

Electronic Supplementary Information for:

Theoretical View on a Linear End-on Manganese-Dioxygen
Complex Bearing a Calix[4]arene Ligand †

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Cartesian coordinates of all structures described in this work.

Table S1 Experimental and calculated structural parameters (angle in degrees and bond distances in Å) of sextet [MnL(O₂)(H₂O)]²⁺ with different functional at B1 level.^a

Method	Mn-O2-O1	O2-Mn-O _w	<i>d</i> _{O1-O2}	<i>d</i> _{Mn-O2}	<i>d</i> _{Mn-O_w}	<i>d</i> _{O_e-O_e}	<i>d</i> _{Mn-O_e}	RMSD ^b
<i>Exp.</i>	180.0°	180.0°	1.249	2.444	2.210	3.773	1.887	
wB97X-D	129.9°	170.1°	1.308	2.229	2.293	3.828	1.915	0.110
B3LYP	129.3°	170.6°	1.321	2.245	2.335	3.858	1.928	0.118
B97-D	128.6°	171.6°	1.300	2.299	2.288	3.985	1.993	0.131
M06-2X	127.6°	170.3°	1.309	2.199	2.243	3.852	1.927	0.120
TPSSh	126.6°	169.2°	1.323	2.202	2.325	3.845	1.924	0.129
BP86	125.8°	169.9°	1.323	2.269	2.362	3.867	1.934	0.119
B3LYP-D3	128.2°	169.4°	1.321	2.268	2.310	3.854	1.928	0.104

^aB1: polarized triple- ζ basis sets 6-311+G(d) for Mn, O atoms and polarized double- ζ basis sets 6-31G(d) for C, N, H atoms.

^bRMSD: the root-mean-square deviation of the key bond distances as relative to the experimental parameters is calculated by eq. 1.

$$RMSD = \sqrt{\frac{\sum_1^5 (d_{i(cal.)} - d_{i(Exp.)})^2}{5}} \quad (\text{eq. 1})$$

Here the $d_{i(cal.)}$ and $d_{i(Exp.)}$ correspond to the five key bond distances listed in Tables from calculations (cal.) and experiments (Exp.).

Table S2 Optimized structural parameters (angle in degrees and bond distances in Å) of sextet $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+}$ under different basis set levels.

Method	Mn-O2-O1	O2-Mn-O _w	$d_{\text{O1-O2}}$	$d_{\text{Mn-O2}}$	$d_{\text{Mn-O}_w}$	$d_{\text{O}_e\text{-O}_e}$	$d_{\text{Mn-O}_e}$	RMSD
B3LYP/B1	129.3°	170.6°	1.321	2.245	2.335	3.858	1.928	0.118
B3LYP/B2	129.3°	170.4°	1.321	2.244	2.358	3.855	1.928	0.123
B3LYP/B3	129.2°	170.3°	1.320	2.263	2.335	3.872	1.936	0.115
B3LYP/B4	130.7°	167.6°	1.319	2.271	2.357	3.851	1.927	0.113
B3LYP/B5	128.7°	171.7°	1.321	2.238	2.331	3.857	1.929	0.119
B3LYP/B6	123.5°	168.3°	1.323	2.181	2.348	3.837	1.920	0.140
B3LYP/B7	122.8°	167.0°	1.321	2.209	2.368	3.854	1.929	0.137

B1: 6-311+G(d) for Mn, O atoms, 6-31G(d) for C, H, N atoms;

B2: 6-311+G(d) for Mn, O atoms, 6-31G(d, p) for C, H, N atoms;

B3: LanL2DZ for Mn atom, 6-311+G(d) for O atoms, 6-31G(d) for C, H, N atoms;

B4: LanL2DZ for Mn atom, 6-311+G (d) for O1, O2 atom, 6-31G(d) for the rest atoms;

B5: 6-311+G(d) for Mn, O atoms, 6-31G+(d) for C, H, N atoms;

B6: 6-31G(d) for the whole system;

B7: LanL2DZ for Mn atom, 6-31G(d) for the rest.

Table S3 Optimized structural parameters (bond distances in Å and angles in degrees) of sextet $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+} - n\text{H}_2\text{O}$ complex at B3LYP/B1 level. The stretching vibration frequencies of dioxygen ligand ($\nu_{\text{O1-O2}}$) were scaled by 0.946.

	$n = 1$	$n = 4$	$n = 6$	$n = 8$	$n = 8(\text{B3LYP-D3})$
$\nu_{\text{O1-O2}}/\text{cm}^{-1}$	1151.4	1156.2	1156.5	1160.3	1173.9
$\angle \text{MnO2O1}$	132.1°	140.5°	150.6°	162.6°	156.4°
$\angle \text{O2MnO}_w$	178.9°	171.0°	172.5°	174.9°	172.9°
$d_{\text{O1-O2}}/\text{Å}$	1.322	1.325	1.324	1.325	1.321
$d_{\text{Mn-O2}}/\text{Å}$	2.366	2.458	2.462	2.552	2.431
$d_{\text{Mn-O}_w}/\text{Å}$	2.300	2.262	2.265	2.234	2.224
$d_{\text{Mn-O}_e}/\text{Å}$	1.927	1.922	1.914	1.914	1.917
$d_{\text{O}_e\text{-O}_e}/\text{Å}$	3.853	3.843	3.828	3.826	3.832
RMSD	0.074	0.054	0.050	0.066	0.045
$d_{\text{O1-O2}}/(\text{p})$	0.887	1.022	1.153	1.264	1.211


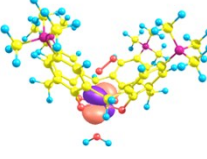
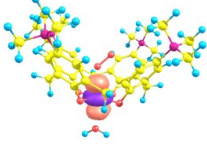
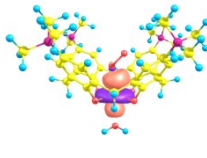
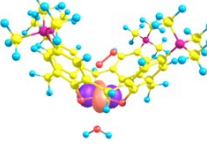
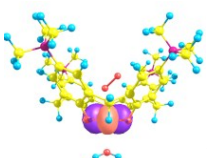
Table S4 Calculated structural parameters (bond distances in Å and angles in degrees) of sextet $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+} - 8\text{H}_2\text{O}$ complex at different basis set levels using B3LYP method and in CPCM model with water as solvent (*).


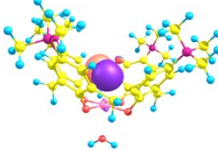
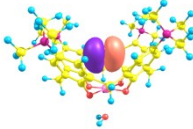
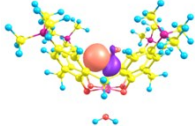
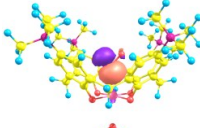
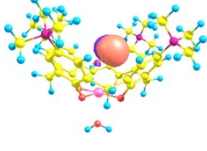
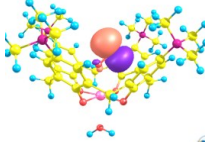
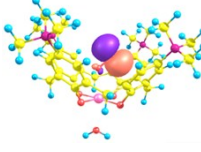
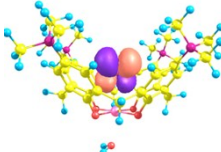
	B2	B8	B1*	B2*	B8*
$\angle \text{MnO2O1}$	164.6°	168.6°	153.1°	159.6°	161.3°
$\angle \text{O2MnO}_w$	175.7°	178.4°	173.0°	174.2°	174.9°
$d_{\text{O1-O2}}/\text{Å}$	1.326	1.328	1.321	1.323	1.324
$d_{\text{Mn-O2}}/\text{Å}$	2.586	2.692	2.402	2.467	2.478
$d_{\text{Mn-O}_w}/\text{Å}$	2.245	2.226	2.325	2.333	2.311

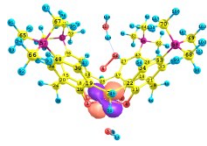
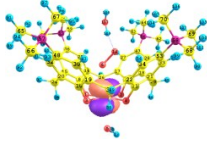
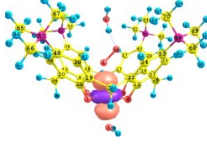
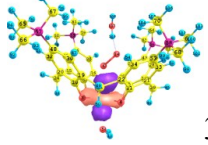
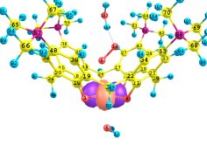
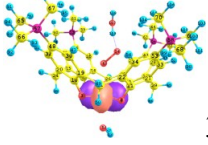

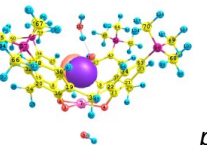
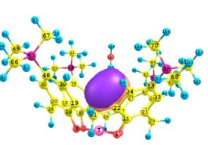
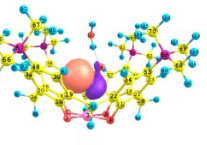
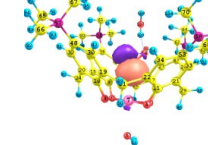
$d_{\text{Mn-O}_e}/\text{\AA}$	1.913	1.911	1.922	1.918	1.921
$d_{\text{O}_e\text{-O}_e}/\text{\AA}$	3.823	3.818	3.843	3.837	3.842
<i>RMSD</i>	0.078	0.119	0.073	0.073	0.068
$d_{\text{O1-O2(p)}}$	1.278	1.302	1.179	1.240	1.254

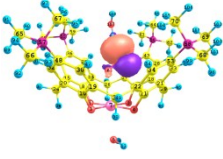
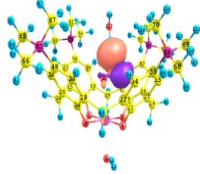
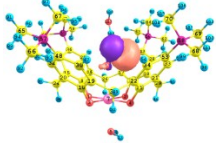
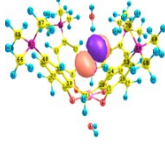
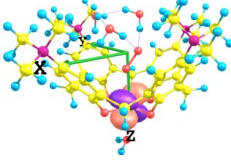
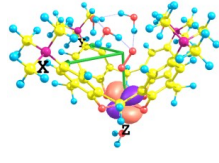
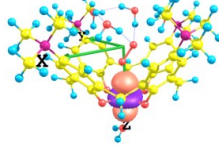

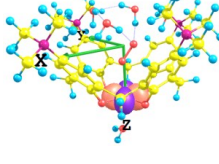
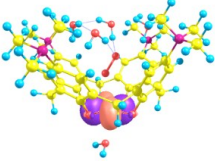
B8: 6-311+G(d) for Mn, O atoms, 6-31G(d, p) for H of the additional waters, and 6-31G(d) for C, N and the rest of H atoms.

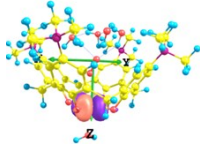
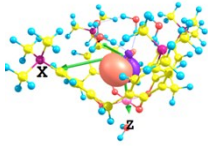
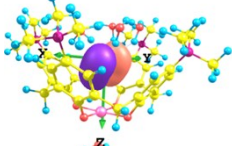
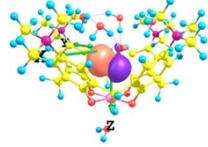
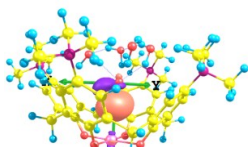
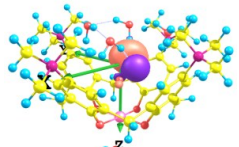
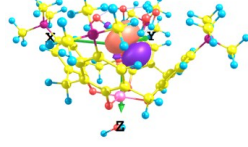
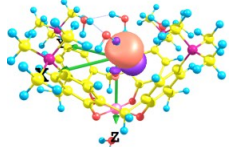
Table S5. Relevant natural bond orbitals of Mn 3d orbitals and O₂ lone pair orbitals and their occupation numbers (unit: e) in both α and β spaces. (The subscript ip or op denote orbitals in the plane or out of the plane of MnO2O1)

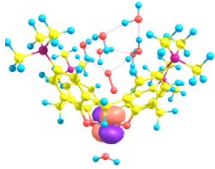
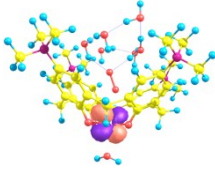
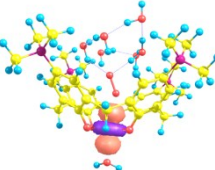
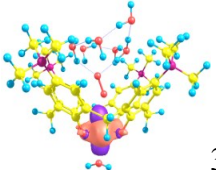
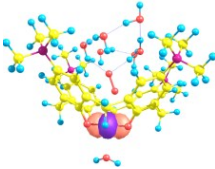
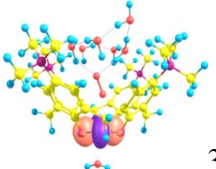
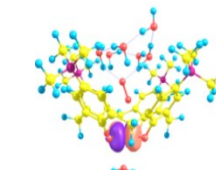
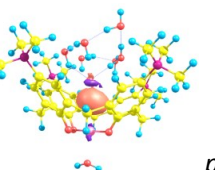
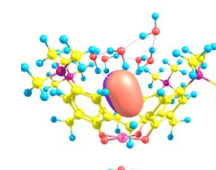
[MnL(O₂)(H₂O)]²⁺				
α		β		
 $3d_{xz}$	0.97880	-	-	Mn(α - β)=3.25
 $3d_{yz}$	0.97859	-	-	
 $3d_{z^2}$	0.97368	 $3d_{z^2}$	0.22936	
 $3d_{xy}$	0.97179	 $3d_{xy}$	0.16863	

