

SUPPORTING INFORMATION FOR

Triplet Oxygen Evolution Catalyzed by a
Biomimetic Oxomanganese Complex: Functional
Role of the Carboxylate Buffer

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1. Computational details

Electronic structure calculations were performed with the hybrid B3LYP exchange-correlation functional^{1,2,3} implemented in the *Gaussian* 09 software.⁴ All density functional theory (DFT) calculations were performed with a pruned grid having 99 radial shells and 590 angular points for each shell, which is called the ultrafine grid in *Gaussian* 09. The geometry optimization and subsequent frequency analysis are performed with a mixed basis set (denoted BS1): the LanL2DZ pseudopotential and LanNL2DZ basis set⁵ for Mn atoms, the 6-31G(d) basis set⁶ for O atoms, the 6-31G basis set⁷ for N atom, the 3-21G basis set⁸ for C and H atoms. The optimized stationary points were confirmed to be minimums with all real frequencies and to be transition states with one imaginary frequency. The calculated frequencies were used to evaluate the thermal correction to Gibbs free energy G_{cor} . Single-point calculations were performed at optimized geometries with LanL2DZ pseudopotential and LanL2DZ basis set for Mn atoms and Dunning's correlation consistent polarized valence triple-zeta basis set⁹ by removing the f functions (cc-PVTZ(-f)) for other atoms (denoted BS2).

The ground states of the manganese dimers in our study involves the anti-ferromagnetic coupling of the two high-spin Mn centers which require the broken-symmetry (BS) solution,¹⁰ with α and β electronic densities localized on different metal centers, for proper description. Initial guesses of the broken-symmetry solutions were built from separated fragment SCF solutions with *Gaussian* 09. The converged broken-symmetry solutions were confirmed by atomic spin densities using Mulliken population analysis.

The solvation effects were considered with the polarizable continuum model (PCM) of Tomasi and coworkers¹¹ with the same mixed basis set at optimized geometry. The default

universal force field (UFF) atomic radius were used for solute molecules. The solvation free energy is considered by taking the difference between single-point energies in gas phase ($E(\text{gas})$) and in PCM water solution ($E(\text{PCM})$) with BS1. The final free energy in aqueous solution is calculated by adding the thermal correction G_{cor} calculated with BS1, the calculated solvation free energy ΔG_{solv} with BS1 to the single-point electronic energy at BS2 (E_{BS2}). The equations to calculate the final free energy are given below:

$$\Delta G_{\text{solv}} = E(\text{PCM}, \text{BS1}) - E(\text{gas}, \text{BS1}) \quad (\text{S-1})$$

$$G_{\text{aq}} = E_{\text{BS2}} + G_{\text{cor}} + \Delta G_{\text{solv}} \quad (\text{S-2})$$

For transition states, intrinsic reaction coordinate (IRC)¹² calculations with local quadratic approximation (LQA) algorithm^{13,14} were performed to map out the reaction path to confirm the transition states are indeed connect the desired reactants and products.

2. Energetics

Table S1. Relative energetics of complexes in the nucleophilic attack of water to oxyl radicals (in kcal/mol)^a

	$\Delta E(\text{BS1})$	$\Delta G(\text{BS1})$	$\Delta G_{\text{sol}}(\text{BS1})$	$\Delta E(\text{BS2})$	$\Delta G_{\text{cor}}(\text{BS1})$	$\Delta \Delta G_{\text{sol}}(\text{BS1})$	ΔG_{aq}
AcO–Mn(IV)–Mn(IV)–Odot2_OH2_R	0.0	0.0	-121.6	0.0	0.0	0.0	0.0
AcO–Mn(IV)–Mn(IV)–Odot2_OH2_TS	20.7	20.5	-120.9	21.8	-0.2	0.7	22.3
AcO–Mn(IV)–Mn(IV)–Odot2_OH2_P1	6.3	6.5	-120.1	7.4	0.1	1.4	9.0
AcO–Mn(IV)–Mn(IV)–Odot2_OH2_P2	-2.4	-4.5	-118.0	-4.7	-2.1	3.5	-3.2
AcO–Mn(IV)–Mn(IV)–Odot1_OH2_R	6.7	6.7	-122.3	6.6	0.0	-0.7	5.8
AcO–Mn(IV)–Mn(IV)–Odot1_OH2_TS	30.5	28.1	-121.4	29.7	-2.4	0.2	27.4
AcO–Mn(IV)–Mn(IV)–Odot1_OH2_P	-5.8	-8.1	-120.4	-7.0	-2.2	1.2	-8.0
AcO–Mn(IV)–Mn(III)–OOH_OH	-8.6	-10.8	-118.9	-7.9	-2.2	2.7	-7.4

^a The nomenclature of complexes is giving in section 3 (Cartesian coordinates of optimized stationary points).

Table S2. The calculated absolute energies of complexes in the nucleophilic attack of water to oxyl radicals (in hartree)^a

	$E(\text{BS1})$	$G(\text{BS1})$	$E(\text{PCM, BS1})$	$E(\text{BS2})$	$G_{\text{cor}}(\text{BS1})$
AcO–Mn(IV)–Mn(IV)–Odot2_OH2_R	-2216.13910	-2215.65766	-2216.33285	-2223.70254	0.48144
AcO–Mn(IV)–Mn(IV)–Odot2_OH2_TS	-2216.10604	-2215.62500	-2216.29869	-2223.66776	0.48104
AcO–Mn(IV)–Mn(IV)–Odot2_OH2_P1	-2216.12899	-2215.64732	-2216.32045	-2223.69079	0.48168
AcO–Mn(IV)–Mn(IV)–Odot2_OH2_P2	-2216.14299	-2215.66485	-2216.33109	-2223.71006	0.47814
AcO–Mn(IV)–Mn(IV)–Odot1_OH2_R	-2216.12839	-2215.64702	-2216.32326	-2223.69202	0.48137
AcO–Mn(IV)–Mn(IV)–Odot1_OH2_TS	-2216.09053	-2215.61296	-2216.28402	-2223.65525	0.47757
AcO–Mn(IV)–Mn(IV)–Odot1_OH2_P	-2216.14839	-2215.67050	-2216.34019	-2223.71370	0.47790
AcO–Mn(IV)–Mn(III)–OOH_OH	-2216.15279	-2215.67492	-2216.34223	-2223.71509	0.47788

^a The nomenclature of complexes is giving in section 3 (Cartesian coordinates of optimized stationary points).

Table S3. Relative energetics of complexes in the acetate-assisted nucleophilic attack of water to oxyl radicals (in kcal/mol)^a

	$\Delta E(\text{BS1})$	$\Delta G(\text{BS1})$	$\Delta G_{\text{sol}}(\text{BS1})$	$\Delta E(\text{BS2})$	$\Delta G_{\text{cor}}(\text{BS1})$	$\Delta \Delta G_{\text{sol}}(\text{BS1})$	ΔG_{aq}
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_PT_R	0.0	0.0	-58.6	0.0	0.0	0.0	0.0
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_PT_TS	0.5	-1.6	-58.1	0.5	-2.1	0.5	-1.1
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_PT_P	-2.0	-2.4	-56.5	-1.7	-0.4	2.1	0.0
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_TS	-1.0	-1.2	-55.4	-0.1	-0.3	3.2	2.8
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_P	-31.4	-33.0	-50.8	-34.0	-1.6	7.8	-27.8
AcO–Mn(IV)–Mn(IV)–Od ₁ OH ₂ OAc_R	2.2	0.3	-55.1	2.5	-1.9	3.5	4.2
AcO–Mn(IV)–Mn(IV)–Od ₁ OH ₂ OAc_P	-28.9	-30.4	-51.3	-32.2	-1.6	7.3	-26.5

^a The nomenclature of complexes is giving in section 3 (Cartesian coordinates of optimized stationary points).

^b The proton-transfer (PT) from the substrate H₂O molecule to acetate have a small barrier of 0.5kcal/mol on the UB3LYP/BS1 potential energy surface. However, this barrier disappears on the free energy surface.

Table S4. The calculated absolute energies of complexes in the acetate-assisted nucleophilic attack of water to oxyl radicals (in hartree)^a

	$E(\text{BS1})$	$G(\text{BS1})$	$E(\text{PCM, BS1})$	$E(\text{BS2})$	$G_{\text{cor}}(\text{BS1})$
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_PT_R	-2444.42992	-2443.90591	-2444.52329	-2452.52013	0.52401
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_PT_TS	-2444.42912	-2443.90847	-2444.52174	-2452.51934	0.52065
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_PT_P	-2444.43310	-2443.90980	-2444.52311	-2452.52276	0.52330
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_TS	-2444.43146	-2443.90788	-2444.51981	-2452.52029	0.52358
AcO–Mn(IV)–Mn(IV)–Od ₂ OH ₂ OAc_P	-2444.48001	-2443.95853	-2444.56097	-2452.57431	0.52149
AcO–Mn(IV)–Mn(IV)–Od ₁ OH ₂ OAc_R	-2444.42646	-2443.90542	-2444.51422	-2452.51612	0.52104
AcO–Mn(IV)–Mn(IV)–Od ₁ OH ₂ OAc_P	-2444.47596	-2443.95443	-2444.55788	-2452.57152	0.52153

^a The nomenclature of complexes is giving in section 3 (Cartesian coordinates of optimized stationary points).

Table S5. Relative energetics of complexes involved in the intramolecular proton-coupled electron transfer (IPCET) of hydroxo to superoxo (in kcal/mol)^a

	$\Delta E(\text{BS1})$	$\Delta G(\text{BS1})$	$\Delta G_{\text{sol}}(\text{BS1})$	$\Delta E(\text{BS2})$	$\Delta G_{\text{cor}}(\text{BS1})$	$\Delta \Delta G_{\text{sol}}(\text{BS1})$	ΔG_{aq}
AcO–Mn(III)–Mn(IV)–OOH_R	0.0	0.0	-50.9	0.0	0.0	0.0	0.0
AcO–Mn(III)–Mn(IV)–OOH_TS1	4.2	1.9	-49.6	3.6	-2.3	1.3	2.7
AcO–Mn(III)–Mn(IV)–OOH_P1	-12.6	-16.9	-47.3	-13.9	-4.3	3.7	-14.4
AcO–Mn(III)–Mn(IV)–OOH_TS2	11.0	6.9	-48.4	12.4	-4.1	2.5	10.7
AcO–Mn(III)–Mn(IV)–OOH_P2	3.7	2.4	-48.8	5.2	-1.2	2.1	6.0
AcO–Mn(IV)–Mn(III)–OOH_R	2.7	2.1	-51.2	2.7	-0.6	-0.3	1.8
AcO–Mn(IV)–Mn(III)–OOH_TS	12.5	9.3	-52.6	10.9	-3.2	-1.6	6.1
AcO–Mn(IV)–Mn(III)–OOH_P	-10.1	-14.3	-46.5	-11.0	-4.1	4.5	-10.7

^a The nomenclature of complexes is giving in section 3 (Cartesian coordinates of optimized stationary points).

Table S6. The calculated absolute energies of complexes involved in the intramolecular proton-coupled electron transfer (IPCET) of hydroxo to superoxo (in hartree)^a

	<i>E</i> (BS1)	<i>G</i> (BS1)	<i>E</i> (PCM, BS1)	<i>E</i> (BS2)	<i>G</i> _{cor} (BS1)
AcO–Mn(III)–Mn(IV)–OOH_R	-2215.81310	-2215.34623	-2215.89426	-2223.38020	0.46687
AcO–Mn(III)–Mn(IV)–OOH_TS1	-2215.80640	-2215.34315	-2215.88546	-2223.37446	0.46325
AcO–Mn(III)–Mn(IV)–OOH_P1	-2215.83320	-2215.37311	-2215.90850	-2223.40229	0.46008
AcO–Mn(III)–Mn(IV)–OOH_TS2	-2215.79556	-2215.33521	-2215.87277	-2223.36052	0.46035
AcO–Mn(III)–Mn(IV)–OOH_P2	-2215.80722	-2215.34234	-2215.88500	-2223.37195	0.46488
AcO–Mn(IV)–Mn(III)–OOH_R	-2215.80873	-2215.34289	-2215.89034	-2223.37585	0.46584
AcO–Mn(IV)–Mn(III)–OOH_TS	-2215.79314	-2215.33140	-2215.87689	-2223.36279	0.46174
AcO–Mn(IV)–Mn(III)–OOH_P	-2215.82923	-2215.36896	-2215.90326	-2223.39781	0.46026

^a The nomenclature of complexes is giving in section 3 (Cartesian coordinates of optimized stationary points).

Table S7. Relative energetics of the complexes involved in the triplet oxygen evolution (in kcal/mol)^a

	$\Delta E(\text{BS1})$	$\Delta G(\text{BS1})$	$\Delta G_{\text{sol}}(\text{BS1})$	$\Delta E(\text{BS2})$	$\Delta G_{\text{cor}}(\text{BS1})$	$\Delta \Delta G_{\text{sol}}(\text{BS1})$	ΔG_{aq}
AcO–Mn(III)–Mn(IV)–OOH_P2 + AcOH	0.0	0.0	-51.5	0.0	0.0	0.0	0.0
AcO–Mn(III)–Mn(IV)–OOH_P + AcOH	2.5	2.6	-50.7	2.8	-2.3	0.8	3.7
AcO–Mn(III)–Mn(II)– ³ O ₂ + AcO ⁻	135.0	128.4	-178.9	131.6	-3.2	-127.4	-2.3
AcO–Mn(II)–Mn(III)– ³ O ₂ + AcO ⁻	146.9	138.2	-182.5	143.1	-4.1	-131.1	3.3

^a The nomenclature of complexes is giving in section 3 (Cartesian coordinates of optimized stationary points).

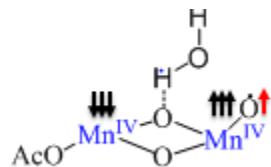
Table S8. The calculated absolute energies of the complexes involved in the triplet oxygen evolution (in kcal/mol)^a

	$E(\text{BS1})$	$G(\text{BS1})$	$E(\text{PCM, BS1})$	$E(\text{BS2})$	$G_{\text{cor}}(\text{BS1})$
AcO ⁻	-2215.81310	-2215.34623	-2215.89426	-2223.38020	0.46687
AcOH	-2215.80640	-2215.34315	-2215.88546	-2223.37446	0.46325
AcO–Mn(III)–Mn(IV)–OOH_P2	-2215.83320	-2215.37311	-2215.90850	-2223.40229	0.46008
AcO–Mn(IV)–Mn(III)–OOH_P	-2215.79556	-2215.33521	-2215.87277	-2223.36052	0.46035
AcO–Mn(III)–Mn(II)– ³ O ₂	-2215.80722	-2215.34234	-2215.88500	-2223.37195	0.46488
AcO–Mn(II)–Mn(III)– ³ O ₂	-2215.82923	-2215.36896	-2215.90326	-2223.39781	0.46026

^a The nomenclature of complexes is giving in section 3 (Cartesian coordinates of optimized stationary points).

3. Cartesian coordinates of optimized stationary points

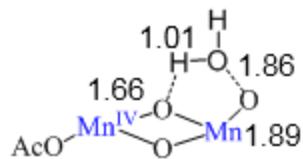
Cartesian coordinates of optimized stationary point in Å:



AcO–Mn(IV)–Mn(IV)–Od₁–OH₂–R:

Mn	1.34338000	0.05436200	-0.77398800
Mn	-1.09727400	-0.05243000	0.49584600
O	0.59907200	-0.01079100	0.93191400
O	-0.38023200	0.00117900	-1.22921600
O	2.06364600	0.19000300	-2.45044200
O	-1.84854000	-0.06530700	2.20759500
N	1.79280800	-1.89809200	-0.99523400
N	3.14537700	-0.02923000	0.09059500
N	1.83981300	2.02335300	-0.72425900
N	-1.51007800	1.94331200	0.55121300
N	-2.92891900	0.00831500	-0.34361800
N	-1.52774700	-2.03831100	0.33714700
C	1.08513900	-2.73198000	-1.77945400
C	1.48879400	-4.05377800	-1.96721300
C	2.63569200	-4.51070000	-1.31574600
C	3.36929200	-3.63446300	-0.50876000
C	2.94064700	-2.31637300	-0.37441900
C	3.68363500	-1.24059200	0.31224100
C	4.86498400	-1.34100800	1.05186000
C	5.45184300	-0.16093800	1.52466400
C	4.88946800	1.08697500	1.23360900
C	3.70633500	1.12390800	0.48808200
C	2.99042800	2.30783900	-0.02922000
C	3.45568800	3.61607500	0.05675900
C	2.75882800	4.63393800	-0.60491500
C	1.61567100	4.31813000	-1.33626700
C	1.16921100	2.99376400	-1.37774400
C	-0.75967300	2.82186700	1.23792300
C	-1.15600200	4.15187000	1.37601300
C	-2.35011000	4.56729000	0.78396400
C	-3.13228300	3.64198300	0.08773200
C	-2.69864200	2.32144100	-0.00483700
C	-3.47719100	1.21178800	-0.58872800
C	-4.68282200	1.28905100	-1.29057900
C	-5.28151200	0.09815600	-1.71435200
C	-4.69220200	-1.13944200	-1.43235000

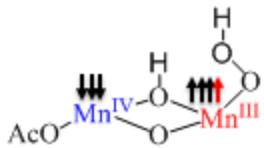
C	-3.48505400	-1.15441300	-0.72761700
C	-2.71270400	-2.33208400	-0.28556800
C	-3.14435700	-3.65122900	-0.39722200
C	-2.36488600	-4.67326600	0.15492900
C	-1.17453000	-4.35216500	0.80449400
C	-0.77689800	-3.01481700	0.88024600
H	0.20543500	-2.30901700	-2.24549900
H	0.91794100	-4.70212000	-2.61805300
H	2.97088300	-5.53189600	-1.44725200
H	4.27579200	-3.96697400	-0.02086600
H	5.32163700	-2.30000700	1.25495100
H	6.36281900	-0.21370400	2.10729200
H	5.36647700	1.99522400	1.57547100
H	4.36374600	3.83820500	0.60128500
H	3.12285400	5.65295500	-0.56311300
H	1.07073500	5.07638700	-1.88249400
H	0.28283700	2.69943700	-1.94064100
H	0.14556500	2.42864400	1.68069800
H	-0.54490800	4.83824400	1.94649200
H	-2.68186300	5.59359000	0.87860600
H	-4.07429200	3.94027100	-0.35201300
H	-5.14097200	2.24297400	-1.51153600
H	-6.21343700	0.13378300	-2.26429500
H	-5.16457100	-2.05693900	-1.75519100
H	-4.08511500	-3.87955300	-0.87993300
H	-2.69858500	-5.70152100	0.09294100
H	-0.56471000	-5.11527000	1.26883800
H	0.10418400	-2.69293100	1.41392800
C	-1.36006200	-0.70167700	3.28584800
O	-0.43568500	-1.49804500	3.26185100
C	-2.11768200	-0.31681300	4.55447600
H	-3.17277400	-0.58923200	4.44811000
H	-1.68233700	-0.83770100	5.40746800
H	-2.06187500	0.76587400	4.70479100
O	-1.31273600	1.94253400	-2.91553200
H	-1.16640800	1.85726200	-3.87285700
H	-1.00894400	1.09369900	-2.52092800



AcO–Mn(IV)–Mn(IV)–Odotted1_OH2_TS:

Mn	1.27952000	-0.03140700	-0.76264500
Mn	-1.20534100	-0.00802700	0.43575200
O	0.45367600	-0.10000800	0.93925400
O	-0.44644200	0.08397100	-1.27704000
O	1.85338100	-0.13594000	-2.56464000
O	-2.03198300	-0.04288700	2.11418700
N	1.93517200	-2.10871000	-0.80769300
N	3.16172100	-0.02405100	0.14942100
N	1.88071400	2.06777800	-0.76103200
N	-1.48034900	2.01420500	0.57961000
N	-3.02394600	0.22027200	-0.41469100
N	-1.76394900	-1.94589500	0.17231900
C	1.32232800	-3.07798700	-1.50758800
C	1.76920800	-4.39896200	-1.46563100
C	2.87488200	-4.70808700	-0.67069300
C	3.51749200	-3.69175800	0.04105500
C	3.03376800	-2.38571900	-0.05667100
C	3.69426900	-1.20111400	0.53582200
C	4.81531100	-1.22559500	1.36999300
C	5.37386500	-0.01092200	1.77509200
C	4.83108600	1.19588600	1.32908300
C	3.70591600	1.15873200	0.49912200
C	3.04294800	2.33529600	-0.10601000
C	3.57637100	3.62574800	-0.09508600
C	2.91217800	4.64090300	-0.78804900
C	1.73211200	4.34596700	-1.47245100
C	1.24113500	3.04047300	-1.43303900
C	-0.66752800	2.81061600	1.29340000
C	-0.97355500	4.15767300	1.49392400
C	-2.14314100	4.67606000	0.93662500
C	-2.99088300	3.83578600	0.20799200
C	-2.64581500	2.49450000	0.05242700
C	-3.50026000	1.46700400	-0.58027100
C	-4.71104300	1.65727200	-1.25197900
C	-5.39100600	0.52901900	-1.72589900
C	-4.87694500	-0.75555300	-1.52099400
C	-3.65996900	-0.88342900	-0.84231700
C	-2.96236100	-2.13026500	-0.46645000
C	-3.47670300	-3.41076600	-0.64944500
C	-2.76576500	-4.50873000	-0.15207700

