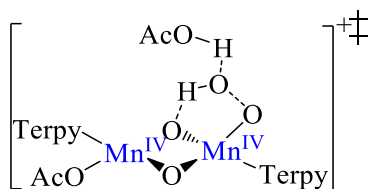


Transition state of HOOSO_3^- nucleophilic attack to the antiparallel-spin $\text{Mn}^{\text{IV}}\text{-O}^\bullet$ oxyl-radical species assisted by AcO^- as a proton acceptor (**III-TS1** in Scheme 2)

E = -3143.30341894 a.u.

Mn	0.62196400	0.05636000	0.09083200
Mn	-2.10946000	-0.06365300	0.34075200
O	-0.82771700	-0.20271200	1.48387700
O	-0.86896300	0.20700500	-0.93034600
O	1.79541600	0.54576000	-1.09094900
N	0.92937100	-1.90914200	-0.09531100
N	1.91053400	-0.24674800	1.56474100
N	0.91150400	1.96353400	0.74183800
N	-2.42172100	-1.98612800	-0.17777200
N	-3.49318500	0.15084900	-1.10386700
N	-2.53495300	1.90954700	0.49636100
C	1.77002400	-2.46675900	0.82510400
C	2.29722500	-1.50968100	1.81223800
C	3.15909400	-1.77191800	2.87943900
C	3.59518200	-0.69260500	3.65668600
C	3.18062800	0.61428400	3.36873100
C	2.31352400	0.80988900	2.29133300
C	1.77929100	2.09020000	1.78939000
C	-3.27233500	-2.18074700	-1.23454900
C	-3.84463600	-0.94270600	-1.79844500
C	-4.68178200	-0.80939100	-2.91061200
C	-5.11792300	0.47669900	-3.25587900
C	-4.73614300	1.59684100	-2.50438600
C	-3.90068700	1.39513200	-1.40230400
C	-3.39523500	2.40206100	-0.44765600
C	-1.88916800	-3.02942700	0.47785900
C	-3.57711200	-3.46636900	-1.66920400
C	-2.17082500	-4.34131200	0.09060300
C	-3.01607000	-4.55965500	-0.99708400
C	-2.08193900	2.68887000	1.49093800
C	-3.78059400	3.73921800	-0.42215300
C	-2.44872500	4.03362000	1.57405100
C	-3.29577700	4.56450900	0.60001900
C	0.49197100	-2.62357400	-1.14350700
C	2.15599300	-3.79915200	0.72313700
C	1.69269900	-4.55436600	-0.35997600
C	0.86162000	-3.95841600	-1.31026100
C	2.15019900	3.34851600	2.25833800

C	0.42963700	3.04911100	0.11552800
C	0.77521900	4.33556100	0.53307500
C	1.63696200	4.48470400	1.62236700
H	3.48374300	-2.78057200	3.09508300
H	3.52007600	1.44942200	3.96544500
H	-4.97936600	-1.67102200	-3.49166800
H	-5.07537000	2.58744300	-2.77318500
H	4.26443800	-0.86905500	4.48873600
H	-5.76049600	0.60760100	-4.11662200
H	-1.72010600	-5.16365800	0.62824600
H	-3.24379000	-5.56665300	-1.32153800
H	-4.24819900	-3.61149500	-2.50471900
H	-1.23193600	-2.78591800	1.29729600
H	-2.06277300	4.64389500	2.37841200
H	-3.58736300	5.60596900	0.63596000
H	-4.45907900	4.12266500	-1.17210100
H	-1.41061500	2.21613700	2.19410200
H	1.98997200	-5.58996400	-0.46349900
H	0.49165600	-4.51329900	-2.16148300
H	0.36745700	5.19299500	0.01587500
H	1.91741300	5.47092800	1.96857300
H	2.82574200	-4.22805600	1.45631200
H	-0.16416000	-2.10577700	-1.82918900
H	2.83707100	3.43821100	3.08922100
H	-0.23797000	2.86375100	-0.71478900
O	3.32711900	-1.57038600	-1.41586100
S	4.89334100	-1.12785600	-0.83265800
O	5.37217200	-2.48523700	-0.47017600
O	5.57390300	-0.49659500	-1.98966700
O	4.67283000	-0.22291900	0.31708200
O	-3.68216300	-0.25183600	1.57078700
C	-3.93548400	-1.11524800	2.51206000
O	-3.15343900	-1.98729900	2.93671600
C	-5.35408700	-0.97187900	3.08236500
H	-6.08166900	-1.19270300	2.29079100
H	-5.50076900	-1.65727000	3.92055300
H	-5.51351400	0.06222400	3.41019100
O	2.68352800	-0.53950300	-2.12320300
H	3.57829900	1.15599700	-2.31652800
O	3.89866100	2.08418500	-2.16377700
C	3.02148400	2.97867400	-2.65104500
O	2.10398900	2.68491700	-3.41234900
C	3.28750600	4.37407700	-2.12493200
H	4.36295500	4.55572400	-2.03712200
H	2.82249500	5.11320500	-2.78081100
H	2.83782800	4.44829300	-1.12523600

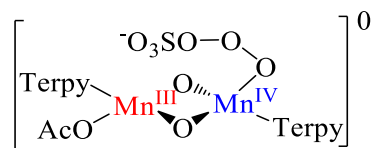


Transition state of H₂O nucleophilic attack to the antiparallel-spin Mn^{IV}-O[•] oxyl-radical species assisted by AcO⁻ as a proton acceptor (**III-TS2** in Scheme 2)

E = -2444.76272434 a.u.

Mn	1.36988100	-0.40047500	-0.74922700
Mn	-0.67791200	0.46689700	0.85290600
O	0.92053900	-0.11630300	1.16688000
O	-0.32928100	0.21777900	-0.89248800
O	1.60829200	-0.67266500	-2.45437300
O	-1.26877800	0.88891200	2.70513500
N	1.09652300	-2.38116700	-0.52880300
N	3.15870100	-0.95073300	-0.11401300
N	2.37326000	1.35834500	-0.87459300
N	-0.32780400	2.45340700	0.74388400
N	-2.47585100	1.14591300	0.25692000
N	-1.79116400	-1.21684300	0.98702300
C	0.00149300	-3.03538600	-0.95302700
C	-0.12142000	-4.41429600	-0.78005200
C	0.91072200	-5.11519900	-0.15127000
C	2.05924500	-4.43144300	0.26102000
C	2.13683100	-3.05717800	0.04586000
C	3.30583200	-2.21482600	0.33462800
C	4.48039400	-2.58535500	0.99539000
C	5.47138100	-1.61612100	1.18463300
C	5.28273700	-0.30337700	0.73237700
C	4.08854500	0.00803900	0.08053400
C	3.66643800	1.32174500	-0.43295200
C	4.47841100	2.44965800	-0.51390500
C	3.95835400	3.61677400	-1.08407300
C	2.64520200	3.62730000	-1.55812900
C	1.87231700	2.47298600	-1.43203200
C	0.79538700	3.03252300	1.19682300
C	0.96960100	4.41526400	1.12183500
C	-0.04008200	5.19367800	0.55327900
C	-1.21592600	4.58276600	0.10076000
C	-1.34800900	3.20307100	0.22421300
C	-2.56329100	2.43487600	-0.10954100
C	-3.73482100	2.89935100	-0.71334800
C	-4.78062500	1.98704000	-0.90959600
C	-4.65575600	0.64893200	-0.51595100
C	-3.45543400	0.24683200	0.07632700

C	-3.08722800	-1.09764900	0.55792300
C	-3.95717700	-2.18071200	0.62467500
C	-3.49234700	-3.39198000	1.15257000
C	-2.17682300	-3.48687200	1.60414900
C	-1.34235700	-2.37087800	1.50491300
H	-0.76064500	-2.43602300	-1.42958600
H	-1.01679400	-4.91591400	-1.11994000
H	0.83240800	-6.18308700	0.00495400
H	2.88493800	-4.95565000	0.72270700
H	4.61254200	-3.59481900	1.35928200
H	6.38739500	-1.87927700	1.69670600
H	6.03698700	0.45386600	0.89492400
H	5.49753600	2.41177100	-0.15423300
H	4.57536900	4.50248300	-1.15960600
H	2.21216600	4.51350500	-2.00010900
H	0.83870100	2.43356600	-1.74306600
H	1.54966700	2.36339800	1.58728400
H	1.88710700	4.85797300	1.48285500
H	0.07722600	6.26593300	0.46815600
H	-2.02100100	5.16814700	-0.32212300
H	-3.83190000	3.93161300	-1.01993300
H	-5.69762900	2.32112800	-1.37709500
H	-5.46234000	-0.05291500	-0.67447000
H	-4.97745600	-2.07738300	0.28148600
H	-4.15651600	-4.24426300	1.21215100
H	-1.78594500	-4.40765600	2.01374700
H	-0.31324200	-2.37788600	1.82792400
C	-1.16459500	0.20259900	3.80930800
O	-0.56146900	-0.87799000	3.94236300
C	-1.88631800	0.86668700	4.98916900
H	-1.74397000	0.28154500	5.90074400
H	-1.49551100	1.88168800	5.13029000
H	-2.95623900	0.94445400	4.75845900
O	0.50713700	0.26092800	-3.46050600
H	-0.63521800	-0.84679200	-3.57081400
H	0.01410200	0.67186100	-2.71062300
O	-1.42286900	-1.50298900	-3.49591900
C	-2.54450500	-0.83784900	-3.18864300
O	-2.61894000	0.38881600	-3.14303400
C	-3.69871800	-1.77454000	-2.88651700
H	-3.49057300	-2.30356500	-1.94862800
H	-4.62283100	-1.20325000	-2.78388400
H	-3.79498900	-2.51810600	-3.68503500

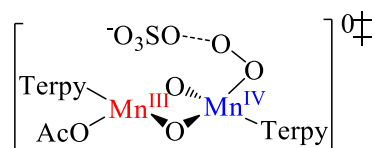


Complexes generated by HOOSO_3^- nucleophilic attack to the antiparallel-spin $\text{Mn}^{\text{IV}}\text{-O}^\bullet$ oxyl-radical species (**IV** in Scheme 2)

E = -2914.64432868 a.u.