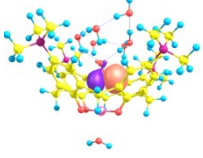
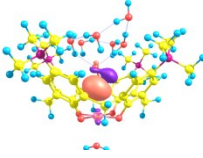
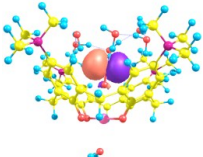
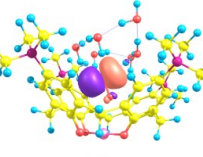
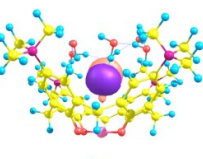
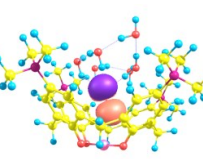
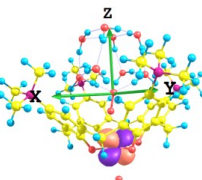
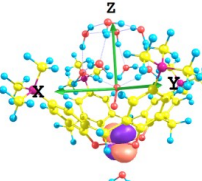
$3d_{x^2-y^2}$	-	 $3d_{x^2-y^2}$ y^2	0.25009	
 $p_{op}(O2)$	0.98792	 $\pi_{op}(O1-O2)$	0.98371	$O_2(\alpha-\beta)=1.17$
 $p_{ip}(O2)$	0.98883	 $p_{ip}(O2)$	0.84316	
 $p_{op}(O1)$	0.99571	 $p_{ip}(O1)$	0.96698	
 $p_{ip}(O1)$	0.99011	 π^*_{op} (O1-O2)	0.00444	
[MnL(O₂)(H₂O)]²⁺-1H₂O				
α		β		

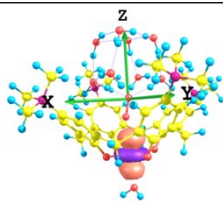
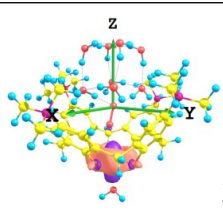
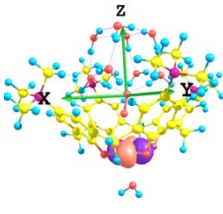
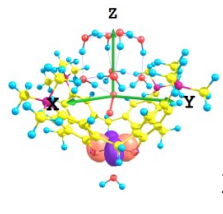
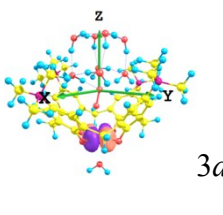
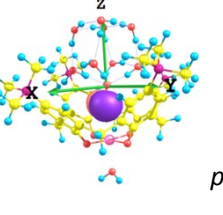
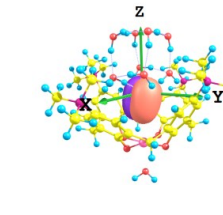
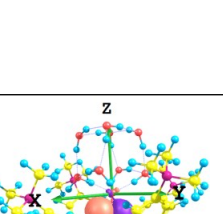
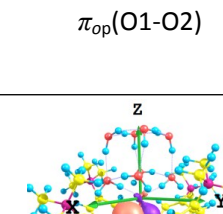
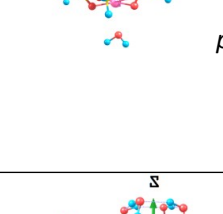
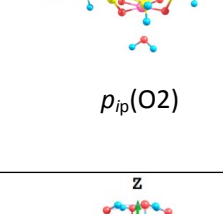
 $3d_{xz}$	0.97880			Mn(α - β)=3.29
 $3d_{yz}$	0.97805			
 $3d_{z^2}$	0.97553	 $3d_{z^2}$	0.19476	
 $3d_{xy}$	0.97153	 $3d_{xy}$	0.17160	
$3d_{x^2-y^2}$		 $3d_{x^2-y^2}$	0.25197	
 $p_{op}(O_2)$	0.99022	 $\pi_{op}(O$ 1-O2)	0.98843	O_2 (α - β)=1.13
 $p_{ip}(O_2)$	0.99172	 $p_{ip}(O_2)$	0.87375	

 $p_{op}(O1)$	0.95995	 $p_{ip}(O1)$	0.94664	
 $p_{ip}(O1)$	0.99538	 $\pi^*_{op}(O1-O2)$	0.00563	
[MnL(O₂)(H₂O)]²⁺-4H₂O				
α		β		
 $3d_{xz}$	0.97669			Mn(α - β)=3.30
 $3d_{yz}$	0.97779			
 $3d_{z^2}$	0.97570	 $3d_{z^2}$	0.17059	
 $3d_{xy}$	0.97076	 $3d_{xy}$	0.17470	

$3d_{x^2-y^2}$			0.25324	
		$3d_{x^2-y^2}$		
 $p_{op}(O2)$	0.99058		0.98950	$O_2(\alpha-\beta)=1.13$
		$\pi_{op}(O1-O2)$		
 $p_{ip}(O2)$	0.99186		0.90642	
		$p_{ip}(O2)$		
 $p_{op}(O1)$	0.98463		0.95383	
		$p_{ip}(O1)$		
 $p_{ip}(O1)$	0.96325			
$[MnL(O_2)(H_2O)]^{2+} \cdot 6H_2O$				
α		β		

 $3d_{xz}$	0.97735			Mn(α - β)=3.30
 $3d_{yz}$	0.97647			
 $3d_{z^2}$	0.97485	 $3d_{z^2}$	0.16751	
 $3d_{xy}$	0.97026	 $3d_{xy}$	0.17719	
$3d_{x^2-y^2}$		 $3d_{x^2-y^2}$	0.25621	
 $p_{op}(O_2)$	0.96563	 $\pi_{op}(O_1-O_2)$	0.99134	O ₂ (α - β)=1.05

 $\rho_{ip}(O2)$	0.98828	 $\rho_{ip}(O2)$	0.91143	
 $\rho_{ip}(O1)$	0.99005	 $\rho_{ip}(O1)$	0.95835	
 $\rho_{op}(O1)$	0.96776	 $\pi^*_{op}(O1-O2)$	0.00739	
[MnL(O₂)(H₂O)]²⁺-8H₂O				
α		β		
 $3d_{xz}$	0.97416	--	--	Mn(α - β)=3.31
 $3d_{yz}$	0.97796	--	--	

 <p>$3d_{z^2}$</p>	0.97570	 <p>$3d_{z^2}$</p>	0.15567	
 <p>$3d_{xy}$</p>	0.96976	 <p>$3d_{xy}$</p>	0.17717	
<p>$3d_{x^2-y^2}$</p>		 <p>$3d_{x^2-y^2}$</p>	0.25466	
 <p>$p_{op}(O2)$</p>	0.99275	 <p>$\pi_{op}(O1-O2)$</p>	0.99390	$O_2(\alpha-\beta)=1.01$
 <p>$p_{ip}(O2)$</p>	0.98846	 <p>$p_{ip}(O2)$</p>	0.97902	
 <p>$p_{op}(O1)$</p>	0.99347	 <p>$p_{ip}(O1)$</p>	0.94235	

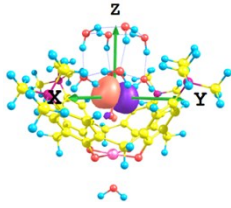
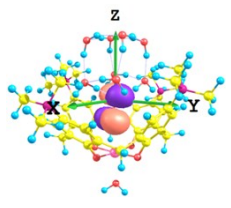
 <p>$p_{ip}(O1)$</p>	0.94942	 <p>$\pi^*_{op}(O1-O2)$</p>	0.01111	
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Table S6 Mulliken spin populations on Mn-O₂ unit (e.g., S_{Mn}) and Wiberg bond indices (e.g., B_{O1-O2}) of $[MnL(O_2)(H_2O)]^{2+}-nH_2O$ complexes. The results of $[MnL(O_2)(H_2O)]^{2+}-8H_2O$ in CPCM model is based on B3LYP/B2 method.

	$n = 0$	$n = 1$	$n = 4$	$n = 6$	$n = 8$	$n = 8$ (CPCM)
S_{Mn}/e	3.91	3.96	3.98	3.97	3.99	4.00
S_{O1}/e	0.61	0.54	0.47	0.49	0.48	0.51
S_{O2}/e	0.50	0.54	0.56	0.55	0.53	0.53
B_{O1-O2}	1.49	1.50	1.49	1.49	1.48	1.49
B_{Mn-O1}	0.07	0.04	0.03	0.03	0.02	0.03
B_{Mn-O2}	0.42	0.34	0.26	0.26	0.20	0.25

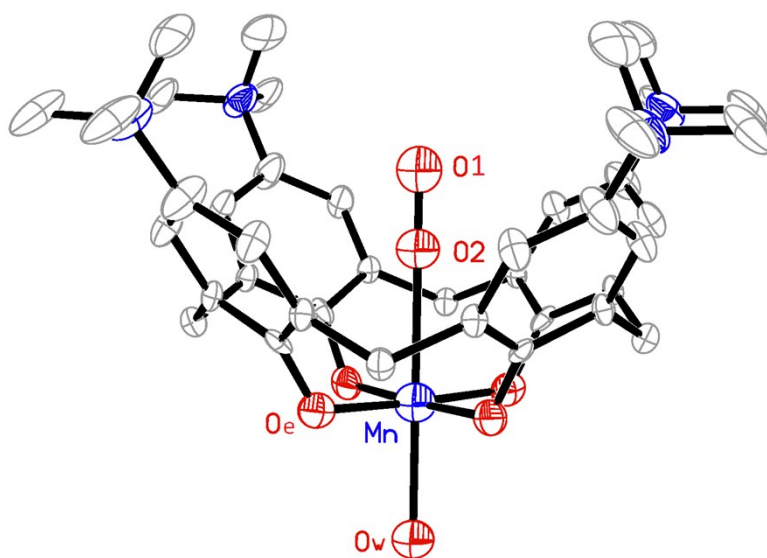


Fig. S1 View of the bowl-shaped cationic structure of $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})](\text{PF}_6)_2$ with 50% thermal ellipsoids.

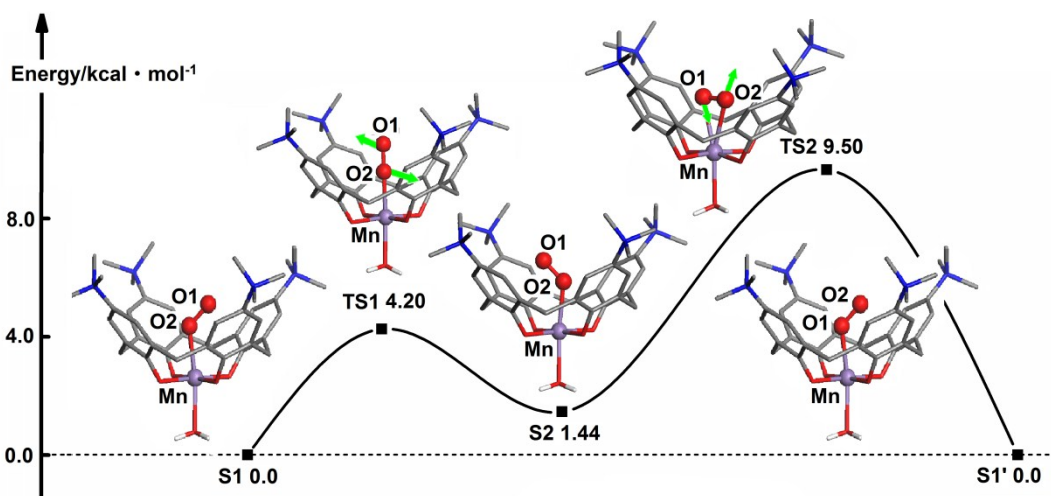


Fig. S2 Potential energy surface of three binding configurations of $S = 5/2$.

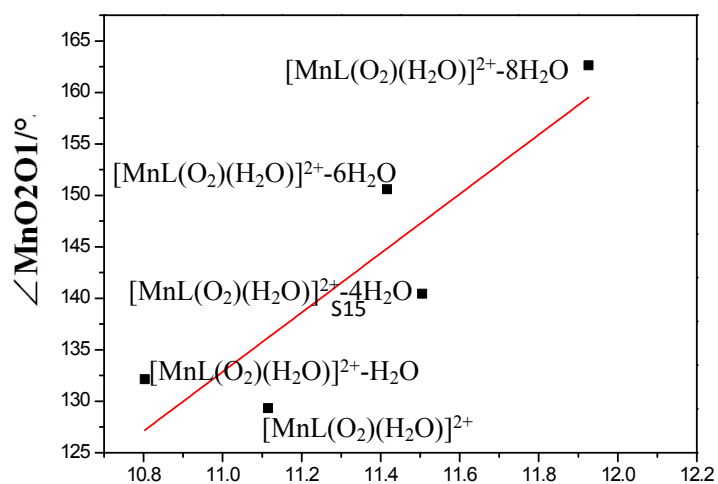


Fig. S3 Linear relationship of Mn-O2-O1 (\angle MnO2O1) bonding angle of optimized sextet $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+} \cdot n\text{H}_2\text{O}$ ($n = 0, 1, 4, 6, 8$) with $d_{\text{C}_\text{N}-\text{C}_\text{N}}$ ($R^2 = 0.713$).