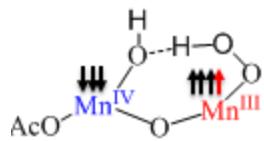
C	-1.56193100	-4.29885400	0.51644200
C	-1.08076700	-2.99469300	0.66546600
H	0.47483700	-2.77292500	-2.10698900
H	1.26894700	-5.15925300	-2.05039200
H	3.24699000	-5.72357600	-0.61873400
H	4.39203400	-3.91406400	0.63708700
H	5.24638700	-2.16075500	1.69894300
H	6.23769700	-0.00571100	2.42767300
H	5.27356900	2.13617200	1.62707100
H	4.50713200	3.83385500	0.41503800
H	3.32270600	5.64268000	-0.80634400
H	1.20690100	5.10420500	-2.03769400
H	0.33705800	2.75186500	-1.95092700
H	0.21445400	2.33798500	1.70404800
H	-0.31238400	4.77679400	2.08512600
H	-2.40687800	5.71610800	1.08202100
H	-3.91716400	4.21493300	-0.20264400
H	-5.12004200	2.64681100	-1.40331100
H	-6.33046400	0.65193600	-2.24997700
H	-5.41446600	-1.62340000	-1.87746400
H	-4.42720600	-3.55358600	-1.14572500
H	-3.16300500	-5.50896700	-0.27102500
H	-1.00344300	-5.12256800	0.93978500
H	-0.18424600	-2.75824300	1.21668500
C	-1.62751200	-0.76293000	3.17381500
O	-0.77989000	-1.63956700	3.13809700
C	-2.37957300	-0.35977800	4.44119900
H	-3.45322400	-0.51832100	4.29760400
H	-2.02262700	-0.95919700	5.27889700
H	-2.21846700	0.70382900	4.64339800
O	0.55164000	0.73260100	-3.56384100
H	0.57372400	0.07288500	-4.28441300
H	-0.12058300	0.43104100	-2.86993900



AcO–Mn(IV)–Mn(IV)–Od1_OH2_P:

Mn	1.31781700	0.12220600	-0.94686000
Mn	-1.30752700	0.11417200	0.37249600
O	0.37850900	0.20078000	0.71480700
O	-0.65712000	-0.09719100	-1.46186400
O	1.89266600	0.08857400	-2.69136900
O	-1.97703300	0.33756900	2.06724800
N	1.71688500	-2.09148400	-1.05403400
N	3.16969200	-0.25020800	0.14967500
N	2.29199400	2.14550000	-0.57980000
N	-1.76534900	2.09746000	0.10629900
N	-3.19319100	0.01370700	-0.34644900
N	-1.64920500	-1.87337900	0.47571400
C	1.04269400	-2.90192200	-1.88923700
C	1.41825500	-4.23336000	-2.07389100
C	2.52027200	-4.72291800	-1.36934000
C	3.22243200	-3.87310100	-0.51032900
C	2.79928500	-2.54794000	-0.37893100
C	3.51494600	-1.52444100	0.42207800
C	4.50229700	-1.80456700	1.37270300
C	5.12392500	-0.73924500	2.02544900
C	4.77483800	0.57410900	1.70686000
C	3.78242400	0.79081800	0.74426400
C	3.36007100	2.12837700	0.25910200
C	4.04667000	3.30637800	0.57237600
C	3.63400200	4.51073400	0.00139200
C	2.54689100	4.51447300	-0.87513900
C	1.90005200	3.30810200	-1.13971900
C	-0.97448500	3.09435800	0.54023200
C	-1.39339300	4.42444400	0.48396400
C	-2.65707800	4.71499200	-0.03161400
C	-3.48244400	3.67113700	-0.46162800
C	-3.02062200	2.35977000	-0.37106900
C	-3.81960000	1.15573600	-0.68516800
C	-5.10202700	1.10055700	-1.23689600
C	-5.69468500	-0.15597900	-1.41222500
C	-5.02249900	-1.32366900	-1.03741400
C	-3.73952400	-1.20644700	-0.49108100
C	-2.86739400	-2.28951800	0.00505900
C	-3.22622100	-3.63248100	0.06683700
C	-2.33386800	-4.55108100	0.63143500
C	-1.10815800	-4.10488000	1.11970500

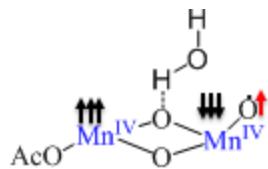
C	-0.78934500	-2.74717100	1.02799700
H	0.20540900	-2.45414400	-2.40859000
H	0.87083400	-4.86167800	-2.76383100
H	2.84457100	-5.74769900	-1.50085100
H	4.09920800	-4.23070800	0.01252500
H	4.77377200	-2.82389900	1.60963300
H	5.88091100	-0.93080900	2.77531500
H	5.26241800	1.40033700	2.20451500
H	4.90572800	3.28645400	1.22843600
H	4.16457600	5.42777000	0.22492400
H	2.21542700	5.42634900	-1.35435000
H	1.06142000	3.24797500	-1.82099200
H	-0.01566500	2.79649500	0.94104300
H	-0.74280800	5.20790500	0.84842600
H	-3.00763000	5.73809700	-0.08351700
H	-4.47604500	3.87792800	-0.83611000
H	-5.63013700	1.99969300	-1.52319600
H	-6.68742400	-0.22376000	-1.83906900
H	-5.48995300	-2.28983400	-1.16800400
H	-4.19008100	-3.95975700	-0.29912200
H	-2.60566700	-5.59699000	0.69877400
H	-0.40643900	-4.78561800	1.58177700
H	0.12478900	-2.32990400	1.41833100
C	-1.44465500	-0.15274100	3.21211900
O	-0.55704900	-0.98151300	3.26149500
C	-2.12604100	0.45897500	4.43271200
H	-2.01000200	1.54716200	4.41437800
H	-3.19650000	0.23116500	4.40962100
H	-1.67692400	0.04854100	5.33732000
O	1.19328300	1.20251500	-3.28403500
H	1.94430000	1.72605200	-3.62832400
H	-0.97926900	0.45738100	-2.19367200



AcO–Mn(IV)–Mn(III)–OOH_OH:

Mn	1.87606200	-0.00357000	-1.06804400
Mn	-1.50756900	0.15389700	-0.12713300
O	0.19919600	0.16785000	-0.20926300
O	-1.62306900	0.31683100	-1.99257400
O	1.41290500	0.16766800	-2.81656100
O	-1.60645900	0.01578200	1.75528800
N	2.45248500	-2.08650500	-0.85516400
N	3.13089500	-0.04138100	0.58893000
N	2.75402000	1.94625800	-1.02109200
N	-1.82035700	2.16149300	0.08869800
N	-3.52365000	0.24378100	-0.02652100
N	-2.00530300	-1.81781200	-0.23322800
C	2.18783600	-3.05858900	-1.75090100
C	2.47228900	-4.39789000	-1.47557800
C	3.01885000	-4.72914300	-0.23443400
C	3.28805100	-3.71794900	0.69325400
C	3.01024900	-2.39509500	0.35256100
C	3.37481700	-1.22345800	1.18505600
C	4.02579900	-1.25268900	2.42285500
C	4.43548500	-0.04264000	2.98911300
C	4.24268000	1.16429000	2.30710800
C	3.58270300	1.13211200	1.07636400
C	3.39525500	2.26876500	0.14164100
C	3.88766200	3.55721200	0.34486500
C	3.73710500	4.50981100	-0.66897700
C	3.09594300	4.15884100	-1.85848700
C	2.60586900	2.85939900	-2.00016600
C	-0.82909400	3.06451600	0.12742000
C	-1.09694800	4.42617900	0.27370600
C	-2.42211900	4.84813300	0.37973700
C	-3.44926100	3.90100400	0.34092200
C	-3.12421900	2.55391700	0.19566800
C	-4.10052500	1.44722700	0.15479100
C	-5.48795300	1.53178100	0.30035400
C	-6.23446400	0.34896600	0.26330300
C	-5.60454000	-0.88819400	0.09542300
C	-4.21327100	-0.91235500	-0.04457600
C	-3.34499600	-2.09687100	-0.18814800
C	-3.79887800	-3.41188000	-0.25076800
C	-2.86749500	-4.44944300	-0.35556900
C	-1.50807000	-4.14588300	-0.38556400

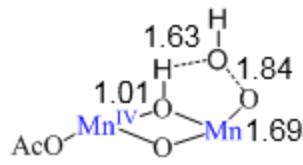
C	-1.10553000	-2.81078000	-0.31633100
H	1.73709500	-2.73714600	-2.68167100
H	2.27806500	-5.15453300	-2.22426900
H	3.24749600	-5.75951100	0.00780300
H	3.72054200	-3.96161800	1.65404200
H	4.22213900	-2.18680800	2.92995200
H	4.93719300	-0.04193200	3.94855400
H	4.61265700	2.09144500	2.72255100
H	4.39885500	3.81419300	1.26297300
H	4.13091500	5.50942500	-0.53330500
H	2.98373300	4.86855500	-2.66721400
H	2.09443700	2.52067600	-2.89371400
H	0.17120600	2.66708400	0.04149400
H	-0.28052600	5.13482000	0.30285500
H	-2.65818300	5.89865600	0.49250100
H	-4.48241400	4.21064800	0.42284300
H	-5.97858900	2.48408300	0.44670800
H	-7.31057000	0.39130000	0.37494000
H	-6.18425500	-1.80076900	0.08414900
H	-4.85806900	-3.62839900	-0.21629300
H	-3.20476100	-5.47691600	-0.40618800
H	-0.76039500	-4.92382000	-0.45430800
H	-0.07090900	-2.51514600	-0.30138900
C	-0.78048400	-0.71046200	2.51043900
O	0.04695700	-1.51184000	2.09619600
C	-1.00931700	-0.43955100	4.00065200
H	-0.86982700	0.62580500	4.20886100
H	-2.03864100	-0.70146700	4.26604600
H	-0.31290800	-1.03542300	4.59122700
O	0.44330000	-0.81583900	-3.07153300
H	-0.41942900	-0.35012800	-2.78060600
H	-2.51703700	0.19860500	-2.35729900



AcO–Mn(IV)–Mn(IV)–Od₂–OH₂_R:

Mn	1.33667500	0.06153500	-0.88621900
Mn	-1.06523600	-0.06367600	0.49238100
O	0.62957400	-0.01952600	0.88069500
O	-0.39058100	-0.00085300	-1.26927800
O	1.95995300	0.18785000	-2.50126600
O	-1.78987600	-0.08569200	2.21133000
N	1.78108700	-1.92025000	-1.00563800
N	3.14585900	-0.00407200	0.00702200
N	1.79941300	2.05733200	-0.74741800
N	-1.48996900	1.93149800	0.56440700
N	-2.91353700	-0.00518400	-0.32274200
N	-1.49903000	-2.05015300	0.33854300
C	1.06859000	-2.78502300	-1.74952600
C	1.47650000	-4.11103900	-1.89524100
C	2.63501100	-4.53805700	-1.24425300
C	3.37256300	-3.62922800	-0.47884400
C	2.93617800	-2.30935500	-0.38515200
C	3.67455800	-1.21174600	0.27084000
C	4.82892800	-1.30331400	1.05247500
C	5.39841100	-0.11890800	1.53406400
C	4.83514000	1.12337600	1.22420400
C	3.67931900	1.15112800	0.43694300
C	2.95123400	2.33696000	-0.05807200
C	3.40380300	3.64830400	0.05612700
C	2.68801900	4.67459200	-0.57056300
C	1.53982900	4.36395400	-1.29617600
C	1.11007300	3.03507900	-1.36764500
C	-0.74110000	2.80783400	1.25559800
C	-1.14843000	4.13181800	1.41721100
C	-2.35206000	4.54447100	0.84280600
C	-3.13269000	3.62160000	0.14166500
C	-2.68833700	2.30628200	0.02700400
C	-3.46733000	1.19718400	-0.55841900
C	-4.67837400	1.27397400	-1.25121100
C	-5.27620400	0.08285900	-1.67574700
C	-4.68128700	-1.15422500	-1.40282300
C	-3.46896900	-1.16780100	-0.70686500
C	-2.69111200	-2.34456400	-0.27079900
C	-3.12731800	-3.66320000	-0.37036800
C	-2.34713300	-4.68390600	0.18329900

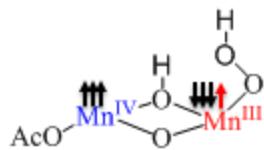
C	-1.15138700	-4.36189200	0.82231200
C	-0.74789200	-3.02557100	0.88351900
H	0.18100600	-2.38535500	-2.22140400
H	0.90024500	-4.78493100	-2.51461400
H	2.97531200	-5.56108100	-1.34452200
H	4.28805200	-3.93802200	0.00772400
H	5.27394100	-2.26050600	1.28716400
H	6.28883900	-0.16463900	2.14819500
H	5.28663800	2.03531000	1.58991000
H	4.31658100	3.86649700	0.59421100
H	3.04112600	5.69632500	-0.50723000
H	0.97930800	5.12918600	-1.81631200
H	0.22306300	2.74351700	-1.93122100
H	0.17264100	2.41681900	1.68233300
H	-0.53817200	4.81567000	1.99159600
H	-2.69251300	5.56610200	0.95551000
H	-4.08236200	3.91680800	-0.28345500
H	-5.14099400	2.22732700	-1.46524900
H	-6.21201400	0.11781700	-2.21909800
H	-5.15333600	-2.07177400	-1.72605100
H	-4.07312200	-3.89168300	-0.84305100
H	-2.68499700	-5.71139100	0.13166700
H	-0.54127300	-5.12340100	1.28889700
H	0.13846300	-2.70202200	1.40745500
C	-1.27195400	-0.70539800	3.28614700
O	-0.33930900	-1.49130200	3.25300400
C	-2.01127100	-0.31610300	4.56435600
H	-3.06445400	-0.60331600	4.48039800
H	-1.55366800	-0.82218900	5.41462600
H	-1.96693800	0.76877600	4.70206000
O	-1.36014100	1.96880300	-2.91103700
H	-1.23354400	1.90188300	-3.87261500
H	-1.04937200	1.11282200	-2.53898500



AcO–Mn(IV)–Mn(IV)–Od₂–OH₂–TS:

Mn	1.41481400	-0.00250500	-0.87718800
Mn	-1.16936600	0.03285600	0.47847600
O	0.48008600	-0.04709600	0.91093100
O	-0.38785400	-0.03216500	-1.34703500
O	1.90481700	0.07635200	-2.49783700
O	-1.94683800	0.11552100	2.13583300
N	1.74637600	-2.00524800	-0.91116200
N	3.13866500	-0.13157100	0.10261700
N	1.92943200	1.98129800	-0.68463200
N	-1.48474500	2.05999300	0.43519500
N	-2.99200300	0.15482000	-0.40530600
N	-1.68067700	-1.93101000	0.34843800
C	1.01763700	-2.85972900	-1.65145400
C	1.35974100	-4.20822900	-1.74169600
C	2.47586800	-4.67378100	-1.04229800
C	3.23137000	-3.77984600	-0.27995300
C	2.85262500	-2.43810700	-0.23870100
C	3.59991600	-1.35890300	0.42509200
C	4.68977400	-1.49040000	1.28910100
C	5.27571400	-0.33243200	1.80707000
C	4.78103900	0.92756200	1.45676100
C	3.69107500	1.00060100	0.58665800
C	3.05206200	2.21847600	0.05836200
C	3.56704900	3.50735500	0.18372200
C	2.94010400	4.55762300	-0.49306200
C	1.82361800	4.29098300	-1.28538700
C	1.33981800	2.98369500	-1.36151100
C	-0.70558100	2.93253400	1.09687100
C	-1.05176600	4.28100100	1.19382000
C	-2.22607000	4.72326900	0.58351500
C	-3.04030400	3.80663400	-0.08902400
C	-2.65827100	2.46731800	-0.13704500
C	-3.48610500	1.37272000	-0.68917900
C	-4.68745400	1.48152200	-1.39520300
C	-5.34001800	0.30328200	-1.77758200
C	-4.80767800	-0.94895300	-1.45249100
C	-3.60048800	-0.99363000	-0.74647100
C	-2.87832600	-2.19051600	-0.26612100
C	-3.36470900	-3.49238200	-0.34440700
C	-2.62688800	-4.53206300	0.23316500
C	-1.42181900	-4.24543100	0.87057800

C	-0.96817500	-2.92396600	0.91104900
H	0.16848800	-2.43381700	-2.16759300
H	0.76916200	-4.87243700	-2.35825100
H	2.76733000	-5.71471500	-1.10341100
H	4.11476500	-4.11635700	0.24600100
H	5.06884300	-2.46606900	1.56043400
H	6.11694400	-0.41117400	2.48378100
H	5.23394100	1.82425700	1.85680500
H	4.46152500	3.68614900	0.76524500
H	3.33948600	5.56169300	-0.42410800
H	1.34167600	5.07317700	-1.85630300
H	0.51154200	2.71106200	-1.99824800
H	0.18366200	2.51950000	1.55331200
H	-0.41647100	4.96080900	1.74532200
H	-2.51976500	5.76359700	0.64581200
H	-3.97085000	4.12751100	-0.53780300
H	-5.10842800	2.44592400	-1.64434600
H	-6.27097900	0.36224000	-2.32728100
H	-5.32244900	-1.85426300	-1.74336800
H	-4.31382200	-3.69481300	-0.82233100
H	-3.00327300	-5.54672500	0.19706200
H	-0.84116200	-5.02219100	1.34926900
H	-0.06607400	-2.62589900	1.42238500
C	-1.51767600	-0.50778200	3.25845300
O	-0.66112700	-1.36952300	3.29013900
C	-2.27556500	0.00313400	4.48100100
H	-3.34667400	-0.18432000	4.35495500
H	-1.90898900	-0.51072800	5.36984200
H	-2.12943800	1.08302100	4.58248500
O	0.58297700	0.95887400	-3.43258700
H	0.78331900	0.42953300	-4.22775500
H	-0.39743400	0.34325500	-2.28749900



AcO–Mn(IV)–Mn(IV)–Od₂–OH₂–P1:

Mn	1.43083500	-0.01672700	-0.80150800
Mn	-1.21850800	0.04569900	0.41271600
O	0.44032300	-0.01984300	0.84450500
O	-0.46900500	-0.06202000	-1.40524200
O	2.10370500	-0.00226600	-2.50535300
O	-1.98044000	0.14757800	2.08361900
N	1.72665100	-2.03554400	-0.87756700
N	3.11536200	-0.14852600	0.18310400
N	1.94026000	1.99581400	-0.66108600
N	-1.53868800	2.07529400	0.35746400
N	-3.05228800	0.16023200	-0.44018900
N	-1.72208800	-1.91468600	0.30948900
C	1.02605500	-2.89136400	-1.63965800
C	1.37404700	-4.24068800	-1.72096700
C	2.46961200	-4.70043200	-0.98771000
C	3.20277300	-3.80262600	-0.20540300
C	2.81831100	-2.46267800	-0.17717400
C	3.56515300	-1.38061300	0.50130300
C	4.65697900	-1.51717600	1.36014700
C	5.25662700	-0.35807500	1.86628300
C	4.78202100	0.90509000	1.50360100
C	3.68688800	0.98265600	0.63642300
C	3.07465300	2.20562200	0.07805000
C	3.63765400	3.47658500	0.18961900
C	3.04912300	4.54510400	-0.49183300
C	1.91393500	4.31530900	-1.26805900
C	1.38441900	3.02499300	-1.32630500
C	-0.75073500	2.95184800	1.00416700
C	-1.10637600	4.29676000	1.11666400
C	-2.30064800	4.73142900	0.54093800
C	-3.12575700	3.81042800	-0.11256200
C	-2.73284000	2.47522700	-0.17794400
C	-3.56616100	1.37422600	-0.70851000
C	-4.78752500	1.47279100	-1.38037100
C	-5.43962900	0.28884200	-1.74616000
C	-4.88746500	-0.95838600	-1.43654900
C	-3.66108700	-0.99369800	-0.76339200
C	-2.92243900	-2.18422800	-0.29531000
C	-3.39824400	-3.48991700	-0.37010000
C	-2.64688200	-4.52343200	0.20115000
C	-1.44050700	-4.22613700	0.83040400

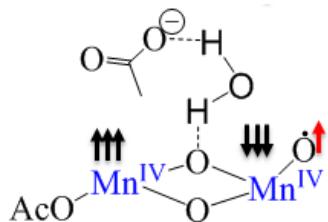
C	-0.99746900	-2.90079000	0.86768100
H	0.19414900	-2.46278000	-2.18247500
H	0.80689900	-4.90770800	-2.35630100
H	2.76652100	-5.74054400	-1.03823300
H	4.07253200	-4.13843000	0.34326900
H	5.03222000	-2.49280800	1.63675700
H	6.09930000	-0.44149600	2.54086600
H	5.25366500	1.79786000	1.89023200
H	4.53865800	3.62831600	0.76865900
H	3.48557400	5.53416600	-0.43175900
H	1.44893800	5.11351700	-1.83106400
H	0.51652000	2.79598300	-1.92459100
H	0.15261900	2.54455900	1.43659400
H	-0.46201000	4.97958900	1.65370900
H	-2.60150600	5.76884700	0.61626100
H	-4.07233100	4.12452500	-0.53173700
H	-5.22462400	2.43370300	-1.61497400
H	-6.38617200	0.33970300	-2.26944500
H	-5.40262400	-1.86812000	-1.71241200
H	-4.34890100	-3.70060100	-0.84125600
H	-3.01409100	-5.54147000	0.16648800
H	-0.84899600	-4.99760800	1.30418200
H	-0.09436700	-2.59615200	1.37250700
C	-1.54451600	-0.46620000	3.20703300
O	-0.69723900	-1.33817800	3.23635700
C	-2.27633400	0.06566700	4.43645400
H	-3.35125400	-0.11242100	4.33040800
H	-1.90034400	-0.44159100	5.32515700
H	-2.11813400	1.14519800	4.52314400
O	1.35733500	0.95200300	-3.30722000
H	1.59715500	0.63398000	-4.19863000
H	-0.65126900	0.57438400	-2.11886900