Mn	0.81701500	0.83055200	-0.04247800
Mn	-1.45451500	-0.43219100	0.69663800
O	-0.24499700	0.78321600	1.39037400
O	-0.27088200	-0.34622200	-0.75390600
O	2.13534600	0.96818300	-1.52432000
N	2.19959100	-0.31609400	0.88440000
N	1.95056400	2.23373500	0.79910900
N	-0.00914400	2.49445100	-0.81985600
N	-1.14519400	-2.68286000	0.79210600
N	-2.91602600	-1.30314400	-0.62288500
N	-2.86674700	1.22506200	0.12392200
C	3.12613400	0.37077500	1.61934700
C	2.95473900	1.83609400	1.60120500
C	3.69317200	2.79496700	2.30005500
C	3.34766700	4.14285200	2.13832000
C	2.29495600	4.52331900	1.29493700
C	1.59640700	3.52001300	0.61949900
C	0.48432000	3.67504900	-0.33772300
C	-1.80349900	-3.37856100	-0.16839700
C	-2.81124000	-2.61132500	-0.93856700
C	-3.63025600	-3.17072400	-1.92680000
C	-4.54975000	-2.34954100	-2.58096000
C	-4.64471800	-0.99825300	-2.24277300
C	-3.80425400	-0.49473500	-1.24495800
C	-3.80996800	0.91656000	-0.79480300
C	-0.24913100	-3.30428300	1.58053300
C	-1.54286800	-4.73519500	-0.38390700
C	0.05913100	-4.65687600	1.41971200
C	-0.59343000	-5.37665200	0.41623400
C	-2.78722200	2.46187500	0.64027700
C	-4.70854200	1.88467300	-1.25347000
C	-3.65875800	3.47443900	0.23740100
C	-4.62565600	3.17791900	-0.72837100
C	2.25480400	-1.65137500	0.78101400
C	4.14031000	-0.30636000	2.29041000
C	4.19613900	-1.70259200	2.20014900
C	3.24513700	-2.38338300	1.43857200
C	-0.02136700	4.88963300	-0.79231900

C	-0.95252500	2.47715900	-1.77572900
C	-1.48473600	3.66489200	-2.27769100
C	-1.02277300	4.88097800	-1.77025400
H	4.50428000	2.50327000	2.95244800
H	2.03115900	5.56427600	1.17127700
H	-3.55585400	-4.21790800	-2.18094900
H	-5.35150500	-0.35472000	-2.74639500
H	3.90187500	4.90263100	2.67342800
H	-5.18930200	-2.76062100	-3.35096700
H	0.79308500	-5.12390400	2.06259500
H	-0.37326200	-6.42463500	0.25860900
H	-2.06219900	-5.28324000	-1.15709100
H	0.21432000	-2.69412300	2.34196900
H	-3.57069000	4.46686900	0.65776800
H	-5.30956600	3.94342400	-1.07162800
H	-5.45772100	1.64213600	-1.99397800
H	-1.98967700	2.62340000	1.35345200
H	4.97681000	-2.24561300	2.71671300
H	3.25898000	-3.46086900	1.34700700
H	-2.25331800	3.62639400	-3.03638600
H	-1.42892700	5.81559300	-2.13409000
H	4.87135500	0.24383800	2.86712100
H	1.50191200	-2.11246500	0.16143000
H	0.36734700	5.82008700	-0.40165900
H	-1.27910700	1.50018600	-2.10167100
O	2.28230300	-1.29750700	-2.18079800
S	3.93171900	-1.63925900	-2.42689200
O	3.88550400	-3.09802700	-2.14529200
O	4.22136200	-1.28085400	-3.83860300
O	4.69639700	-0.84670900	-1.43390500
O	-2.59497200	-0.59195500	2.30798600
C	-2.20948700	-1.03843400	3.47037800
O	-1.03113800	-1.30398600	3.78001400
C	-3.35808700	-1.22672200	4.46676800
H	-4.04704300	-1.98751800	4.07800700
H	-2.97211000	-1.53969600	5.43960700
H	-3.91411800	-0.28700500	4.56775800
O	1.93658900	0.10313000	-2.58707700

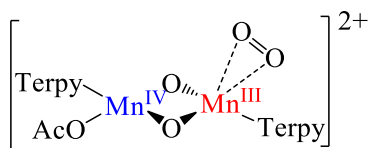


Transition state of O–O cleavage for triplet O₂ evolution (**IV-TS** in Scheme 2)

E = -2914.62221595 a.u.

Mn	0.84330100	0.84793400	-0.00515900
Mn	-1.58631000	-0.28668000	0.42456800
O	-0.51590200	0.70660200	1.36459900
O	-0.37700900	-0.19378600	-0.88614300
O	2.21569200	0.97686100	-1.40764500
N	2.02905100	-0.56748300	0.85766200
N	1.94510400	1.96528200	1.17904000
N	0.26049800	2.66436800	-0.58903500
N	-1.07221300	-2.16850300	0.94655700
N	-2.74371500	-1.35869700	-0.82396600
N	-2.76891700	1.16365300	-0.37159200
C	2.88337800	-0.09545900	1.81583200
C	2.78610800	1.35952100	2.04343900
C	3.45429900	2.11781100	3.00530500
C	3.22122600	3.50005000	3.04417900
C	2.34324900	4.10313700	2.13741800
C	1.70277400	3.29213700	1.19553500
C	0.76767400	3.70606800	0.13989900
C	-1.62353100	-3.16084300	0.17869800
C	-2.54795800	-2.68630200	-0.86851200
C	-3.21981600	-3.44794000	-1.82930900
C	-4.07683500	-2.78301600	-2.71614100
C	-4.26177800	-1.39573200	-2.63914400
C	-3.56094400	-0.69228900	-1.65614100
C	-3.61511200	0.75375100	-1.36516100
C	-0.28561900	-2.46626700	1.99327800
C	-1.34598000	-4.49753600	0.44319400
C	0.01231000	-3.79314000	2.31303600
C	-0.51370500	-4.81542000	1.52406400
C	-2.79188700	2.42810500	0.07652800
C	-4.48030800	1.65790800	-1.97418400
C	-3.65624200	3.37215900	-0.48102000
C	-4.49600500	2.98475200	-1.52658500
C	2.06026200	-1.85711400	0.49019100
C	3.78024100	-0.94593800	2.45444900
C	3.80986100	-2.29616200	2.08160400
C	2.94846500	-2.75591500	1.08554900
C	0.44222900	5.02333700	-0.17696600
C	-0.51883800	2.89668200	-1.66125700

C	-0.85953200	4.19536900	-2.03670700
C	-0.38590800	5.26837600	-1.27666200
H	4.13148100	1.64958500	3.70588600
H	2.16045300	5.16837400	2.16290000
H	-3.08034400	-4.51834200	-1.88783600
H	-4.92575900	-0.88465500	-3.32197200
H	3.72596700	4.10633000	3.78476000
H	-4.60480600	-3.34935000	-3.47203700
H	0.65784000	-4.00529000	3.15369600
H	-0.28828800	-5.85044900	1.74531400
H	-1.78128200	-5.27302600	-0.17217200
H	0.09865000	-1.62790100	2.55218000
H	-3.64958400	4.38743300	-0.11027900
H	-5.16463000	3.70077000	-1.98610000
H	-5.13915500	1.32939800	-2.76662600
H	-2.08965600	2.66299200	0.86462400
H	4.50358100	-2.97337300	2.56268300
H	2.94661000	-3.79165500	0.77559900
H	-1.49677900	4.35304700	-2.89559100
H	-0.64792600	6.28458300	-1.54059600
H	4.44910400	-0.56317900	3.21340800
H	1.36616200	-2.14889400	-0.28298000
H	0.84283700	5.83738800	0.41199900
H	-0.87794600	2.02091500	-2.18429000
O	2.45363000	-1.31042500	-2.39215700
S	4.06528800	-1.54440600	-2.58686500
O	4.12700500	-3.03644300	-2.52266700
O	4.44110700	-0.98648200	-3.91855400
O	4.76406900	-0.87324400	-1.45537000
O	-3.10936100	-0.46764100	1.72933800
C	-3.11955500	-0.81933100	2.98233200
O	-2.11954400	-0.93370200	3.71785400
C	-4.53164000	-1.10655200	3.51198100
H	-4.93278000	-1.98769600	2.99431200
H	-4.50601600	-1.29165800	4.58854200
H	-5.18739000	-0.25621500	3.29127000
O	2.06360100	0.31131300	-2.54488500



Complex with triplet O₂ weakly binding to Mn^{III} (V in Scheme 2)

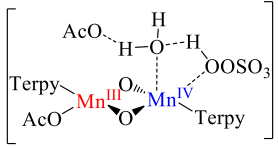
E = -2215.29454031 a.u.

Mn	1.23056900	-0.03570400	-0.37599000
Mn	-1.32438200	0.07306700	0.43291900
O	0.20242600	-0.07791500	1.24895200
O	-0.36331600	0.07983500	-1.14057800
O	4.14384100	-0.10902400	-2.49100900
N	1.72027500	-2.04924000	-0.69209800
N	3.07995600	-0.14368800	0.37399900
N	1.90472400	1.93357300	-0.57924300
N	-1.85620400	-1.84203500	0.16465500
N	-2.96116600	0.31046400	-0.67680400
N	-1.47497500	2.08335400	0.41906600
C	2.82085500	-2.46424400	0.00763400
C	3.61646400	-1.36427900	0.59038000
C	4.85793900	-1.47034300	1.21995500
C	5.52081200	-0.29194800	1.58483700
C	4.97233700	0.96188100	1.28643200
C	3.72768200	1.00793900	0.65607100
C	3.03820600	2.20729600	0.13776100
C	-2.95549100	-2.03611200	-0.63070400
C	-3.58071500	-0.79509400	-1.12349800
C	-4.69394900	-0.66486900	-1.95871100
C	-5.11475700	0.62677600	-2.30129700
C	-4.44242400	1.75842700	-1.82008900
C	-3.33795300	1.56318100	-0.98712100
C	-2.49083300	2.58738300	-0.34772400
C	-1.20489500	-2.88146300	0.71127100
C	-3.40938600	-3.32183800	-0.90373900
C	-1.62384500	-4.19209200	0.47381400
C	-2.73227100	-4.41247500	-0.34391100
C	-0.66765300	2.89462000	1.12143700
C	-2.67998900	3.96188300	-0.44907300
C	-0.82481100	4.28053500	1.06890300
C	-1.83342800	4.81698400	0.26692500
C	0.95619900	-2.93534800	-1.35470700
C	3.15591100	-3.81311400	0.07631100
C	2.35773000	-4.74044600	-0.60567400
C	1.25396700	-4.29954900	-1.33825600
C	3.49489100	3.51424700	0.27678400
C	1.22709200	2.91942700	-1.19295500

C	1.64984500	4.24700900	-1.10708400
C	2.78729800	4.54531600	-0.35453800
H	5.30391500	-2.43765500	1.40268200
H	5.50865500	1.87031500	1.52119100
H	-5.21624900	-1.53523900	-2.32989300
H	-4.77054500	2.75422600	-2.08370300
H	6.48382300	-0.35027300	2.07446100
H	-5.97298900	0.75288600	-2.94795400
H	-1.07659300	-5.01313400	0.91502500
H	-3.07176100	-5.41955300	-0.54733400
H	-4.27349400	-3.46844500	-1.53702900
H	-0.35443900	-2.63859900	1.32927000
H	-0.15572500	4.91466000	1.63290400
H	-1.96747800	5.88837900	0.19923200
H	-3.47727900	4.35511000	-1.06468100
H	0.10692600	2.41200300	1.70126100
H	2.60200400	-5.79379400	-0.56500600
H	0.62177700	-4.99224300	-1.87581800
H	1.08507900	5.02225700	-1.60518900
H	3.12710000	5.56808500	-0.25823800
H	4.01997500	-4.13500600	0.64132200
H	0.09869600	-2.53183000	-1.87660800
H	4.38349300	3.72621800	0.85513600
H	0.33407000	2.62453400	-1.72778000
O	-2.52040200	0.14881500	1.95605700
C	-2.51024900	-0.59905300	3.03544000
O	-1.69940900	-1.50414000	3.27793000
C	-3.64559200	-0.23798900	3.99745200
H	-4.60769000	-0.40099900	3.49617400
H	-3.58574800	-0.85298900	4.89821400
H	-3.57543200	0.82395700	4.26136400
O	2.95599100	-0.08254800	-2.74550300

Vibrational Frequencies for ^{16}O and ^{18}O Isotopologues of Relevant Species in Scheme 2

HSO_5^-	
$\text{H}^{16}\text{OOSO}_3$	$\text{H}^{18}\text{OOSO}_3$
111.0759	108.8926
214.4583	211.4369
272.7586	269.0138
369.0338	362.5440
381.2678	380.9582
488.2048	487.8238
511.1852	511.0973
557.4638	555.8531
658.2161	657.6055
917.6353	893.7312
987.8196	987.7534
1169.9727	1169.9661
1183.5699	1183.4777
1389.6571	1385.6036
3652.0983	3639.7583

 I₀-TS in Scheme 2	
H¹⁶OOSO₃	H¹⁸OOSO₃
78.2498 <i>i</i>	77.3867 <i>i</i>
16.3900	16.3890
27.3832	27.3792
28.4961	28.4937
29.8531	29.8496
36.5039	36.5030
39.5030	39.4832
41.2760	41.2538
44.2491	44.1788
47.3493	47.3344
47.7637	47.7538
54.5974	54.5667
61.9070	61.9032
62.7962	62.5818
66.0294	65.9963
70.4079	70.3346
76.1786	76.1534
77.8500	77.4612
86.8105	86.7089
89.5166	89.4176
96.1069	96.0539
101.3914	100.5462
107.9813	107.8260
111.3640	111.2297
115.6332	115.5913
120.6672	120.6239
122.0937	121.9626
128.4078	128.3749
133.8230	133.7833
140.3226	140.1411
144.7717	144.2539
151.1861	151.1687
156.1724	156.0262
161.1678	160.9125
168.9971	168.7688
178.1279	178.0411
189.1959	189.1831
198.7190	198.7032
209.0618	209.0284