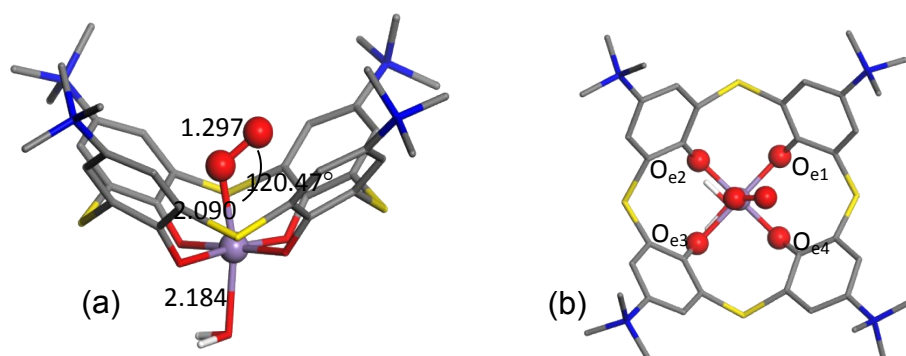
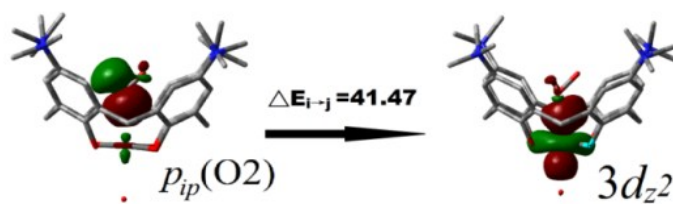
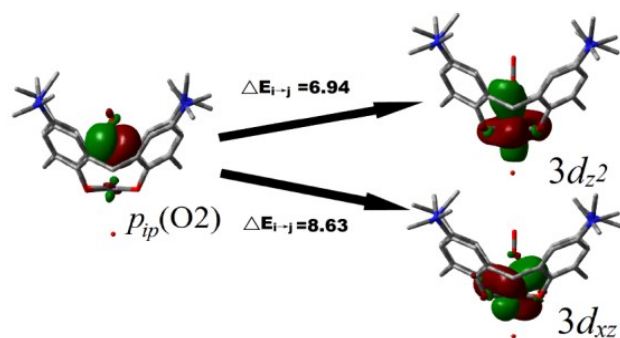


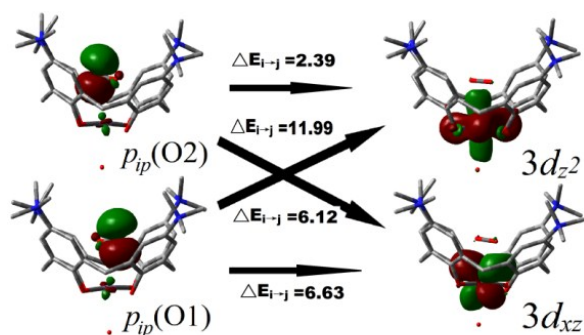
Fig. S4 Optimized structure of $[\text{MnL}^{\text{S}}(\text{O}_2)(\text{H}_2\text{O})]^{2+}$ complex (a) side view and (b) top view. The distances of $\text{O}_{\text{e}1}-\text{O}_{\text{e}3}$ and $\text{O}_{\text{e}2}-\text{O}_{\text{e}4}$ are 3.829 Å and 4.125 Å, respectively.



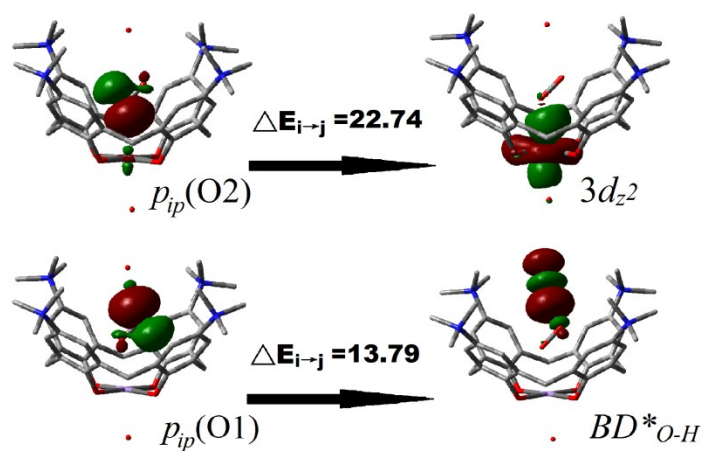
(a) Bent end-on $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+}$



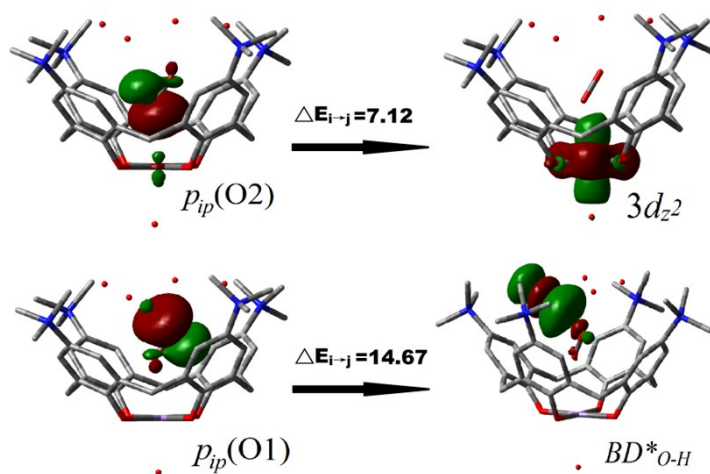
(b) Linear end-on $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+}$



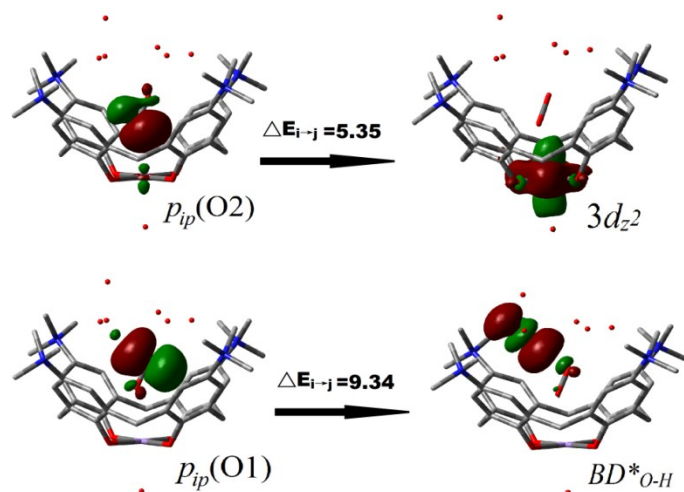
(c) Side-on $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+}$



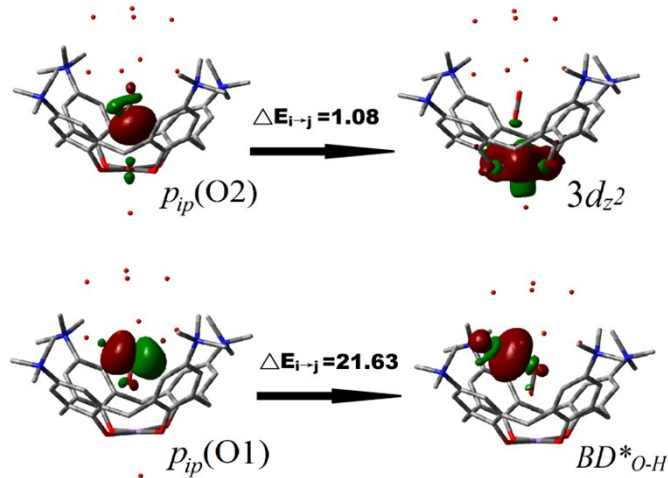
(d) Bent end-on $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+} - 1\text{H}_2\text{O}$



(e) Bent end-on $[MnL(O_2)(H_2O)]^{2+} \cdot 4H_2O$



(f) Bent end-on $[MnL(O_2)(H_2O)]^{2+} \cdot 6H_2O$



(g) Bent end-on $[MnL(O_2)(H_2O)]^{2+} \cdot 8H_2O$

Fig. S5 NBOs of superoxo donors (left) and Mn(III) acceptors (right) for sextet

$[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+}$ in three different binding configurations (a-c) and $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+}\text{-nH}_2\text{O}$ ($n = 1, 4, 6, 8$) complexes (d-g), as well as second-order perturbation energies ($\Delta E_{i \rightarrow j}$ in kcal/mol). All hydrogen atoms are omitted for clarity.

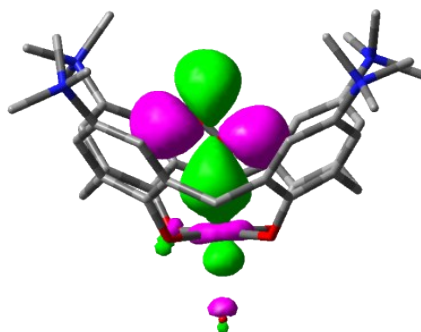


Fig. S6. HOMO of the sextet bent end-on $[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+}$ in β space, corresponding to a bonding interaction of superoxo π^*_{ip} with Mn $3d_{z^2}$

Cartesian coordinates of all structures described in this work:

$[\text{MnL}(\text{O}_2)(\text{H}_2\text{O})]^{2+}$ (Bent end-on)

Charge=2 S=5/2

Gibbs free energy: -3452.089338 Ha

O	1.93646200	-0.27991800	2.52997400
O	0.30755900	1.90003100	2.52276400
O	-0.26410600	-1.91470700	2.53806700
O	-1.87793800	0.26734400	2.52074600
O	0.16112300	-0.22296400	4.79456000
O	0.23003300	0.12314400	0.24342400
Mn	0.01371400	0.00030300	2.47471800
C	2.64784100	-0.38238600	1.44135800
C	0.40304500	2.62518100	1.44479900

C	-0.37728600	-2.62685400	1.44826000
C	-2.61314600	0.38185100	1.44957200
H	1.09495500	-0.15819100	5.04122700
H	-0.13099300	-1.11999100	5.01244500
O	-0.53731900	-0.39073000	-0.70176800
C	2.87189800	-1.66040900	0.84841700
C	3.23034000	0.78367700	0.85148600
C	1.67989500	2.86668400	0.85482000
C	-0.76669900	3.21360000	0.87009000
C	-1.65956200	-2.85388600	0.86692600
C	0.78471900	-3.20457800	0.85012200
C	-2.84934300	1.66398400	0.87508900
C	-3.21660100	-0.77931300	0.87519200
C	3.77396000	-1.77407000	-0.20883700
C	2.17268300	-2.89732500	1.41158500
C	4.12497700	0.62887400	-0.19986700
C	2.91866100	2.16912000	1.41541200
C	1.78855000	3.78761200	-0.18505600
C	-0.61736300	4.12371100	-0.16994100
C	-2.14600500	2.89542100	1.44492600
C	-1.77942000	-3.75564400	-0.18848500
C	-2.89670100	-2.16255600	1.43856200
C	0.62518200	-4.09150900	-0.20897000
C	-3.77693100	1.78473600	-0.15985800
C	-4.14119200	-0.61774900	-0.14802700
H	3.96828900	-2.76484300	-0.60403500
C	4.41268800	-0.64082200	-0.71796900
H	2.81638500	-3.76847400	1.23423400
H	2.07725000	-2.76729200	2.49349200
H	4.60641900	1.51920500	-0.59812400
H	3.78800700	2.81560800	1.23970500
H	2.78750300	2.07226300	2.49726400
H	2.77772400	3.99458300	-0.57782900
C	0.64940800	4.42656000	-0.68437600
H	-1.51000700	4.61149500	-0.55519000
H	-2.79432200	3.76695300	1.28766800
H	-2.03548900	2.75011400	2.52397400
H	-2.77242400	-3.94990300	-0.57739800
C	-0.64718500	-4.38320600	-0.71343000
H	-3.76422800	-2.81283100	1.26815300
H	-2.76116000	-2.06288400	2.51970600
H	1.51367300	-4.56771300	-0.61741100
H	-3.98068600	2.77794200	-0.54384500
C	-4.43281300	0.65552600	-0.65492500

H	-4.63877500	-1.50380000	-0.53540100
N	5.47892100	-0.74466200	-1.78999000
N	0.74671700	5.51501900	-1.73477800
N	-0.75543500	-5.42923400	-1.80497100
N	-5.52026100	0.76721900	-1.70475300
C	6.80101800	-0.24095400	-1.24782900
C	5.69700000	-2.15735000	-2.26014200
C	5.08263600	0.07673400	-2.99500600
C	0.24976500	6.82608200	-1.15999300
C	2.15613900	5.74026700	-2.21123600
C	-0.08450900	5.14691000	-2.94174500
C	-0.21871500	-6.75364200	-1.30315800
C	-2.17398000	-5.66196200	-2.25027900
C	0.03359000	-4.98998000	-3.01681800
C	-6.83396200	0.27163900	-1.13568500
C	-5.73864800	2.18138500	-2.16999500
C	-5.15269800	-0.05597600	-2.91769500
H	7.06647200	-0.84986900	-0.38357800
H	6.68752400	0.79653300	-0.94024700
H	7.56167900	-0.32359200	-2.02751200
H	6.02107700	-2.76894100	-1.41922900
H	4.76612200	-2.54220300	-2.67502500
H	6.47072900	-2.14365000	-3.02891100
H	4.12730300	-0.29941300	-3.36140300
H	4.97471500	1.11708900	-2.69592300
H	5.85655900	-0.01407600	-3.76056300
H	0.86427000	7.07032000	-0.29345000
H	-0.78614300	6.70782400	-0.84874500
H	0.32963400	7.60415400	-1.92270400
H	2.77417400	6.04968300	-1.36955800
H	2.53705600	4.81606700	-2.64435900
H	2.13749500	6.52700100	-2.96658600
H	-1.12285800	5.03403100	-2.63776000
H	0.28726700	4.19956200	-3.33245600
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H	-0.80432800	-7.04786200	-0.43214000
H	0.82346100	-6.63058900	-1.01614100
H	-0.30650200	-7.49835100	-2.09745600
H	-2.76310100	-6.00822700	-1.40211500
H	-2.58152100	-4.73118100	-2.64286800
H	-2.16361600	-6.42358600	-3.03109700
H	-0.36316500	-4.03034600	-3.34874600
H	1.07841500	-4.87441400	-2.73645400
H	-0.06309900	-5.74508700	-3.80037000

H	-7.07807700	0.88202500	-0.26615800
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H	-4.81338600	2.56025200	-2.60257800
H	-6.52722200	2.17272100	-2.92360700
H	-5.04998200	-1.09780100	-2.62214800
H	-4.19943700	0.31086600	-3.29863300
H	-5.93884400	0.04411700	-3.66951900

[MnL(O₂)(H₂O)]²⁺ (Bent end-on)