AcO–Mn(IV)–Mn(IV)–O(OH)₂ P2:

Mn	1.44966600	-0.15295400	-0.77879400
Mn	-1.14911700	-0.07116200	0.51354600
O	0.68044500	-0.03543000	0.80487100
O	-0.31798600	-0.09609700	-1.34941600
O	2.02978500	-0.36373900	-2.55119100
O	-1.60243900	-0.24828700	2.29879400
N	1.80659800	-2.14328600	-0.57175300
N	3.27232600	-0.13974700	-0.00232800
N	1.90604000	1.81890300	-0.91387800
N	-1.26844600	2.19322900	0.86684000
N	-3.08133700	0.61641900	-0.26050500
N	-2.39233600	-1.94268100	-0.04018000
C	0.99811700	-3.09959400	-1.05369400
C	1.29626500	-4.45166700	-0.87553300
C	2.45126200	-4.80465900	-0.17803700
C	3.29648600	-3.80115800	0.30548100
C	2.95781500	-2.46899000	0.08515700
C	3.79011400	-1.30550900	0.43686400
C	5.01653500	-1.30687800	1.10462400
C	5.67843500	-0.08882500	1.28933400
C	5.12462000	1.10191500	0.80915700
C	3.89123600	1.04782600	0.15533800
C	3.13698500	2.16831500	-0.43102600
C	3.60241200	3.47514800	-0.55129200
C	2.79837100	4.42761400	-1.18510000
C	1.54915800	4.05154300	-1.67695600
C	1.12765100	2.72971400	-1.52227000
C	-0.37987600	2.83386500	1.64703800
C	-0.61792100	4.12631500	2.11647300
C	-1.81214800	4.75851900	1.76240100
C	-2.73601500	4.08487600	0.95985200
C	-2.43482800	2.78893400	0.52981100
C	-3.36644000	1.94042800	-0.25006400
C	-4.49153200	2.43525300	-0.91672800
C	-5.32477900	1.54044800	-1.58743300
C	-5.03887200	0.17671800	-1.56045200
C	-3.90262400	-0.26636800	-0.87210900
C	-3.55152800	-1.69717900	-0.70090500
C	-4.38661500	-2.74133800	-1.11034500
C	-4.02744600	-4.05691000	-0.81167000
C	-2.85259300	-4.29690200	-0.09953700

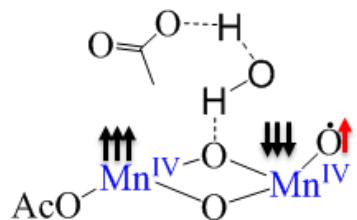
C	-2.05670400	-3.21170600	0.27183200
H	0.11500800	-2.76405200	-1.57843800
H	0.63454200	-5.20443900	-1.28199700
H	2.70280800	-5.84597800	-0.02231600
H	4.20753900	-4.05730800	0.82915100
H	5.44866200	-2.22743500	1.47167600
H	6.63000700	-0.06839300	1.80529400
H	5.64078700	2.04188000	0.94715600
H	4.58105800	3.74480800	-0.17748600
H	3.15091800	5.44487000	-1.29917700
H	0.90791600	4.76205700	-2.18071500
H	0.17145400	2.38162800	-1.88114400
H	0.51398700	2.27548500	1.89424700
H	0.10521200	4.61588600	2.75529000
H	-2.03293000	5.75592800	2.12156900
H	-3.68014700	4.55010300	0.71079300
H	-4.70973000	3.49398700	-0.92140400
H	-6.19593100	1.90218600	-2.11892400
H	-5.69151700	-0.52268200	-2.06252900
H	-5.31386800	-2.54258800	-1.62913700
H	-4.66904600	-4.87592600	-1.11166300
H	-2.56409300	-5.30074100	0.18339600
H	-1.15910000	-3.32357400	0.86394200
C	-1.08964000	-1.25707700	3.01450700
O	-0.41897900	-2.16074900	2.53070900
C	-1.44946200	-1.15490100	4.49138600
H	-1.07590800	-0.20937100	4.89687000
H	-2.53845800	-1.16274700	4.60404000
H	-1.01154800	-1.99526600	5.03022100
O	1.17853500	0.38999200	-3.44820100
H	1.44034800	-0.00786900	-4.30134800
H	-0.39514300	-0.02955000	-2.32473900



AcO–Mn(IV)–Mn(IV)–Od₂–OH₂–OAc_PT_R:

Mn	0.91847100	-0.94086500	-0.75353400
Mn	-0.12671500	1.04508300	0.90043900
O	1.10325600	-0.13221400	1.10267700
O	-0.23229700	0.39582700	-0.83164700
O	0.75418300	-1.51363600	-2.32159400
O	-0.04134400	1.93543500	2.57610800
N	-0.24862900	-2.47006700	-0.11391200
N	2.30886600	-2.24055000	-0.09678800
N	2.66251300	-0.02600600	-1.33208800
N	0.93686700	2.68964500	0.25090500
N	-1.60537000	2.27421900	0.21940700
N	-1.77890300	0.05661100	1.51077600
C	-1.56294500	-2.54117900	-0.38083000
C	-2.28378600	-3.70291100	-0.07755000
C	-1.63236900	-4.78157400	0.51253000
C	-0.26094400	-4.69400900	0.78132600
C	0.41696400	-3.52734000	0.44341900
C	1.87601700	-3.33553000	0.55262700
C	2.79932900	-4.15210800	1.21451400
C	4.14922400	-3.79325400	1.18088500
C	4.56755500	-2.64663500	0.49628900
C	3.60120800	-1.86979500	-0.14620100
C	3.81366500	-0.64382600	-0.94389100
C	5.05248400	-0.16634900	-1.37056800
C	5.09334900	0.93759700	-2.22655400
C	3.90082000	1.53246000	-2.64170200
C	2.69045000	1.02075800	-2.17148400
C	2.23934600	2.87258200	0.52022000
C	2.88486800	4.06303400	0.18539500
C	2.15253600	5.07420800	-0.44009700
C	0.79483600	4.88018900	-0.70524900
C	0.19721500	3.67407700	-0.33797000
C	-1.23999000	3.35647900	-0.48902000
C	-2.18233500	4.00890400	-1.28495000
C	-3.47594300	3.47138600	-1.35219300
C	-3.81352100	2.32114800	-0.63617000
C	-2.83242800	1.73558600	0.17195900
C	-2.96042700	0.53714700	1.02175600
C	-4.16807600	-0.04995100	1.38854900

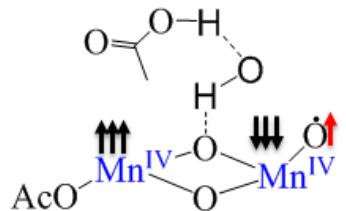
C	-4.15780600	-1.11146100	2.29482700
C	-2.94293000	-1.56712300	2.80834200
C	-1.75689100	-0.96637300	2.38678200
H	-2.04945600	-1.67759500	-0.83776400
H	-3.33593100	-3.73861400	-0.32395900
H	-2.17105100	-5.69127600	0.74668400
H	0.27086300	-5.53179700	1.21246200
H	2.47711500	-5.03382700	1.75090300
H	4.87933600	-4.40643000	1.69375600
H	5.61226100	-2.36832500	0.47674800
H	5.96492300	-0.66377100	-1.06985700
H	6.04530300	1.31081600	-2.58271100
H	3.90004100	2.36712300	-3.32951300
H	1.72799300	1.41647700	-2.46646300
H	2.73772000	2.04756200	1.01230400
H	3.93275600	4.19252100	0.42026600
H	2.62670800	6.01123500	-0.70411900
H	0.20435200	5.66348900	-1.16163600
H	-1.91911100	4.88160000	-1.86726900
H	-4.21335900	3.93764600	-1.99304600
H	-4.78082500	1.85589200	-0.74842700
H	-5.09518400	0.31997700	0.97654000
H	-5.08996600	-1.56859000	2.60236100
H	-2.90389000	-2.37182500	3.52988700
H	-0.78223000	-1.23865300	2.76415300
C	0.25275100	1.40636600	3.75931000
O	0.34747800	0.21233800	4.01122700
C	0.45305700	2.49171100	4.82554600
H	0.70897500	2.02521200	5.77726900
H	1.25060000	3.17263000	4.51131400
H	-0.46812000	3.07444100	4.92834400
O	-0.74274200	-0.37973100	-3.33081100
H	-1.54505600	-1.04775300	-3.31386700
H	-0.85239400	0.12110300	-2.48771700
O	-2.89010900	-1.76004900	-3.31989800
C	-3.77191800	-1.22065600	-2.58083200
O	-3.55564000	-0.54492600	-1.53294900
C	-5.23592800	-1.43204300	-3.02861800
H	-5.39048600	-2.48130600	-3.29546300
H	-5.92967500	-1.13054600	-2.24117000
H	-5.42042200	-0.83327000	-3.92801800



AcO–Mn(IV)–Mn(IV)–O^{···}H₂OAc_PT_TS:

Mn	0.92444100	-0.91478200	-0.74357400
Mn	-0.19758500	1.00434400	0.94622900
O	1.07930900	-0.11901900	1.14114500
O	-0.29724300	0.37071200	-0.77536700
O	0.71976700	-1.47185900	-2.30709300
O	-0.15709200	1.88043300	2.64252900
N	-0.12540000	-2.52476100	-0.08130500
N	2.40618300	-2.12174800	-0.10361600
N	2.58610200	0.09183600	-1.37161100
N	0.82588200	2.68037300	0.32603600
N	-1.70724300	2.21028100	0.27718200
N	-1.83713000	-0.03882500	1.52514700
C	-1.43222400	-2.69362500	-0.34322000
C	-2.07224400	-3.89068800	-0.00394600
C	-1.34564900	-4.90647300	0.61349100
C	0.01763400	-4.72076800	0.86796200
C	0.61302500	-3.51858100	0.49550900
C	2.05768600	-3.22509700	0.58160600
C	3.04083900	-3.95691900	1.25543500
C	4.36232800	-3.50569600	1.19813100
C	4.69257000	-2.35014200	0.48154200
C	3.66826100	-1.66002800	-0.17073900
C	3.78397000	-0.43751500	-0.99365400
C	4.97877500	0.11379600	-1.45525800
C	4.92672000	1.19721800	-2.33665900
C	3.68823800	1.69438700	-2.74621900
C	2.52424800	1.11196400	-2.24225300
C	2.12557600	2.88184800	0.59372100
C	2.74746300	4.09052700	0.27882500
C	1.99428000	5.09954800	-0.32433500
C	0.63946000	4.88466900	-0.58953700
C	0.06681700	3.66066200	-0.24372100
C	-1.36388000	3.31551300	-0.40397500
C	-2.31790400	3.96629300	-1.18877800
C	-3.60001300	3.40590500	-1.26886600
C	-3.91463200	2.23296400	-0.57847300
C	-2.92196000	1.64601300	0.21361200
C	-3.02536000	0.42043500	1.02996100
C	-4.22051600	-0.21152900	1.35969200

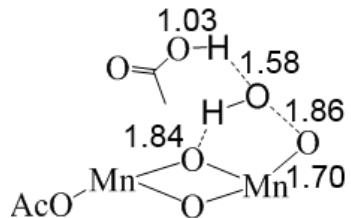
C	-4.19416500	-1.29826300	2.23691300
C	-2.97587700	-1.72936900	2.76015600
C	-1.80076000	-1.08104400	2.37540100
H	-1.96129400	-1.87694300	-0.83662200
H	-3.12134300	-4.00714800	-0.23934500
H	-1.82132300	-5.84279600	0.87747800
H	0.60762500	-5.50988900	1.31493600
H	2.78577700	-4.84309300	1.82000300
H	5.13796300	-4.05227000	1.71940300
H	5.71441700	-1.99796300	0.44635300
H	5.92879500	-0.31368200	-1.16322100
H	5.84377600	1.62711900	-2.71960000
H	3.61734700	2.50553600	-3.45811300
H	1.53078500	1.41752300	-2.54242900
H	2.63966500	2.05562100	1.06720700
H	3.79383700	4.23488000	0.51173400
H	2.44985900	6.05009700	-0.57219200
H	0.03334800	5.66484800	-1.03055500
H	-2.07122300	4.85651600	-1.75134900
H	-4.34775300	3.87356800	-1.89664200
H	-4.88175400	1.76541500	-0.69097500
H	-5.15419900	0.14588900	0.94956100
H	-5.11755900	-1.79019100	2.51589000
H	-2.92413000	-2.55121000	3.46125300
H	-0.82535200	-1.33246300	2.76525700
C	0.12537700	1.33422000	3.81783600
O	0.22396800	0.13550500	4.05144900
C	0.30828700	2.39952300	4.90796700
H	0.54912600	1.91588200	5.85507500
H	1.11112900	3.08551700	4.61900400
H	-0.61407500	2.98109800	5.00660300
O	-0.59861600	-0.20500700	-3.33940800
H	-1.51359400	-0.90427400	-3.50342600
H	-0.79260200	0.19056800	-2.45462100
O	-2.61756300	-1.49886400	-3.75218400
C	-3.53629400	-1.29297700	-2.87646900
O	-3.37877100	-0.78487700	-1.74082500
C	-4.93869800	-1.74003400	-3.32638600
H	-4.90070700	-2.78318500	-3.65502800
H	-5.65629400	-1.62434100	-2.51238900
H	-5.24872600	-1.13639300	-4.18606000



AcO–Mn(IV)–Mn(IV)–Od₂–OH₂–OAc_PT_P:

Mn	-0.96836600	-0.89386500	0.66609900
Mn	0.346444800	1.01627700	-0.89306100
O	-1.01295000	0.02438200	-1.18792400
O	0.40141700	0.25464000	0.75899600
O	-0.81646400	-1.53687900	2.19675100
O	0.40559200	2.01492100	-2.54238600
N	-0.06784900	-2.56386000	-0.08438200
N	-2.54028300	-1.90159100	-0.11969300
N	-2.55746100	0.19478300	1.34266300
N	-0.57949300	2.70605600	-0.18159900
N	1.92529300	2.11373400	-0.19769100
N	1.93181200	-0.08907100	-1.53743000
C	1.19843700	-2.89650000	0.21886500
C	1.73563100	-4.11232900	-0.21390400
C	0.94426000	-4.98141100	-0.96472100
C	-0.37905900	-4.63313400	-1.25243500
C	-0.87033000	-3.41541600	-0.78560800
C	-2.27044800	-2.96062000	-0.90386300
C	-3.27851800	-3.50366200	-1.70618700
C	-4.54374300	-2.91021200	-1.67643100
C	-4.79070600	-1.79823700	-0.86463900
C	-3.74380500	-1.30047400	-0.08457900
C	-3.77913100	-0.15348200	0.84681100
C	-4.93516400	0.48030300	1.30022500
C	-4.82395200	1.45344900	2.29799300
C	-3.57059900	1.74707300	2.83684500
C	-2.44301300	1.08911500	2.33956500
C	-1.87523800	2.97296300	-0.40376900
C	-2.43922400	4.18723100	-0.00949000
C	-1.63211600	5.13090400	0.62722200
C	-0.28058100	4.84888000	0.84297000
C	0.23238600	3.62426900	0.41678100
C	1.65576000	3.22498200	0.50357700
C	2.68032300	3.85777800	1.21273800
C	3.95875500	3.28805500	1.17379900
C	4.20259600	2.12173800	0.44272000
C	3.13525200	1.53996600	-0.25091800
C	3.15701000	0.32304400	-1.09085900
C	4.31459000	-0.34363300	-1.48285800

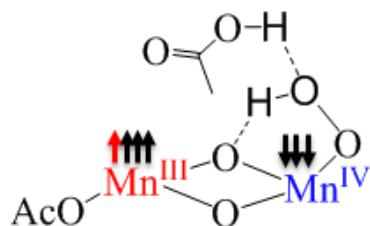
C	4.21087700	-1.42658000	-2.36104800
C	2.95652800	-1.81334700	-2.82693900
C	1.82326100	-1.12106700	-2.39090400
H	1.75747700	-2.19733300	0.83478900
H	2.75297400	-4.36432200	0.05323900
H	1.33877300	-5.93117400	-1.30389700
H	-1.02176900	-5.31094100	-1.79844900
H	-3.08285800	-4.35074400	-2.34920600
H	-5.33717000	-3.30817600	-2.29625000
H	-5.76565600	-1.33027800	-0.85458500
H	-5.90482000	0.19453800	0.91436200
H	-5.71226900	1.94593500	2.67367900
H	-3.46147200	2.45457400	3.64779600
H	-1.44853400	1.19258900	2.76254600
H	-2.43200000	2.19285000	-0.90560800
H	-3.48426500	4.38448700	-0.20640100
H	-2.04267600	6.08278700	0.93993000
H	0.36600500	5.57931600	1.31065200
H	2.49413700	4.75035400	1.79422700
H	4.76622100	3.75025300	1.72735600
H	5.18633100	1.67366900	0.43491500
H	5.28125400	-0.01469900	-1.12663600
H	5.10337400	-1.94686200	-2.68541000
H	2.84372100	-2.63084100	-3.52575900
H	0.82521600	-1.33612600	-2.73988700
C	0.16246500	1.54007100	-3.75293600
O	0.05081600	0.35689600	-4.05682200
C	0.04221200	2.66335300	-4.79440800
H	-0.15585100	2.23293400	-5.77652600
H	-0.76952100	3.34038500	-4.50878600
H	0.97200100	3.24098500	-4.81709000
O	0.20258600	-0.12452900	3.40422400
H	1.22613600	-1.19705200	3.90146600
H	0.63774100	0.10810600	2.54869700
O	1.96657500	-1.80769600	4.28888100
C	2.97336900	-1.95236100	3.44709200
O	3.02810500	-1.48195600	2.30986100
C	4.09662200	-2.78938900	4.05335800
H	3.70464100	-3.76907100	4.34458200
H	4.90549200	-2.90443500	3.33148300
H	4.46751400	-2.29854300	4.95870800



AcO–Mn(IV)–Mn(IV)–Od₂–OH₂–OAc_TS:

Mn	-1.05693500	-0.81553100	0.57139500
Mn	0.47485100	1.03441100	-0.82430100
O	-0.95432700	0.16906100	-1.20363800
O	0.41570900	0.20092800	0.78611100
O	-0.99627200	-1.56251200	2.09277200
O	0.65789700	2.09704600	-2.43052000
N	-0.27375900	-2.51851300	-0.20407400
N	-2.67511800	-1.66751300	-0.25881700
N	-2.57057000	0.37501800	1.27030300
N	-0.32345300	2.76974700	-0.06852000
N	2.12341000	1.97188300	-0.06052000
N	1.98133400	-0.16981400	-1.48890600
C	0.95544500	-2.96235800	0.11563600
C	1.41098000	-4.19462900	-0.35780100
C	0.57906100	-4.96697300	-1.17026000
C	-0.70474700	-4.50699100	-1.47373100
C	-1.11786700	-3.27683900	-0.96283900
C	-2.47485000	-2.71658200	-1.08110300
C	-3.51059800	-3.15802600	-1.91053000
C	-4.73160500	-2.48086600	-1.87108100
C	-4.90781500	-1.38353300	-1.02079200
C	-3.83867700	-0.98754100	-0.21525900
C	-3.80786000	0.12624100	0.75342700
C	-4.92321800	0.82600900	1.21258500
C	-4.75844400	1.76123300	2.23815500
C	-3.49353500	1.95720800	2.79423700
C	-2.40891500	1.23871800	2.28698300
C	-1.58540500	3.15459200	-0.31153000
C	-2.05405700	4.39920200	0.11227600
C	-1.18663100	5.24808600	0.80087700
C	0.13025400	4.84425400	1.03675600
C	0.54820400	3.59520800	0.57883100
C	1.93218300	3.07708300	0.67511700
C	2.99342700	3.60367800	1.41648100
C	4.22468000	2.93864600	1.36969400
C	4.38764600	1.78422900	0.59838500
C	3.28713500	1.31045200	-0.12527000
C	3.22817300	0.12959600	-1.01364100
C	4.33753500	-0.60573500	-1.42200200

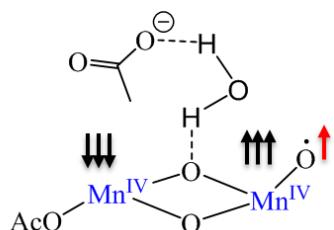
C	4.16380400	-1.64118000	-2.34560900
C	2.89000400	-1.91300400	-2.83859900
C	1.80641900	-1.15492800	-2.38525600
H	1.54524200	-2.33900200	0.78092300
H	2.39739100	-4.53637000	-0.07472600
H	0.91148000	-5.92777800	-1.54308100
H	-1.38111600	-5.10887600	-2.06612500
H	-3.36643500	-3.99429900	-2.58084000
H	-5.54433900	-2.80034000	-2.51081200
H	-5.84808400	-0.84948000	-1.00062500
H	-5.90490900	0.61963200	0.80717600
H	-5.61547300	2.30286800	2.61875700
H	-3.34474000	2.63711000	3.62223800
H	-1.41382300	1.27990900	2.71133500
H	-2.19298000	2.44329300	-0.85494400
H	-3.07282600	4.69221100	-0.10234900
H	-1.52266600	6.22081100	1.13751800
H	0.82467400	5.50126500	1.54321600
H	2.86992600	4.48863900	2.02564800
H	5.05872500	3.31815400	1.94627000
H	5.33547400	1.26462900	0.58059300
H	5.32194600	-0.36489400	-1.04436300
H	5.01875300	-2.21357800	-2.68306800
H	2.72468300	-2.69088700	-3.57131400
H	0.79959700	-1.28124800	-2.75150800
C	0.42606000	1.69451100	-3.66847300
O	0.23960200	0.53732400	-4.03065800
C	0.42603000	2.86754600	-4.66153100
H	0.23394300	2.49557400	-5.66840800
H	-0.34491500	3.58954700	-4.37300800
H	1.39524100	3.37558500	-4.62636800
O	-0.07090200	-0.50111900	3.31018400
H	0.84045500	-1.67079100	3.85175300
H	0.51616500	-0.18467300	2.58227500
O	1.50212400	-2.35051200	4.25399600
C	2.58354700	-2.47008200	3.50180300
O	2.76785600	-1.90101200	2.42611700
C	3.60386000	-3.41336000	4.13115900
H	3.14235400	-4.39171800	4.29829800
H	4.47165100	-3.50996700	3.47845900
H	3.90895500	-3.01979100	5.10599000