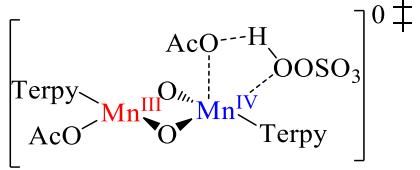
224.7445	224.7367
234.6168	234.0317
241.2573	237.4706
244.4105	243.8307
249.0695	248.0092
253.5637	252.9687
260.2490	259.6224
265.0115	263.6949
269.2301	269.0210
280.8508	280.4882
287.3257	286.8901
295.5312	295.4867
300.1209	300.0811
310.0723	309.8950
320.3721	320.2556
335.9209	335.8271
348.5469	345.6521
351.7929	349.1765
365.7344	365.7333
373.7105	373.0500
382.6129	382.3035
396.3711	393.2925
402.4077	396.9019
422.5472	422.4919
435.7752	435.7730
441.4543	441.4495
444.3243	444.3105
455.0637	455.0536
459.6389	459.4907
460.5830	460.5375
463.9879	463.9852
468.3365	468.3342
473.0172	473.0146
481.0437	481.0332
484.0424	483.9841
498.6342	497.9502
510.8242	510.8190
519.9421	519.9419
533.2883	533.2883
543.2771	543.2770
544.8523	544.8490
553.3494	553.3035
554.9476	554.9440
561.3233	559.1512
569.6815	569.5354

614.9716	614.9620
616.1486	616.1486
639.2838	639.2757
646.3583	646.3565
650.5711	650.5711
652.6941	652.6936
662.4857	662.4857
674.3298	674.3297
682.0088	682.0085
685.4894	685.4751
686.8355	686.7529
688.7180	688.4373
694.4151	694.4148
696.4994	696.4974
703.5901	703.5830
717.5474	717.5448
753.7919	753.7913
756.0304	756.0280
762.1424	762.1422
767.4588	767.4549
775.2487	775.2483
776.4757	776.4728
778.2683	778.2679
781.8438	781.8429
786.2030	786.1641
792.0556	792.0556
795.1969	795.1945
811.9345	811.9326
818.3448	818.3444
827.6382	825.9635
852.6399	852.6395
855.5103	855.4956
857.6741	857.6735
859.7475	859.7475
866.8476	863.2812
897.0281	896.3495
898.2857	898.2751
931.1384	920.9809
934.7846	931.1386
935.6214	934.7848
938.0683	935.6235
939.6465	938.0952
957.9546	957.9496
959.4153	959.4153
987.8909	987.8812

1012.5326	1012.5326
1014.1674	1014.1674
1021.8148	1021.8148
1022.5874	1022.5874
1033.4632	1033.4631
1034.2739	1034.2731
1038.1628	1038.1628
1047.6232	1047.6227
1047.9325	1047.9325
1052.9266	1052.9259
1054.6434	1054.6433
1056.3166	1056.3166
1057.6961	1057.6961
1059.6521	1059.6521
1060.2379	1060.2379
1061.2446	1061.2446
1063.5666	1063.5666
1065.6649	1065.6640
1069.1419	1069.1419
1073.8769	1073.8769
1078.6772	1078.6772
1081.4475	1081.4471
1090.2505	1090.2505
1093.7342	1093.7341
1104.8167	1104.8166
1110.5123	1110.5123
1117.7475	1117.7472
1120.6240	1120.6238
1125.2871	1125.2871
1129.1001	1129.1001
1141.3097	1141.3095
1144.0544	1144.0544
1163.7380	1163.7353
1170.4070	1170.4070
1173.0508	1173.0493
1173.6505	1173.5678
1205.6316	1205.6316
1207.6986	1207.6986
1210.9626	1210.9625
1217.3526	1217.3526
1229.0001	1228.9998
1246.7023	1246.7023
1280.9117	1280.9117
1285.0223	1285.0220
1288.5943	1288.5942

1290.9251	1290.9250
1304.9394	1304.9390
1307.6280	1307.6280
1310.3326	1310.3326
1338.0315	1338.0314
1339.3796	1339.3794
1344.4920	1344.4920
1353.5341	1353.5339
1356.1303	1356.1303
1358.2811	1358.2805
1372.1029	1372.1025
1372.7835	1372.7835
1376.0717	1376.0717
1403.9202	1403.9202
1418.9494	1418.9494
1443.7096	1443.7096
1449.0390	1449.0387
1484.6961	1484.6961
1486.4546	1486.4545
1492.5442	1492.5442
1493.8763	1493.8761
1494.5087	1494.5086
1497.9764	1497.9740
1498.0918	1498.0911
1500.3382	1500.3325
1510.1311	1510.1311
1510.6408	1510.6408
1512.8024	1512.8024
1523.1337	1523.1331
1534.2304	1534.2303
1535.1737	1535.1737
1561.3521	1559.3339
1573.3772	1572.2016
1585.4718	1585.4718
1586.7965	1586.7964
1590.5558	1590.5556
1594.7654	1594.7654
1600.1433	1600.1433
1600.8311	1600.8311
1611.8867	1611.8867
1614.9766	1614.9766
1618.5489	1618.5487
1620.3016	1620.3016
1623.1610	1623.1609
1626.7512	1626.7511

1627.2828	1627.2827
1664.3865	1664.3692
2920.6484	2917.2289
3033.6706	3033.6706
3045.9256	3045.9061
3062.2978	3054.4653
3101.6523	3101.6523
3124.6714	3124.6707
3144.8844	3144.8844
3149.6571	3149.6568
3221.3635	3221.3635
3222.4981	3222.4981
3225.8968	3225.8968
3226.3675	3226.3675
3227.4272	3227.4271
3227.4768	3227.4768
3228.3086	3228.3086
3234.0432	3234.0432
3235.4262	3235.4262
3236.3411	3236.3411
3238.2070	3238.2070
3240.8400	3240.8400
3242.0476	3242.0476
3243.3475	3243.3475
3243.7128	3243.7128
3245.1646	3245.1646
3246.7203	3246.7203
3252.1058	3252.1058
3254.3711	3254.3711
3259.1068	3259.1068
3270.5145	3270.5140
3319.5347	3319.5347
3792.5548	3792.5516

 I-TS in Scheme 2	
$\text{H}^{16}\text{OOSO}_3$	$\text{H}^{18}\text{OOSO}_3$
-72.7942	-71.9581
11.6768	11.6727
14.5561	14.5564
18.1010	18.0944
28.9578	28.9528
33.4290	33.4136
36.5791	36.5444
39.9182	39.8946
41.9481	41.9332
45.5268	45.5085
49.8823	49.8632
53.5984	53.4724
60.6657	60.5060
62.1169	62.0404
66.1067	66.0513
71.6736	71.4574
76.9160	76.8790
90.2172	90.1478
92.2859	92.1768
98.1771	98.1712
106.3756	105.7531
108.7261	108.5921
114.7397	114.7224
119.8723	119.5414
124.6317	124.6303
127.6421	127.2485
131.8441	131.7811
137.5732	137.5631
140.6085	140.4956
141.8852	141.8410
150.5384	150.0023
161.7066	161.6362
165.2889	165.2804
180.0748	180.0417
184.6459	184.6237
191.2659	191.2344
204.9796	204.9791
222.3379	222.3357
235.8916	235.7446

240.2886	238.0470
246.9267	244.8165
249.2645	248.8909
257.8353	256.4314
263.6553	262.9664
271.5588	270.7279
276.4108	276.3705
296.0050	295.9424
302.9581	302.9204
306.6839	306.4894
318.8848	316.9442
326.3458	318.8854
335.5193	335.4441
348.5398	348.5089
363.0370	363.0369
377.6373	376.8781
384.9317	381.0912
389.8185	386.0057
398.6314	398.6247
421.8999	421.8407
434.6495	434.6474
439.0328	439.0263
444.6679	444.6401
451.6534	451.6409
459.8458	459.8206
465.7114	465.7109
467.1787	467.1771
471.1475	471.1444
474.4345	474.3722
479.2189	479.1902
484.2951	484.2313
500.0464	499.2412
511.7798	511.7526
524.0880	524.0877
531.5664	531.5664
541.0574	541.0528
543.0204	543.0201
553.8604	553.8593
560.2073	558.3862
564.4899	564.4168
613.8222	613.8222
624.0380	624.0107
644.6575	644.6211
648.0088	647.4200
648.3787	648.3177

651.2397	651.2366
663.0822	663.0822
675.0634	675.0634
681.4289	681.4288
684.9811	684.9809
686.6646	686.6553
693.0247	692.6529
694.6202	694.5845
695.3280	695.3254
704.3740	704.3613
720.3238	720.3187
753.0895	753.0895
754.4045	754.4025
760.6373	760.6372
769.7914	769.7880
773.7399	773.7399
775.9340	775.9330
778.5002	778.4998
781.4154	781.4143
787.0694	787.0641
790.3908	790.3907
793.9185	793.9165
810.3020	810.3009
816.0765	816.0765
852.3453	852.3453
855.7495	855.7492
856.6271	856.6232
861.3616	861.3616
887.4086	885.4995
898.2717	895.9862
913.8367	898.2811
925.9591	925.9591
929.4608	929.4552
931.0063	931.0058
939.6906	939.6906
956.5697	956.5697
964.9289	964.9279
983.4116	980.4318
989.7535	988.2636
1007.2784	1007.2783
1007.8504	1007.8504
1012.4362	1012.4361
1022.1301	1022.1301
1028.3051	1028.3035
1034.1963	1034.1959

1038.5840	1038.5840
1047.7002	1047.6994
1047.9615	1047.9615
1055.6909	1055.6909
1056.2902	1056.2901
1056.9325	1056.9325
1057.9482	1057.9482
1058.8476	1058.8476
1062.2713	1062.2712
1062.4746	1062.4746
1066.9993	1066.9987
1067.5238	1067.5237
1069.4014	1069.3426
1072.3857	1072.3857
1077.3828	1077.3822
1079.2376	1079.2361
1086.0482	1086.0478
1089.9185	1089.9185
1103.5639	1103.5636
1109.6902	1109.6902
1119.2620	1119.2616
1120.1235	1120.1234
1123.8462	1123.8462
1125.0775	1125.0775
1140.8963	1140.8963
1142.2246	1142.2242
1159.9468	1159.9447
1169.9695	1169.9695
1170.6455	1170.5630
1172.3594	1172.3590
1206.9556	1206.9556
1208.8043	1208.8043
1211.4809	1211.4809
1214.5781	1214.5781
1229.2585	1229.2583
1242.2798	1242.2798
1280.4908	1280.4908
1284.4968	1284.4964
1287.2406	1287.2402
1289.8749	1289.8748
1303.9669	1303.9669
1305.8486	1305.8482
1309.3857	1309.3857
1334.3871	1334.3871
1339.4479	1339.4470