Charge=2 S=3/2

Gibbs free energy: -3452.086475 Ha

O	1.96944300	-0.10808000	2.53804600
O	0.13822200	1.91043100	2.51739400
O	-0.08932800	-1.94499300	2.54871200
O	-1.89044800	0.08875000	2.50482100
O	0.17032900	-0.20411500	4.76660400
O	0.24046500	0.07831700	0.29934000
Mn	0.02246100	-0.00866300	2.45189100
C	2.69075900	-0.14846600	1.45311500
C	0.17168700	2.63534600	1.43453700
C	-0.14159700	-2.64524800	1.44581000
C	-2.64842700	0.14182700	1.44677300
H	1.09168900	-0.04673900	5.01851100
H	-0.03155500	-1.12669300	4.98050000
O	-0.54707400	-0.32658000	-0.68160100
C	3.02480300	-1.40196500	0.85908500
C	3.16752000	1.06414500	0.86188700
C	1.42375400	2.98923900	0.84834200
C	-1.04502600	3.11438700	0.85496300
C	-1.39850200	-2.97397600	0.85695300
C	1.06748300	-3.10812300	0.83902200
C	-3.00047700	1.39935400	0.87708900
C	-3.15873100	-1.06730800	0.88082100
C	3.94484100	-1.43670100	-0.18801900
C	2.42342600	-2.69323600	1.41152500
C	4.08170000	0.98847500	-0.18172200
C	2.72046300	2.41525300	1.41837800
C	1.45184000	3.90979900	-0.19670300
C	-0.97478400	4.02719700	-0.19135000
C	-2.39258000	2.68503000	1.43605500
C	-1.43663700	-3.86456800	-0.21430000
C	-2.69727700	-2.41301900	1.43646600

C	0.98787100	-3.98633100	-0.23609100
C	-3.95666400	1.43956500	-0.13770700
C	-4.11199400	-0.98671100	-0.12527100
H	4.22887900	-2.40692300	-0.57996800
C	4.48848300	-0.25210300	-0.69140100
H	3.13547900	-3.50956500	1.23437400
H	2.31004200	-2.57711000	2.49324200
H	4.48316100	1.91766200	-0.58006300
H	3.52465000	3.14188000	1.24561500
H	2.59167300	2.30863100	2.49960100
H	2.41967100	4.20413200	-0.58671800
C	0.26129400	4.44024100	-0.70332700
H	-1.90646400	4.42861200	-0.58383600
H	-3.10913200	3.50159700	1.28008100
H	-2.26396400	2.55321300	2.51494000
H	-2.40848300	-4.13927600	-0.60797700
C	-0.25398300	-4.38044400	-0.74793800
H	-3.49494200	-3.14770500	1.26781100
H	-2.56596000	-2.30329100	2.51716000
H	1.91521800	-4.37480600	-0.65109000
H	-4.25343700	2.41162400	-0.51507800
C	-4.52377000	0.25841700	-0.62135000
H	-4.53654400	-1.91221100	-0.50768800
N	5.57343900	-0.26546900	-1.74987100
N	0.26565200	5.51993300	-1.76734200
N	-0.27182500	-5.41820100	-1.85290700
N	-5.63330300	0.27900800	-1.65385600
C	6.83458300	0.36858800	-1.19924800
C	5.93183100	-1.65617200	-2.19845400
C	5.11614600	0.50060100	-2.96967700
C	-0.37483300	6.78022100	-1.22235700
C	1.65313800	5.88431100	-2.22077400
C	-0.49993800	5.05043000	-2.98289500
C	0.37374800	-6.69850600	-1.36481200
C	-1.66501200	-5.76384900	-2.30435400
C	0.47912500	-4.90038100	-3.05783900
C	-6.88401900	-0.35174000	-1.07688500
C	-5.99657700	1.67203600	-2.09115000
C	-5.20470900	-0.48544400	-2.88520900
H	7.14364000	-0.20036200	-0.32242000
H	6.61969700	1.39509000	-0.90987000
H	7.61047100	0.34650000	-1.96791600
H	6.30113000	-2.22318200	-1.34497100
H	5.04752100	-2.13364800	-2.61855700

H	6.71070200	-1.57785300	-2.95804100
H	4.20880100	0.02782400	-3.34604300
H	4.90016900	1.52785800	-2.68356700
H	5.90671600	0.47990300	-3.72327800
H	0.19329200	7.09687400	-0.34769300
H	-1.39981500	6.56122100	-0.93073700
H	-0.35802300	7.55234200	-1.99496600
H	2.21939900	6.26265400	-1.37075300
H	2.13538000	5.00038100	-2.63622000
H	1.56838000	6.65799400	-2.98495600
H	-1.52551600	4.83067100	-2.69371100
H	-0.02332300	4.14277500	-3.35358500
H	-0.48443800	5.83612900	-3.74173200
H	-0.18654700	-7.05066700	-0.49868400
H	1.40119600	-6.49076700	-1.07374800
H	0.35023800	-7.43911800	-2.16745000
H	-2.22383500	-6.16861500	-1.46159900
H	-2.14868100	-4.86536200	-2.68549300
H	-1.58965600	-6.51200900	-3.09451900
H	0.00204100	-3.97502600	-3.38117900
H	1.50992100	-4.69869900	-2.77394300
H	0.44859100	-5.65280300	-3.84925800
H	-7.17206600	0.21645400	-0.19240300
H	-6.66686700	-1.37962300	-0.79422400
H	-7.67633900	-0.32552600	-1.82845300
H	-6.34446900	2.23853200	-1.22835700
H	-5.12022300	2.14703500	-2.53021700
H	-6.79282100	1.59798100	-2.83295500
H	-4.98963400	-1.51485700	-2.60643300
H	-4.30107800	-0.01751300	-3.27633900
H	-6.00980300	-0.45680500	-3.62306500

[MnL(O₂)(H₂O)]²⁺ (Bent end-on)

Charge=2 S=1/2

Gibbs free energy: -3452.064504 Ha

O	0.54894100	-1.89549400	2.52963600
O	1.88538200	0.50580600	2.51376800
O	-1.83638300	-0.54764900	2.48374200
O	-0.51597700	1.81703600	2.45864600
O	-0.08923800	-0.11372000	4.46949300
O	0.24974900	-0.14728000	0.49213900
Mn	0.02954900	-0.01758800	2.39440700

C	0.74511100	-2.58773700	1.44507400
C	2.58592700	0.71248900	1.44042900
C	-2.55809600	-0.74324500	1.41934800
C	-0.71777200	2.54465100	1.40360100
H	0.35327900	-0.92899200	4.75134300
H	-1.02939200	-0.19331200	4.69416000
O	-0.59542400	0.31298000	-0.39274600
C	-0.33173500	-3.30550300	0.83985500
C	2.04636900	-2.63241400	0.84673400
C	3.32328100	-0.35891900	0.84813700
C	2.63603100	2.01625200	0.84771100
C	-3.29677400	0.33256700	0.83880900
C	-2.62006200	-2.04639600	0.83326600
C	0.35519300	3.29085400	0.83144100
C	-2.02732600	2.62022600	0.82902700
C	-0.06359400	-4.17449700	-0.21761500
C	-1.75294000	-3.17561200	1.39503300
C	2.27225200	-3.51065300	-0.20616600
C	3.18204900	-1.77529300	1.40958600
C	4.21639400	-0.08478100	-0.18570700
C	3.53637900	2.24820200	-0.18569200
C	1.76742500	3.14658900	1.40461200
C	-4.19530700	0.05937400	-0.19003300
C	-3.15496700	1.75269800	1.39238800
C	-3.52384800	-2.27680200	-0.19875400
C	0.08002000	4.20283500	-0.18737500
C	-2.26185700	3.54395800	-0.18063100
H	-0.88840800	-4.75443500	-0.61676800
C	1.23293700	-4.29494700	-0.72481900
H	-2.27543200	-4.12570200	1.22383800
H	-1.67454900	-3.02693600	2.47601800
H	3.28209600	-3.58306500	-0.60454300
H	4.12742500	-2.30761700	1.24227900
H	3.03174500	-1.68900100	2.48973000
H	4.81190500	-0.90467200	-0.57223800
C	4.33951500	1.21506000	-0.68765300
H	3.61479200	3.25998200	-0.57815600
H	2.29876800	4.09454900	1.24947500
H	1.67054200	2.98749100	2.48319400
H	-4.78646900	0.88201200	-0.57654200
C	-4.32193300	-1.23889600	-0.69595100
H	-4.10450500	2.27843600	1.22783000
H	-2.99966300	1.67423300	2.47293000
H	-3.60879300	-3.28814200	-0.59080200

H	0.90018300	4.80389300	-0.56428500
C	-1.22138600	4.34340900	-0.67805900
H	-3.27519800	3.63922600	-0.56508400
N	1.57739300	-5.32139400	-1.78559200
N	5.39438400	1.57079000	-1.71644700
N	-5.37023800	-1.58325100	-1.73579200
N	-1.57251900	5.41235400	-1.69397400
C	2.56618200	-6.32271400	-1.22379400
C	0.37636000	-6.09435800	-2.25915000
C	2.18108900	-4.64180100	-2.99247200
C	6.37902000	2.55482900	-1.11754200
C	6.18148000	0.37514900	-2.17970700
C	4.74883600	2.18598300	-2.93593100
C	-6.35791100	-2.57529400	-1.15651800
C	-6.15531000	-0.38268300	-2.19092800
C	-4.71391200	-2.18210700	-2.95772100
C	-2.55521700	6.39206800	-1.08547000
C	-0.37454800	6.20227900	-2.14647900
C	-2.18663500	4.78203400	-2.92209300
H	2.10886400	-6.79905000	-0.35662700
H	3.46739500	-5.79638500	-0.91625500
H	2.80217100	-7.06266500	-1.99212200
H	-0.05765900	-6.63307800	-1.41797000
H	-0.34919000	-5.40045300	-2.68205200
H	0.70663000	-6.80107700	-3.02160200
H	1.45441200	-3.92592800	-3.37709200
H	3.08598500	-4.11835100	-2.69122600
H	2.41947200	-5.39608400	-3.74577500
H	6.82992900	2.09031300	-0.24067100
H	5.84357900	3.45321600	-0.81761200
H	7.14090200	2.79742700	-1.86210200
H	6.69929100	-0.06494600	-1.32867800
H	5.49978900	-0.34824500	-2.62560800
H	6.90677400	0.71249500	-2.92133600
H	4.21343800	3.08576900	-2.64048300
H	4.04718400	1.46162000	-3.34992600
H	5.52427500	2.43528200	-3.66378100
H	-6.81772300	-2.12117200	-0.27881100
H	-5.82383900	-3.47631000	-0.86208400
H	-7.11283600	-2.81105000	-1.91024900
H	-6.67864100	0.04769200	-1.33829300
H	-5.47154500	0.34581000	-2.62506700
H	-6.87580500	-0.71292300	-2.94039600
H	-4.00676300	-1.45306700	-3.35383600

H	-4.18329500	-3.08715100	-2.66969200
H	-5.48272300	-2.41931900	-3.69659700
H	-2.09052700	6.83273600	-0.20349600
H	-3.45493800	5.85524000	-0.79223400
H	-2.79572000	7.16235200	-1.82196900
H	0.06355000	6.71183500	-1.28945400
H	0.34933300	5.52390800	-2.59651900
H	-0.70909700	6.93476700	-2.88227100
H	-3.08839600	4.24571600	-2.63453900
H	-1.46321500	4.08267000	-3.34156000
H	-2.43197300	5.56609400	-3.64209200

[MnL(O₂)(H₂O)]²⁺ (Linear end-on)

Charge=2 S=5/2

Gibbs free energy: -3452.082648 Ha

Mn	-0.00474100	-0.00243600	2.49888700
O	-0.02374600	-0.01492200	0.32598600
O	-0.02580700	0.00223100	-0.99400900
O	-1.93611400	0.13232300	2.54829900
O	-0.15118100	-1.94966500	2.58264600
O	0.12631400	1.92235200	2.58130100
O	1.90486100	-0.15268700	2.52800300
O	-0.13733000	-0.20471400	4.78454100
C	-2.65285900	0.19253900	1.45932100
C	-0.19913000	-2.64751500	1.47860400
C	0.18628500	2.63421100	1.48909100
C	2.63709200	-0.20023400	1.45181200
H	-0.17062400	-1.15788700	4.95473000
H	-0.95595300	0.17897900	5.12920300
C	-2.97077100	1.45329000	0.87589900
C	-3.15041100	-1.00870400	0.86656900
C	-1.45548100	-2.96157600	0.87921400
C	1.00416600	-3.13832800	0.88039000
C	1.44713000	2.95620800	0.90358700
C	-1.01265200	3.14102800	0.89594300
C	2.96984300	-1.45712800	0.86895600
C	3.14593800	1.00659200	0.88127300
C	-3.86916000	1.50549800	-0.18879100
C	-2.37301300	2.73302100	1.45531900
C	-4.04288100	-0.91651500	-0.19478300
C	-2.74392000	-2.36400500	1.44004100
C	-1.50296600	-3.85354700	-0.19066200
C	0.91614300	-4.02350100	-0.18723100
C	2.36555800	-2.73642900	1.44253200

C	1.50100200	3.86842400	-0.14878400
C	2.73095300	2.35305900	1.46853300
C	-0.91848700	4.04721700	-0.15303200
C	3.89298000	-1.50186100	-0.17435800
C	4.06263600	0.92211600	-0.15978500
H	-4.13272400	2.48118600	-0.58092500
C	-4.41669400	0.33085000	-0.70997600
H	-3.07993400	3.55491500	1.28464600
H	-2.26765100	2.59962100	2.53593900
H	-4.45450000	-1.83784600	-0.60058400
H	-3.56192600	-3.07431500	1.26464900
H	-2.62385000	-2.25030600	2.52116800
H	-2.47710300	-4.11350200	-0.58928100
C	-0.32695500	-4.39946200	-0.70896800
H	1.84051600	-4.42792800	-0.59349500
H	3.06907700	-3.56094000	1.27045700
H	2.26171100	-2.60356600	2.52344300
H	2.47775000	4.13509200	-0.53638000
C	0.32894600	4.42819700	-0.66177500
H	3.54927100	3.06728400	1.31176900
H	2.59848800	2.22348600	2.54692700
H	-1.83941100	4.46538100	-0.55329900
H	4.17035900	-2.47449300	-0.56470600
C	4.45000400	-0.32180700	-0.67460800
H	4.48588500	1.84622000	-0.54696800
N	-5.46391700	0.36350300	-1.80484500
N	-0.35234600	-5.43709400	-1.81226500
N	0.36412900	5.49269400	-1.73906700
N	5.53110900	-0.34552000	-1.73647900
C	-6.75431700	-0.24828500	-1.29927200
C	-5.78164500	1.76039800	-2.26570300
C	-4.97560000	-0.40983400	-3.00823000
C	0.26700400	-6.72811200	-1.31799500
C	-1.74687600	-5.75916300	-2.27632100
C	0.41890700	-4.93273800	-3.01050100
C	-0.24669900	6.77543600	-1.21334400
C	1.76195200	5.81607500	-2.19251800
C	-0.40819800	5.02481300	-2.95102400
C	6.80708800	0.25454800	-1.18176300
C	5.85798900	-1.73789700	-2.20427400
C	5.08569800	0.44461600	-2.94536100
H	-7.08589100	0.32710900	-0.43488900
H	-6.56778800	-1.27787100	-1.00111700
H	-7.50138700	-0.21462400	-2.09554500