AcO–Mn(IV)–Mn(IV)–Od₂–OH₂–OAc_P:

Mn	-1.28876900	-0.38310600	0.38741500
Mn	0.86067000	0.70109900	-0.90246500
O	-0.95516600	0.46110800	-1.14958800
O	0.40663800	-0.08739100	0.75736500
O	-1.57012900	-1.32875700	2.01647100
O	1.19142900	1.35236000	-2.67158600
N	-1.27530200	-2.20684000	-0.52547800
N	-3.21826500	-0.58166900	-0.16228300
N	-2.13362100	1.20714200	1.31884300
N	0.49591700	2.94868800	-0.40779900
N	2.67744400	1.54050600	0.12724000
N	2.59774100	-0.81805400	-1.08627800
C	-0.23616300	-3.05298700	-0.46911600
C	-0.28006200	-4.28066800	-1.13759700
C	-1.41953700	-4.62088600	-1.86315000
C	-2.51194400	-3.74743300	-1.87839600
C	-2.42064400	-2.54349200	-1.18617200
C	-3.52748200	-1.57940400	-1.00833600
C	-4.80404600	-1.62509000	-1.57661200
C	-5.71876100	-0.62294400	-1.23672700
C	-5.36496100	0.40111200	-0.35201600
C	-4.07100200	0.39968400	0.17737400
C	-3.47275000	1.37724000	1.11025600
C	-4.17439400	2.37201200	1.78745600
C	-3.49162600	3.18415200	2.69776700
C	-2.12831000	2.98257000	2.90939700
C	-1.47162100	1.97780600	2.19610800
C	-0.55957500	3.60014100	-0.92223600
C	-0.65366100	4.99215100	-0.86765400
C	0.38259100	5.71000300	-0.26544700
C	1.48028800	5.02585300	0.26120300
C	1.50788900	3.63019600	0.16902800
C	2.63665700	2.78910700	0.63815400
C	3.61030500	3.22769200	1.54157500
C	4.62767600	2.34640600	1.90801700
C	4.66934800	1.06804500	1.35563900
C	3.67165200	0.68867800	0.44701200
C	3.65498400	-0.61294900	-0.26605300
C	4.68964500	-1.54838400	-0.17247900

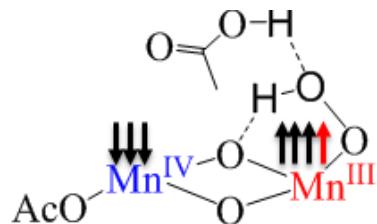
C	4.63417200	-2.70169800	-0.95583300
C	3.55927000	-2.88461600	-1.82439200
C	2.55243000	-1.91745800	-1.86325400
H	0.60410300	-2.75199900	0.14387300
H	0.56774100	-4.94903700	-1.07355100
H	-1.47333200	-5.56267100	-2.39445200
H	-3.41962600	-4.01163100	-2.40418200
H	-5.08012600	-2.41009900	-2.26686900
H	-6.71219800	-0.63817100	-1.66701600
H	-6.07340100	1.17727700	-0.09704800
H	-5.23718600	2.49685800	1.62810400
H	-4.02419600	3.95372600	3.24209000
H	-1.57646000	3.58376300	3.61914800
H	-0.42004900	1.76058700	2.31192400
H	-1.31254800	2.97076800	-1.38021600
H	-1.50842100	5.49804000	-1.29703800
H	0.34592300	6.79143800	-0.21952200
H	2.30503600	5.57117900	0.70052400
H	3.56706000	4.22284000	1.96236500
H	5.38473100	2.65535700	2.61783200
H	5.45910300	0.38372800	1.63008000
H	5.53235700	-1.38246500	0.48397200
H	5.42896900	-3.43490300	-0.89813500
H	3.50043800	-3.75087700	-2.47034700
H	1.70595000	-1.96962100	-2.53606200
C	0.87902700	0.59712600	-3.70364400
O	0.55058800	-0.58944600	-3.63486700
C	0.97206000	1.33973100	-5.04022800
H	0.71506600	0.66490900	-5.85720000
H	0.28916900	2.19554700	-5.02834800
H	1.98919200	1.72267500	-5.17284400
O	-0.56550400	-0.95861800	2.99553100
H	-0.10650700	-2.49363800	3.56798700
H	0.20815300	-0.78010400	2.39365700
O	0.27046300	-3.37168400	3.88105700
C	1.26545000	-3.74178300	3.07312000
O	1.63674000	-3.10509900	2.09436500
C	1.88549200	-5.05590000	3.52470200
H	1.11553600	-5.83338000	3.55234700
H	2.68561200	-5.33971700	2.84130300
H	2.28012800	-4.94246500	4.53940200



AcO–Mn(IV)–Mn(IV)–Od₁–OH₂–OAc–R:

Mn	1.08850600	-0.78870200	-0.76080900
Mn	-0.37152800	0.89048800	0.95277200
O	1.07956500	0.02135200	1.16462200
O	-0.38914100	0.23929800	-0.75293800
O	0.99119700	-1.34070600	-2.34141700
O	-0.49282200	1.77299400	2.66317700
N	0.35356000	-2.57551600	-0.11843900
N	2.76492100	-1.71086800	-0.10685900
N	2.55280000	0.50505300	-1.37231400
N	0.36634700	2.71107000	0.34428700
N	-2.06684500	1.87022400	0.36180700
N	-1.82412200	-0.40356000	1.55264200
C	-0.89777000	-2.98234900	-0.39143100
C	-1.31727500	-4.27136600	-0.05195900
C	-0.42279400	-5.13756400	0.57652700
C	0.88194200	-4.70863300	0.83797000
C	1.25315500	-3.41761600	0.46657200
C	2.61885600	-2.86238000	0.57188300
C	3.70839700	-3.40208800	1.26188800
C	4.92348800	-2.71103100	1.22948200
C	5.04292500	-1.51050800	0.52216900
C	3.91839900	-1.02094000	-0.14848000
C	3.82017400	0.20561400	-0.96802500
C	4.90454800	0.96623500	-1.40551100
C	4.67579000	2.02260900	-2.29100000
C	3.37692200	2.28006600	-2.73311700
C	2.32726400	1.49369200	-2.25491900
C	1.63222700	3.09364700	0.56966000
C	2.06155400	4.38478900	0.25836800
C	1.15016400	5.28290200	-0.29854200
C	-0.16969400	4.87926000	-0.51756100
C	-0.54685800	3.58128100	-0.17455700
C	-1.92536800	3.04704300	-0.26627000
C	-3.02454300	3.61979000	-0.91180400
C	-4.23924700	2.92327300	-0.88872700
C	-4.34900200	1.69302000	-0.23422700
C	-3.21279800	1.17680000	0.39958000
C	-3.09478800	-0.08578000	1.16034800
C	-4.17210600	-0.88330400	1.53614900

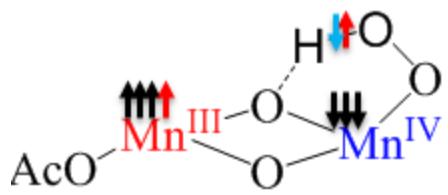
C	-3.94102200	-2.00091000	2.34356900
C	-2.64277800	-2.29228100	2.75580200
C	-1.59316300	-1.46977800	2.33712500
H	-1.54464300	-2.27399600	-0.89888900
H	-2.32605500	-4.57871100	-0.29202300
H	-0.72474400	-6.14285200	0.84276000
H	1.60146900	-5.37693300	1.29209300
H	3.61410300	-4.32310100	1.82061500
H	5.77852700	-3.10551700	1.76371600
H	5.98076200	-0.97217200	0.50739300
H	5.91001900	0.71802800	-1.09223800
H	5.50697000	2.61410500	-2.65413100
H	3.17469500	3.06153800	-3.45319500
H	1.30489100	1.59839800	-2.59894700
H	2.27500000	2.34136700	1.00745400
H	3.08451100	4.67454200	0.45702700
H	1.45525700	6.29195300	-0.54593700
H	-0.89660600	5.57085400	-0.92212700
H	-2.94212000	4.56329500	-1.43383500
H	-5.10174000	3.33816700	-1.39477400
H	-5.28277200	1.14855300	-0.23910600
H	-5.17504100	-0.62917500	1.22173500
H	-4.77050800	-2.62291000	2.65594900
H	-2.43310300	-3.13484400	3.40042900
H	-0.56935100	-1.60871500	2.64790600
C	-0.17747900	1.25259600	3.83792000
O	0.05104800	0.06985600	4.06809500
C	-0.13787100	2.31979000	4.94296900
H	0.12055800	1.85299100	5.89396500
H	0.60220200	3.08442400	4.68501900
H	-1.11585300	2.80650400	5.01582200
O	-0.60566500	0.41946000	-3.36226700
H	-1.75358200	-0.69752700	-3.85396300
H	-0.66456000	0.31738900	-2.36471800
O	-2.49974000	-1.27288700	-4.22523400
C	-3.29807100	-1.71849300	-3.26253700
O	-3.15734700	-1.48970500	-2.06436700
C	-4.43064900	-2.56327400	-3.83312000
H	-4.00943200	-3.42396800	-4.36261700
H	-5.08348300	-2.90000300	-3.02776700
H	-4.99838000	-1.97311500	-4.55909700



AcO–Mn(IV)–Mn(III)–OOH–OAc (or AcO–Mn(IV)–Mn(IV)–O^{dot1}–OH₂–OAc_P) :

Mn	-1.12756400	0.45279300	-0.52528300
Mn	0.95974300	-0.82589300	0.71504400
O	-0.64359900	-0.31171800	1.14781500
O	0.56858900	-0.24161900	-0.92823800
O	-1.19158400	1.35655700	-2.15691000
O	1.48271000	-1.57127300	2.42233000
N	-1.46068500	2.51653300	0.37486200
N	-3.20499500	0.54881300	0.27868400
N	-2.35760300	-1.28578200	-1.43030200
N	0.55686300	-2.77777500	0.24848000
N	2.74631900	-1.46034200	-0.00641900
N	2.13242800	0.79076500	1.07688700
C	-0.62833000	3.55056400	0.15530200
C	-0.83293500	4.78721200	0.77497300
C	-1.92444800	4.94075300	1.63009600
C	-2.80052000	3.87015200	1.82597000
C	-2.54601200	2.66334900	1.16957200
C	-3.46751700	1.49926400	1.19647700
C	-4.57336800	1.38075000	2.04665100
C	-5.40673800	0.27042100	1.91118100
C	-5.14116100	-0.68556400	0.92976500
C	-4.01464200	-0.51565800	0.11715600
C	-3.62521300	-1.43515100	-0.98131400
C	-4.49875000	-2.35189400	-1.57433300
C	-4.04588600	-3.10784000	-2.65807500
C	-2.74256700	-2.92836600	-3.12569400
C	-1.92166700	-2.00080900	-2.48115400
C	-0.60361900	-3.37480400	0.55758800
C	-0.80217200	-4.73397000	0.30746700
C	0.22969600	-5.47190000	-0.27314500
C	1.43908800	-4.84249500	-0.58067400
C	1.58530700	-3.48449800	-0.30123400
C	2.82469600	-2.70253800	-0.50892000
C	4.00205900	-3.11719300	-1.13756600
C	5.06169500	-2.20630900	-1.22268100
C	4.94569200	-0.91950500	-0.68930900
C	3.74185300	-0.56343300	-0.06928000
C	3.40357600	0.72051700	0.57944200
C	4.28927900	1.78084300	0.74587100

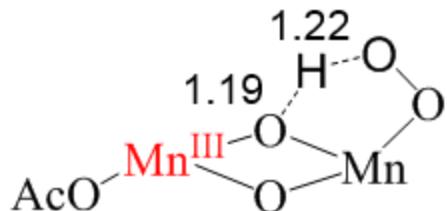
C	3.86469000	2.91749600	1.44036200
C	2.57461900	2.95891600	1.96108400
C	1.72288700	1.86827600	1.76406500
H	0.19127700	3.37601900	-0.53452400
H	-0.15497600	5.60679000	0.57603200
H	-2.10857600	5.88711200	2.12348800
H	-3.67303200	3.98893300	2.45393600
H	-4.77620600	2.12736900	2.80160300
H	-6.26113600	0.15211400	2.56571000
H	-5.78518300	-1.54654700	0.81372900
H	-5.51870900	-2.45064900	-1.22695100
H	-4.71084000	-3.81170900	-3.14314900
H	-2.37221600	-3.48111400	-3.97890600
H	-0.90979100	-1.79393900	-2.80305700
H	-1.34983300	-2.73580800	1.00989300
H	-1.74345200	-5.19713100	0.57060300
H	0.10331800	-6.52831600	-0.47405800
H	2.25743700	-5.40449000	-1.01055200
H	4.09618500	-4.10997300	-1.55569300
H	5.98220000	-2.50186400	-1.71010200
H	5.76616600	-0.21915700	-0.76104500
H	5.29427100	1.72244700	0.35043000
H	4.54138800	3.75111700	1.57845800
H	2.22024500	3.81428400	2.51948100
H	0.72767100	1.81388600	2.17478200
C	1.24540100	-1.02536200	3.60438200
O	0.82662200	0.10914900	3.80546700
C	1.57250200	-1.99011900	4.75513200
H	1.37298000	-1.50223300	5.70970900
H	0.96058200	-2.89294000	4.65839400
H	2.62482400	-2.28637800	4.69621500
O	-0.26365700	0.80488600	-3.13782300
H	0.44879800	2.24643400	-3.65606400
H	0.43021800	0.42972400	-2.52879600
O	0.92243100	3.04980000	-4.03706300
C	1.67777200	3.63961300	-3.11262600
O	1.78152500	3.26783900	-1.94914600
C	2.40612800	4.84748400	-3.68676500
H	1.67268400	5.57412300	-4.05098100
H	3.03309200	5.29956900	-2.91839800
H	3.01717100	4.53615400	-4.53961700



AcO–Mn(III)–Mn(IV)–OOH_R:

Mn	1.33610200	-0.14794900	-0.75470900
Mn	-1.04451800	-0.17187200	0.58646500
O	0.75654900	-0.05924500	0.94508700
O	-0.37568200	-0.18620300	-1.18312500
O	1.90175500	-0.30199500	-2.54950300
O	-1.57339600	-0.37613000	2.42366900
N	1.80473100	-2.13733400	-0.54339900
N	3.25162100	-0.06840500	-0.11417000
N	1.73780100	1.82279000	-0.94623700
N	-1.20185400	2.11373200	1.04566300
N	-2.99995000	0.64468100	-0.23509600
N	-2.44079700	-1.94457500	-0.03647300
C	0.99350800	-3.13155300	-0.92932500
C	1.34988800	-4.46842400	-0.74176800
C	2.57132600	-4.76340600	-0.13794800
C	3.41897600	-3.72020500	0.24452000
C	3.01560200	-2.40563500	0.02116000
C	3.83641600	-1.20696300	0.29537900
C	5.10483100	-1.15724600	0.88045100
C	5.72623100	0.08889500	1.01442900
C	5.09511300	1.25426600	0.56922800
C	3.82393600	1.14229100	-0.00314900
C	2.98335000	2.22369000	-0.55466400
C	3.39602500	3.54025000	-0.74361300
C	2.52346300	4.44357600	-1.35853300
C	1.26507700	4.00907000	-1.77043600
C	0.89807400	2.67986000	-1.54758100
C	-0.32834700	2.69274300	1.88527600
C	-0.55074500	3.97218300	2.39862600
C	-1.71298500	4.65117600	2.02504400
C	-2.61966300	4.03969700	1.15637200
C	-2.33209600	2.75491600	0.68336800
C	-3.23465700	1.97367900	-0.19736600
C	-4.27255400	2.54284000	-0.94362000
C	-5.06728600	1.70911300	-1.72936800
C	-4.83146300	0.33585400	-1.73771800
C	-3.78185400	-0.17696400	-0.96326000
C	-3.49204100	-1.62706900	-0.82809200
C	-4.28554900	-2.62160300	-1.41018000
C	-3.99594500	-3.96134000	-1.14848400

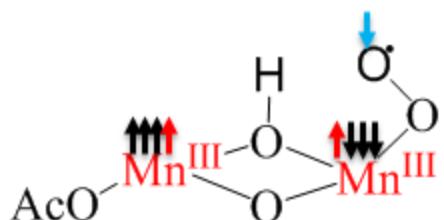
C	-2.93562000	-4.27591000	-0.29898300
C	-2.17561200	-3.23647700	0.24228500
H	0.06088400	-2.83031100	-1.38499900
H	0.67986000	-5.25309900	-1.06567300
H	2.86983800	-5.79109200	0.02519400
H	4.37888500	-3.93075400	0.69642800
H	5.59689800	-2.05610100	1.22516800
H	6.70793100	0.15102000	1.46672800
H	5.57929300	2.21561400	0.67214900
H	4.38693100	3.85182300	-0.44141200
H	2.83263400	5.46792500	-1.52366600
H	0.57487100	4.67932200	-2.26447700
H	-0.05763600	2.27433500	-1.84160500
H	0.53964700	2.09331400	2.13006500
H	0.161112700	4.41658200	3.08175600
H	-1.92082900	5.63932100	2.41661700
H	-3.53935200	4.54082100	0.88498100
H	-4.44643900	3.60988300	-0.92478400
H	-5.86830000	2.12580900	-2.32697000
H	-5.45330900	-0.31661200	-2.33352000
H	-5.12478300	-2.36578200	-2.04185200
H	-4.60331900	-4.74321900	-1.58727700
H	-2.70541500	-5.30254400	-0.04541800
H	-1.36167400	-3.39529900	0.93871900
C	-1.11379400	-1.41794400	3.07889900
O	-0.52480800	-2.37099000	2.55859500
C	-1.38400300	-1.35604700	4.58507400
H	-1.001112500	-2.25556600	5.06793900
H	-0.89882300	-0.46802900	5.00347700
H	-2.46116500	-1.26356600	4.75787100
O	0.97521000	0.37707400	-3.41382800
H	0.12027500	0.06156500	-3.03464300



AcO–Mn(III)–Mn(IV)–OOH_TS1:

Mn	1.41266200	-0.11897200	-0.73465900
Mn	-1.05240900	-0.14553700	0.57634500
O	0.73244100	-0.01933000	0.92887300
O	-0.36925300	-0.06444700	-1.22735500
O	1.70950500	-0.38589400	-2.67797300
O	-1.55265600	-0.41512000	2.40264900
N	1.89230800	-2.10076500	-0.49961700
N	3.30038800	-0.00338200	-0.14480600
N	1.78805700	1.82858300	-1.03234400
N	-1.25055300	2.12078300	1.06498400
N	-3.04315600	0.62702900	-0.19913800
N	-2.41713100	-1.95576400	-0.07927500
C	1.09984000	-3.11942100	-0.86183400
C	1.45410200	-4.44326800	-0.59499500
C	2.65423200	-4.69973000	0.06672300
C	3.48662000	-3.63432400	0.42067200
C	3.08708700	-2.33570200	0.11304400
C	3.89791600	-1.11957200	0.32690600
C	5.17124400	-1.03863400	0.88997800
C	5.80419200	0.21031700	0.93812500
C	5.17202000	1.34654500	0.43044900
C	3.88896300	1.21178600	-0.11155400
C	3.03627800	2.26512800	-0.67715900
C	3.41388700	3.59298600	-0.88221300
C	2.50282100	4.47613900	-1.46148100
C	1.23387000	4.01299500	-1.82261300
C	0.90438500	2.68034200	-1.58945000
C	-0.36193300	2.71478100	1.87763400
C	-0.59177900	3.99015500	2.39806000
C	-1.77703400	4.64773400	2.06054100
C	-2.69772400	4.02104200	1.21774100
C	-2.40099200	2.74224800	0.73413800
C	-3.30894300	1.94984000	-0.13098500
C	-4.37923200	2.50678300	-0.83979800
C	-5.17325000	1.66973900	-1.62213400
C	-4.90313400	0.30376000	-1.66502300
C	-3.82286400	-0.19853200	-0.92669900
C	-3.49599500	-1.64430900	-0.83478600
C	-4.28223900	-2.64299300	-1.42028200