1341.9469	1341.9467
1351.6152	1351.6150
1354.6330	1354.6330
1357.7508	1357.6889
1368.3021	1368.3020
1370.5653	1370.5649
1374.6984	1374.6983
1414.5523	1414.5365
1420.6981	1420.6981
1442.1611	1442.1611
1449.7493	1449.7488
1484.0472	1484.0472
1486.3782	1486.3782
1493.1415	1493.1415
1493.6376	1493.6376
1494.6692	1494.6692
1497.1553	1497.1553
1498.6430	1498.6429
1505.6943	1505.6753
1509.9680	1509.9680
1510.5819	1510.5818
1510.8263	1510.8263
1527.5913	1527.5863
1530.9094	1530.9094
1534.4963	1534.4963
1553.2261	1552.6500
1585.0607	1585.0607
1586.2309	1586.2308
1589.8950	1589.8949
1594.1841	1594.1841
1599.7625	1599.7624
1600.6985	1600.6985
1611.0827	1611.0827
1614.5188	1614.5187
1616.3463	1616.3463
1619.6305	1619.6304
1621.8823	1621.8820
1625.5731	1625.5676
1627.1246	1627.1204
1641.4403	1639.5198
2561.4424	2550.2018
3033.6760	3033.6760
3034.3495	3034.3493
3101.4280	3101.4280
3110.2603	3110.2603

3134.5210	3134.5207
3145.3312	3145.3312
3221.0300	3221.0300
3221.8236	3221.8236
3224.5871	3224.5871
3226.1679	3226.1679
3226.5287	3226.5287
3228.1200	3228.1200
3228.1357	3228.1357
3233.7392	3233.7392
3234.9186	3234.9186
3236.1891	3236.1891
3237.6961	3237.6961
3241.5827	3241.5827
3242.4550	3242.4550
3242.6056	3242.6056
3244.2891	3244.2891
3246.5483	3246.5483
3247.9217	3247.9217
3248.2331	3248.2331
3252.0833	3252.0833
3257.1553	3257.1553
3274.4080	3274.4080
3275.9084	3275.9084

$\left[\begin{array}{c} \text{Terpy} \diagup \text{Mn}^{\text{III}} \text{O} \diagdown \text{Mn}^{\text{IV}} \text{OOSO}_3^- \\ \text{AcO} \diagdown \text{Mn}^{\text{III}} \diagup \text{O} \diagup \text{Mn}^{\text{IV}} \diagdown \text{Terpy} \end{array} \right]^{-0}$ II in Scheme 2	
$\text{Mn}^{\text{IV}}\text{-}^{16}\text{OOSO}_3$	$\text{Mn}^{\text{IV}}\text{-}^{18}\text{OOSO}_3$
14.0143	14.0100
19.2427	19.2421
21.3900	21.3873
27.0585	27.0383
35.1054	35.0989
40.4110	40.3985
45.9362	45.8603
46.1582	46.1534
48.8364	48.7691
56.1408	56.0698
62.3393	62.3162
73.5609	73.5036
79.6190	79.6002
90.4719	90.4436
96.5295	96.2593
100.0633	99.9941
107.9879	107.8965
113.5680	112.6909
114.1715	113.9621
124.6787	124.6739
129.3850	129.1503
140.0776	140.0252
141.5072	141.3631
152.1599	152.1345
161.1896	160.7250
163.7973	163.7006
179.7850	179.4521
191.7934	191.5778
194.5082	194.3933
198.7044	198.6193
221.1085	221.0926
227.2967	227.1505
242.0586	241.3770
244.5429	242.4004
249.3065	247.8251
259.9929	259.0434
264.2840	261.9202
271.7204	271.4108
281.9242	281.6821
286.3476	286.1927

302.8798	302.5415
311.2089	310.0111
312.9806	312.6858
332.3324	330.6108
340.5812	338.4813
355.8939	353.9080
363.6687	363.6652
382.9625	382.7468
389.5667	388.6963
410.1601	406.5471
434.0521	433.9110
436.5830	436.5306
443.0189	442.9956
452.0077	451.9660
457.9517	457.8260
463.4804	458.7905
465.0343	463.4129
465.9812	465.0393
472.2413	467.7316
476.8294	475.4051
486.0941	485.5570
498.5274	498.0338
504.3852	503.1921
511.5589	511.3624
515.6834	515.3462
534.8491	534.8490
539.9772	539.9704
541.6825	541.6821
553.6331	553.6269
558.4756	556.0206
594.7112	594.0603
614.7185	614.6675
637.3299	636.9242
642.2965	642.2960
646.8598	646.8212
649.7677	649.7671
662.5720	662.5715
673.7843	673.7818
681.9535	681.9534
684.4457	684.4448
685.3674	685.3650
693.3068	692.2067
694.4580	694.2474
694.9045	694.4806
705.3396	705.3341

725.2226	725.1304
752.9789	752.9788
754.9397	754.9337
763.2347	763.2344
770.7748	770.7671
773.6312	773.6309
778.1059	778.1058
782.5310	782.5287
783.7138	783.7120
790.6948	790.6936
791.9119	791.9110
808.9658	808.9650
818.1643	818.1643
851.9032	851.9032
856.4567	856.4540
857.5318	857.5240
862.6593	862.6591
894.1817	871.1788
894.9180	894.1877
930.1839	930.1839
930.5594	930.5594
932.1646	932.1541
935.2029	935.1989
960.0061	960.0061
960.4499	960.4490
981.3505	981.2978
1009.8503	1009.8502
1010.6174	1010.6174
1015.6676	1015.6676
1016.5353	1016.5328
1022.3380	1022.3380
1034.6979	1034.6976
1037.7231	1037.7231
1046.1012	1046.1011
1049.3577	1049.3563
1053.8455	1053.8455
1056.1001	1056.0999
1056.7232	1056.7232
1057.0050	1057.0048
1057.4774	1057.4774
1058.8185	1058.8182
1062.1304	1062.1303
1065.2672	1065.2601
1066.5228	1066.5227
1070.5290	1070.5288

1072.7572	1072.7478
1079.2896	1079.2893
1088.5701	1088.5701
1104.6788	1104.6778
1110.0731	1110.0731
1115.4426	1115.4391
1120.9955	1120.9954
1123.5774	1123.5774
1126.1136	1126.1136
1140.1191	1140.1191
1141.5633	1141.5615
1144.7141	1144.6876
1164.5119	1164.4862
1168.9129	1168.9129
1173.2131	1173.2128
1205.8790	1205.8790
1207.1967	1207.1967
1209.9219	1209.9218
1213.3313	1213.3313
1227.3412	1227.3411
1242.3674	1242.3674
1278.6717	1278.6717
1283.9828	1283.9826
1286.7324	1286.7319
1289.6231	1289.6230
1302.3803	1302.3803
1303.0667	1303.0665
1329.5824	1329.5823
1332.1250	1332.1249
1335.1107	1335.1096
1337.7286	1337.7280
1347.7115	1347.7114
1352.2163	1352.2163
1364.5098	1364.5097
1366.3077	1366.3077
1372.5163	1372.5162
1417.2565	1417.2565
1440.3075	1440.3075
1445.8502	1445.8485
1483.3925	1483.3925
1485.4360	1485.4360
1492.2962	1492.2962
1492.6645	1492.6644
1494.6427	1494.6426
1496.6084	1496.6084

1499.0541	1499.0541
1509.6946	1509.6943
1509.9407	1509.9407
1512.4624	1512.4624
1529.4284	1529.4284
1532.3608	1532.3608
1584.8768	1584.8768
1585.8027	1585.8027
1590.1198	1590.1197
1595.0337	1595.0337
1600.6251	1600.6251
1600.9172	1600.9172
1609.6254	1609.6254
1610.7821	1610.7819
1613.3559	1613.3558
1615.3141	1615.3138
1616.7174	1616.7174
1621.3372	1621.3371
1626.9268	1626.9268
3030.6367	3030.6367
3099.0188	3099.0188
3139.9356	3139.9356
3219.0436	3219.0436
3220.7302	3220.7302
3224.4849	3224.4849
3225.4751	3225.4751
3225.7053	3225.7053
3227.0807	3227.0807
3229.0492	3229.0492
3231.8046	3231.8046
3235.2607	3235.2607
3236.5090	3236.5090
3236.6232	3236.6232
3240.4374	3240.4374
3240.8084	3240.8084
3242.4830	3242.4830
3242.5570	3242.5570
3244.4257	3244.4257
3247.6730	3247.6730
3250.4496	3250.4496
3250.8615	3250.8615
3254.0917	3254.0917
3256.2179	3256.2179
3264.6970	3264.6970

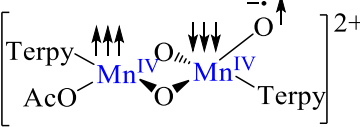
 II-TS in Scheme 2	
Mn^{IV} - ¹⁶OOSO₃	Mn^{IV} - ¹⁸OOSO₃
-702.3289	-680.1819
15.7301	15.7253
17.1499	17.1434
24.7919	24.7919
27.8060	27.7995
35.5313	35.5257
41.2224	41.1871
44.0699	44.0628
49.5843	49.5260
51.1657	51.1099
60.9091	60.8741
64.8095	64.7355
69.4226	69.3864
77.9530	77.9337
93.0321	93.0230
99.0408	98.7840
101.9007	101.8290
113.1747	112.5212
121.0629	121.0196
122.3119	122.3031
130.6829	130.5268
137.3364	137.3020
142.3563	142.2577
161.1659	161.1547
165.5614	165.2528
176.0894	175.7222
178.1041	177.9741
196.2419	195.9880
207.9641	207.1249
218.3340	218.1617
224.9139	223.8059
230.4036	226.3853
233.4410	231.1460
250.2877	250.0701
253.9707	253.8123
261.6522	260.5049
272.7268	271.9829
281.6094	281.4482
289.4950	288.7253
304.3074	303.1289

305.0835	304.7195
309.9912	309.9311
325.2963	324.5170
340.4381	340.3990
346.1343	345.8871
349.2014	349.1660
361.7019	360.9879
379.1853	377.6434
388.5490	388.3657
392.7385	392.6615
420.1234	419.1227
433.0793	431.7423
450.6309	450.6028
451.4399	451.3694
456.1588	456.1483
457.3231	457.3038
460.9102	460.9095
464.0934	464.0626
483.4012	483.2614
484.5645	484.5093
490.5796	490.5518
495.0778	494.3514
506.7329	506.6393
517.9401	516.3905
529.1139	528.4720
538.8243	538.7730
540.4441	540.4385
540.6111	540.5746
553.0730	553.0661
553.5849	553.5656
615.4999	614.7256
615.9890	615.6676
639.6527	628.4747
641.8363	639.9725
643.0675	641.9592
644.5741	643.0818
650.3325	645.9893
681.4434	681.3033
681.9133	681.8745
682.2955	682.2921
683.4762	683.4749
690.1537	689.8997
691.6367	691.6300
705.0226	705.0157
705.5152	705.4966

753.7965	752.8166
754.2546	754.0407
756.1799	755.1464
767.6529	767.6109
770.1741	770.1584
779.1510	779.0765
780.1636	780.0876
781.8858	781.8701
783.0810	783.0576
786.6262	786.5193
792.5876	792.5862
793.4881	793.4450
808.2528	808.2485
810.6477	810.6437
855.1069	855.1069
856.4957	856.4948
857.7407	857.7398
858.2631	858.2626
893.2867	893.2867
929.0102	929.0101
930.1405	930.1394
934.0287	934.0280
935.5742	935.5741
958.7979	958.3026
960.1965	960.1964
960.9168	960.9163
1004.0685	1004.0685
1009.6075	1009.6066
1016.8966	1016.8962
1020.5817	1020.5817
1032.6754	1032.6754
1033.8656	1033.8622
1046.4227	1046.4226
1047.3081	1047.3043
1054.9850	1054.9849
1055.3334	1055.3334
1055.7887	1055.7887
1056.2867	1056.2867
1057.6447	1057.6447
1059.2746	1059.2746
1061.0063	1061.0062
1063.1999	1063.1958
1063.7659	1063.7654
1069.3150	1069.2975
1071.7805	1071.7804