H	-6.16776300	2.33586300	-1.42540700
H	-4.87554900	2.22030700	-2.65826000
H	-6.53730300	1.69516900	-3.04959100
H	-4.04162100	0.04122900	-3.34386300
H	-4.79732300	-1.44296900	-2.71768000
H	-5.73436600	-0.36690900	-3.79291800
H	-0.30795900	-7.07193900	-0.45812000
H	1.29456800	-6.53746600	-1.01559300
H	0.24032200	-7.46767900	-2.12154500
H	-2.32133800	-6.15190400	-1.43837100
H	-2.21059900	-4.85326600	-2.66477900
H	-1.67742100	-6.51048600	-3.06402200
H	1.45128500	-4.75365500	-2.71771000
H	-0.03527800	-3.99632700	-3.33494200
H	0.37880100	-5.68290900	-3.80361400
H	0.32842500	7.09237500	-0.34331100
H	-1.27651500	6.58488100	-0.91856500
H	-0.21206600	7.53524400	-1.99749400
H	2.33687300	6.18622900	-1.34469300
H	2.22082100	4.91611500	-2.60011300
H	1.69914200	6.58543400	-2.96318700
H	0.04087300	4.09457100	-3.29947800
H	-1.44223500	4.84483900	-2.66469600
H	-0.36216700	5.79511400	-3.72426700
H	7.10734800	-0.33210600	-0.31352700
H	6.61496000	1.28143200	-0.87783300
H	7.57979200	0.22650600	-1.95344700
H	6.21888600	-2.32418900	-1.36029800
H	4.96198800	-2.19053500	-2.62736600
H	6.63567800	-1.66604900	-2.96571200
H	4.90074200	1.47465400	-2.64819500
H	4.16256000	0.00066400	-3.31841000
H	5.87026900	0.40926300	-3.70460900

[MnL(O₂)(H₂O)]²⁺ (Linear end-on)

Charge=2 S=3/2

Gibbs free energy: -3452.081853 Ha

Mn	0.00355300	-0.00202500	2.46591900
O	0.02387800	-0.01025100	0.35799300
O	0.02501900	-0.01302400	-0.96031300
O	0.83582500	-1.76284000	2.55926400
O	1.77109800	0.82199100	2.57007100
O	-1.73587300	-0.82962400	2.56128600
O	-0.80421500	1.74511200	2.54521700

O	0.23506900	-0.06020400	4.76199500
C	1.13305800	-2.41132400	1.46666200
C	2.40910900	1.12491800	1.47155300
C	-2.39160200	-1.12854400	1.47468600
C	-1.11840900	2.40145600	1.46493800
H	1.03711000	0.44571200	4.95913300
H	0.40135500	-0.97547100	5.02963800
C	0.18716500	-3.29898600	0.87419700
C	2.42242600	-2.25122100	0.86937300
C	3.29989000	0.18356000	0.87497300
C	2.24956600	2.41617800	0.87740500
C	-3.29282000	-0.18692200	0.89461400
C	-2.24800300	-2.42323300	0.88442400
C	-0.18271000	3.30148000	0.87533500
C	-2.41697500	2.24853700	0.88651800
C	0.58098900	-4.10208900	-0.19504800
C	-1.22433400	-3.40624000	1.44715100
C	2.77811000	-3.06958900	-0.19618000
C	3.40647700	-1.23184500	1.43927900
C	4.10659700	0.58225300	-0.18951200
C	3.07030600	2.77619500	-0.18453400
C	1.23091700	3.40259500	1.44393100
C	-4.12190400	-0.58915900	-0.15109300
C	-3.39117800	1.22579000	1.46641800
C	-3.09176600	-2.78740800	-0.15760000
C	-0.59330900	4.12328400	-0.17286000
C	-2.78915800	3.08460900	-0.15937500
H	-0.14213200	-4.80534100	-0.59222400
C	1.87358800	-4.00389800	-0.71530500
H	-1.59162500	-4.42609900	1.27570400
H	-1.16468000	-3.24797000	2.52794100
H	3.78249600	-2.97476700	-0.60268600
H	4.42576500	-1.59942800	1.26495100
H	3.24885300	-1.17861500	2.52024700
H	4.81304600	-0.13801800	-0.58646000
C	4.00914200	1.87698600	-0.70402600
H	2.97412100	3.78189500	-0.58754700
H	1.60228800	4.42095400	1.27238300
H	1.17016500	3.24477200	2.52475600
H	-4.83674900	0.13000600	-0.53477800
C	-4.03850700	-1.88684300	-0.66158000
H	-4.41336000	1.59343200	1.31040500
H	-3.21478200	1.16674800	2.54471300
H	-3.00996000	-3.79657000	-0.55524000

H	0.12079400	4.83792100	-0.56617600
C	-1.89395700	4.03023100	-0.67532600
H	-3.80051100	2.99769700	-0.55015300
N	2.35871000	-4.93125100	-1.81131300
N	4.93587700	2.36815100	-1.79732500
N	-4.99651400	-2.38274700	-1.72560800
N	-2.40115700	4.98201300	-1.74011500
C	3.51860700	-5.76270400	-1.30279000
C	1.29438200	-5.88652600	-2.27948400
C	2.80244600	-4.12551700	-3.01060000
C	5.76062400	3.53173600	-1.28652000
C	5.89726300	1.30937800	-2.26477100
C	4.12932400	2.80900300	-2.99726400
C	-5.81619900	-3.53445700	-1.18048600
C	-5.96210500	-1.32188700	-2.17979700
C	-4.22539900	-2.84280500	-2.94120200
C	-3.54881300	5.80295700	-1.18789200
C	-1.34600500	5.94662700	-2.20960900
C	-2.87213900	4.20441000	-2.94739800
H	3.17321700	-6.33434300	-0.44132900
H	4.32606900	-5.09960300	-0.99927900
H	3.85606800	-6.42986300	-2.09925000
H	0.97653200	-6.50702100	-1.44266600
H	0.45324800	-5.31683100	-2.67266800
H	1.72162300	-6.51208400	-3.06427400
H	1.95592600	-3.52734800	-3.34827400
H	3.61797100	-3.46887200	-2.71520300
H	3.13659300	-4.80757900	-3.79570500
H	6.33383800	3.18804600	-0.42542500
H	5.09291600	4.33487500	-0.98173700
H	6.42614000	3.87447800	-2.08213200
H	6.51599500	0.99203000	-1.42643000
H	5.33253400	0.46680900	-2.66199000
H	6.52378500	1.74104400	-3.04637400
H	3.46992400	3.62239100	-2.70210600
H	3.53338800	1.96065300	-3.33425300
H	4.81056800	3.14505500	-3.78230700
H	-6.36268500	-3.17734900	-0.30756500
H	-5.14658900	-4.33976700	-0.88570100
H	-6.50597100	-3.87977900	-1.95404100
H	-6.55902900	-0.99322700	-1.33012400
H	-5.40165900	-0.48643600	-2.59763900
H	-6.60955900	-1.75653100	-2.94247000
H	-3.63465600	-2.00196500	-3.30512000

H	-3.56275900	-3.65649800	-2.65422900
H	-4.92943400	-3.18452800	-3.70335500
H	-3.18439300	6.35341400	-0.32051100
H	-4.35080200	5.13383800	-0.88308700
H	-3.90159000	6.48914800	-1.96123300
H	-1.01155100	6.55010600	-1.36686900
H	-0.51291500	5.38504700	-2.63068500
H	-1.78832500	6.58805400	-2.97294400
H	-3.68047700	3.54023600	-2.64916900
H	-2.03340300	3.61537800	-3.31887600
H	-3.22451800	4.90443700	-3.70834300

[MnL(O₂)(H₂O)]²⁺ (Side-on)

Charge=2 S=5/2

Gibbs free energy: -3452.074199 Ha

O	0.03001900	-1.93270400	2.44973000
O	1.93521800	0.02238900	2.54249500
O	-1.94976100	-0.05509700	2.54546900
O	-0.04030000	1.89977200	2.43454400
O	-0.17573600	-0.10020200	4.65194300
O	0.64411000	-0.12599300	-0.03077200
Mn	0.00454600	-0.00578000	2.33586000
C	0.05111500	-2.63569200	1.35212200
C	2.71102400	0.03952800	1.49816500
C	-2.71791700	-0.05717400	1.49304800
C	-0.05290200	2.61807200	1.34988900
H	0.24767200	-0.89564100	5.00306700
H	-1.13059300	-0.19334400	4.78798400
O	-0.65726700	0.10164600	-0.03833600
C	-1.17544400	-3.04469700	0.75196800
C	1.30407500	-3.00267900	0.76943200
C	3.17623600	-1.18437000	0.92393600
C	3.11653900	1.28609900	0.91877000
C	-3.17038500	1.17212200	0.91993100
C	-3.12032800	-1.29787300	0.89969900
C	1.17802100	3.03900100	0.76833900
C	-1.30320600	2.99888900	0.77145800
C	-1.13380700	-3.89804600	-0.34993700
C	-2.50942000	-2.61715200	1.37628600
C	1.30011000	-3.85499800	-0.32785200
C	2.61276200	-2.52221800	1.40684300
C	4.18018400	-1.14596500	-0.04164100
C	4.11769600	1.28207800	-0.04531400
C	2.50282300	2.60071800	1.40387900

C	-4.16225900	1.14118300	-0.05866400
C	-2.60922000	2.50949300	1.40801600
C	-4.11006200	-1.28619200	-0.07629100
C	1.14243400	3.91661400	-0.31419900
C	-1.29363600	3.87601100	-0.30596600
H	-2.07613500	-4.23654300	-0.76547900
C	0.09337700	-4.31033900	-0.87760000
H	-3.23948500	-3.41664100	1.19548300
H	-2.35460800	-2.54508700	2.45701500
H	2.25719500	-4.16935800	-0.73791800
H	3.37409700	-3.29539800	1.24127800
H	2.44330800	-2.44565300	2.48511200
H	4.56633700	-2.09031000	-0.40928200
C	4.67218000	0.07920900	-0.50248100
H	4.47144200	2.24016600	-0.42027500
H	3.23708200	3.40061700	1.24320600
H	2.33280100	2.51293900	2.48159300
H	-4.53872100	2.08919200	-0.42668100
C	-4.65432500	-0.07864000	-0.53251800
H	-3.37418900	3.28035500	1.24854300
H	-2.43438500	2.42955000	2.48533900
H	-4.46049000	-2.24081100	-0.46298600
H	2.08681800	4.26637100	-0.71553900
C	-0.08246100	4.34179000	-0.83863900
H	-2.24788800	4.20417300	-0.71197900
N	0.16612800	-5.31225300	-2.01361000
N	5.85556400	0.15460400	-1.44641800
N	-5.82149200	-0.14201500	-1.49719800
N	-0.14722700	5.37431500	-1.94766100
C	0.87030200	-6.56888300	-1.54365900
C	-1.19109200	-5.72169700	-2.51795500
C	0.92033300	-4.71798400	-3.18081200
C	7.00230500	0.87982700	-0.77156200
C	6.36290200	-1.20237300	-1.85289300
C	5.46923400	0.89026200	-2.70824800
C	-6.98116600	-0.87183800	-0.85040300
C	-6.31930700	1.22018800	-1.89841700
C	-5.41401500	-0.86529200	-2.75964900
C	-0.85129800	6.61937500	-1.44756500
C	1.21338400	5.79462600	-2.43351300
C	-0.89626200	4.81368200	-3.13447400
H	0.30894600	-6.97673000	-0.70302200
H	1.87672200	-6.31277100	-1.21912400
H	0.90922000	-7.28606000	-2.36680000

H	-1.74727900	-6.19380300	-1.70918700
H	-1.71765300	-4.83856200	-2.87772000
H	-1.04947600	-6.43114600	-3.33426700
H	0.39622900	-3.81641800	-3.49834100
H	1.92745600	-4.46018400	-2.86034900
H	0.96045600	-5.45066600	-3.98998800
H	7.26490200	0.32996900	0.13220200
H	6.68022100	1.88434900	-0.50502800
H	7.85083200	0.92336400	-1.45828500
H	6.68175200	-1.74561700	-0.96446300
H	5.56680600	-1.74273900	-2.36379300
H	7.20949300	-1.06064300	-2.52600700
H	5.15128200	1.89789900	-2.44909600
H	4.64204400	0.35344100	-3.17300500
H	6.33144100	0.93123700	-3.37780600
H	-7.25966800	-0.33002900	0.05346000
H	-6.66564200	-1.87947900	-0.58772300
H	-7.81699400	-0.90750400	-1.55293400
H	-6.65081600	1.75555400	-1.00981300
H	-5.51405400	1.76357300	-2.39139300
H	-7.15548400	1.08689400	-2.58608600
H	-4.57682500	-0.32597600	-3.20311100
H	-5.10375700	-1.87655600	-2.50525200
H	-6.26377200	-0.89650100	-3.44545200
H	-0.29414100	7.00217300	-0.59249100
H	-1.86034100	6.35708900	-1.13636900
H	-0.88327700	7.35913700	-2.25079400
H	1.76552900	6.24431500	-1.60938900
H	1.74084500	4.92044100	-2.81328800
H	1.07742800	6.52556100	-3.23161500
H	-1.90546900	4.54895300	-2.82630900
H	-0.37178900	3.92038000	-3.47402700
H	-0.93128100	5.56795400	-3.92386700