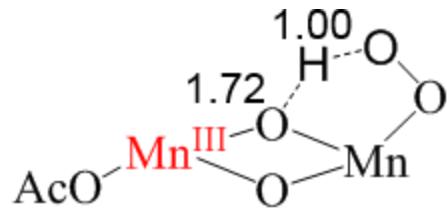
C	-3.95601700	-3.98136800	-1.19830700
C	-2.86830200	-4.29135600	-0.38236300
C	-2.11830200	-3.24737700	0.16388000
H	0.17978500	-2.85140300	-1.36218700
H	0.79870300	-5.24746500	-0.90039300
H	2.94847800	-5.71590700	0.29631300
H	4.43029500	-3.81668100	0.91687500
H	5.66541300	-1.91885700	1.27734700
H	6.79377600	0.29301500	1.36915900
H	5.66220400	2.30993800	0.46315600
H	4.40593700	3.92669500	-0.60781700
H	2.78177800	5.50734200	-1.63673200
H	0.51016500	4.67058000	-2.28515300
H	-0.05601300	2.25259900	-1.84023100
H	0.52318200	2.12952100	2.09422000
H	0.13278700	4.44773500	3.05875700
H	-1.99096600	5.63181600	2.45904100
H	-3.63280200	4.50717200	0.97317900
H	-4.57791800	3.56865800	-0.79589700
H	-5.99898500	2.07808700	-2.19116300
H	-5.52193400	-0.35187500	-2.26038300
H	-5.14325800	-2.39239800	-2.02402800
H	-4.55655200	-4.76650600	-1.64064300
H	-2.61013900	-5.31819300	-0.15825000
H	-1.28706400	-3.40378200	0.83982700
C	-1.08269200	-1.46506700	3.04173600
O	-0.48667600	-2.40566400	2.51096200
C	-1.35740400	-1.42225800	4.54810200
H	-0.97500700	-2.32777100	5.01999400
H	-0.87317200	-0.53963100	4.97876400
H	-2.43492200	-1.33243100	4.71952600
O	0.55918400	-0.27388700	-3.36312300
H	-0.18758400	-0.17862500	-2.40267200



AcO–Mn(III)–Mn(IV)–OOH_P1:

Mn	1.44409400	-0.09057500	-0.74780100
Mn	-1.07982500	-0.07645000	0.53646700
O	0.69554000	0.03298800	0.87854300
O	-0.43034100	0.10137700	-1.31412200
O	1.94812900	-0.39970200	-2.66906800
O	-1.57796500	-0.34563200	2.35206600
N	1.81909700	-2.11445600	-0.52637300
N	3.27490200	-0.04039900	-0.07245500
N	1.87696100	1.86483000	-1.06156500
N	-1.29099100	2.19119900	0.96289100
N	-3.09702200	0.63658300	-0.20827700
N	-2.38218600	-1.92599100	-0.09953200
C	1.07665200	-3.13215100	-0.98637100
C	1.41612100	-4.46190100	-0.72968100
C	2.55550000	-4.73290700	0.02671400
C	3.34952500	-3.67348200	0.47139500
C	2.96846200	-2.36757000	0.16670300
C	3.79061200	-1.17149500	0.44717100
C	5.02379600	-1.12546700	1.10571000
C	5.69311600	0.09886000	1.18523100
C	5.14121900	1.25299900	0.61836800
C	3.89889500	1.15445100	-0.01200200
C	3.12084700	2.24186600	-0.64220300
C	3.57173000	3.54760300	-0.83453100
C	2.73252900	4.46505700	-1.47170100
C	1.46604900	4.06054200	-1.89839000
C	1.06529900	2.74286500	-1.67383900
C	-0.39029300	2.82562700	1.73041800
C	-0.61618900	4.12253500	2.19622700
C	-1.81015800	4.75961400	1.85054100
C	-2.74314700	4.09134700	1.05461000
C	-2.45035300	2.79260100	0.62478000
C	-3.37140700	1.95921400	-0.18601900
C	-4.46230000	2.47944000	-0.89140900
C	-5.26608800	1.60738600	-1.62386600
C	-4.98466500	0.24294700	-1.62193000
C	-3.88518200	-0.22138300	-0.88780900
C	-3.53578000	-1.65826600	-0.75710500
C	-4.36722400	-2.68869200	-1.20907100

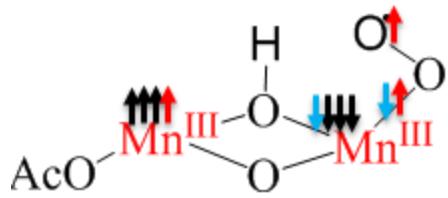
C	-4.00437500	-4.01278800	-0.95900900
C	-2.83480600	-4.27626800	-0.24677400
C	-2.04623700	-3.20289400	0.17299200
H	0.21576600	-2.86034300	-1.57964500
H	0.79780900	-5.25979800	-1.11837200
H	2.83628900	-5.75362900	0.25301600
H	4.25594100	-3.86586700	1.02942500
H	5.45586900	-2.01532800	1.54195000
H	6.64999300	0.15443400	1.68867400
H	5.66290600	2.19825300	0.67947500
H	4.56155600	3.84091400	-0.51070700
H	3.06990000	5.47997900	-1.64069200
H	0.80131200	4.74694600	-2.40541100
H	0.10333400	2.34817700	-1.97382400
H	0.50182300	2.25558900	1.95838500
H	0.11826200	4.61245900	2.82184800
H	-2.02108200	5.76037600	2.20681000
H	-3.68400300	4.56311500	0.80445200
H	-4.66844500	3.54071900	-0.88523200
H	-6.10578800	1.98803500	-2.19160400
H	-5.60432000	-0.43979200	-2.18535000
H	-5.29223500	-2.47142300	-1.72473400
H	-4.63920900	-4.82220400	-1.29744600
H	-2.54222600	-5.28926500	-0.00346400
H	-1.15583700	-3.32513200	0.77517800
C	-1.08425800	-1.36606100	3.02658700
O	-0.46802500	-2.30886100	2.52861100
C	-1.36624700	-1.27625100	4.52935200
H	-0.97222300	-2.15968500	5.03249700
H	-0.89636700	-0.37267400	4.93164300
H	-2.44551200	-1.19658800	4.69427500
O	0.96845400	-1.04108800	-3.27323900
H	-0.51177800	-0.54094400	-2.05349100



AcO–Mn(III)–Mn(IV)–OOH_TS2:

Mn	1.30998400	-0.11329200	-0.74074800
Mn	-1.08648200	-0.18038900	0.57212400
O	0.71053300	-0.05169700	0.94314700
O	-0.41430700	-0.15238400	-1.19441700
O	1.77051100	-0.27021900	-2.67417100
O	-1.63774300	-0.37995800	2.39985200
N	1.98093300	-2.18602000	-0.54738500
N	3.30017700	0.01481100	-0.11713800
N	1.78755500	1.92612600	-1.01163200
N	-1.31007600	2.10336100	1.00420400
N	-3.07020400	0.55222500	-0.23753700
N	-2.38966900	-2.00950300	-0.05460400
C	1.23802000	-3.24709200	-0.89164500
C	1.66572200	-4.55092500	-0.63181100
C	2.89049500	-4.73976900	0.00813600
C	3.66483100	-3.62946800	0.35338600
C	3.18552500	-2.35345500	0.05361800
C	3.93186900	-1.09822500	0.30122400
C	5.20081500	-1.00312000	0.88332100
C	5.78779400	0.25728100	1.00813100
C	5.11935100	1.39534400	0.55116500
C	3.85137300	1.24013000	-0.01692700
C	3.00844400	2.32539800	-0.56659500
C	3.40345800	3.65866200	-0.68318900
C	2.53047500	4.57476700	-1.27589200
C	1.28824400	4.14105200	-1.73979700
C	0.94543500	2.79636900	-1.58847200
C	-0.44293200	2.72635700	1.81825600
C	-0.70299500	4.00370500	2.31901100
C	-1.89768400	4.63268600	1.96056600
C	-2.79785700	3.97500900	1.11940900
C	-2.47121400	2.69557100	0.65671400
C	-3.36211100	1.86970500	-0.19549000
C	-4.44521500	2.38936700	-0.91327200
C	-5.22512200	1.51858600	-1.67308900
C	-4.92677800	0.15768000	-1.68839100
C	-3.83184200	-0.30529500	-0.94592600
C	-3.46428700	-1.73984800	-0.83151000
C	-4.20449800	-2.76898100	-1.42372800
C	-3.83347700	-4.09357200	-1.18860200

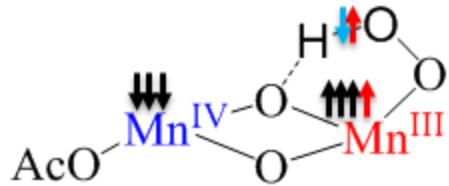
C	-2.74740100	-4.35996100	-0.35523100
C	-2.04514500	-3.28706300	0.19895400
H	0.29399400	-3.03066100	-1.37381700
H	1.05067800	-5.39113600	-0.92465100
H	3.24549000	-5.73788800	0.23126600
H	4.62193000	-3.76291700	0.83908100
H	5.72033200	-1.88483800	1.23112200
H	6.76839900	0.35251600	1.45705400
H	5.57559200	2.37138400	0.64035700
H	4.37795800	3.97686700	-0.33821300
H	2.82466500	5.61132600	-1.38240300
H	0.59747900	4.82368400	-2.21594000
H	0.00451600	2.38654800	-1.92840400
H	0.45014700	2.16203800	2.05669500
H	0.00469700	4.48395300	2.98193900
H	-2.13544900	5.61750200	2.34345100
H	-3.74129900	4.43743800	0.86134100
H	-4.66598000	3.44759800	-0.89215300
H	-6.06239700	1.89711800	-2.24588900
H	-5.53613200	-0.52379500	-2.26426800
H	-5.06253700	-2.55244600	-2.04477200
H	-4.39796600	-4.90230500	-1.63593400
H	-2.45440500	-5.37562300	-0.12330900
H	-1.22048700	-3.40905400	0.88990200
C	-1.17849300	-1.40493300	3.08337400
O	-0.56139900	-2.35675400	2.59760900
C	-1.49180400	-1.31999400	4.58077400
H	-1.10850400	-2.20458600	5.09018600
H	-1.03195100	-0.41710400	4.99593200
H	-2.57465000	-1.24185100	4.72216700
O	0.75299000	0.28788100	-3.42929300
H	-0.04533800	0.05045300	-2.86713300



AcO–Mn(III)–Mn(IV)–OOH_P2:

Mn	1.36105500	0.08130800	-0.96713000
Mn	-1.14857100	0.18819300	0.44768100
O	0.63411100	0.31655800	0.66988200
O	-0.62673400	-0.13997000	-1.43968500
O	1.88992800	0.10754100	-2.83168800
O	-1.59384900	0.49124800	2.26210900
N	1.51622200	-2.18854200	-1.07627700
N	3.26155300	-0.52681200	0.00319600
N	2.64783100	1.94970400	-0.70695000
N	-1.62902600	2.42990900	0.11526000
N	-3.24217600	0.34065100	-0.24482600
N	-2.06519700	-1.92868000	0.50239700
C	0.66758300	-2.93257300	-1.80618700
C	0.83503200	-4.31263500	-1.93672500
C	1.90797100	-4.92215400	-1.28403700
C	2.78309900	-4.14376500	-0.52312700
C	2.56177700	-2.76603100	-0.44076800
C	3.44638500	-1.82803600	0.29333800
C	4.41583200	-2.21984000	1.22343000
C	5.18512000	-1.23418200	1.84123500
C	4.99127300	0.10827100	1.51493300
C	4.00743800	0.43613000	0.57485600
C	3.72045000	1.81665600	0.10957700
C	4.51924700	2.91870400	0.43094300
C	4.20452400	4.16676500	-0.10842500
C	3.10898500	4.28626300	-0.96432600
C	2.35153900	3.14741600	-1.24164300
C	-0.78834500	3.39920900	0.51266100
C	-1.19520300	4.73206700	0.59333100
C	-2.51299200	5.04962500	0.25812700
C	-3.38618500	4.03546200	-0.14026400
C	-2.91025400	2.72138000	-0.19919400
C	-3.75502100	1.55284800	-0.55399200
C	-5.00884600	1.66596800	-1.16395400
C	-5.72801100	0.50416500	-1.44076700
C	-5.19616600	-0.73668200	-1.09801500
C	-3.93479200	-0.79276000	-0.48990900
C	-3.29458900	-2.05753500	-0.04664900
C	-3.91985300	-3.30631400	-0.12862900
C	-3.25807200	-4.42709900	0.37704700

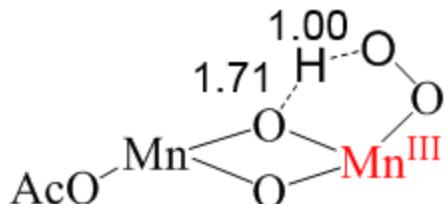
C	-2.00067200	-4.27555500	0.96079600
C	-1.43129000	-3.00054100	1.00966900
H	-0.14590900	-2.38916300	-2.26877900
H	0.14499900	-4.88809100	-2.53928900
H	2.07065700	-5.98911900	-1.37302800
H	3.63054900	-4.59995200	-0.02945500
H	4.55357100	-3.26154400	1.47739500
H	5.92994100	-1.51005500	2.57690800
H	5.58395700	0.87508700	1.99326000
H	5.38268800	2.80801700	1.07227200
H	4.81699100	5.02863900	0.12527700
H	2.85055800	5.23373100	-1.41831100
H	1.50525300	3.16659000	-1.91568600
H	0.20961400	3.07308100	0.77622700
H	-0.50154300	5.49471400	0.92169200
H	-2.86379100	6.07225300	0.31992400
H	-4.41758300	4.26580500	-0.37033200
H	-5.40833700	2.63408700	-1.43142000
H	-6.69681000	0.56600600	-1.92024300
H	-5.75223400	-1.63990600	-1.30341700
H	-4.90615900	-3.41146200	-0.55889400
H	-3.72960700	-5.40091400	0.32911300
H	-1.47301300	-5.11958000	1.38460800
H	-0.48692100	-2.79547600	1.49414600
C	-1.06941800	-0.20392500	3.25988300
O	-0.39425400	-1.22123800	3.14100900
C	-1.41170100	0.39992300	4.62762200
H	-0.98577000	-0.21775900	5.41882000
H	-1.00954300	1.41673700	4.68539300
H	-2.49907100	0.45973600	4.73920700
O	1.20349700	1.14785900	-3.22607200
H	-0.86968700	0.55409600	-2.07822500



AcO-Mn(IV)-Mn(III)-OOH_R:

Mn	1.22221200	0.08936200	-0.94369100
Mn	-1.20856500	0.13191800	0.34799000
O	0.46707500	0.13627600	0.81000400
O	-0.64620500	0.06168500	-1.33114600
O	1.64437300	0.12590800	-2.74974600
O	-1.97857600	0.30982100	2.13615500
N	1.67613800	-2.16394700	-1.08734300
N	3.14610100	-0.33562600	0.12177800
N	2.35730500	2.07051300	-0.64621200
N	-1.55481200	2.14851700	0.25778300
N	-3.11976700	0.20199800	-0.34222500
N	-1.72012900	-1.83545700	0.37023800
C	1.01239600	-2.96910000	-1.93259200
C	1.36912300	-4.30930300	-2.09493400
C	2.44287900	-4.80990300	-1.35541900
C	3.13587200	-3.96404900	-0.48608800
C	2.72878900	-2.63068600	-0.37902000
C	3.42831900	-1.61242100	0.44397500
C	4.33258900	-1.90861000	1.46938000
C	4.93726400	-0.85221900	2.15174200
C	4.65487000	0.46428100	1.78768500
C	3.74541400	0.69383500	0.74819000
C	3.40577800	2.03520900	0.21071100
C	4.15767900	3.18340800	0.47858100
C	3.82725000	4.37504700	-0.16986500
C	2.77143000	4.38831800	-1.08233900
C	2.05604000	3.20856700	-1.29793400
C	-0.69650900	3.05868300	0.74113000
C	-1.00291500	4.42094600	0.71999200
C	-2.22551100	4.83007900	0.18780300
C	-3.12123500	3.87217900	-0.29558300
C	-2.76670000	2.52514400	-0.24173000
C	-3.64398200	1.40113300	-0.63833000
C	-4.90576600	1.47175400	-1.23645200
C	-5.57905300	0.27423500	-1.50316500
C	-5.00693600	-0.95825700	-1.17362900
C	-3.74024200	-0.96325400	-0.57793000
C	-2.95818500	-2.13374300	-0.12499100
C	-3.42362900	-3.44659500	-0.12727700
C	-2.60957200	-4.45535800	0.39740600

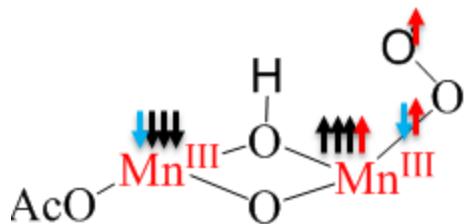
C	-1.35867500	-4.12756900	0.91468100
C	-0.93867400	-2.79418800	0.89209600
H	0.19648200	-2.51009700	-2.47622000
H	0.82707100	-4.93624900	-2.79041400
H	2.75121000	-5.84212700	-1.46648700
H	3.99156500	-4.32914400	0.06613400
H	4.54485000	-2.93255800	1.74460900
H	5.62451100	-1.05423800	2.96355200
H	5.12097700	1.28745500	2.31108000
H	5.00437000	3.14643000	1.15062100
H	4.40510400	5.27179900	0.01665300
H	2.51469700	5.28512100	-1.63070800
H	1.25601200	3.12949200	-2.02233400
H	0.22544500	2.66195800	1.14318600
H	-0.29590300	5.13619200	1.11776200
H	-2.48894700	5.87987500	0.15988200
H	-4.08391000	4.17003200	-0.68897100
H	-5.35355200	2.42209000	-1.49255900
H	-6.55565300	0.30281000	-1.96970800
H	-5.53293700	-1.88018500	-1.37970700
H	-4.40756800	-3.67855200	-0.51222300
H	-2.95984300	-5.47984100	0.41230400
H	-0.71465200	-4.88091700	1.34691600
H	-0.00253200	-2.46151900	1.30957500
C	-1.58685700	-0.34549900	3.21253600
O	-0.82235400	-1.30593800	3.24033000
C	-2.21729200	0.22337800	4.49513100
H	-1.88042700	-0.35348200	5.35707900
H	-1.92667400	1.27304500	4.60793100
H	-3.30849000	0.18115000	4.41649800
O	0.82804200	1.21330800	-3.26268900
H	-0.06881700	0.85635900	-3.06589400



AcO–Mn(IV)–Mn(III)–OOH_TS:

Mn	1.21740800	-0.07708700	-0.81693100
Mn	-1.19237800	0.00335900	0.44425800
O	0.52992100	-0.02793300	0.88687100
O	-0.56564600	0.04377200	-1.26784700
O	1.66893200	-0.09365800	-2.72823900
O	-1.89173400	-0.01447200	2.24281500
N	1.91936000	-2.27087400	-0.80416200
N	3.21474700	-0.12957900	0.06345400
N	2.06241000	2.08427800	-0.85969500
N	-1.45153100	2.14602600	0.61037000
N	-3.13022900	0.37952900	-0.30643200
N	-2.02186100	-1.94934600	0.12197900
C	1.31058500	-3.27107200	-1.46158200
C	1.76454300	-4.58859600	-1.37644100
C	2.87908800	-4.85938000	-0.58084400
C	3.51823800	-3.81314800	0.08730200
C	3.01656100	-2.51515100	-0.05231700
C	3.67088300	-1.31317100	0.52506400
C	4.72207400	-1.36091500	1.44652100
C	5.30184200	-0.16429300	1.86784700
C	4.84700700	1.04727500	1.34989600
C	3.78878700	1.03409900	0.43349900
C	3.24269100	2.25002100	-0.21889000
C	3.91141000	3.47875100	-0.24464100
C	3.34692700	4.53933400	-0.95567600
C	2.13840400	4.34958400	-1.62881600
C	1.52321400	3.09892900	-1.55673700
C	-0.56361700	2.91858900	1.25153300
C	-0.82106400	4.27118100	1.48646700
C	-2.02811400	4.81244200	1.04084000
C	-2.95087100	3.99472300	0.38308100
C	-2.63715600	2.64846500	0.18517000
C	-3.54465800	1.65333900	-0.43250300
C	-4.74426400	1.93805700	-1.09276300
C	-5.48795000	0.87469300	-1.61031900
C	-5.03964900	-0.43881600	-1.46010600
C	-3.83110200	-0.66106400	-0.78876200
C	-3.22386800	-1.98374500	-0.51326700
C	-3.83574300	-3.20116900	-0.81528900

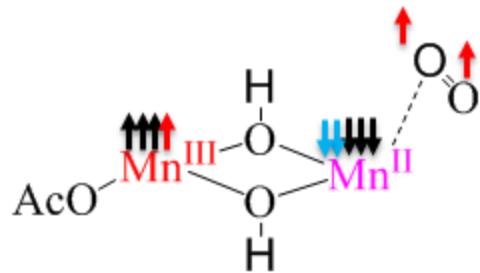
C	-3.20039600	-4.38963900	-0.44627000
C	-1.98058700	-4.33400100	0.22546300
C	-1.41427800	-3.08616800	0.50190400
H	0.45535200	-2.99303400	-2.06424900
H	1.26329700	-5.37383400	-1.92665400
H	3.25912700	-5.86959300	-0.49340900
H	4.40062200	-4.00805400	0.68119400
H	5.07384500	-2.30476100	1.83837800
H	6.10569600	-0.17725000	2.59296500
H	5.29406400	1.97948700	1.66586000
H	4.86612900	3.60175500	0.24878100
H	3.85543000	5.49445800	-0.99877800
H	1.68751600	5.14496700	-2.20732000
H	0.59819900	2.87981900	-2.07366900
H	0.34156900	2.41758700	1.57024400
H	-0.09537600	4.87705100	2.01227600
H	-2.25829300	5.85625900	1.21424100
H	-3.90105500	4.39513100	0.05572900
H	-5.08729500	2.95649600	-1.21194500
H	-6.41641300	1.07027600	-2.13180900
H	-5.61571400	-1.26160800	-1.85964600
H	-4.79573900	-3.22770200	-1.31267900
H	-3.66460500	-5.34262600	-0.66747200
H	-1.47510400	-5.23385400	0.54904800
H	-0.50528500	-2.96357800	1.07165100
C	-1.47866000	-0.84365400	3.18370900
O	-0.76530300	-1.82866200	3.01111900
C	-2.00594200	-0.45458200	4.57273400
H	-1.65415500	-1.17327800	5.31358900
H	-1.65381100	0.55071700	4.82639600
H	-3.10045200	-0.43520000	4.55610300
O	0.67321600	0.53645300	-3.48008100
H	-0.11469100	0.45384300	-2.86255600