1072.9002	1072.9002
1077.7168	1077.7115
1086.3947	1086.3947
1095.6098	1095.6021
1102.0647	1102.0645
1103.5933	1103.5926
1111.8545	1111.8523
1113.4034	1113.4034
1118.8305	1118.8304
1119.7423	1119.7373
1121.8022	1121.8003
1139.0597	1139.0597
1139.6894	1139.6883
1170.1841	1170.1840
1171.1936	1171.1932
1205.6982	1205.6982
1207.2321	1207.2320
1207.3337	1207.3335
1208.4158	1208.4157
1219.8665	1219.8664
1221.1361	1221.1361
1279.5952	1279.5951
1282.4203	1282.4203
1284.7912	1284.7911
1287.3325	1287.3323
1298.4354	1298.4353
1299.8292	1299.8291
1322.2329	1322.2322
1328.6835	1328.6831
1332.3622	1332.3608
1343.3762	1343.3761
1344.5138	1344.5135
1358.6137	1358.6131
1362.5445	1362.5444
1366.3768	1366.3766
1370.5056	1370.5036
1415.0214	1415.0214
1443.5528	1443.5519
1446.8592	1446.8589
1483.8822	1483.8822
1485.7074	1485.7069
1492.6458	1492.6458
1493.1950	1493.1949
1493.3940	1493.3939
1497.1100	1497.1100

1499.0120	1499.0120
1505.7456	1505.7455
1507.2007	1507.2003
1512.5964	1512.5964
1525.3454	1525.3454
1527.8439	1527.8435
1584.9561	1584.9560
1586.9936	1586.9936
1590.3868	1590.3868
1591.4559	1591.4559
1599.0026	1599.0025
1603.1559	1603.1559
1610.5390	1610.5390
1614.2409	1614.2399
1614.7930	1614.7921
1620.0230	1620.0223
1620.2719	1620.2718
1623.6992	1623.6992
1627.0331	1627.0320
3029.7681	3029.7681
3098.5366	3098.5366
3138.4077	3138.4077
3222.2696	3222.2696
3224.2520	3224.2520
3224.7452	3224.7452
3226.1064	3226.1064
3226.3876	3226.3876
3227.5297	3227.5297
3232.7281	3232.7281
3234.1583	3234.1583
3235.1578	3235.1578
3237.1339	3237.1339
3237.4203	3237.4203
3240.0197	3240.0197
3240.1123	3240.1123
3240.9719	3240.9719
3242.0441	3242.0441
3243.8598	3243.8598
3244.9343	3244.9343
3245.2202	3245.2202
3248.2064	3248.2064
3252.5199	3252.5199
3258.4752	3258.4751
3279.6992	3279.6992

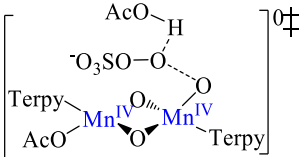
 III in Scheme 2	
Mn^{IV} - ¹⁶O[•]	Mn^{IV} - ¹⁸O[•]
18.8935	18.8843
25.3091	25.3099
35.7481	35.7368
37.0296	37.0271
48.8546	48.8278
51.6040	51.5451
54.1302	54.0879
60.7010	60.6588
73.4662	73.4354
77.6468	77.5696
95.9467	95.9465
105.0396	104.9961
117.1887	113.5941
125.4549	125.0795
129.4410	129.3606
134.3621	133.8244
139.9565	139.2501
150.2309	149.7220
157.6747	156.8949
167.2225	167.0737
170.7872	170.1295
193.5732	193.2045
197.3632	197.1594
214.0386	211.9522
223.9795	223.8742
228.2246	227.9486
232.9058	230.7572
240.9916	239.5922
256.7111	256.7060
262.0803	261.7037
278.4201	277.5013
280.4986	279.7289
294.2227	291.8421
294.7193	294.4609
300.0831	299.9035
307.0914	307.0862
327.5599	327.4832
337.1328	336.2560
349.7752	349.2763
350.3035	350.1978

370.5143	370.0629
389.1650	389.0404
401.7938	401.0649
410.0433	406.6012
448.4423	448.2935
452.0935	452.0622
456.8605	456.8494
458.9793	458.9352
459.6945	459.6289
464.0582	464.0056
483.4032	483.2665
485.9550	485.6394
488.9158	488.8561
491.1159	490.5590
512.1350	507.1285
527.8722	526.0154
535.5730	535.2779
539.2482	537.7606
553.3198	541.5122
554.2710	554.2301
556.6794	556.6092
611.1304	611.1298
637.2386	637.2338
641.4093	641.4089
643.2753	643.2315
681.2101	681.2100
681.9134	681.9132
685.4117	685.4099
686.4816	686.4643
692.8079	692.8022
695.0481	695.0479
705.7437	705.6565
706.0922	706.0837
726.3643	725.4944
755.0344	755.0335
757.3649	757.3634
762.6485	762.4721
770.9675	770.9546
775.6129	775.6037
778.9435	778.9342
782.6496	782.6165
783.5535	783.5296
785.2859	785.2793
794.1713	794.1655
795.8126	795.8126

805.1787	805.1754
809.8273	809.8272
854.0222	854.0153
855.6147	855.6146
856.3169	856.3154
859.3829	859.3828
898.5023	898.5023
930.6762	930.6762
933.4552	933.4545
936.8609	936.8605
938.7373	938.7373
956.1561	956.1559
966.8884	966.8884
1010.3488	1010.3486
1017.3319	1017.3318
1017.5033	1017.5031
1024.7633	1024.7633
1033.7432	1033.7431
1035.8053	1035.7999
1048.6619	1048.6619
1049.6507	1049.6451
1056.8500	1056.8500
1058.7053	1058.7053
1059.7541	1059.7541
1060.9764	1060.9764
1061.6978	1061.6977
1062.3294	1062.3294
1062.6560	1062.6560
1065.8902	1065.8887
1066.6800	1066.6799
1075.4678	1075.4651
1076.3975	1076.3938
1076.4397	1076.4341
1078.2211	1078.2159
1087.7884	1087.7884
1103.3000	1103.2969
1104.0562	1104.0557
1115.7865	1115.7856
1116.2974	1116.2971
1121.3823	1121.3821
1121.7799	1121.7792
1141.7018	1141.7013
1142.6604	1142.6603
1172.1736	1172.1735
1172.7952	1172.7950

1210.6486	1210.6485
1211.0330	1211.0329
1212.7618	1212.7617
1214.3209	1214.3209
1225.8742	1225.8739
1228.3526	1228.3526
1281.1815	1281.1814
1281.8718	1281.8716
1285.3149	1285.3148
1286.4136	1286.4136
1291.1966	1291.1964
1301.7729	1301.7727
1303.0468	1303.0468
1332.2492	1332.2488
1336.4114	1336.4111
1348.2000	1348.1996
1349.5627	1349.5627
1364.3488	1364.3488
1366.2527	1366.2527
1372.0702	1372.0701
1374.0053	1374.0050
1418.9804	1418.9804
1445.3045	1445.3041
1448.1823	1448.1823
1486.3288	1486.3286
1487.0523	1487.0515
1494.3135	1494.3135
1495.0715	1495.0714
1495.3386	1495.3385
1498.7336	1498.7335
1499.3042	1499.3028
1509.0215	1509.0215
1509.3650	1509.3650
1510.7077	1510.7072
1530.6922	1530.6919
1530.7896	1530.7895
1585.3729	1585.3729
1586.7189	1586.7189
1589.8616	1589.8616
1590.7148	1590.7147
1596.5741	1596.5741
1600.9268	1600.9268
1612.5100	1612.5092
1613.1014	1613.1013
1619.7164	1619.7155

1621.1116	1621.1116
1622.5191	1622.5186
1624.1334	1624.1334
1642.3881	1642.3880
3034.2950	3034.2950
3103.8304	3103.8304
3144.7467	3144.7467
3227.3988	3227.3988
3229.6192	3229.6192
3230.4380	3230.4380
3230.6161	3230.6161
3230.6276	3230.6276
3233.0007	3233.0007
3236.7234	3236.7234
3238.6857	3238.6857
3240.2824	3240.2824
3240.6540	3240.6540
3241.2957	3241.2957
3242.6420	3242.6420
3243.3323	3243.3323
3244.8745	3244.8745
3246.0205	3246.0205
3247.1559	3247.1559
3249.2841	3249.2841
3250.2604	3250.2604
3253.4011	3253.4011
3253.6664	3253.6664
3254.3205	3254.3205
3276.0725	3276.0725

 III-TS1 in Scheme 2		
Mn^{IV}–¹⁶O•---¹⁶OOSO₃	Mn^{IV}–¹⁶O•---¹⁸OOSO₃	Mn^{IV}–¹⁸O•---¹⁶OOSO₃
-622.6774	-608.0655	-603.7196
14.3035	14.2923	14.2952
16.2608	16.2524	16.2549
18.9892	18.9844	18.9889
24.5753	24.5748	24.5737
27.4596	27.4461	27.4515
34.6057	34.5958	34.5940
43.1140	43.1059	43.1072
43.7998	43.7782	43.7796
49.8704	49.8522	49.8425
52.1753	52.1071	52.0850
54.6172	54.6091	54.5798
59.3461	59.3027	59.3150
59.9063	59.8874	59.8910
63.8598	63.8363	63.8425
67.7073	67.6596	67.6832
72.9935	72.8909	72.9515
78.8077	78.7939	78.8048
86.9817	86.7764	86.9255
87.8276	87.8254	87.8271
98.7209	97.8930	98.5888
102.3931	101.9666	102.2985
105.8161	105.7601	105.7942
117.8989	117.8737	117.7639
124.0924	124.0140	123.9379
131.4009	131.3971	131.3286
137.0790	136.8638	137.0160
140.2607	140.2311	139.9867
143.1191	143.0468	142.9824
150.7110	150.5544	150.5019
151.4047	151.3176	150.9231
158.8044	158.7722	158.7102
167.7906	167.7800	167.6935
172.8440	172.6643	172.3587
185.5333	185.4468	184.7064
195.7261	195.6475	195.6925
213.9804	213.9578	212.2253
218.6987	218.6808	217.2318
223.3479	223.2900	222.9182

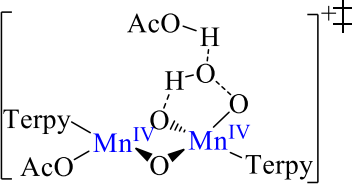
233.6896	233.6134	230.5187
248.4477	248.3412	248.3760
251.1924	249.6212	250.8505
254.8215	254.5764	253.9533
262.5546	258.8373	261.9751
271.9111	270.5433	271.7711
281.4804	280.9068	281.4029
286.6554	286.3438	286.1707
297.5980	297.2581	296.5354
306.8609	306.5864	306.7047
310.4522	309.3201	309.6551
320.0174	319.1629	318.9297
326.6367	326.5730	325.9807
345.7328	345.6499	345.6659
347.3005	347.1619	346.9746
355.2016	354.7795	354.7517
368.0517	365.4733	367.9259
379.4481	375.9682	378.6605
388.1607	388.0884	387.8493
399.8554	398.3072	399.6071
420.4224	420.0465	420.1489
447.2536	444.7001	446.1739
448.6919	447.8909	447.9238
452.9600	452.9390	452.9494
454.1398	454.1273	454.1144
456.4008	455.9097	456.1222
458.5439	457.4905	457.5824
462.1423	462.0963	462.0942
466.9697	466.9124	466.8886
484.7987	484.7758	484.7739
486.3156	485.8304	485.6253
490.7910	490.7738	490.7487
491.4081	490.8653	491.1117
499.0467	498.8219	498.4634
506.8897	506.8855	506.8335
516.8862	515.2787	516.3191
540.4119	540.4101	540.4105
542.1587	542.1490	542.1444
551.4630	551.4629	551.4629
552.8495	552.7998	552.7848
557.9127	556.5249	556.9254
586.7941	586.7855	586.7237
600.0526	599.9508	598.0845
610.6844	609.6516	603.0807
613.9723	613.9437	613.7667