[MnL(O₂)(H₂O)]²⁺ (Side-on)

Charge=2 S=3/2

Gibbs free energy: -3452.066645 Ha

O	-0.01600500	-1.92804900	2.45418100
O	1.92717400	-0.03254400	2.53008900
O	-1.94490300	0.00271800	2.53583700
O	0.00387700	1.89704200	2.44330200
O	-0.18263700	-0.10595000	4.69063600
O	0.65742600	-0.02504900	-0.06941700
Mn	0.00231600	-0.00580000	2.41451300

C	-0.01971300	-2.61976800	1.34408100
C	2.70939100	-0.03248100	1.48568600
C	-2.71737600	0.01814700	1.48196500
C	0.01723000	2.60429800	1.34610500
H	0.19341400	-0.92023900	5.05314100
H	-1.13501000	-0.11794800	4.86884100
O	-0.66755800	-0.00130100	-0.06918100
C	-1.25785900	-2.99701000	0.75098900
C	1.21787000	-3.02016200	0.75613600
C	3.13697800	-1.26448200	0.90822700
C	3.14900500	1.20401000	0.91764100
C	-3.13183800	1.25532200	0.90590600
C	-3.15180000	-1.21227600	0.89710600
C	1.25986000	2.99294000	0.77104800
C	-1.21733100	3.01832500	0.76202900
C	-1.24604400	-3.86077200	-0.34447800
C	-2.57746700	-2.54227900	1.38137400
C	1.18746400	-3.88115000	-0.33576100
C	2.54228700	-2.58651600	1.39010200
C	4.14299100	-1.25033200	-0.05817600
C	4.15063800	1.17910800	-0.04676300
C	2.57104000	2.52868200	1.41133200
C	-4.12491100	1.24929200	-0.07438000
C	-2.53989700	2.57643400	1.39447200
C	-4.14070700	-1.17927700	-0.08039100
C	1.25440100	3.87773900	-0.30718700
C	-1.18073600	3.90062600	-0.31222400
H	-2.19958900	-4.17758400	-0.75100200
C	-0.03308700	-4.30628300	-0.87639500
H	-3.32702300	-3.32480500	1.20581200
H	-2.41863400	-2.47031600	2.46143100
H	2.13415500	-4.22635800	-0.74470300
H	3.27986900	-3.38056700	1.21589500
H	2.38288600	-2.51184500	2.47004700
H	4.50316500	-2.20330500	-0.42913000
C	4.66630200	-0.03707100	-0.51307400
H	4.53072900	2.12902500	-0.41584800
H	3.32378900	3.31211500	1.25487800
H	2.39835500	2.44177500	2.48852400
H	-4.47562600	2.20596700	-0.44463500
C	-4.64654300	0.04157500	-0.54448100
H	-3.28058100	3.36881500	1.22594500
H	-2.37619100	2.49785000	2.47358900
H	-4.51592100	-2.12562600	-0.46332800

H	2.21025600	4.20441800	-0.70028400
C	0.04423700	4.33473400	-0.83706800
H	-2.12434500	4.25809400	-0.71791300
N	0.00711000	-5.31993800	-2.00423200
N	5.84691500	0.00960100	-1.46313200
N	-5.80890400	0.00661900	-1.51726400
N	0.01223800	5.37411300	-1.94170200
C	0.68257900	-6.58951200	-1.52809300
C	-1.36307200	-5.69933900	-2.49626900
C	0.76836900	-4.75376100	-3.18055800
C	7.01781400	0.69615300	-0.78950600
C	6.31180500	-1.35877600	-1.88199400
C	5.47506900	0.76525700	-2.71731200
C	-6.99191500	-0.68996900	-0.87642200
C	-6.26725800	1.38019400	-1.92648000
C	-5.41111900	-0.73167600	-2.77396400
C	-0.66452500	6.63350400	-1.44074700
C	1.38587700	5.76304500	-2.41632900
C	-0.74234000	4.83622600	-3.13531300
H	0.11602400	-6.97630200	-0.68102900
H	1.69671300	-6.35573800	-1.21114800
H	0.69882100	-7.31410800	-2.34548200
H	-1.92544200	-6.14907400	-1.67909100
H	-1.86946700	-4.80635500	-2.86059900
H	-1.24502100	-6.41983700	-3.30666300
H	0.26565300	-3.84100500	-3.50068000
H	1.78387600	-4.51966900	-2.86835300
H	0.78398700	-5.49259100	-3.98504100
H	7.26782500	0.13352200	0.10999200
H	6.72749700	1.70850800	-0.51605100
H	7.86419000	0.71764700	-1.47990600
H	6.62150200	-1.91673300	-0.99948200
H	5.49643500	-1.87256500	-2.38984900
H	7.15707500	-1.23699400	-2.56065500
H	5.18752400	1.77961300	-2.44923000
H	4.63030600	0.25588200	-3.18138500
H	6.33456700	0.78597500	-3.39124500
H	-7.26117000	-0.13892600	0.02468100
H	-6.70592000	-1.70543700	-0.61008700
H	-7.82398900	-0.70379800	-1.58414100
H	-6.59258500	1.92647200	-1.04224500
H	-5.44341400	1.90086600	-2.41310700
H	-7.10032900	1.26680600	-2.62145600
H	-4.55765700	-0.21538200	-3.21383200

H	-5.12778200	-1.74923100	-2.51347800
H	-6.25678100	-0.74393500	-3.46539900
H	-0.10341700	6.99909700	-0.58075000
H	-1.68134700	6.39436600	-1.13664300
H	-0.67357500	7.37707000	-2.24103700
H	1.94294100	6.19442500	-1.58577300
H	1.89424900	4.87785500	-2.79655300
H	1.27361700	6.50116900	-3.21153100
H	-1.75956900	4.59493600	-2.83429100
H	-0.23775500	3.93135000	-3.47437000
H	-0.75368400	5.59365600	-3.92242400

[MnL(O₂)(H₂O)]²⁺ (Side-on)

Charge=2 S=1/2

Gibbs free energy: -3452.024996 Ha

O	-0.01961100	-1.93881200	2.41699000
O	1.94295200	-0.04731900	2.52130200
O	-1.93763100	0.00979500	2.52372100
O	0.00974000	1.89146200	2.38562100
O	-0.07215200	-0.10650600	4.34183900
O	0.63480500	-0.02871300	0.32510100
Mn	0.02097700	-0.01104300	2.24256200
C	-0.02934300	-2.62981200	1.31321000
C	2.74630100	-0.05117400	1.49716300
C	-2.74362200	0.02870100	1.49900900
C	0.02641200	2.60458400	1.30060300
H	0.12734000	-1.03174100	4.55647100
H	-1.01515200	0.03528100	4.52780000
O	-0.69006300	0.00662800	0.15204600
C	-1.27384900	-2.99105900	0.71893800
C	1.20720000	-3.02527500	0.71484700
C	3.16511300	-1.28505700	0.91106700
C	3.18310200	1.18552900	0.91990800
C	-3.15709000	1.26800400	0.91930200
C	-3.18770600	-1.20248300	0.91650000
C	1.27408200	2.98250500	0.72345100
C	-1.20906200	3.02354600	0.71700100
C	-1.26886300	-3.84319900	-0.38506300
C	-2.58839900	-2.53632200	1.36909900
C	1.16739000	-3.87234400	-0.38718400
C	2.53558000	-2.60668300	1.36010900
C	4.19309100	-1.27361100	-0.03235700
C	4.20703700	1.15650800	-0.02077100
C	2.58003600	2.51478200	1.38144000

C	-4.18022900	1.26229600	-0.02973200
C	-2.53070500	2.59175400	1.36793900
C	-4.20618800	-1.16653900	-0.02985900
C	1.27152600	3.86669700	-0.35444600
C	-1.16727500	3.90550400	-0.35668600
H	-2.22459900	-4.15300700	-0.79256600
C	-0.05842200	-4.28905400	-0.92638200
H	-3.33785600	-3.32039900	1.19922200
H	-2.41001800	-2.47451200	2.44666500
H	2.11025100	-4.21853300	-0.80489600
H	3.26393700	-3.40886400	1.18325300
H	2.36519100	-2.54446300	2.43917000
H	4.55295200	-2.22708800	-0.40317300
C	4.73608400	-0.06149400	-0.46953800
H	4.59399400	2.10509600	-0.38684300
H	3.33343000	3.29937300	1.23243200
H	2.38591500	2.43560200	2.45572900
H	-4.53318600	2.21909500	-0.39828300
C	-4.72633700	0.05563700	-0.47659800
H	-3.26639200	3.38917600	1.20039700
H	-2.34805200	2.52828600	2.44514100
H	-4.59360800	-2.11201000	-0.40327800
H	2.22802600	4.19017300	-0.74953900
C	0.06162500	4.33267800	-0.88259700
H	-2.10812200	4.27099000	-0.76264400
N	-0.02647900	-5.30214900	-2.05535500
N	5.95811800	-0.01790600	-1.36599700
N	-5.93551700	0.02303600	-1.39056400
N	0.03475000	5.38106000	-1.97925100
C	0.63976800	-6.57704300	-1.57963700
C	-1.39984500	-5.67172100	-2.54614900
C	0.73793300	-4.74404000	-3.23317500
C	7.10405400	0.64439300	-0.62724400
C	6.42497200	-1.38689600	-1.78140400
C	5.65808000	0.75887300	-2.62588300
C	-7.09296600	-0.64673500	-0.67744000
C	-6.39545000	1.39715200	-1.79725200
C	-5.61627200	-0.73949300	-2.65456600
C	-0.63037700	6.64197600	-1.46619900
C	1.41002600	5.76348800	-2.45425200
C	-0.72734400	4.86141600	-3.17590500
H	0.07182400	-6.95828600	-0.73103600
H	1.65627700	-6.35082500	-1.26478200
H	0.64873600	-7.30255600	-2.39637200

H	-1.96389300	-6.11947600	-1.72908800
H	-1.90133900	-4.77492400	-2.90800400
H	-1.28774600	-6.39143900	-3.35809500
H	0.23915400	-3.83074100	-3.55792900
H	1.75454500	-4.51357600	-2.92178200
H	0.75089200	-5.48557100	-4.03522300
H	7.29938300	0.06971900	0.27814900
H	6.81394700	1.65814700	-0.35832900
H	7.98489200	0.65980200	-1.27340300
H	6.68833500	-1.96000600	-0.89362400
H	5.62713200	-1.88413400	-2.33199000
H	7.30103300	-1.26738800	-2.42028300
H	5.36896300	1.77315200	-2.35944800
H	4.83344300	0.26482800	-3.14002800
H	6.55047700	0.77922200	-3.25549900
H	-7.30356600	-0.08107100	0.23020900
H	-6.80756900	-1.66331600	-0.41423900
H	-7.96304900	-0.65561900	-1.33807300
H	-6.66942200	1.96093300	-0.90668500
H	-5.59014400	1.89931100	-2.33217900
H	-7.26341500	1.28540400	-2.44846000
H	-4.78258100	-0.24085900	-3.14932500
H	-5.33274800	-1.75714000	-2.39487100
H	-6.49843900	-0.75114900	-3.29868000
H	-0.06499500	6.99449600	-0.60360000
H	-1.64877600	6.40872200	-1.16280200
H	-0.63418400	7.39298600	-2.25961800
H	1.97161300	6.18585000	-1.62214600
H	1.91194300	4.87738100	-2.84090000
H	1.30149000	6.50734800	-3.24463200
H	-1.74448800	4.62118900	-2.87365400
H	-0.22815900	3.95882100	-3.52879800
H	-0.73887400	5.62786600	-3.95428500

[MnL(O₂)(H₂O)]²⁺-1H₂O

Charge=2 S=5/2

SCF energy: -3529.37616764 Ha

O	0.58700200	-1.76666300	2.79266900
O	1.71875600	0.73571100	2.79418300
O	-1.87033100	-0.63271500	2.53516700
O	-0.76749600	1.83658800	2.56021500
O	-0.18831500	0.33889800	4.91546200
O	0.00846900	-0.25844800	0.29252400
Mn	-0.07381800	0.03104200	2.63879600

C	0.91153400	-2.45985200	1.72932900
C	2.45161100	0.93851400	1.72472500
C	-2.50966700	-0.93701700	1.44410300
C	-0.96520200	2.47953200	1.44052200
H	0.69882100	0.38232200	5.30030900
H	-0.61814100	1.18990800	5.08479800
O	0.47809200	0.50501700	-0.67961900
C	-0.06694300	-3.25956100	1.06391100
C	2.24244900	-2.41151000	1.22935800
C	3.29381300	-0.09620900	1.23133100
C	2.40686800	2.19604900	1.05143700
C	-3.31976700	0.04476100	0.79368500
C	-2.45059500	-2.26536800	0.92634400
C	0.07091100	3.29466800	0.89616000
C	-2.23156500	2.40949300	0.78153100
C	0.31199900	-4.00278500	-0.04749200
C	-1.50987900	-3.28424400	1.56546000
C	2.58510800	-3.17336900	0.11440100
C	3.26529100	-1.48024900	1.87158700
C	4.10885200	0.15058700	0.12844500
C	3.23488800	2.40514800	-0.04545200
C	1.45842600	3.29157900	1.53398300
C	-4.16057400	-0.35654600	-0.23903300
C	-3.32647700	1.48290000	1.30892100
C	-3.31097100	-2.62969900	-0.10761700
C	-0.21776100	4.14026100	-0.17292600
C	-2.47823100	3.26282500	-0.28988700
H	-0.44493600	-4.60362000	-0.54549000
C	1.62832900	-3.96314200	-0.52095900
H	-1.91852000	-4.28851400	1.39706200
H	-1.49577800	-3.10297000	2.64426500
H	3.60695600	-3.11965300	-0.24156900
H	4.26140900	-1.93217700	1.78729900
H	3.02847100	-1.37527900	2.93290200
H	4.74887000	-0.65231100	-0.21681300
C	4.08392900	1.39264700	-0.50344300
H	3.19141200	3.36962900	-0.54528800
H	1.92855600	4.26497400	1.34581000
H	1.33656500	3.18168100	2.61525200
H	-4.82642600	0.38434300	-0.67585300
C	-4.17701500	-1.68823800	-0.67398300
H	-4.29966700	1.92975200	1.06944800
H	-3.23551300	1.44448300	2.39901000
H	-3.29887900	-3.66307800	-0.43541700