AcO–Mn(IV)–Mn(III)–OOH_P:

Mn	1.36698300	0.15237400	-1.01694500
Mn	-1.14822800	0.21941300	0.41669700
O	0.64102500	0.45001000	0.58972800
O	-0.66144700	-0.16438600	-1.45021400
O	1.94235500	0.17570400	-2.90902000
O	-1.55521100	0.59353000	2.22418000
N	1.46427600	-2.13637600	-1.17008500
N	3.22508100	-0.54326800	-0.00241300
N	2.73805200	1.97095100	-0.67185000
N	-1.73014600	2.41675700	-0.02452900
N	-3.26825200	0.24984100	-0.19999300
N	-1.95879400	-1.92592900	0.60127500
C	0.61767400	-2.84230800	-1.94050400
C	0.77790100	-4.21564300	-2.13369500
C	1.84170300	-4.86235300	-1.50222100
C	2.71340900	-4.12576500	-0.69775000
C	2.49861900	-2.75173500	-0.55264400
C	3.38008300	-1.85902300	0.23736600
C	4.31904900	-2.31052400	1.17183300
C	5.09343400	-1.36958000	1.84878300
C	4.93516700	-0.01181500	1.57290400
C	3.98097100	0.37718800	0.62548800
C	3.74754400	1.78271000	0.20938700
C	4.53676000	2.85469300	0.63959800
C	4.27849600	4.13158600	0.14015600
C	3.24892500	4.30900400	-0.78500500
C	2.49789900	3.19709500	-1.16849000
C	-0.90904100	3.43991400	0.26382400
C	-1.36186500	4.76021800	0.27312400
C	-2.70472200	5.00789800	-0.01830200
C	-3.55608900	3.93899500	-0.30487400
C	-3.03425100	2.64117500	-0.29773700
C	-3.84787600	1.42274400	-0.54036200
C	-5.13728100	1.45304800	-1.08227500
C	-5.82068100	0.25066000	-1.25743500
C	-5.21783300	-0.94839700	-0.88467100
C	-3.92323300	-0.92176300	-0.34883400
C	-3.20382300	-2.13508500	0.11621600

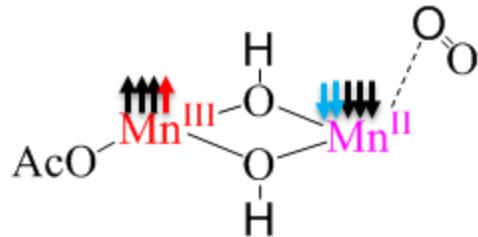
C	-3.76999600	-3.41442400	0.11274400
C	-3.03176200	-4.48081100	0.62970800
C	-1.75780200	-4.24616500	1.14639600
C	-1.25038300	-2.94490600	1.11865800
H	-0.18967500	-2.27287300	-2.38076900
H	0.08939800	-4.75760500	-2.76830300
H	1.99962800	-5.92473500	-1.64093200
H	3.55485200	-4.60891100	-0.21969000
H	4.42884000	-3.36495700	1.38319000
H	5.81512400	-1.69159100	2.58872100
H	5.53550500	0.72108400	2.09266000
H	5.34774800	2.70130900	1.33786700
H	4.88310600	4.97144200	0.45891800
H	3.03690600	5.28084800	-1.21074900
H	1.70057200	3.26326400	-1.89684300
H	0.11224400	3.16861500	0.49894600
H	-0.68297800	5.56763700	0.51339200
H	-3.09049400	6.01968600	-0.01016700
H	-4.60423200	4.11775600	-0.50258100
H	-5.59255700	2.38868000	-1.37477200
H	-6.81689000	0.24873100	-1.68151800
H	-5.74575400	-1.88249700	-1.01090500
H	-4.76785100	-3.58383900	-0.26740500
H	-3.45625500	-5.47709300	0.64171600
H	-1.17036600	-5.04640500	1.57638400
H	-0.29538500	-2.67688100	1.54795200
C	-0.97343300	-0.03245400	3.23686800
O	-0.25461100	-1.02173700	3.14198600
C	-1.30902600	0.61518900	4.58566300
H	-0.83247100	0.05491200	5.39060100
H	-0.95653900	1.65184500	4.58754000
H	-2.39473000	0.62728100	4.72541300
O	1.17660300	1.24101200	-3.03569600
H	-0.92907000	0.53651200	-2.07053200



AcO–Mn(III)–Mn(II)– ${}^3\text{O}_2$:

Mn	1.50573500	0.06845400	-0.30250400
Mn	-1.51679000	0.12106600	0.45753100
O	0.17486300	0.13600000	1.26891100
O	-0.41081600	0.09780700	-1.14750300
O	2.30412400	0.19145300	-2.92128500
O	-2.45788700	0.15437200	2.09319400
N	2.10685000	-2.08130500	-0.59569000
N	3.64381700	-0.07796800	0.18202500
N	2.33970300	2.16861700	-0.32850500
N	-2.17763200	2.28509800	0.16979700
N	-3.30701700	0.03603600	-0.70302600
N	-2.07192600	-2.09932400	0.31847500
C	1.29519400	-3.01651800	-1.12638400
C	1.68749000	-4.34943500	-1.24861100
C	2.95553400	-4.71665900	-0.79556900
C	3.79816700	-3.74572600	-0.24887800
C	3.35164100	-2.42462700	-0.16693900
C	4.19559700	-1.30070800	0.31990200
C	5.48748500	-1.43634300	0.84002900
C	6.18983700	-0.28193600	1.19261900
C	5.61677400	0.97698300	1.00043500
C	4.32078600	1.04984700	0.47728100
C	3.60355200	2.31278000	0.15555100
C	4.18225800	3.57826700	0.28306900
C	3.45484300	4.70421300	-0.10798100
C	2.16515500	4.54421700	-0.61704000
C	1.63926400	3.25594400	-0.70628200
C	-1.62690800	3.33665800	0.80264500
C	-2.18755700	4.61262300	0.72953200
C	-3.35025900	4.78895200	-0.02333600
C	-3.92489700	3.69210200	-0.66956700
C	-3.31518600	2.43928700	-0.54838100
C	-3.88435400	1.19003700	-1.11614500
C	-4.97614900	1.16169600	-1.99005800
C	-5.47134600	-0.07166300	-2.41231900
C	-4.89391100	-1.24966400	-1.94079600
C	-3.80332300	-1.17074300	-1.06691700
C	-3.16312800	-2.35696700	-0.44207500

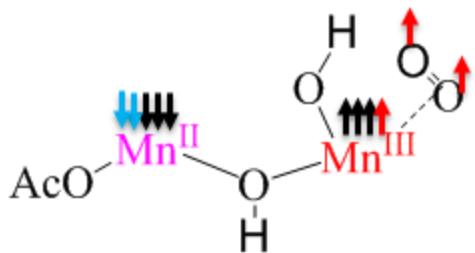
C	-3.67356800	-3.65488100	-0.54908200
C	-3.05193500	-4.68718900	0.15787400
C	-1.94307600	-4.40340100	0.95681300
C	-1.47710200	-3.08834000	1.01098200
H	0.32383300	-2.66855000	-1.45386200
H	1.01826200	-5.07511300	-1.69097700
H	3.29208100	-5.74276200	-0.87479100
H	4.78829300	-4.01881000	0.08912500
H	5.94169400	-2.40843400	0.97035400
H	7.18785800	-0.36267700	1.60459500
H	6.17225700	1.86892100	1.25332500
H	5.18632400	3.69226800	0.66754900
H	3.89447600	5.69000900	-0.02279300
H	1.58100200	5.39473100	-0.94212700
H	0.64135700	3.07322300	-1.08461400
H	-0.73514500	3.13234800	1.38256600
H	-1.73364100	5.43863200	1.26087600
H	-3.81600400	5.76384900	-0.09436300
H	-4.84164700	3.81600100	-1.22925100
H	-5.43161100	2.07789900	-2.33768400
H	-6.31040900	-0.11437000	-3.09523300
H	-5.28847300	-2.20715000	-2.24891300
H	-4.55100600	-3.86407500	-1.14512100
H	-3.44307500	-5.69515500	0.09833600
H	-1.45728300	-5.17593500	1.53801000
H	-0.63898700	-2.79996100	1.63223700
C	-2.04928900	-0.34285600	3.24853300
O	-0.91710400	-0.80345800	3.44785500
C	-3.11005500	-0.29539700	4.33695000
H	-2.71145500	-0.72351500	5.25650700
H	-3.41043200	0.74383200	4.50629100
H	-3.99504200	-0.85157500	4.01156500
O	3.47957400	0.25499800	-3.22067500
H	-0.80424900	0.33403500	-2.00152100
H	0.04959500	-0.22644900	2.19358400



AcO–Mn(III)–Mn(II)– $^1\text{O}_2$:

Mn	1.53755500	0.04666600	-0.33768600
Mn	-1.46840800	0.09605500	0.48235600
O	0.23964000	0.08537300	1.25918200
O	-0.39214800	0.10958300	-1.14366800
O	2.36772400	0.17204700	-2.83806600
O	-2.37532000	0.09193800	2.13701200
N	2.14512500	-2.09905900	-0.63332200
N	3.67496100	-0.08525000	0.13788600
N	2.34870100	2.15422100	-0.34960200
N	-2.12316800	2.26952800	0.26319700
N	-3.28072000	0.04894400	-0.64472000
N	-2.03853800	-2.11797200	0.29907500
C	1.33608600	-3.04026400	-1.15742600
C	1.73728500	-4.36988300	-1.28495600
C	3.01235700	-4.72771800	-0.84432500
C	3.85231800	-3.75081100	-0.30455200
C	3.39667300	-2.43314800	-0.21690500
C	4.23758400	-1.30415600	0.26338300
C	5.53717100	-1.43178300	0.76627700
C	6.23529800	-0.27347500	1.11411500
C	5.65024500	0.98170300	0.93412700
C	4.34708800	1.04663500	0.42809500
C	3.61684300	2.30550300	0.12028900
C	4.18741600	3.57493700	0.24577600
C	3.44719000	4.69668600	-0.13312900
C	2.15284000	4.52903000	-0.62785300
C	1.63556900	3.23717900	-0.71544200
C	-1.55491100	3.30179000	0.91211700
C	-2.11082900	4.58161600	0.88344300
C	-3.28727600	4.78256200	0.15865000
C	-3.87973400	3.70553100	-0.50467000
C	-3.27380500	2.44740600	-0.42825400
C	-3.85976200	1.21592500	-1.01718700
C	-4.96770200	1.21517800	-1.87099100
C	-5.47695000	-0.00455900	-2.31554200
C	-4.89707400	-1.19700300	-1.88510100
C	-3.79019700	-1.14573000	-1.02986100
C	-3.14554400	-2.35053700	-0.44667500

C	-3.66656900	-3.64226600	-0.57523300
C	-3.03892300	-4.69523800	0.09493500
C	-1.91364900	-4.43766100	0.87964200
C	-1.43783700	-3.12727100	0.95651700
H	0.35861300	-2.70082200	-1.47564500
H	1.06953300	-5.10011900	-1.72201700
H	3.35614000	-5.75106800	-0.92787400
H	4.84757700	-4.01663400	0.02391000
H	6.00068600	-2.40074600	0.88645600
H	7.23931100	-0.34813400	1.51243300
H	6.20232600	1.87693800	1.18271900
H	5.19506900	3.69517700	0.61875900
H	3.88063100	5.68539200	-0.04989900
H	1.55871900	5.37630400	-0.94319900
H	0.63469400	3.04750700	-1.08248000
H	-0.65256800	3.07867900	1.46819700
H	-1.64239900	5.39148700	1.42688400
H	-3.74969500	5.76095400	0.12238400
H	-4.80667400	3.84800800	-1.04274100
H	-5.42479600	2.14216800	-2.18639500
H	-6.32864500	-0.02574400	-2.98366700
H	-5.30222700	-2.14438000	-2.21024600
H	-4.55635100	-3.83147700	-1.15952000
H	-3.43783600	-5.69900600	0.01851100
H	-1.42251300	-5.22692700	1.43322100
H	-0.58641600	-2.85956300	1.56883600
C	-1.94509300	-0.43676200	3.27042900
O	-0.81155500	-0.90816200	3.43355300
C	-2.98215500	-0.41142200	4.38208400
H	-2.56686200	-0.86557300	5.28154300
H	-3.27214900	0.62482100	4.58462500
H	-3.87742900	-0.95370700	4.06144500
O	1.74846300	0.89023800	-3.60176100
H	-0.80082500	0.35797400	-1.98715900
H	0.13272900	-0.30253700	2.17589400



AcO–Mn(II)–Mn(III)– $^3\text{O}_2$:

Mn	1.87539400	-0.88750200	0.09324100
Mn	-1.78564600	0.14428200	-0.55722200
O	0.24469100	0.10251000	-0.18968900
O	1.40644900	-2.53834100	-0.45383600
O	4.59811800	-3.19391400	0.20743400
O	-1.59986300	0.80499500	-2.46995500
N	1.81576800	-1.21708700	2.13863500
N	3.02172000	0.61464400	0.79706000
N	2.93014700	-0.30994900	-1.59588700
N	-2.48043800	-1.99830000	-0.71268100
N	-3.83904800	0.06323300	0.27208400
N	-2.24159400	2.17878900	0.36273400
C	1.16474100	-2.24706300	2.71213100
C	1.00834200	-2.32188900	4.09661200
C	1.53128400	-1.30055500	4.89134100
C	2.20313100	-0.23060300	4.29029100
C	2.33876000	-0.21024800	2.90434500
C	3.06077800	0.82304200	2.13206800
C	3.79298700	1.89794900	2.64084900
C	4.48303700	2.72028200	1.74290500
C	4.46448400	2.45247000	0.37038600
C	3.71798200	1.36334800	-0.08729400
C	3.63132800	0.85874100	-1.47323800
C	4.20871900	1.46102400	-2.58651200
C	4.06595200	0.85143600	-3.83765600
C	3.34942100	-0.34048600	-3.94680000
C	2.78417300	-0.89598000	-2.79861600
C	-1.72406600	-2.98371200	-1.23896200
C	-2.25802300	-4.23459000	-1.55121400
C	-3.61187900	-4.46599100	-1.30856700
C	-4.38979800	-3.45178400	-0.74634900
C	-3.79704200	-2.22138900	-0.45201400
C	-4.53703900	-1.08590400	0.15871600
C	-5.86047800	-1.15861000	0.60868000
C	-6.43881500	-0.02178500	1.17434200
C	-5.70163600	1.15788600	1.28352400
C	-4.38286500	1.17300800	0.81483100
C	-3.49551900	2.36558400	0.84933200

C	-3.90474600	3.61680400	1.31933800
C	-3.00760600	4.68577700	1.27632600
C	-1.72595300	4.48523000	0.76202800
C	-1.37785000	3.21145800	0.31207000
H	0.77873400	-2.99863700	2.03530800
H	0.49100900	-3.16449600	4.53518500
H	1.42292500	-1.33425900	5.96808000
H	2.61318500	0.56628900	4.89610200
H	3.84418800	2.08521300	3.70449600
H	5.05869000	3.55735800	2.11747700
H	5.03046900	3.06712900	-0.31574400
H	4.75452000	2.38996400	-2.49078300
H	4.50918300	1.30649700	-4.71430600
H	3.22452000	-0.83445600	-4.90090400
H	2.20465000	-1.80984300	-2.81340200
H	-0.67415300	-2.76049900	-1.38118800
H	-1.62581600	-5.00237100	-1.97691200
H	-4.05980300	-5.42164700	-1.55043200
H	-5.44005600	-3.62179500	-0.55428800
H	-6.43010000	-2.07337100	0.52829700
H	-7.46116300	-0.05510800	1.52925400
H	-6.15036900	2.03812000	1.72119100
H	-4.90465400	3.76778600	1.70179100
H	-3.31190900	5.66278700	1.63025800
H	-1.01406800	5.29738800	0.69937600
H	-0.40916800	3.00016600	-0.12314400
C	-0.61332400	1.52051200	-2.88659100
O	0.43906700	1.73908300	-2.22527800
C	-0.77642100	2.13211600	-4.27508300
H	0.12696200	2.66766300	-4.56677900
H	-1.00282100	1.34121800	-4.99680600
H	-1.62885000	2.81996500	-4.26440100
O	5.10715900	-2.22336300	0.73092800
H	2.15431800	-3.16611100	-0.42104100
H	0.43269400	0.77202500	-0.93492200

4. IRC analysis of transition states

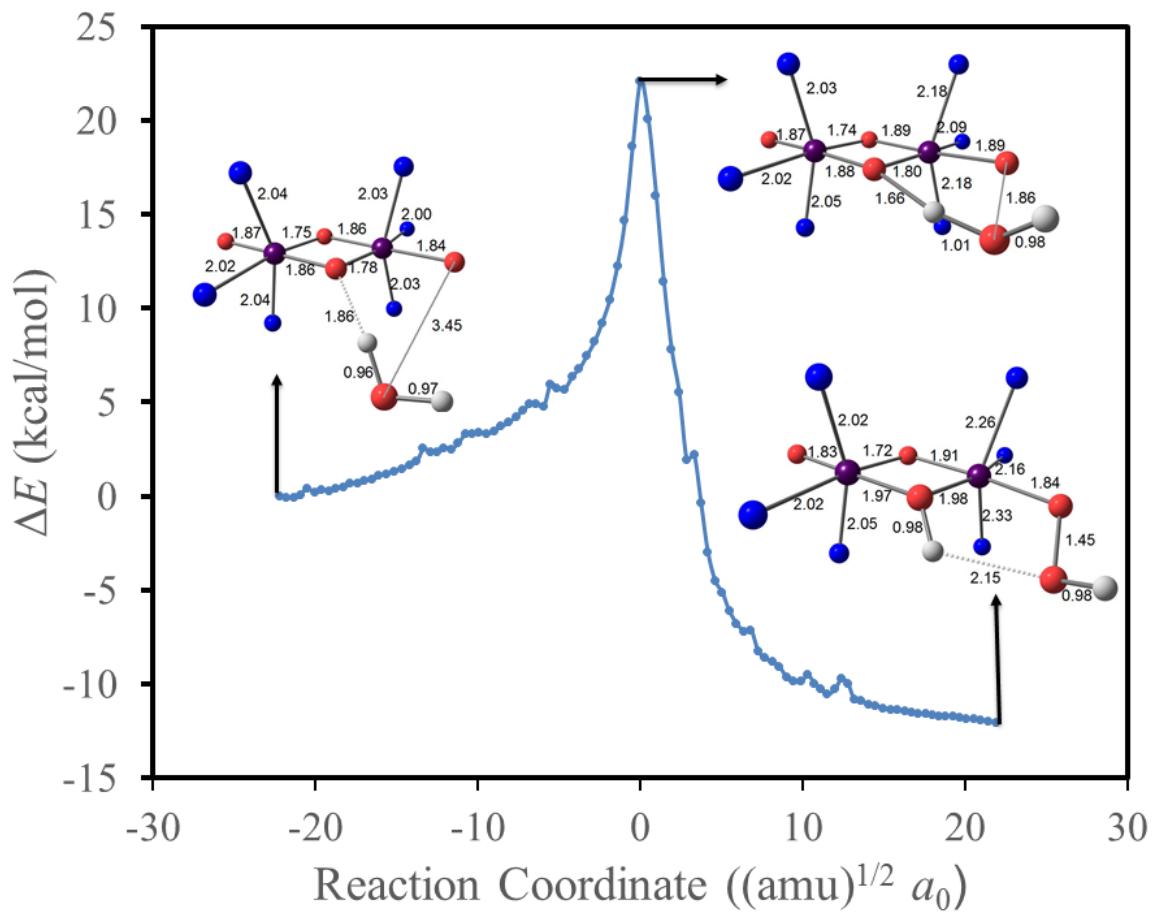


Figure S1. Reaction path of the nucleophilic attack of water to the parallel-spin Mn(IV)-O[•] radical. The C and H atoms in terpy and acetate are omitted for clarity and key bond lengths are shown in Å.