628.1685	626.7595	618.2225
632.0999	630.8832	631.8583
639.8053	639.7590	639.6329
641.4490	641.4446	641.4278
643.3712	643.3228	643.2527
649.0650	647.8798	646.2905
680.8162	680.7986	680.7091
681.5175	681.5087	681.4781
682.0100	682.0091	682.0063
683.4460	683.4456	683.4450
688.8738	688.8560	688.7953
691.5780	691.5775	691.5753
705.0896	705.0891	705.0864
706.1547	706.1543	706.1479
726.2879	726.2208	726.0979
753.7190	753.7189	753.7183
754.1300	754.1289	754.1193
767.4512	767.4484	767.4305
769.2842	769.2840	769.2804
779.6128	779.6102	779.5240
780.2958	780.2749	780.2904
781.6251	781.6177	781.5891
782.8323	782.8275	782.8217
785.3047	785.2612	785.2714
792.7112	792.7082	792.7081
793.6316	793.6220	793.6263
809.2437	809.2436	809.2424
813.1389	813.1385	813.1348
854.7805	854.7803	854.7805
856.4631	856.3912	856.4623
857.2329	857.1452	857.2311
857.8834	857.8622	857.8824
858.8765	857.9462	858.8747
882.5884	861.3050	882.4167
892.9661	892.9635	892.9659
929.0533	929.0533	929.0533
934.6320	934.6284	934.6305
936.8162	936.8161	936.8161
938.8807	938.8807	938.8804
955.9175	955.9175	955.9173
962.5885	962.5885	962.5885
985.7272	985.3076	985.6490
1004.5046	1004.5046	1004.5045
1016.9342	1016.9340	1016.9341
1022.3205	1022.3193	1022.3197

1027.9522	1027.9522	1027.9519
1032.6159	1032.6159	1032.6159
1033.6673	1033.6670	1033.6630
1045.9651	1045.9651	1045.9651
1046.8394	1046.8388	1046.8385
1049.9438	1049.9356	1049.9423
1053.1141	1053.1140	1053.1139
1056.1062	1056.1061	1056.1062
1056.6677	1056.6677	1056.6676
1057.2455	1057.2454	1057.2453
1058.3675	1058.3675	1058.3675
1059.8474	1059.8474	1059.8474
1061.2000	1061.2000	1061.2000
1062.9252	1062.9250	1062.9250
1064.5465	1064.5462	1064.5380
1069.9586	1069.9585	1069.9564
1070.2915	1070.2915	1070.2851
1073.2777	1073.2774	1073.2769
1074.8388	1074.8377	1074.8271
1086.0723	1086.0723	1086.0723
1101.3627	1101.3624	1101.3626
1103.3320	1103.3316	1103.3311
1105.1913	1105.1913	1105.1913
1111.7067	1111.7067	1111.7067
1114.7537	1114.7535	1114.7503
1118.7568	1118.7568	1118.7568
1120.8123	1120.8122	1120.8118
1138.4771	1138.4771	1138.4770
1138.7605	1138.7605	1138.7586
1169.8502	1169.8502	1169.8502
1170.7279	1170.7276	1170.7275
1172.2648	1172.2390	1172.2645
1181.4585	1181.4556	1181.4565
1204.4379	1204.4378	1204.4378
1206.0231	1206.0231	1206.0231
1206.4519	1206.4518	1206.4518
1208.3487	1208.3487	1208.3487
1220.3816	1220.3816	1220.3816
1222.9072	1222.9070	1222.9069
1244.0326	1244.0017	1244.0289
1279.5860	1279.5859	1279.5859
1281.9883	1281.9882	1281.9882
1284.7151	1284.7151	1284.7150
1288.0421	1288.0415	1288.0418
1298.1620	1298.1620	1298.1620

1301.5434	1301.5433	1301.5433
1322.8240	1322.8237	1322.8238
1329.0193	1329.0191	1329.0188
1331.3260	1331.3242	1331.3246
1342.1896	1342.1896	1342.1895
1342.8751	1342.8750	1342.8750
1360.5496	1360.5485	1360.5481
1361.6788	1361.6787	1361.6787
1366.3215	1366.3213	1366.3214
1369.6389	1369.6382	1369.6373
1403.2608	1403.2405	1403.2526
1415.0802	1415.0802	1415.0802
1439.4153	1439.4141	1439.4149
1445.6107	1445.6106	1445.6104
1446.5460	1446.5459	1446.5439
1483.0239	1483.0239	1483.0239
1485.0975	1485.0973	1485.0973
1492.5295	1492.5295	1492.5295
1492.7839	1492.7839	1492.7839
1493.5009	1493.5009	1493.5007
1495.9014	1495.9014	1495.9014
1498.8608	1498.8608	1498.8606
1499.8367	1499.8365	1499.8366
1504.8460	1504.8460	1504.8460
1507.4436	1507.4436	1507.4430
1512.7861	1512.7861	1512.7861
1514.1663	1514.1663	1514.1663
1524.9335	1524.9335	1524.9335
1527.8715	1527.8711	1527.8710
1585.9054	1585.9054	1585.9053
1586.7850	1586.7850	1586.7849
1589.9891	1589.9891	1589.9891
1591.5775	1591.5775	1591.5775
1602.0544	1602.0544	1602.0541
1602.5226	1602.5226	1602.5226
1609.7916	1609.7915	1609.7916
1611.4551	1611.4545	1611.4546
1617.4816	1617.4814	1617.4807
1619.2717	1619.2717	1619.2717
1620.8130	1620.8130	1620.8124
1623.3376	1623.3376	1623.3376
1626.7022	1626.7019	1626.7012
1720.5032	1720.4975	1720.5014
3029.4796	3029.4796	3029.4796
3039.7833	3039.7833	3039.7833

3098.5324	3098.5324	3098.5324
3115.0658	3115.0658	3115.0658
3138.0106	3138.0106	3138.0106
3154.7939	3154.7939	3154.7939
3220.9631	3220.9631	3220.9631
3223.2502	3223.2502	3223.2502
3224.3095	3224.3095	3224.3095
3224.4046	3224.4046	3224.4046
3224.7736	3224.7736	3224.7736
3226.8356	3226.8356	3226.8356
3231.2619	3231.2619	3231.2619
3232.8191	3232.8191	3232.8191
3233.8133	3233.8133	3233.8133
3235.4796	3235.4796	3235.4796
3235.9591	3235.9591	3235.9591
3236.8919	3236.8919	3236.8919
3238.8164	3238.8163	3238.8164
3240.0956	3240.0956	3240.0956
3241.3183	3241.3183	3241.3183
3243.5224	3243.5224	3243.5224
3244.7121	3244.7121	3244.7121
3246.6880	3246.6880	3246.6880
3247.2223	3247.2223	3247.2223
3250.1026	3250.1026	3250.1026
3251.1663	3251.1663	3251.1663
3280.6102	3280.6102	3280.6102
3406.8926	3406.8846	3406.8765

 III-TS2 in Scheme 2		
Mn^{IV}-¹⁶O[•]---¹⁶OH₂	Mn^{IV}-¹⁶O[•]---¹⁸OH₂	Mn^{IV}-¹⁸O[•]---¹⁶OH₂
-745.2905	-726.5531	-723.9243
15.3840	15.3680	15.3830
24.5264	24.5264	24.5264
33.4193	33.4009	33.4051
40.8760	40.7959	40.8698
44.3042	44.2779	44.2777
47.1472	47.1301	47.1429
51.7738	51.5806	51.7464
54.0627	53.8275	53.9868
58.9852	58.8899	58.9068
63.9529	63.8171	63.8464
72.6297	72.5071	72.5990
73.5961	73.4586	73.5594
77.2412	77.2138	77.2114
86.8043	86.4862	86.7852
94.1365	94.0608	94.1342
95.2114	94.6743	95.0697
100.4834	100.3610	100.4619
115.6013	115.1486	115.4919
122.4395	122.3487	122.3404
124.5329	124.3931	124.3632
128.4257	127.7598	127.7868
132.0262	131.7354	131.9004
134.9214	133.9161	134.2122
146.4788	145.4409	146.2252
150.8813	150.6438	150.8800
159.0496	158.8569	157.8150
165.3283	164.9568	165.1624
171.8922	171.8235	171.8530
186.7300	186.5590	186.2029
189.5082	189.4191	188.4300
201.7651	201.7443	199.8085
218.4224	218.1688	217.9953
223.3498	223.2315	222.7017
228.3215	228.2304	227.9279
239.9760	235.7673	239.0970
256.3320	252.5502	256.1639
258.2799	257.3240	258.0089

261.1494	260.2999	260.3338
270.1852	269.2250	269.6959
273.8859	273.4076	272.7944
287.8356	287.6478	286.9584
288.9571	288.5979	288.4715
306.8238	306.7383	306.6337
309.3600	309.3470	309.2897
326.0532	325.3347	325.2611
330.5649	330.5613	329.4759
341.8510	341.4467	341.1430
349.1289	349.1207	349.1051
357.9109	357.4480	356.9567
368.5930	368.2299	367.8360
395.1148	395.1017	394.9468
408.6549	407.2952	407.2484
446.6513	446.1207	446.3400
448.3937	448.2624	448.3896
449.9169	449.3825	449.8729
451.5356	451.3412	451.4030
456.4705	456.4639	456.4650
460.2914	460.1558	460.2055
462.8516	462.8312	462.8372
465.1328	465.0476	465.0770
483.4590	483.4425	483.3409
484.8332	484.8133	484.6839
490.1548	490.1463	490.1312
493.6614	493.5346	492.4428
510.1556	510.1327	510.0749
539.9849	539.9747	539.9813
541.0199	541.0174	541.0193
552.9805	552.9804	552.9801
554.8382	554.8365	554.8171
595.0169	594.1337	594.0407
607.3669	607.1446	605.5141
613.2854	613.2851	613.2807
621.2082	620.8715	613.8007
629.3915	626.9659	621.8321
639.0004	638.9888	638.9938
640.5815	640.5470	640.5105
641.6939	641.6929	641.6922
661.0301	660.6151	656.0704
680.7136	680.6652	680.6894
680.9288	680.8969	680.9169
682.3287	682.3219	682.3244
682.9500	682.9494	682.9431

690.2052	690.2025	690.1404
691.8980	691.8969	691.8977
698.4488	697.3651	697.7548
704.4356	704.4023	704.4287
706.2847	706.1829	705.8735
753.2359	753.2351	753.2355
755.1601	755.1600	755.1256
762.9589	762.9282	762.9048
768.4730	768.4716	768.4656
774.2786	774.2177	774.2328
780.7985	780.7981	780.7952
782.3436	782.3358	782.3304
783.0997	783.0987	783.0640
784.5162	784.5155	784.5153
792.4043	792.4029	792.4015
793.7637	793.7561	793.7379
808.7298	808.7261	808.7230
811.0330	811.0308	811.0292
854.6549	854.6549	854.6549
855.3689	855.3686	855.3682
856.0190	856.0183	856.0175
857.3891	857.3890	857.3873
866.3730	866.3427	866.3479
894.0062	894.0059	894.0051
932.2639	932.2639	932.2639
933.9928	933.9902	933.9899
936.8109	936.8108	936.8108
937.7856	937.7855	937.7855
959.4754	959.4754	959.4754
961.9168	961.9168	961.9167
1010.7906	1010.7765	1010.7686
1011.3932	1011.3912	1011.3908
1016.8124	1016.8063	1016.8020
1019.8766	1019.8681	1019.8696
1032.3810	1032.3449	1032.3436
1033.7214	1033.6432	1033.6619
1039.4831	1037.9065	1037.6456
1046.6652	1046.6640	1046.6638
1048.0133	1047.9773	1047.9750
1052.8123	1052.7795	1052.7802
1053.4635	1053.4629	1053.4624
1055.4138	1055.4130	1055.4134
1057.9326	1057.9317	1057.9322
1057.9881	1057.9818	1057.9824
1059.2136	1059.2129	1059.2133