H	0.56917600	4.79810100	-0.52372200
C	-1.48995800	4.14012300	-0.75133800
H	-3.47002300	3.25027300	-0.73604200
N	1.95704300	-4.72695200	-1.78397400
N	4.90890500	1.65372600	-1.74485100
N	-5.22417100	-2.09134100	-1.69388500
N	-1.86759500	5.13985100	-1.82720600
C	3.41328500	-4.64190900	-2.15406800
C	1.62126300	-6.19152500	-1.61897100
C	1.16464300	-4.13279000	-2.93173200
C	5.76770000	2.88393200	-1.55843900
C	5.83203500	0.51375400	-2.08173000
C	3.97375700	1.84218400	-2.92226200
C	-5.13231400	-3.54329200	-2.08079500
C	-6.60845400	-1.86529400	-1.11869100
C	-5.06530700	-1.27665100	-2.95587900
C	-2.96671700	6.04961200	-1.31539300
C	-0.71471700	6.01676900	-2.23684100
C	-2.34750300	4.41834400	-3.06458700
H	4.01566300	-5.02898100	-1.33263300
H	3.66478000	-3.60324300	-2.36290000
H	3.56886700	-5.24785900	-3.04754500
H	2.21841600	-6.58920000	-0.79787200
H	0.56410100	-6.29556200	-1.38481900
H	1.85061800	-6.71437900	-2.54991500
H	0.10487700	-4.28773600	-2.73482100
H	1.37955300	-3.06028600	-2.97104700
H	1.45136900	-4.63996300	-3.85655000
H	6.42894800	2.71360400	-0.70838700
H	5.13045900	3.74252100	-1.35889200
H	6.34662200	3.05298800	-2.46884100
H	6.49699000	0.32932100	-1.23838800
H	5.23704300	-0.37051200	-2.30442600
H	6.41299400	0.79925500	-2.95959800
H	3.36658600	2.72773000	-2.74103300
H	3.32806000	0.96166800	-2.98750600
H	4.57021800	1.97438400	-3.82858900
H	-5.29518600	-4.16099400	-1.19875100
H	-4.14782400	-3.73762500	-2.50488200
H	-5.90597100	-3.74636100	-2.82238800
H	-6.69831300	-2.46169200	-0.21078900
H	-6.72438000	-0.81107800	-0.87525600
H	-7.35560200	-2.16849900	-1.85573600
H	-5.18198800	-0.22176900	-2.71668000

H	-4.06516800	-1.45526200	-3.35111600
H	-5.82674000	-1.58181500	-3.67703300
H	-2.59913300	6.55445100	-0.42206100
H	-3.83749800	5.44838800	-1.06158000
H	-3.22036800	6.77445200	-2.09221000
H	-0.37319400	6.58705700	-1.37420200
H	0.08922400	5.39045400	-2.62173600
H	-1.06477200	6.69586800	-3.01526300
H	-3.21677400	3.81520800	-2.81136500
H	-1.54175400	3.77240300	-3.41377300
H	-2.61289200	5.15425500	-3.82687100
O	1.57190100	-0.72384500	-2.82444800
H	0.99955900	-0.45192000	-3.55400500
H	1.13936100	-0.36313000	-1.98845800

[MnL(O₂)(H₂O)]²⁺-4H₂O

Charge=2 S=5/2

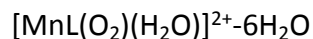
SCF energy: -3758.77427747 Ha

O	-0.07100100	-1.95366500	2.89968400
O	2.00929900	-0.22930500	2.73636800
O	0.30554000	1.87574100	2.80444400
O	0.29808100	0.10369700	5.11422200
O	0.20563700	-0.06158700	0.41255600
Mn	0.08445100	-0.04693900	2.86771700
C	-0.20694100	-2.64785000	1.79292200
C	2.72514700	-0.31483000	1.65305600
C	-2.57333700	0.23178100	1.88998000
C	0.33710600	2.57507700	1.70155600
H	1.05541100	-0.35565800	5.50334500
H	0.30774800	1.01653900	5.43588900
O	-0.53057200	-0.37060900	-0.64484800
C	-1.50452100	-2.91322800	1.27320300
C	0.94360400	-3.14663600	1.11076200
C	3.01180600	-1.59448100	1.08036200
C	3.25806400	0.86329400	1.04792500
C	-2.87322100	1.48397500	1.28021800
C	-3.14477000	-0.96249700	1.36804500
C	1.58059000	2.84570300	1.05519000
C	-0.87183700	3.10870200	1.15542900
C	-1.63698300	-3.69485900	0.12599000
C	-2.73912000	-2.31605000	1.94357500
C	0.76959700	-3.91902000	-0.03508400
C	2.34542800	-2.84666100	1.64466600
C	3.92646600	-1.67544500	0.03387000

C	4.16626900	0.74131700	-0.00416400
C	2.87541000	2.23753500	1.59473700
C	-3.79016700	1.52639400	0.23102200
C	-2.21590300	2.76371300	1.79313200
C	-4.06057200	-0.87965600	0.32143600
C	1.61053100	3.72575300	-0.02930300
C	-0.79896700	3.98005700	0.07201200
H	-2.63668100	-3.88971100	-0.24223600
C	-0.51035200	-4.18937300	-0.53129400
H	-3.57633400	-3.01491300	1.82840800
H	-2.53797200	-2.20035800	3.01159300
H	1.65452600	-4.30493600	-0.53449900
H	2.98942300	-3.70893600	1.43280500
H	2.27685800	-2.73830700	2.73081200
H	4.18083200	-2.66082100	-0.34801500
C	4.51417400	-0.51950600	-0.50339500
H	4.59540900	1.64998100	-0.41025800
H	3.69671700	2.93395700	1.38565300
H	2.77767300	2.15256600	2.68097900
H	-4.03340400	2.49416300	-0.19457900
C	-4.37859900	0.35375300	-0.25211900
H	-2.90447400	3.60066600	1.62492900
H	-2.06721000	2.66300200	2.87201800
H	-4.50411800	-1.80037300	-0.03779400
H	2.57432000	3.95283300	-0.46957900
C	0.43109000	4.30026600	-0.51634600
H	-1.72330800	4.41868500	-0.29389500
N	-0.63657300	-5.01013100	-1.79565700
N	5.57898700	-0.68527200	-1.56732600
N	-5.41656900	0.43939200	-1.35059200
N	0.45174500	5.33134900	-1.62547900
C	0.09699400	-4.31852400	-2.92862400
C	-0.05949100	-6.38941400	-1.57205400
C	-2.06847100	-5.17387500	-2.24358400
C	6.07377800	0.63230500	-2.10557300
C	6.77096600	-1.41451800	-0.97949600
C	5.03752700	-1.47355300	-2.74262400
C	-5.56452000	-0.87272400	-2.08813500
C	-6.75417700	0.80436000	-0.74481500
C	-5.03821500	1.48324100	-2.38271300
C	-0.48268600	4.92801300	-2.75027400
C	0.02473900	6.67302100	-1.06780700
C	1.81909100	5.49986600	-2.23756800
H	1.14628300	-4.21191200	-2.66220400

H	-0.36009400	-3.33804600	-3.06953600
H	-0.00176300	-4.93131900	-3.82737900
H	0.99014900	-6.30013500	-1.29763200
H	-0.61131100	-6.86493500	-0.76065300
H	-0.15798300	-6.96772700	-2.49301700
H	-2.63055200	-5.68874100	-1.46485400
H	-2.48158000	-4.18667800	-2.45324700
H	-2.06144500	-5.77963200	-3.15077000
H	6.52866300	1.20424500	-1.29796400
H	5.23611500	1.17778600	-2.53952200
H	6.81979100	0.42366800	-2.87312400
H	7.14891800	-0.82819600	-0.14179700
H	6.44950900	-2.39256900	-0.62610800
H	7.53676100	-1.52403200	-1.75046400
H	4.16252500	-0.95591500	-3.13731400
H	4.75224100	-2.46770100	-2.40533700
H	5.81916200	-1.55204400	-3.50089800
H	-6.01712500	-1.60892700	-1.42591600
H	-4.57866700	-1.20728400	-2.41734300
H	-6.22770700	-0.70514800	-2.93760300
H	-7.02278500	0.03859900	-0.01684300
H	-6.65734700	1.76731100	-0.24383300
H	-7.50375700	0.85966800	-1.53774500
H	-5.11157600	2.47221700	-1.93449500
H	-4.01572400	1.29657000	-2.71813700
H	-5.75003800	1.41500600	-3.20687200
H	-1.49494300	4.84011400	-2.36172600
H	-0.14273400	3.96944500	-3.14396400
H	-0.44835500	5.70282500	-3.51878300
H	-0.98252000	6.58501800	-0.66413600
H	0.71635300	6.94884400	-0.27135700
H	0.04640900	7.41385300	-1.86992000
H	2.13705200	4.54433600	-2.65464000
H	2.51498200	5.84968300	-1.47610400
H	1.74013700	6.24551700	-3.02951500
O	1.59063900	-0.62791300	-2.25488000
H	0.72608800	-0.63529200	-1.74831000
H	2.26181100	-0.68068400	-1.55861800
O	0.93514300	1.96678600	-2.77279100
H	1.30864900	1.05345500	-2.82537500
H	0.92366400	2.15445900	-1.82035900
O	-1.80713300	1.03196900	-2.70787400
H	-0.96286700	1.39982500	-3.03585500
H	-1.60885800	0.79957800	-1.77946200

O	-2.20649200	-1.82019300	-2.50817800
H	-1.85530400	-1.64252200	-1.61607400
H	-2.06759700	-0.97423000	-2.97554200
O	-1.79984300	0.17842900	2.94886300



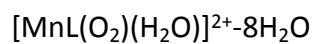
Charge=2 S=5/2

SCF energy: -3911.69937183 Ha

O	1.94305800	-0.45169200	2.84094300
O	0.31047500	1.69022900	2.98253700
O	-1.84446000	0.05335000	2.98007400
O	0.18440500	-0.46490100	5.18040300
O	0.19749500	0.03722800	0.49017700
Mn	0.03904900	-0.19716000	2.93558800
C	2.67388400	-0.49063300	1.75947000
C	0.39042600	2.46362800	1.92934200
C	-0.33136900	-2.75220900	1.72557600
C	-2.60332500	0.19994100	1.92477900
H	-0.06914400	-1.36354700	5.43679000
H	1.06721900	-0.29647300	5.53933200
O	-0.32660700	-0.10030200	-0.71821100
C	2.92613000	-1.73638000	1.11356100
C	3.26731200	0.70533300	1.25173500
C	1.66209300	2.74801100	1.34769700
C	-0.78589200	3.06290000	1.39203700
C	-1.62937600	-2.97366200	1.17352200
C	0.81729900	-3.27305300	1.05907900
C	-2.86553400	1.50009200	1.40145900
C	-3.21544800	-0.94171800	1.32817600
C	3.89046900	-1.79436700	0.10226500
C	2.22147200	-3.00165000	1.60467800
C	4.22033000	0.60649900	0.24323600
C	2.91997100	2.05686300	1.87392400
C	1.74534400	3.71763500	0.35451700
C	-0.65981500	4.02621700	0.38699500
C	-2.15469800	2.72167100	1.98436900
C	-1.76090400	-3.81186000	0.06873500
C	-2.86095200	-2.34312800	1.82250900
C	0.64154400	-4.09969300	-0.05192000
C	-3.83095200	1.64496000	0.40324100
C	-4.17449900	-0.75381000	0.33618500
H	4.12516700	-2.76547700	-0.31944300
C	4.55200300	-0.63345500	-0.31939900
H	2.85456300	-3.86396500	1.36213200

H	2.14814400	-2.93953400	2.69475200
H	4.71332100	1.51735500	-0.08378200
H	3.77099500	2.73214700	1.72290900
H	2.79713300	1.91166300	2.95150300
H	2.72867500	3.96685400	-0.03247000
C	0.59911300	4.36636500	-0.11880400
H	-1.56121000	4.52136900	0.04277600
H	-2.81034000	3.59235900	1.86028100
H	-2.02256900	2.55390000	3.05776500
H	-2.76220900	-4.02049200	-0.29628500
C	-0.63738100	-4.38151900	-0.53940500
H	-3.72084300	-3.00090500	1.64674900
H	-2.69248700	-2.29242400	2.90198700
H	1.52722200	-4.51872200	-0.51439000
H	-4.06116400	2.64805700	0.06292600
C	-4.49122000	0.52924000	-0.12118000
H	-4.67199700	-1.63059700	-0.06531600
N	5.71252000	-0.69261400	-1.29353300
N	0.77888100	5.53554400	-1.06538700
N	-0.84511800	-5.36551100	-1.67152900
N	-5.61783500	0.68980200	-1.11917700
C	5.53262300	0.30719900	-2.41975800
C	6.99499900	-0.38585800	-0.54851700
C	5.86547800	-2.04702500	-1.93801000
C	-0.52533600	6.03309400	-1.63334400
C	1.42227000	6.67908400	-0.30901700
C	1.65132600	5.16031300	-2.24697500
C	0.43881300	-5.69427800	-2.39040300
C	-1.41867500	-6.64870300	-1.11117600
C	-1.78821100	-4.80352300	-2.71697300
C	-5.54152400	-0.37245800	-2.19868100
C	-6.94140400	0.56529900	-0.39548500
C	-5.58100300	2.03169900	-1.81354200
H	5.47540400	1.31061800	-2.00414500
H	4.61008700	0.05677800	-2.94525300
H	6.39702000	0.23363100	-3.08272100
H	6.92356200	0.61260500	-0.12005100
H	7.11181000	-1.11954400	0.24949700
H	7.83324700	-0.43926400	-1.24665400
H	6.07676400	-2.79161500	-1.17188700
H	4.95092900	-2.28526200	-2.48057800
H	6.70452800	-1.99269600	-2.63255100
H	-1.15619800	6.40186900	-0.82595200
H	-1.00764600	5.21949800	-2.17409400