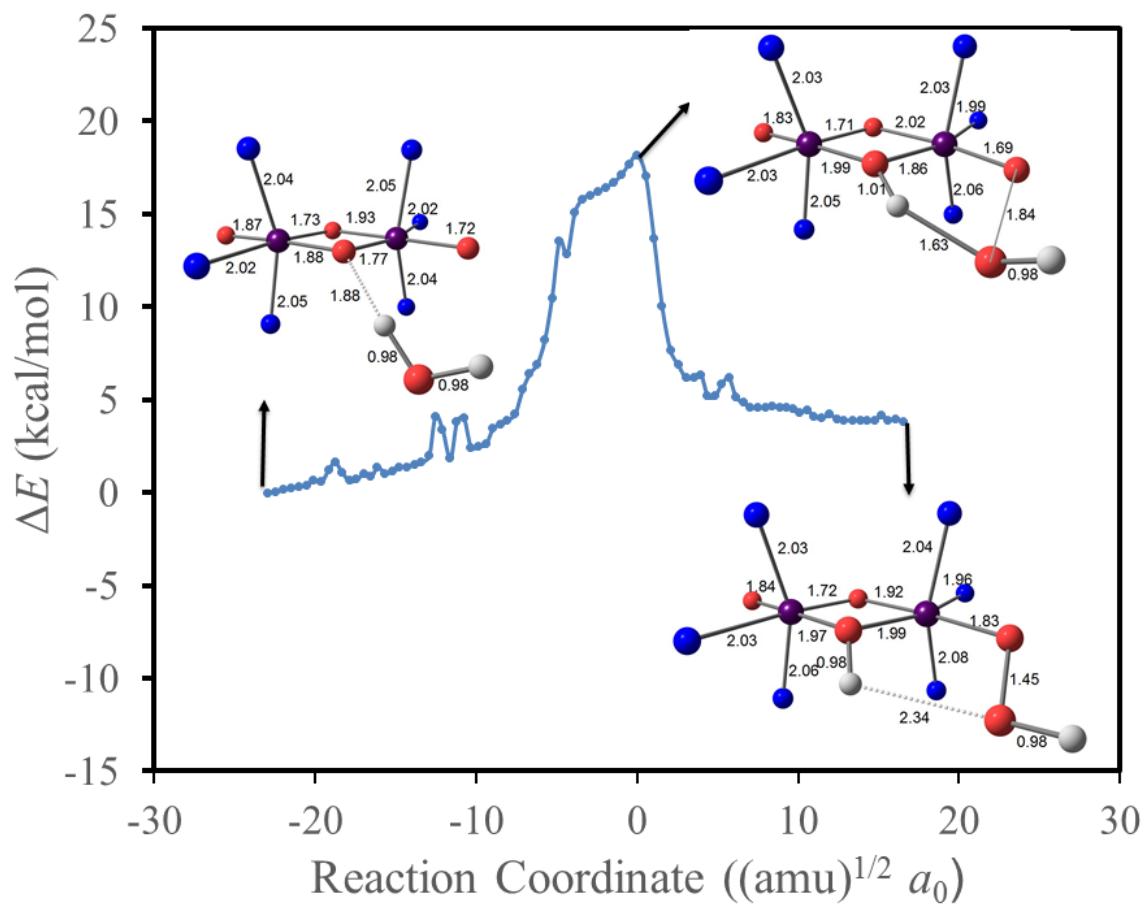


Figure S2. Reaction path of the nucleophilic attack of water to the antiparallel-spin Mn(IV)-O[•] radical. The C and H atoms in terpy and acetate are omitted for clarity and key bond lengths are shown in Å.

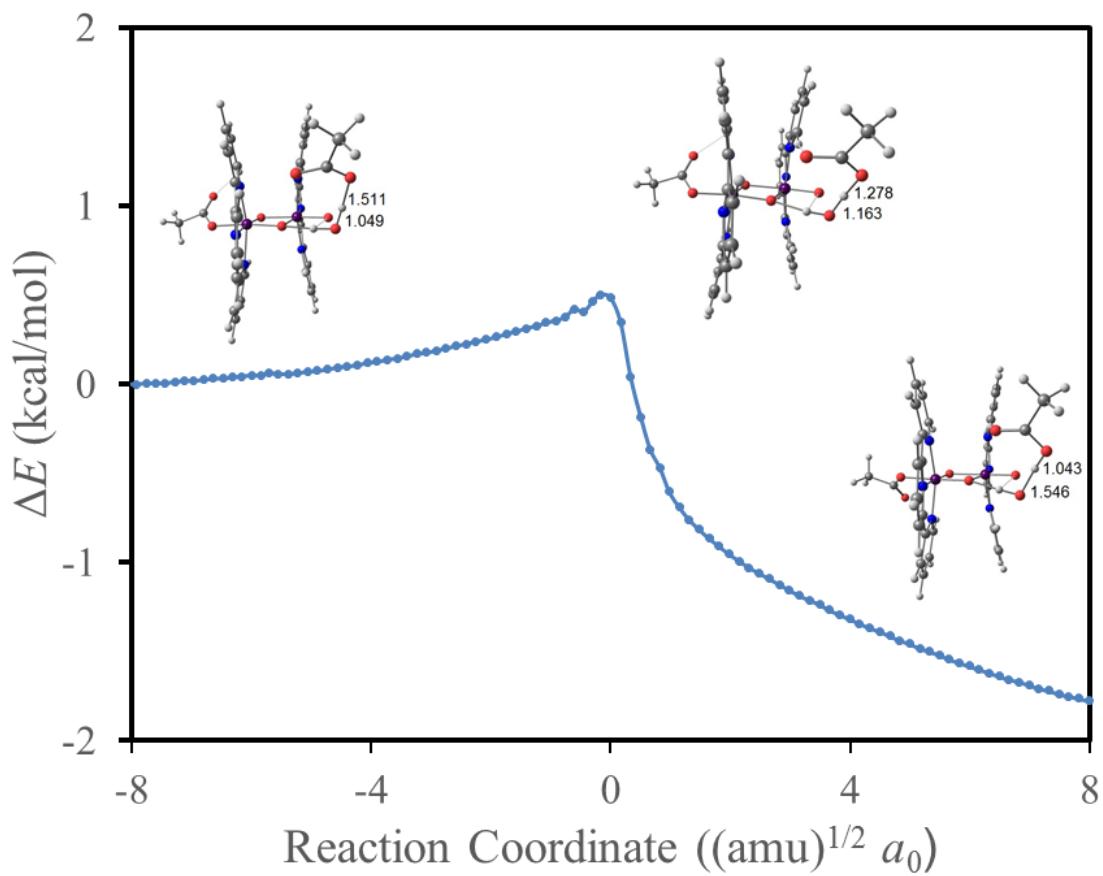


Figure S3. Reaction path of the acetate-assisted proton transfer. The transition state of the acetate-assisted proton-transfer can be located on the potential energy surface with a small barrier of 0.5 kcal/mol. However, the barrier disappears on the free-energy surface as shown in Table S3.

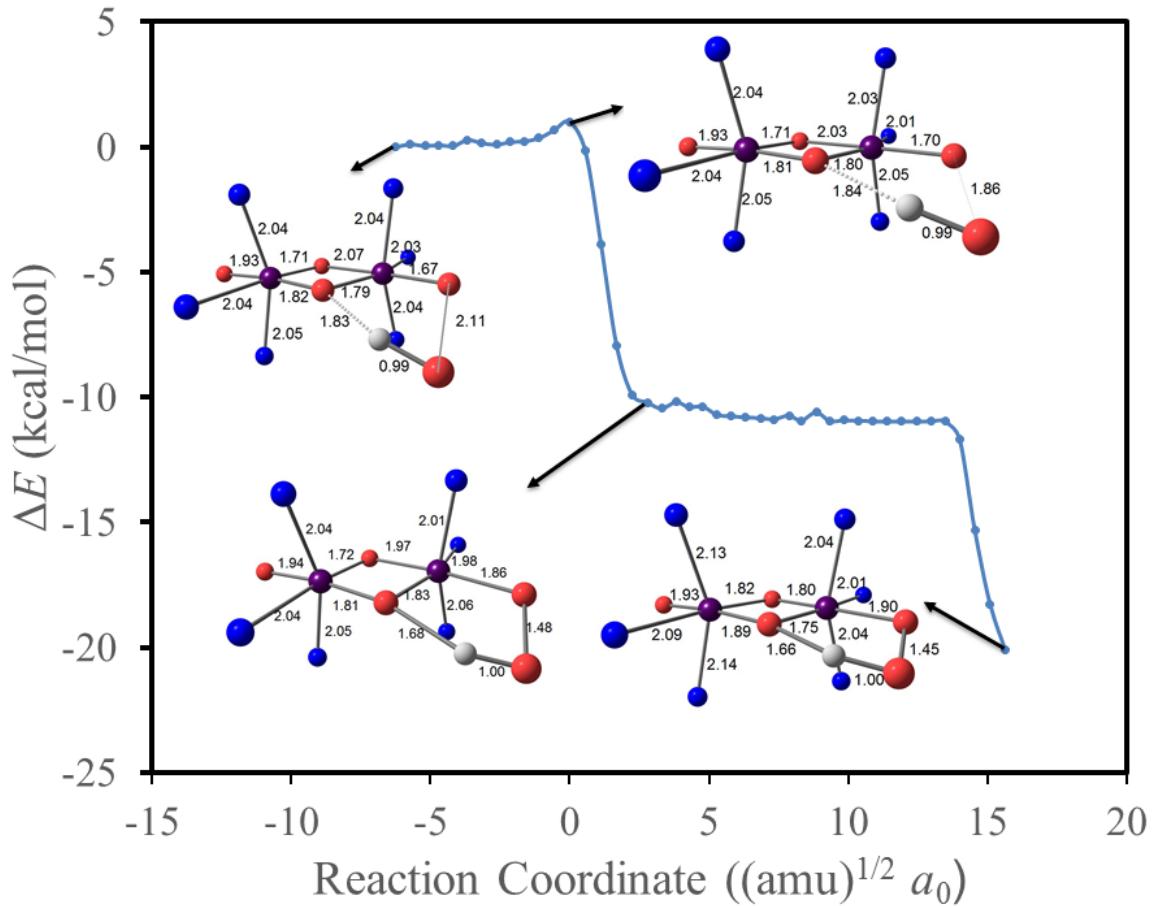


Figure S4. Reaction path of the O–O bond formation and electron transfer to the distal Mn center in the nucleophilic attack of water on the antiparallel-spin Mn(IV)–O[•] radical with the assistance of acetate. Terpy and acetate molecules are omitted for clarity and key bond lengths are shown in Å. After passing the transition state, the potential energy reaches a plateau corresponding to the AcO–Mn(IV)–(μ-O)₂–Mn(III)–OOH ··· HOAc complex with the adjacent Mn(III) center in low-spin triplet state. The potential energy further decreases toward a minimum corresponding to the AcO–Mn(III)–(μ-O)₂–Mn(IV)–OOH ··· HOAc complex with both Mn centers in high-spin states.

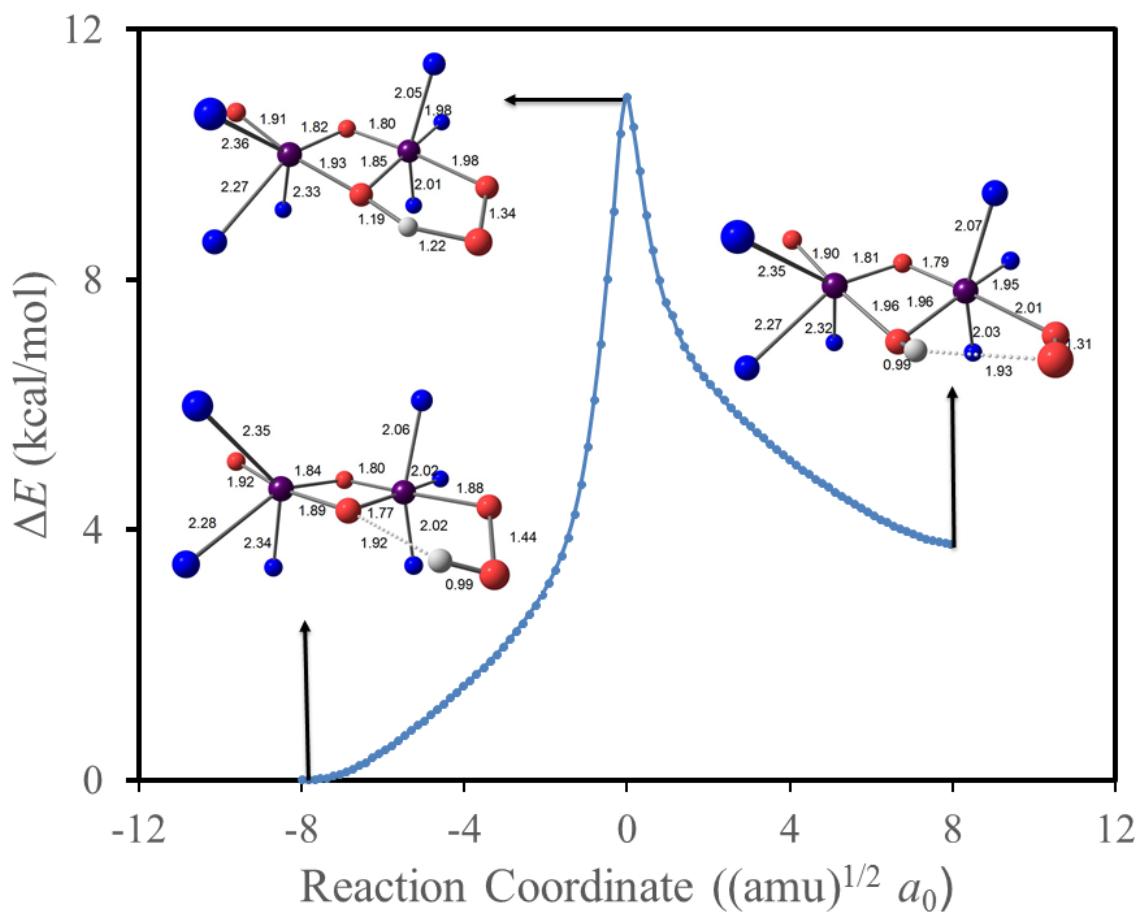


Figure S5. Reaction path of intramolecular proton-coupled electron transfer of AcO-Mn(III)-(μ -O)₂-Mn(IV)-OOH leading to low-spin Mn(III) product. Terpy and acetate molecules are omitted for clarity and key bond lengths are shown in Å.

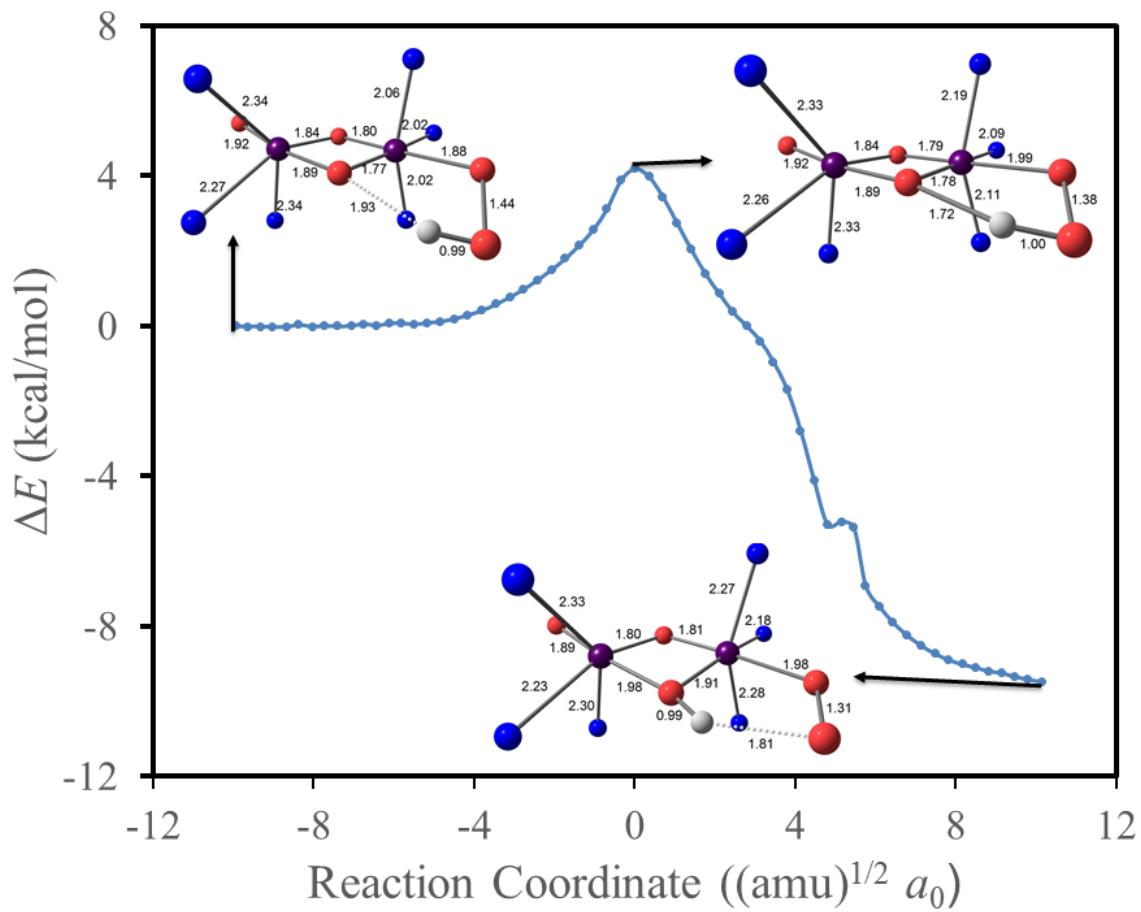


Figure S6. Reaction path of intramolecular proton-coupled electron transfer of AcO-Mn(III)-(μ -O)₂-Mn(IV)-OOH leading to high-spin Mn(III) product. Terpy and acetate molecules are omitted for clarity and key bond lengths are shown in Å.

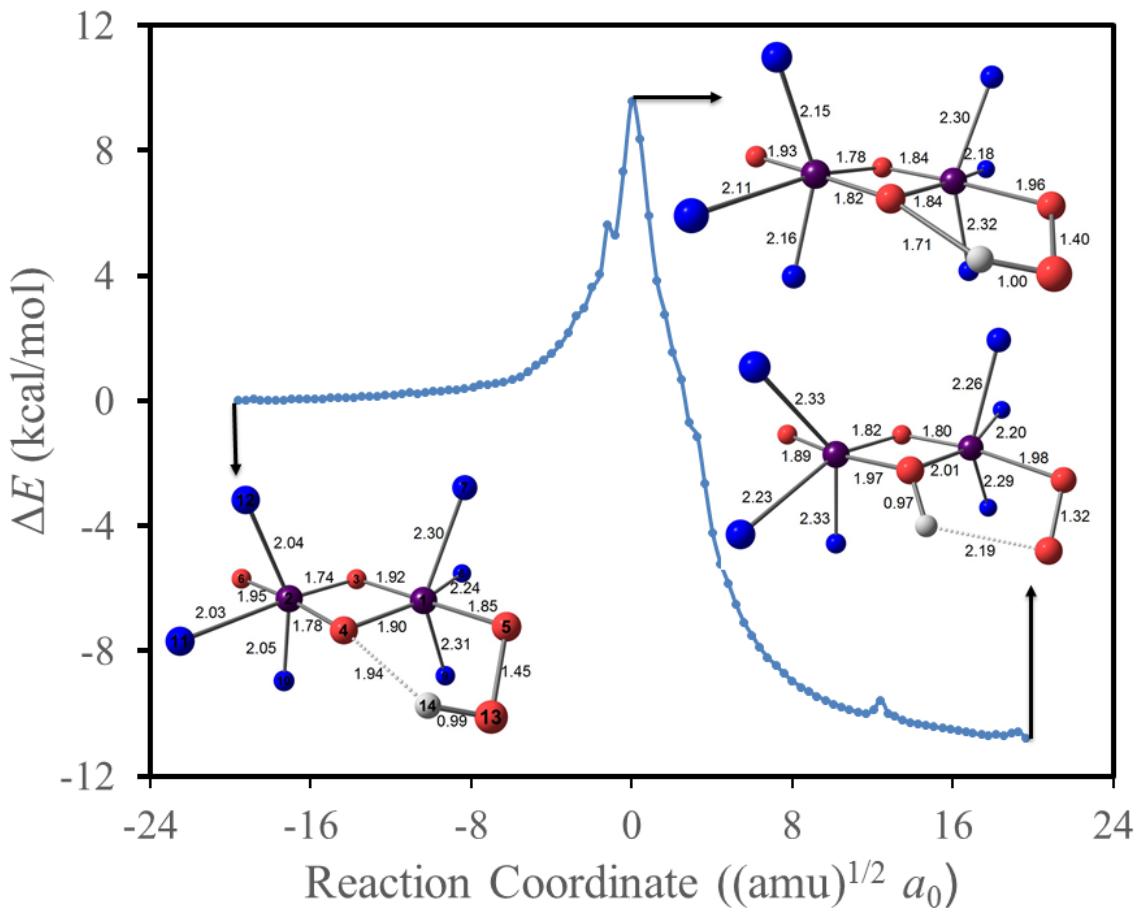


Figure S7. Reaction path of intramolecular proton-coupled electron transfer of AcO-Mn(IV)-(μ -O)₂-Mn(III)-OOH. Terpy and acetate molecules are omitted for clarity and key bond lengths are shown in Å.