1060.5316	1060.5305	1060.5303
1061.8031	1061.8023	1061.8027
1062.6900	1062.6801	1062.6654
1064.6796	1064.6744	1064.6779
1072.1161	1071.4265	1071.9817
1072.5234	1072.4346	1072.4836
1073.7851	1073.7451	1073.7733
1077.2189	1076.9650	1077.1275
1079.1726	1079.0513	1079.1665
1086.3763	1086.3763	1086.3763
1102.9388	1102.9370	1102.9384
1103.6464	1103.6368	1103.6452
1105.2762	1105.2550	1105.2708
1113.8066	1113.8044	1113.8005
1116.3373	1116.3371	1116.3373
1120.0677	1120.0676	1120.0677
1122.1027	1122.1005	1122.1025
1140.1775	1140.1775	1140.1774
1141.6166	1141.6160	1141.6151
1170.8300	1170.8300	1170.8299
1171.6802	1171.6801	1171.6799
1207.1818	1207.1816	1207.1816
1207.4073	1207.4072	1207.4072
1208.6696	1208.6693	1208.6692
1210.5660	1210.5658	1210.5660
1226.4422	1226.4420	1226.4413
1227.4515	1227.4515	1227.4515
1276.2924	1276.2482	1276.2867
1281.3853	1281.3849	1281.3850
1282.1624	1282.1621	1282.1619
1286.0958	1286.0957	1286.0955
1288.1184	1288.1170	1288.1170
1301.2392	1301.2390	1301.2387
1303.6989	1303.6989	1303.6989
1318.9624	1318.9578	1318.9609
1331.5175	1331.5171	1331.5147
1335.3672	1335.3635	1335.3666
1346.0790	1346.0790	1346.0790
1347.3121	1347.3120	1347.3116
1358.1561	1358.1541	1358.1527
1364.5426	1364.5426	1364.5426
1369.9582	1369.9578	1369.9580
1373.0535	1373.0529	1373.0534
1415.8811	1415.8811	1415.8811
1436.1934	1436.1896	1436.1931

1439.3877	1439.3874	1439.3841
1447.3308	1447.3302	1447.3305
1484.1708	1484.1708	1484.1708
1487.7626	1487.7622	1487.7619
1492.5964	1492.5963	1492.5963
1493.0373	1493.0371	1493.0371
1493.1593	1493.1591	1493.1593
1496.6043	1496.5630	1496.6037
1497.4063	1497.4037	1497.4063
1499.5208	1499.5200	1499.5204
1506.2476	1506.2475	1506.2472
1506.9106	1506.9103	1506.9087
1512.5506	1512.5506	1512.5506
1517.7907	1517.7879	1517.7907
1524.5828	1524.3287	1524.5781
1528.3591	1528.3569	1528.3573
1529.1517	1529.1504	1529.1517
1582.7621	1582.7617	1582.7620
1586.5304	1586.5304	1586.5304
1589.3760	1589.3759	1589.3759
1590.4243	1590.4243	1590.4243
1594.3617	1594.3614	1594.3613
1604.0168	1604.0168	1604.0168
1613.2377	1613.2376	1613.2377
1616.7684	1616.7664	1616.7674
1617.6109	1617.6100	1617.6096
1620.7774	1620.7774	1620.7774
1621.4970	1621.4970	1621.4965
1623.6420	1623.6419	1623.6415
1623.9701	1623.9700	1623.9700
1721.9988	1721.9762	1721.9957
2712.5535	2712.3010	2712.4332
3030.3742	3030.3742	3030.3742
3048.9564	3048.9564	3048.9564
3098.9056	3098.9056	3098.9056
3118.9371	3118.9371	3118.9371
3139.7935	3139.7935	3139.7935
3160.8075	3160.8075	3160.8075
3224.6454	3224.6454	3224.6454
3225.0509	3225.0509	3225.0509
3225.7315	3225.7315	3225.7315
3226.1786	3226.1786	3226.1786
3227.4518	3227.4518	3227.4518
3227.5038	3227.5038	3227.5038
3234.4265	3234.4265	3234.4265

3235.5492	3235.5492	3235.5492
3236.2659	3236.2659	3236.2659
3238.0100	3238.0100	3238.0100
3239.1085	3239.1085	3239.1085
3239.6156	3239.6156	3239.6156
3242.0947	3242.0947	3242.0947
3242.4552	3242.4548	3242.4552
3243.1972	3243.1969	3243.1972
3244.9919	3244.9918	3244.9919
3245.0948	3245.0948	3245.0948
3247.1045	3247.1045	3247.1045
3250.7528	3250.7528	3250.7528
3257.0728	3257.0697	3257.0728
3269.1136	3269.1136	3269.1136
3275.3556	3275.3556	3275.3556
3525.7648	3514.0314	3525.7406

$\left[\begin{array}{c} \text{Terpy} \text{---} \text{Mn}^{\text{III}} \text{---} \text{O} \text{---} \text{Mn}^{\text{IV}} \text{---} \text{Terpy} \\ \text{AcO} \text{---} \text{Mn}^{\text{III}} \text{---} \text{O} \text{---} \text{Mn}^{\text{IV}} \text{---} \text{O}_3\text{SO} \end{array} \right]^0$ IV in Scheme 2		
$\text{Mn}^{\text{IV}}\text{--}^{16}\text{O}^{16}\text{OOSO}_3$	$\text{Mn}^{\text{IV}}\text{--}^{16}\text{O}^{18}\text{OOSO}_3$	$\text{Mn}^{\text{IV}}\text{--}^{18}\text{O}^{16}\text{OOSO}_3$
11.5796	11.5709	11.5760
16.3426	16.3414	16.3372
25.3687	25.3610	25.3607
27.8861	27.8815	27.8832
32.5896	32.5814	32.5783
34.8046	34.8025	34.8020
37.2369	37.2053	37.2206
44.1913	44.1528	44.1610
47.4624	47.3383	47.3647
54.0561	54.0328	54.0431
59.6976	59.5707	59.5178
63.3813	63.3443	63.3607
75.6771	75.0449	75.4499
81.4214	80.8327	81.1756
85.3685	84.9692	85.1546
94.3609	94.3385	94.3332
104.9708	104.9452	104.9492
110.8189	110.7914	110.8015
115.5668	115.4974	115.5159
120.9302	120.8924	120.8901
125.7825	125.6683	125.7127
131.9354	131.6934	131.7617
139.1561	139.1220	139.0719
142.3487	142.2608	142.1564
153.2367	153.2227	153.2259
163.2157	163.1597	162.9203
174.2085	174.0808	173.2451
181.2284	181.2135	181.0973
190.9588	190.8819	190.7493
197.5834	197.4768	197.1934
205.6953	204.7286	203.3666
221.9665	221.8891	221.8993
223.1258	222.9996	223.0341
239.5633	239.5433	239.5526
243.4357	242.3252	242.9980
252.9165	251.9621	252.6031
257.2279	256.0271	256.6538
264.6126	263.0738	263.5672
268.4206	268.1370	268.1656

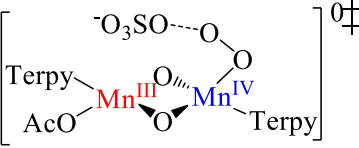
283.4396	283.1292	283.1348
288.0266	287.0202	287.8178
296.6110	295.9418	294.5009
305.3421	304.9844	305.2786
312.5127	312.4282	312.1521
327.9342	325.4853	326.6610
337.7208	335.6434	336.5997
347.4472	347.0501	347.0078
362.5766	357.4184	357.5642
364.9496	364.8886	364.9293
371.3491	369.4894	369.1072
382.3170	382.2803	382.0192
433.3907	433.3752	432.2110
434.7592	434.7177	434.0340
442.2682	442.1984	438.4974
446.5916	446.0994	442.8377
451.6207	451.6123	451.5477
458.0743	456.9047	457.2535
460.0056	459.0736	459.0160
463.5732	463.4025	463.1052
465.9173	465.7022	465.7773
466.8559	466.7058	466.7008
474.3287	474.2155	474.0917
483.5224	483.2042	483.3204
493.7955	493.6961	493.1656
500.8766	500.0011	500.1629
508.4559	508.4535	508.3893
514.2686	512.3409	513.3744
534.4497	534.4497	534.4496
541.9270	541.6416	540.7124
542.6804	542.6284	542.4792
544.9689	544.1643	543.2528
553.1186	553.1152	553.1170
588.9666	582.9377	582.6812
590.4876	589.7332	589.7646
616.0230	616.0156	616.0096
639.9499	639.8691	639.8626
643.5661	643.5618	643.5590
649.6293	649.5658	649.5829
650.6111	650.6013	650.6052
662.6714	662.6704	662.6706
673.6443	673.6435	673.6440
681.5326	681.5323	681.5323
683.8896	683.8883	683.8880
685.4480	685.4478	685.4480

691.2789	691.2677	691.2767
694.5952	694.5950	694.5949
705.8914	701.2774	705.8107
708.4630	706.0195	707.3327
741.2847	741.2569	741.2160
753.3618	753.3612	753.3606
754.8732	754.8723	754.8662
761.6941	761.6938	761.6932
768.5860	768.5815	768.5757
773.2364	773.2364	773.2360
777.6466	777.6435	777.6436
780.8769	780.8676	780.8675
783.3071	783.2898	783.2859
791.3177	791.3159	791.3175
793.7013	793.6924	793.7010
810.2763	810.2745	810.2713
818.7885	818.7885	818.7884
851.8687	851.8687	851.8687
854.7548	854.7546	854.7543
859.1561	859.1549	859.1547
862.7549	862.7549	862.7548
894.3742	894.3741	894.3740
931.0180	931.0179	931.0180
931.3938	931.3027	931.3530
932.2919	932.1141	932.2044
937.2549	936.0170	937.0562
957.3740	937.8085	940.1123
960.0689	957.3740	957.3740
961.5937	961.5896	961.5895
988.0794	985.7906	985.7723
1011.7344	1011.7329	1011.7329
1012.3032	1012.3029	1012.3029
1019.9475	1019.9447	1019.9440
1022.2032	1022.2002	1022.2001
1022.8483	1022.8223	1022.8207
1034.0013	1033.9987	1033.9975
1037.2453	1037.2453	1037.2453
1045.9742	1045.9741	1045.9741
1048.1903	1048.1891	1048.1876
1054.9436	1054.9436	1054.9436
1056.6931	1056.6930	1056.6930
1057.0822	1057.0813	1057.0808
1057.6912	1057.6911	1057.6911
1058.3780	1058.3778	1058.3777
1059.7424	1059.7423	1059.7423

1060.8330	1060.8329	1060.8329
1065.7296	1065.7250	1065.7153
1067.2790	1067.2789	1067.2789
1070.8170	1070.8167	1070.8160
1071.6874	1071.6861	1071.6833
1076.5708	1076.5673	1076.5625
1088.5874	1088.5874	1088.5874
1104.7288	1104.7267	1104.7242
1110.9504	1110.9504	1110.9504
1117.2673	1117.2668	1117.2638
1121.0735	1121.0731	1121.0727
1124.3322	1124.3322	1124.3322
1126.6688	1126.6688	1126.6688
1140.7267	1140.7267	1140.7256
1141.2012	1141.2012	1141.2012
1160.9716	1160.9432	1160.9597
1165.0825	1165.0660	1165.0644
1168.9173	1168.9173	1168.9173
1171.5319	1171.5318	1171.5317
1206.2268	1206.2268	1206.2268
1206.9095	1206.9095	1206.9094
1211.3084	1211.3083	1211.3082
1214.8771	1214.8771	1214.8771
1228.2322	1228.2322	1228.2321
1244.0486	1244.0486	1244.0486
1278.8375	1278.8375	1278.8375
1283.5631	1283.5630	1283.5630
1285.5404	1285.5402	1285.5402
1289.1871	1289.1870	1289.1870
1303.0589	1303.0588	1303.0587
1303.8383	1303.8383	1303.8383
1328.2849	1328.2849	1328.2847
1333.7504	1333.7503	1333.7502
1335.3478	1335.3478	1335.3457
1341.7478	1341.7478	1341.7477
1347.3476	1347.3475	1347.3472
1352.3719	1352.3719	1352.3719
1363.0298	1363.0298	1363.0297
1369.3431	1369.3431	1369.3431
1370.9454	1370.9454	1370.9453
1416.7555	1416.7555	1416.7555
1440.6546	1440.6546	1440.6546
1445.6450	1445.6450	1445.6435
1483.2912	1483.2912	1483.2912
1484.7833	1484.7833	1484.7830