5. Mulliken atomic spin density of all stationary points

Table S1. Mulliken atomic spin densities of stationary points along the reaction path of the nucleophilic attack of water to the parallel-spin Mn(IV)–O[•] radical

index	Atomic Label	R	TS	P	RO
1	Mn	2.59	3.47	3.89	3.97
2	Mn	-2.75	-2.65	-2.65	-2.52
3	O	-0.07	-0.22	-0.29	-0.23
4	O	0.10	-0.07	0.00	-0.07
5	O	1.10	0.32	-0.06	-0.18
6	O	-0.04	-0.02	-0.03	-0.01
7	N	0.00	0.00	0.04	0.01
8	N	-0.02	-0.01	0.02	0.00
9	N	0.00	0.01	0.02	0.00
10	N	0.03	0.02	0.02	0.02
11	N	0.03	0.02	0.02	0.03
12	N	0.03	0.03	0.03	0.03
13	C	0.01	0.01	0.00	0.01
14	C	-0.01	0.00	0.00	0.00
15	C	0.01	0.01	0.00	0.01
16	C	0.00	0.00	0.00	0.00
17	C	0.00	0.01	0.00	0.01
18	C	0.00	0.01	0.01	0.01
19	C	0.00	0.00	0.00	-0.01
20	C	0.00	0.01	0.01	0.01
21	C	0.00	-0.01	0.00	0.00
22	C	0.00	0.01	0.01	0.01
23	C	0.00	0.00	0.00	0.01
24	C	0.00	0.00	0.00	0.00
25	C	0.01	0.00	0.00	0.01
26	C	-0.01	0.00	0.00	-0.01
27	C	0.01	0.00	0.00	0.01
28	C	-0.01	-0.01	-0.01	-0.01
29	C	0.00	0.00	0.00	0.00
30	C	-0.01	0.00	-0.01	0.00
31	C	0.00	0.00	0.00	0.00
32	C	0.00	0.00	0.00	0.00
33	C	-0.01	-0.01	-0.01	-0.01

34	C	0.00	0.00	0.00	0.00
35	C	-0.01	-0.01	-0.01	-0.01
36	C	0.00	0.00	0.00	0.00
37	C	-0.01	-0.01	-0.01	-0.01
38	C	0.00	0.00	0.00	0.00
39	C	0.00	0.00	0.00	0.00
40	C	0.00	0.00	-0.01	0.00
41	C	0.00	0.00	0.01	0.00
42	C	-0.01	-0.01	-0.01	-0.01
43	H	0.00	0.00	0.00	0.00
44	H	0.00	0.00	0.00	0.00
45	H	0.00	0.00	0.00	0.00
46	H	0.00	0.00	0.00	0.00
47	H	0.00	0.00	0.00	0.00
48	H	0.00	0.00	0.00	0.00
49	H	0.00	0.00	0.00	0.00
50	H	0.00	0.00	0.00	0.00
51	H	0.00	0.00	0.00	0.00
52	H	0.00	0.00	0.00	0.00
53	H	0.00	0.00	0.00	0.00
54	H	0.00	0.00	0.00	0.00
55	H	0.00	0.00	0.00	0.00
56	H	0.00	0.00	0.00	0.00
57	H	0.00	0.00	0.00	0.00
58	H	0.00	0.00	0.00	0.00
59	H	0.00	0.00	0.00	0.00
60	H	0.00	0.00	0.00	0.00
61	H	0.00	0.00	0.00	0.00
62	H	0.00	0.00	0.00	0.00
63	H	0.00	0.00	0.00	0.00
64	H	0.00	0.00	0.00	0.00
65	C	0.01	0.01	0.01	0.01
66	O	-0.03	-0.03	-0.03	-0.03
67	C	0.00	0.00	0.00	0.00
68	H	0.00	0.00	0.00	0.00
69	H	0.00	0.00	0.00	0.00
70	H	0.00	0.00	0.00	0.00
71	O	0.00	0.11	0.00	-0.07
72	H	0.00	0.00	0.00	0.00
73	H	0.00	0.00	0.00	0.00

Table S2. Mulliken atomic spin densities of stationary points along the reaction path of the nucleophilic attack of water to the antiparallel-spin Mn(IV)–O[•] radical

index	Atomic Label	R	TS	P1	P2
1	Mn	-2.66	-2.23	-1.84	-2.54
2	Mn	2.73	2.61	2.63	3.84
3	O	0.14	0.36	0.29	-0.27
4	O	-0.12	-0.01	0.01	-0.04
5	O	0.83	-0.22	-0.10	-0.12
6	O	0.03	0.01	0.02	-0.02
7	N	0.04	0.01	0.03	0.02
8	N	0.01	0.02	0.04	0.04
9	N	0.04	0.01	0.02	0.02
10	N	-0.03	-0.02	-0.02	0.05
11	N	-0.02	-0.02	-0.02	0.00
12	N	-0.03	-0.03	-0.03	0.04
13	C	-0.01	0.01	-0.01	0.00
14	C	0.00	0.00	0.01	0.00
15	C	0.00	0.01	-0.01	0.00
16	C	0.00	0.00	0.00	0.00
17	C	0.00	0.01	-0.01	0.00
18	C	0.00	0.00	-0.01	-0.01
19	C	0.00	0.00	0.01	0.00
20	C	-0.01	0.01	-0.01	-0.01
21	C	0.00	0.00	0.01	0.00
22	C	-0.01	0.00	-0.01	-0.01
23	C	0.00	0.00	0.00	0.01
24	C	0.00	0.00	0.00	0.00
25	C	0.00	0.00	0.00	0.00
26	C	0.00	0.00	0.00	0.00
27	C	0.00	0.00	0.00	0.00
28	C	0.01	0.01	0.01	0.00
29	C	0.00	0.00	0.00	0.00
30	C	0.01	0.01	0.01	0.00
31	C	0.00	0.00	0.00	0.00
32	C	0.00	0.00	0.00	0.00
33	C	0.01	0.01	0.01	0.01
34	C	0.00	0.00	0.00	0.00
35	C	0.01	0.01	0.01	0.01

36	C	0.00	0.00	0.00	0.00
37	C	0.01	0.01	0.01	0.01
38	C	0.00	0.00	0.00	0.00
39	C	0.00	0.00	0.00	0.00
40	C	0.00	0.01	0.01	0.00
41	C	0.00	0.00	-0.01	0.00
42	C	0.01	0.01	0.01	0.00
43	H	0.00	0.00	0.00	0.00
44	H	0.00	0.00	0.00	0.00
45	H	0.00	0.00	0.00	0.00
46	H	0.00	0.00	0.00	0.00
47	H	0.00	0.00	0.00	0.00
48	H	0.00	0.00	0.00	0.00
49	H	0.00	0.00	0.00	0.00
50	H	0.00	0.00	0.00	0.00
51	H	0.00	0.00	0.00	0.00
52	H	0.00	0.00	0.00	0.00
53	H	0.00	0.00	0.00	0.00
54	H	0.00	0.00	0.00	0.00
55	H	0.00	0.00	0.00	0.00
56	H	0.00	0.00	0.00	0.00
57	H	0.00	0.00	0.00	0.00
58	H	0.00	0.00	0.00	0.00
59	H	0.00	0.00	0.00	0.00
60	H	0.00	0.00	0.00	0.00
61	H	0.00	0.00	0.00	0.00
62	H	0.00	0.00	0.00	0.00
63	H	0.00	0.00	0.00	0.00
64	H	0.00	0.00	0.00	0.00
65	C	-0.01	-0.01	-0.01	0.00
66	O	0.03	0.03	0.03	0.02
67	C	0.00	0.00	0.00	-0.01
68	H	0.00	0.00	0.00	0.00
69	H	0.00	0.00	0.00	0.00
70	H	0.00	0.00	0.00	0.00
71	O	0.00	0.46	-0.03	-0.04
72	H	0.00	-0.01	0.00	0.00
73	H	0.00	-0.01	0.00	0.00

Table S3. Mulliken atomic spin densities of stationary points along the reaction path of acetate-assisted nucleophilic attack of water to parallel-spin and antiparallel-spin Mn(IV)–O[•] radicals

inde x	Atomic Label	Odot2_PT_ <u>R</u>	Odot2_PT_ <u>TS</u>	Odot2_PT_ <u>P</u>	Odot2_TS_ <u>P</u>	Odot2_ <u>P</u>	Odot1_ <u>R</u>	Odot1_ <u>P</u>
1	Mn	-2.48	-2.43	-2.39	-2.23	-2.55	2.49	3.82
2	Mn	2.62	2.60	2.58	2.60	3.86	-2.66	-2.56
3	O	0.31	0.32	0.33	0.31	-0.20	-0.26	-0.26
4	O	-0.07	-0.05	-0.01	0.00	-0.20	0.08	-0.17
5	O	0.21	0.03	-0.19	-0.22	-0.06	0.98	0.03
6	O	0.01	0.01	0.01	0.01	0.01	-0.02	-0.01
7	N	0.02	0.01	0.00	0.01	0.02	-0.02	0.03
8	N	0.02	0.02	0.01	0.01	0.03	-0.02	0.00
9	N	0.01	0.01	0.01	0.01	0.01	-0.01	0.04
10	N	-0.02	-0.02	-0.02	-0.02	0.04	0.02	0.01
11	N	-0.02	-0.02	-0.02	-0.02	0.00	0.02	0.02
12	N	-0.03	-0.03	-0.02	-0.02	0.03	0.03	0.02
13	C	0.00	0.00	0.00	0.01	0.00	0.00	0.00
14	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	C	0.00	0.00	0.01	0.01	0.00	-0.01	0.00
16	C	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
17	C	0.00	0.01	0.01	0.01	0.00	-0.01	0.00
18	C	-0.01	-0.01	-0.01	0.01	-0.01	0.02	0.01
19	C	0.00	0.00	0.00	0.00	0.00	-0.01	0.00
20	C	-0.01	0.00	0.00	0.01	-0.01	0.02	0.01
21	C	0.00	0.00	0.00	0.00	0.00	-0.01	0.00
22	C	-0.01	-0.01	-0.01	0.01	-0.01	0.02	0.01
23	C	0.01	0.01	0.01	0.00	0.01	-0.01	0.00
24	C	0.00	0.00	0.00	0.00	0.00	0.01	0.00
25	C	0.00	0.00	0.00	0.00	0.01	-0.01	0.00
26	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	C	0.00	0.00	0.00	0.00	0.00	-0.01	0.00
29	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
33	C	0.01	0.01	0.01	0.01	0.01	-0.01	0.00
34	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
35	C	0.01	0.01	0.01	0.01	0.00	-0.01	0.00

36	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
37	C	0.01	0.01	0.01	0.01	0.01	-0.01	0.00
38	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
39	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
40	C	0.01	0.00	0.00	0.00	0.00	0.00	0.00
41	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
42	C	0.01	0.01	0.01	0.00	0.00	-0.01	0.00
43	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
44	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
45	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
46	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
47	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
48	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
49	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
50	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
51	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
52	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
53	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
54	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
55	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
56	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
57	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
58	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
59	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
60	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
61	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
62	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
63	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
64	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
65	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
66	O	0.02	0.02	0.02	0.02	0.01	-0.03	-0.02
67	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
68	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
69	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
70	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
71	O	0.40	0.52	0.68	0.49	-0.03	0.42	0.02
72	H	-0.01	-0.01	-0.01	0.00	0.00	-0.01	0.00
73	H	-0.01	-0.01	-0.02	-0.01	0.00	-0.01	0.00
74	O	0.01	0.01	0.00	0.00	0.00	0.01	0.00
75	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
76	O	0.00	0.00	0.00	0.00	0.00	0.00	0.00

77	C	0.00	0.00	0.00	0.00	0.00	0.00	0.00
78	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
79	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00
80	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S4. Mulliken atomic spin densities of stationary points along the intramolecular proton-coupled electron transfer (IPCET) reaction path of AcO–Mn(III)–Mn(IV)–OOH

index	Atomic Label	R	TS1	P1	TS2	P2
1	Mn	-2.57	-2.09	-1.85	-3.24	-3.93
2	Mn	3.87	3.87	3.87	3.84	3.82
3	O	-0.19	-0.14	-0.15	-0.14	-0.02
4	O	-0.19	-0.05	0.00	-0.05	-0.03
5	O	-0.06	-0.45	-0.39	0.35	0.51
6	O	0.01	0.00	0.00	0.00	0.00
7	N	0.01	0.01	0.01	-0.02	-0.04
8	N	0.02	0.04	0.03	0.01	-0.01
9	N	0.02	0.01	0.02	0.02	-0.02
10	N	0.04	0.04	0.05	0.04	0.04
11	N	0.00	0.00	0.00	0.00	-0.01
12	N	0.02	0.03	0.03	0.03	0.04
13	C	0.00	-0.01	0.00	0.00	0.00
14	C	0.00	0.00	0.00	0.00	0.00
15	C	0.00	0.00	0.00	0.00	0.00
16	C	0.00	0.00	0.00	0.00	0.00
17	C	0.00	0.00	0.00	0.00	0.00
18	C	-0.01	0.00	-0.01	-0.01	-0.01
19	C	0.00	0.00	0.00	0.00	0.00
20	C	0.00	0.01	-0.01	-0.01	0.00
21	C	0.00	0.00	0.00	0.01	0.00
22	C	-0.01	0.00	-0.01	-0.01	-0.01
23	C	0.01	0.03	0.00	-0.01	0.00
24	C	0.00	-0.01	0.00	0.00	0.00
25	C	0.01	0.03	-0.01	-0.01	0.00
26	C	0.00	-0.01	0.01	0.01	0.00
27	C	0.00	0.02	-0.01	-0.01	0.00
28	C	0.00	0.00	0.00	0.00	0.00
29	C	0.00	0.00	0.00	0.00	0.00
30	C	0.00	0.00	0.00	0.00	0.00
31	C	0.00	0.00	0.00	0.00	0.00
32	C	0.00	0.00	0.00	0.00	0.00
33	C	0.01	0.01	0.01	0.01	0.01
34	C	0.00	0.00	0.00	0.00	0.00
35	C	0.00	0.00	0.00	0.00	0.00

36	C	0.00	0.00	0.00	0.00	0.00
37	C	0.01	0.01	0.01	0.01	0.01
38	C	0.00	0.00	0.00	0.00	0.00
39	C	0.00	0.00	0.00	0.00	0.00
40	C	0.00	0.00	0.00	0.00	0.00
41	C	0.00	0.00	0.00	0.00	0.00
42	C	0.00	0.00	0.00	0.00	0.00
43	H	0.00	0.00	0.00	0.00	0.00
44	H	0.00	0.00	0.00	0.00	0.00
45	H	0.00	0.00	0.00	0.00	0.00
46	H	0.00	0.00	0.00	0.00	0.00
47	H	0.00	0.00	0.00	0.00	0.00
48	H	0.00	0.00	0.00	0.00	0.00
49	H	0.00	0.00	0.00	0.00	0.00
50	H	0.00	0.00	0.00	0.00	0.00
51	H	0.00	0.00	0.00	0.00	0.00
52	H	0.00	0.00	0.00	0.00	0.00
53	H	0.00	0.00	0.00	0.00	0.00
54	H	0.00	0.00	0.00	0.00	0.00
55	H	0.00	0.00	0.00	0.00	0.00
56	H	0.00	0.00	0.00	0.00	0.00
57	H	0.00	0.00	0.00	0.00	0.00
58	H	0.00	0.00	0.00	0.00	0.00
59	H	0.00	0.00	0.00	0.00	0.00
60	H	0.00	0.00	0.00	0.00	0.00
61	H	0.00	0.00	0.00	0.00	0.00
62	H	0.00	0.00	0.00	0.00	0.00
63	H	0.00	0.00	0.00	0.00	0.00
64	H	0.00	0.00	0.00	0.00	0.00
65	C	0.00	0.00	0.00	0.00	0.00
66	O	0.01	0.01	0.01	0.02	0.02
67	C	0.00	0.00	0.00	0.00	0.00
68	H	0.00	0.00	0.00	0.00	0.00
69	H	0.00	0.00	0.00	0.00	0.00
70	H	0.00	0.00	0.00	0.00	0.00
71	O	-0.02	-0.38	-0.60	0.17	0.63
72	H	0.00	0.01	0.01	0.00	0.00

Table S5. Mulliken atomic spin densities of stationary points along the intramolecular proton-coupled electron transfer (IPCET) reaction path of AcO–Mn(IV)–Mn(III)–OOH

index	Atomic Label	R	TS	P
1	Mn	3.86	3.73	3.81
2	Mn	-2.55	-3.24	-3.82
3	O	-0.24	-0.03	-0.01
4	O	-0.19	-0.04	0.03
5	O	-0.01	0.31	0.40
6	O	-0.01	0.00	0.00
7	N	0.04	0.04	0.04
8	N	0.00	0.00	0.02
9	N	0.03	0.04	0.02
10	N	0.01	0.00	-0.04
11	N	0.02	0.01	0.01
12	N	0.02	0.01	-0.04
13	C	0.00	0.00	0.00
14	C	0.00	0.00	0.00
15	C	0.00	0.00	0.00
16	C	0.00	0.00	0.00
17	C	0.00	0.00	0.00
18	C	0.01	0.01	0.00
19	C	0.00	0.00	0.00
20	C	0.01	0.00	0.00
21	C	0.00	0.00	0.00
22	C	0.01	0.01	0.00
23	C	0.00	-0.01	0.00
24	C	0.00	0.01	0.00
25	C	0.00	-0.01	0.00
26	C	0.00	0.01	0.00
27	C	0.00	-0.01	0.00
28	C	0.00	0.00	0.00
29	C	0.00	0.00	0.00
30	C	0.00	0.00	0.00
31	C	0.00	0.00	0.00
32	C	0.00	0.00	0.00
33	C	0.00	-0.01	-0.01
34	C	0.00	0.00	0.00
35	C	0.00	0.00	0.00

36	C	0.00	0.00	0.00
37	C	0.00	-0.01	-0.01
38	C	0.00	0.00	0.00
39	C	0.00	0.00	0.00
40	C	0.00	0.00	0.00
41	C	0.00	0.00	0.00
42	C	0.00	0.00	0.00
43	H	0.00	0.00	0.00
44	H	0.00	0.00	0.00
45	H	0.00	0.00	0.00
46	H	0.00	0.00	0.00
47	H	0.00	0.00	0.00
48	H	0.00	0.00	0.00
49	H	0.00	0.00	0.00
50	H	0.00	0.00	0.00
51	H	0.00	0.00	0.00
52	H	0.00	0.00	0.00
53	H	0.00	0.00	0.00
54	H	0.00	0.00	0.00
55	H	0.00	0.00	0.00
56	H	0.00	0.00	0.00
57	H	0.00	0.00	0.00
58	H	0.00	0.00	0.00
59	H	0.00	0.00	0.00
60	H	0.00	0.00	0.00
61	H	0.00	0.00	0.00
62	H	0.00	0.00	0.00
63	H	0.00	0.00	0.00
64	H	0.00	0.00	0.00
65	C	0.00	0.00	0.00
66	O	-0.02	-0.01	-0.02
67	C	0.00	0.00	0.00
68	H	0.00	0.00	0.00
69	H	0.00	0.00	0.00
70	H	0.00	0.00	0.00
71	O	0.01	0.18	0.60
72	H	0.00	0.00	0.00

Table S6. Mulliken atomic spin densities of stationary with O₂ bound to Mn center

index	Atomic Label	Mn(II)- ³ O ₂	Mn(II)- ¹ O ₂	Mn(III)- ³ O ₂
1	Mn	-4.78	4.75	3.64
2	Mn	3.84	-3.84	-4.75
3	O	-0.02	0.02	0.14
4	O	-0.03	0.03	0.08
5	O	0.95	0.02	1.00
6	O	0.00	0.00	-0.05
7	N	-0.02	0.02	-0.02
8	N	-0.01	0.01	-0.02
9	N	-0.02	0.02	-0.02
10	N	0.05	-0.05	-0.02
11	N	-0.01	0.01	-0.01
12	N	0.06	-0.06	-0.02
13	C	-0.01	0.01	0.02
14	C	0.00	0.00	-0.01
15	C	-0.01	0.01	0.02
16	C	0.00	0.00	-0.01
17	C	-0.01	0.01	0.01
18	C	-0.01	0.01	0.02
19	C	0.01	-0.01	-0.01
20	C	-0.01	0.01	0.02
21	C	0.01	-0.01	-0.01
22	C	-0.01	0.01	0.02
23	C	-0.01	0.01	0.01
24	C	0.00	0.00	-0.01
25	C	-0.01	0.01	0.02
26	C	0.00	0.00	-0.01
27	C	-0.01	0.00	0.02
28	C	0.00	0.00	-0.01
29	C	0.00	0.00	0.00
30	C	0.00	0.00	-0.01
31	C	0.00	0.00	0.00
32	C	0.00	0.00	-0.01
33	C	0.01	-0.01	-0.01
34	C	-0.01	0.01	0.01
35	C	0.01	-0.01	-0.01
36	C	-0.01	0.01	0.01
37	C	0.01	-0.01	-0.01

38	C	0.00	0.00	-0.01
39	C	0.00	0.00	0.00
40	C	0.00	0.00	-0.01
41	C	0.00	0.00	0.00
42	C	-0.01	0.01	0.00
43	H	0.00	0.00	0.00
44	H	0.00	0.00	0.00
45	H	0.00	0.00	0.00
46	H	0.00	0.00	0.00
47	H	0.00	0.00	0.00
48	H	0.00	0.00	0.00
49	H	0.00	0.00	0.00
50	H	0.00	0.00	0.00
51	H	0.00	0.00	0.00
52	H	0.00	0.00	0.00
53	H	0.00	0.00	0.00
54	H	0.00	0.00	0.00
55	H	0.00	0.00	0.00
56	H	0.00	0.00	0.00
57	H	0.00	0.00	0.00
58	H	0.00	0.00	0.00
59	H	0.00	0.00	0.00
60	H	0.00	0.00	0.00
61	H	0.00	0.00	0.00
62	H	0.00	0.00	0.00
63	H	0.00	0.00	0.00
64	H	0.00	0.00	0.00
65	C	0.00	0.00	0.00
66	O	0.02	-0.02	-0.01
67	C	-0.01	0.01	0.00
68	H	0.00	0.00	0.00
69	H	0.00	0.00	0.00
70	H	0.00	0.00	0.00
71	O	1.04	0.02	1.01
72	H	0.00	0.00	0.01
73	H	0.00	0.00	0.00

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