1492.2520	1492.2520	1492.2520
1492.5598	1492.5598	1492.5598
1494.5610	1494.5610	1494.5610
1497.0277	1497.0277	1497.0277
1498.1830	1498.1827	1498.1825
1508.1053	1508.1052	1508.1048
1511.0905	1511.0905	1511.0905
1512.4218	1512.4218	1512.4218
1529.9404	1529.9403	1529.9402
1532.9229	1532.9229	1532.9229
1585.2436	1585.2436	1585.2436
1586.0940	1586.0940	1586.0940
1590.9709	1590.9709	1590.9708
1594.9047	1594.9047	1594.9046
1599.4398	1599.4398	1599.4398
1600.5753	1600.5753	1600.5753
1610.4620	1610.4620	1610.4620
1611.2728	1611.2728	1611.2727
1614.1130	1614.1129	1614.1129
1614.2770	1614.2770	1614.2768
1619.3896	1619.3896	1619.3896
1620.8576	1620.8575	1620.8572
1623.9064	1623.9062	1623.9059
3030.7471	3030.7471	3030.7471
3098.8414	3098.8414	3098.8414
3140.9382	3140.9382	3140.9382
3220.1025	3220.1025	3220.1025
3220.3943	3220.3943	3220.3943
3223.0879	3223.0879	3223.0879
3226.1827	3226.1827	3226.1827
3226.9487	3226.9487	3226.9487
3227.0148	3227.0148	3227.0148
3228.7390	3228.7390	3228.7390
3232.0895	3232.0895	3232.0895
3233.1543	3233.1543	3233.1543
3235.7326	3235.7326	3235.7326
3239.6137	3239.6137	3239.6137
3240.2258	3240.2258	3240.2258
3241.3979	3241.3979	3241.3979
3242.3252	3242.3252	3242.3252
3242.8260	3242.8260	3242.8260
3245.2274	3245.2274	3245.2274
3247.3481	3247.3481	3247.3481
3251.0848	3251.0848	3251.0848
3252.4266	3252.4266	3252.4266

3257.3622	3257.3622	3257.3622
3258.2477	3258.2477	3258.2477
3278.4063	3278.4063	3278.4063

 IV-TS in Scheme 2		
Mn ^{IV} - ¹⁶ O ¹⁶ O---OSO ₃	Mn ^{IV} - ¹⁶ O ¹⁸ O---OSO ₃	Mn ^{IV} - ¹⁸ O ¹⁶ O---OSO ₃
-195.7214	-192.0046	-195.5326
16.1861	16.1847	16.1845
18.8461	18.8229	18.8412
22.4479	22.4478	22.4476
30.7101	30.7052	30.6985
39.2892	39.2082	39.2568
43.9922	43.9112	43.9663
46.6702	46.6086	46.5962
48.4976	48.3890	48.4480
50.2112	50.1598	50.1708
56.9227	56.8458	56.8853
63.8227	63.7010	63.6758
68.1631	68.0211	68.1377
70.4900	70.4148	70.4259
79.0364	78.1260	78.7043
82.7914	82.5086	82.7305
91.3367	91.3318	91.3366
109.2218	109.1627	109.1738
115.5327	115.4098	115.4584
120.8941	120.7800	120.7630
127.4553	127.3424	127.1152
135.1785	135.0848	135.0526
146.5288	146.4285	146.5144
147.9956	147.4097	147.6617
155.1387	155.0683	154.7951
162.6794	162.2385	161.5938
169.7556	169.6843	169.7479
180.8857	180.2360	179.1129
195.0701	194.9335	194.8604
202.0168	201.7136	201.4886
219.5228	219.1975	219.3300
224.0933	223.5914	223.9016
231.5436	231.3253	231.2840
242.2039	239.7787	241.2898
252.2952	252.1838	252.1976
256.1418	255.9484	255.9943
263.3961	260.4015	263.1006
269.8489	268.6352	269.7492
283.4188	283.0611	283.2291

285.6043	285.5063	285.5571
303.4880	303.3255	303.3513
309.1784	308.5106	308.8089
313.5221	312.0494	312.8272
327.3788	326.3912	325.9474
332.2367	331.8736	331.8539
343.1586	343.1254	342.8330
349.4756	349.2376	349.0208
355.3446	354.1417	353.3378
364.5029	364.4209	364.0294
374.9202	374.3083	366.8677
389.6333	389.0738	389.2270
397.4710	397.4248	397.2731
416.0384	415.7493	415.0509
437.3584	436.1418	429.9812
451.8894	451.8867	451.8840
454.7958	454.7853	454.6939
458.8126	458.8091	458.8053
460.2504	460.1941	460.2260
464.8597	464.8250	464.7879
469.0959	469.0847	469.0875
478.9892	477.6973	475.9719
484.6999	484.0336	482.6178
485.3017	485.0017	484.9189
491.8436	491.4709	491.1243
499.7736	499.0603	498.0272
505.8267	505.8215	505.7151
522.6001	522.5160	522.4575
532.7267	532.4241	531.6029
543.1895	543.1890	543.1867
545.4653	545.4576	545.4094
552.5815	552.5812	552.5814
554.6458	554.5287	554.5788
561.6862	558.5981	558.4474
593.4725	593.1157	593.3268
612.4042	612.4025	612.4022
640.1941	640.1937	640.1914
643.6583	643.6582	643.6581
644.4308	644.4298	644.4272
647.5535	647.4562	647.4313
679.0594	679.0288	679.0471
681.8216	681.8216	681.8213
681.8733	681.8720	681.8728
682.5555	682.5554	682.5550
689.8779	689.8775	689.8769

691.1785	691.1782	691.1782
702.6204	702.5151	702.6166
704.4380	704.4236	704.4359
715.9682	712.5817	715.7258
752.8794	752.8790	752.8766
754.5886	754.5879	754.5855
757.1603	757.1529	757.1335
769.7595	769.7591	769.7587
772.2501	772.2497	772.2474
780.7616	780.7597	780.7562
780.7982	780.7973	780.7793
781.6938	781.6925	781.6935
783.7585	783.7482	783.7555
792.7509	792.7492	792.7502
794.2122	794.2121	794.2120
810.8339	810.8336	810.8313
814.2207	814.2205	814.2180
855.2296	855.2296	855.2296
856.3930	856.3929	856.3923
858.4287	858.4287	858.4285
859.2869	859.2869	859.2865
892.7469	892.7457	892.7458
930.7071	930.7070	930.7070
932.5416	932.5391	932.5399
938.2296	938.2244	938.2249
939.2185	939.2181	939.2182
960.7721	960.7720	960.7720
962.7743	962.1284	962.4936
964.3029	962.7744	962.7744
1011.1152	1011.0997	1011.1003
1017.8791	1017.8779	1017.8785
1025.2567	1025.1560	1025.1522
1028.9071	1028.8828	1028.8829
1031.5031	1031.3745	1031.3667
1032.0921	1032.0045	1032.0041
1046.1741	1045.9288	1045.8456
1046.2925	1046.2525	1046.2507
1053.5353	1049.4184	1048.5209
1056.3883	1053.5510	1053.5462
1056.5542	1056.4048	1056.4062
1057.5519	1056.5591	1056.5584
1058.5925	1057.5756	1057.5756
1060.0151	1058.6754	1058.6751
1060.5741	1060.1469	1060.1571
1061.8615	1060.6771	1060.7010

1063.9522	1061.8687	1061.8666
1068.9077	1064.1093	1064.0977
1069.8913	1069.7438	1069.7417
1072.5465	1071.2361	1071.1956
1073.3539	1073.1924	1073.1831
1077.4582	1073.9432	1073.9082
1086.9402	1086.9402	1086.9402
1101.9083	1101.7394	1101.7416
1103.5040	1103.5038	1103.5039
1115.1543	1115.1368	1115.1411
1116.1710	1116.1710	1116.1708
1119.1487	1119.1487	1119.1486
1121.0863	1121.0853	1121.0852
1126.7206	1126.0856	1126.1016
1132.9085	1132.6940	1132.6771
1138.7126	1138.7075	1138.7072
1139.6187	1139.6031	1139.5969
1169.7551	1169.7548	1169.7547
1170.6249	1170.6249	1170.6249
1206.7858	1206.7858	1206.7857
1206.9590	1206.9590	1206.9590
1208.7319	1208.7317	1208.7317
1209.3008	1209.2997	1209.3001
1225.6844	1225.6844	1225.6844
1227.6076	1227.6073	1227.6072
1280.2728	1280.2724	1280.2725
1282.0595	1282.0592	1282.0595
1285.8519	1285.8518	1285.8518
1287.2660	1287.2648	1287.2654
1301.2865	1301.2864	1301.2864
1302.7893	1302.7893	1302.7893
1325.4614	1325.4591	1325.4595
1327.9721	1327.9719	1327.9716
1333.8867	1333.8855	1333.8849
1344.8603	1344.8602	1344.8602
1346.2426	1346.2426	1346.2426
1358.1658	1358.1658	1358.1656
1362.9916	1362.9916	1362.9916
1368.5661	1368.5660	1368.5659
1372.4848	1372.4810	1372.4813
1415.6512	1415.6512	1415.6511
1438.1220	1438.1191	1438.1207
1446.8639	1446.8636	1446.8635
1484.4152	1484.4152	1484.4152
1485.2246	1485.2245	1485.2241

1492.3688	1492.3688	1492.3688
1492.6565	1492.6564	1492.6564
1493.0006	1493.0006	1493.0005
1497.3462	1497.3459	1497.3460
1497.9390	1497.9387	1497.9384
1503.2153	1503.2135	1503.2143
1505.6550	1505.6548	1505.6548
1513.1068	1513.1068	1513.1068
1527.2649	1527.2649	1527.2649
1527.6400	1527.6397	1527.6394
1581.4437	1581.4437	1581.4437
1586.6293	1586.6293	1586.6293
1589.7174	1589.7173	1589.7172
1590.6213	1590.6213	1590.6212
1595.3886	1595.3885	1595.3885
1602.6720	1602.6719	1602.6719
1609.6350	1609.6338	1609.6337
1612.5959	1612.5959	1612.5959
1617.9139	1617.9138	1617.9139
1619.8196	1619.8196	1619.8196
1621.2213	1621.2209	1621.2206
1623.7037	1623.7036	1623.7036
1624.0952	1624.0934	1624.0924
3028.9134	3028.9134	3028.9134
3098.5193	3098.5193	3098.5193
3137.7588	3137.7588	3137.7588
3223.1581	3223.1581	3223.1581
3224.1438	3224.1438	3224.1438
3225.5363	3225.5363	3225.5363
3225.7602	3225.7602	3225.7602
3226.8429	3226.8429	3226.8429
3227.2056	3227.2055	3227.2055
3233.8115	3233.8115	3233.8115
3235.8133	3235.8133	3235.8133
3235.9426	3235.9426	3235.9426
3236.7716	3236.7716	3236.7716
3237.2615	3237.2615	3237.2615
3239.4819	3239.4819	3239.4819
3240.1571	3240.1571	3240.1571
3242.2385	3242.2385	3242.2385
3242.6396	3242.6396	3242.6396
3244.6127	3244.6127	3244.6127
3245.8742	3245.8742	3245.8742
3247.0714	3247.0714	3247.0714
3247.8480	3247.8480	3247.8480

3250.1035	3250.1035	3250.1035
3271.3986	3271.3985	3271.3985
3279.9631	3279.9631	3279.9631