H	-0.29993600	6.84993300	-2.31997300
H	0.77879600	6.94003700	0.53161700
H	2.39304100	6.35296900	0.06118700
H	1.53993700	7.53088300	-0.98261700
H	1.14683200	4.37498300	-2.81073500
H	2.61839300	4.81765300	-1.88742400
H	1.78405900	6.05244700	-2.86258400
H	1.11955800	-6.19819100	-1.70595800
H	0.86552800	-4.76459600	-2.76635800
H	0.19687900	-6.36379300	-3.21672500
H	-0.72072100	-7.04337900	-0.37230800
H	-2.37190400	-6.42822700	-0.63226800
H	-1.56009300	-7.36214600	-1.92607000
H	-2.75743200	-4.61087600	-2.26298800
H	-1.34560400	-3.88195800	-3.09631200
H	-1.89931900	-5.54745400	-3.50838100
H	-5.79386900	-1.33919600	-1.76706200
H	-4.52538300	-0.39713400	-2.59481500
H	-6.27214800	-0.12619300	-2.97076800
H	-6.98330000	-0.41001900	0.08844600
H	-6.99626300	1.35070200	0.35861600
H	-7.75503300	0.66840900	-1.11734600
H	-4.59842200	2.16720000	-2.26984800
H	-5.78291400	2.81713700	-1.08681600
H	-6.36760700	2.03714700	-2.56899600
O	1.32502900	1.30016700	-2.46589200
H	0.69134500	0.91772200	-1.80443900
H	0.83138600	1.88143600	-3.07585900
O	-0.28086600	3.13314800	-3.94417500
H	-1.12204300	2.77507800	-3.56003600
H	-0.36500500	3.15457600	-4.90644500
O	-2.26074500	-0.66080100	-2.52765900
H	-1.86183800	-0.63897800	-1.62563200
H	-1.58387300	-1.12391500	-3.05943900
O	0.08785100	-2.22440600	-2.86195100
H	0.95153600	-1.86168000	-3.16609900
H	0.05649600	-1.97295800	-1.92170500
O	-0.20229200	-2.10578400	2.85863100
O	-2.28960100	2.04207900	-2.54074600
H	-2.28469500	1.06042100	-2.69209900
H	-1.99427900	2.14550600	-1.62231100
O	2.54855600	-0.98673700	-2.91723500
H	2.14856100	-0.07107600	-2.91966400
H	2.71333100	-1.16720700	-1.97808000



Charge=2 S=5/2

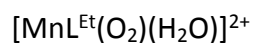
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O	-1.93228600	0.05562100	-3.12312500
O	-0.03794500	0.04619900	-5.46837200
O	0.18500600	-0.13612600	-0.69591600
Mn	-0.03895400	-0.04298300	-3.23599600
C	2.68093600	-0.16128200	-2.16321500
C	-0.13122600	-2.61008800	-2.03050600
C	0.08685900	2.54347700	-2.06950200
C	-2.72468700	0.09762800	-2.09159500
H	0.11737500	0.92016700	-5.85394900
H	0.45739500	-0.60521500	-5.98395500
O	-0.04940100	0.00696400	0.60047400
C	3.19469900	1.05633000	-1.62444000
C	3.10187100	-1.41032400	-1.61802600
C	1.09199800	-3.03562500	-1.42489200
C	-1.37269600	-2.91551800	-1.40258500
C	-1.12373700	2.97482200	-1.44263400
C	1.34226700	2.86809800	-1.47647200
C	-3.23291000	-1.11399700	-1.53278900
C	-3.14606300	1.35469800	-1.56553100
C	4.23270400	0.99642800	-0.69796000
C	2.64837100	2.39505100	-2.11934900
C	4.16250400	-1.42975700	-0.70523800
C	2.43470100	-2.70355000	-2.08273000
C	1.04222400	-3.78315200	-0.25112800
C	-1.37804900	-3.67686100	-0.23016300
C	-2.69238700	-2.45504100	-2.02477400
C	-1.04794400	3.75114900	-0.28769500
C	-2.48324900	2.63700200	-2.06413000
C	1.37193500	3.66703900	-0.32954700
C	-4.27261800	-1.04119600	-0.60971700
C	-4.21459300	1.38670900	-0.66102600
H	4.64056500	1.93107900	-0.32505400
C	4.74462200	-0.23275200	-0.26580100
H	3.41215800	3.16369900	-1.95276400
H	2.48278300	2.31659500	-3.19774000
H	4.53153700	-2.39532300	-0.37691600
H	3.12417600	-3.53686300	-1.90145200
H	2.27079800	-2.63563600	-3.16212600

H	1.97985800	-4.12140100	0.18172600
C	-0.18154900	-4.10145800	0.35183100
H	-2.33723600	-3.92513100	0.20724500
H	-3.45001200	-3.22456300	-1.83570700
H	-2.54863200	-2.38554200	-3.10722000
H	-1.97662100	4.09401300	0.16012000
C	0.18686000	4.09997300	0.27188400
H	-3.16443600	3.47690200	-1.88209400
H	-2.34387000	2.54885200	-3.14587200
H	2.34067000	3.94460100	0.06879100
H	-4.68356900	-1.97111600	-0.22797200
C	-4.79177400	0.19436000	-0.20216600
H	-4.59357800	2.35662200	-0.35704500
N	5.92954500	-0.22096700	0.67701400
N	-0.17289000	-4.95256900	1.60416500
N	0.20144400	4.99270900	1.49474400
N	-5.98969500	0.19192800	0.72426100
C	5.54635000	0.42604500	1.99538100
C	6.44584500	-1.60347500	0.98386300
C	7.07461300	0.55121400	0.05113900
C	-1.55361500	-5.15948400	2.18248100
C	0.39923000	-6.31742500	1.28341600
C	0.66426100	-4.29651100	2.68650500
C	1.59436100	5.24042200	2.02560000
C	-0.39951300	6.33805600	1.14503800
C	-0.59507500	4.36211300	2.62272800
C	-6.49421800	1.57852000	1.03326400
C	-7.13450500	-0.56370100	0.07655100
C	-5.63249300	-0.46748800	2.04318600
H	4.77780600	-0.18647700	2.46703700
H	5.14631500	1.42054500	1.80838300
H	6.43437200	0.48025500	2.62843800
H	5.66753800	-2.17683600	1.48581800
H	6.74675000	-2.09006300	0.05629900
H	7.30570700	-1.50106300	1.64664000
H	7.32175200	0.08424700	-0.90246100
H	6.76926100	1.58272300	-0.11044800
H	7.92951800	0.51934700	0.72911300
H	-2.16610300	-5.70049400	1.46176900
H	-1.99387100	-4.19130800	2.42382500
H	-1.44480100	-5.75525000	3.08937300
H	-0.21490100	-6.77275900	0.50611800
H	1.42075900	-6.20244100	0.92485500
H	0.38664800	-6.92696400	2.18911400

H	0.22676300	-3.32944500	2.92928300
H	1.68051700	-4.15961600	2.32492300
H	0.66358700	-4.94293500	3.56580400
H	2.18019100	5.75952600	1.26749900
H	2.05548200	4.28979100	2.29520000
H	1.50214000	5.87018300	2.91106600
H	0.18543800	6.77540400	0.33554200
H	-1.42914100	6.19729800	0.82081500
H	-0.36984200	6.97777200	2.02923700
H	-1.61934100	4.19961000	2.29597000
H	-0.13815900	3.40965300	2.88573900
H	-0.57764100	5.03776200	3.47951300
H	-6.78311500	2.07203700	0.10566500
H	-5.71431800	2.14230800	1.54390900
H	-7.36097500	1.48220900	1.68791600
H	-7.36600700	-0.08362700	-0.87446200
H	-6.83475300	-1.59544200	-0.09435500
H	-7.99732000	-0.53215500	0.74455100
H	-4.84896600	0.12057600	2.52127500
H	-5.26441000	-1.47402700	1.85591400
H	-6.52497300	-0.49883800	2.67137600
O	2.10808300	-0.90529400	1.75373500
H	2.65099200	-1.21760700	1.01444700
H	1.22024200	-0.65235500	1.34352700
O	-2.20316200	-1.75510600	2.15707600
H	-1.59625700	-1.88213400	1.41061100
H	-2.36837300	-0.78660100	2.15117000
O	-2.17118400	1.00888000	1.75543800
H	-2.82700800	1.27048300	1.09277100
H	-1.34826600	0.76995900	1.23041100
O	2.38468200	1.83260500	2.03888900
H	1.79902900	2.02041500	1.28895200
H	2.44841400	0.84986600	2.04034400
O	0.04681200	1.88092400	-3.20311500
O	-1.35910100	1.41316400	4.45697500
H	-1.42187000	0.48104100	4.77749200
H	-1.71273600	1.39691700	3.54991300
O	1.54980500	-1.21306300	4.53023900
H	1.82398400	-1.23778000	3.59616800
H	1.62482200	-0.26576900	4.79676700
O	1.40810200	1.56331000	4.72801700
H	0.42580400	1.62929400	4.69972600
H	1.73955600	1.84056900	3.85583400
O	-1.21145400	-1.33791700	4.83412400

H	-0.22892700	-1.41337400	4.81707300
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Charge=2 S=5/2

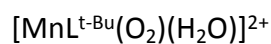
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O	-0.80992900	-1.75561500	2.96945200
O	-1.72507800	0.80498100	2.95557000
O	0.10684500	-0.26666400	5.20775800
O	0.22858900	0.04680700	0.62295200
Mn	0.00682600	-0.00191200	2.88834700
C	2.41369200	-1.13874500	1.85004900
C	1.14532500	2.39337800	1.84990100
C	-1.13387800	-2.40470500	1.88089400
C	-2.39357000	1.12476400	1.88029900
H	1.01941500	-0.51265600	5.41781900
H	-0.44952200	-1.03171100	5.41478400
O	-0.63047700	-0.23918300	-0.34107300
C	2.25256400	-2.42449900	1.25691100
C	3.30706200	-0.19944500	1.25095300
C	2.43138700	2.24853200	1.25225000
C	0.20177800	3.29548300	1.27298400
C	-2.42608700	-2.24697700	1.30288200
C	-0.19763700	-3.29100800	1.27068600
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C	-3.30506300	0.19104200	1.30432200
C	3.07628300	-2.79536400	0.19530000
C	1.22447300	-3.40497300	1.82000700
C	4.11169000	-0.60993100	0.19371400
C	3.41643600	1.22017000	1.80630300
C	2.79620100	3.09087200	0.20468300
C	0.60491900	4.11677400	0.22481700
C	-1.21033600	3.39265100	1.84883200
C	-2.80195600	-3.06354800	0.23905700
C	-3.40661600	-1.22340900	1.87260700
C	-0.60924000	-4.08076500	0.20146700
C	-3.07458800	2.78086800	0.23649900
C	-4.12432900	0.60137800	0.25955500
H	2.95175200	-3.79445300	-0.20256000
C	4.03053400	-1.91234700	-0.32379700
H	1.58373100	-4.42527800	1.63369500
H	1.17887100	-3.26034100	2.90343200

H	4.80718700	0.11376100	-0.21671000
H	4.43513700	1.58390200	1.62018500
H	3.27276700	1.17014200	2.88993000
H	3.79462000	2.97771200	-0.19812500
C	1.90529200	4.04840300	-0.29819700
H	-0.12103500	4.81976900	-0.16869900
H	-1.58065700	4.41241400	1.68289200
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H	-3.80365000	-2.93758900	-0.15110400
C	-1.91508400	-4.00064000	-0.30273900
H	-4.42661000	-1.59089900	1.70232200
H	-3.24885600	-1.16458100	2.95366100
H	0.11611200	-4.76375200	-0.22612800
H	-2.95278800	3.77878900	-0.16485400
C	-4.03809100	1.89944200	-0.26630000
H	-4.82728500	-0.12016000	-0.14106000
N	5.00007900	-2.33835500	-1.40720200
N	2.32406700	5.03754800	-1.36683900
N	-2.32963300	-4.92911500	-1.42510700
N	-4.99284300	2.31066700	-1.36770900
C	6.43271500	-2.51305900	-0.85511300
C	4.61637500	-3.68068900	-2.05753400
C	5.02216800	-1.30223100	-2.53805500
C	2.50285300	6.45984900	-0.78964200
C	3.66162000	4.66483200	-2.03358500
C	1.28047000	5.08117400	-2.49001500
C	-2.45453000	-6.39306100	-0.94738300
C	-3.69263600	-4.55638500	-2.03623600
C	-1.30865500	-4.85605100	-2.56798700
C	-6.43828800	2.47321000	-0.84730400
C	-4.61275700	3.65347600	-2.01742800
C	-4.97503100	1.26674800	-2.49229300
H	6.33403100	-3.23587100	-0.04628600
H	6.99757500	-2.97553300	-1.67047200
H	3.54250300	-3.62739700	-2.22695000
H	5.10968200	-3.67611300	-3.03262500
H	5.34934500	-0.36545000	-2.09419600
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H	3.60792700	3.59344300	-2.21806000
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H	-3.16543500	-6.35916200	-0.12279300
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H	-3.66909400	-3.47671000	-2.17120300
H	-3.69553200	-5.01769900	-3.02699800
H	-0.35721100	-5.17872500	-2.15281800
H	-1.62350200	-5.60463000	-3.30146900
H	-6.36492400	3.20320700	-0.04225400
H	-6.99000500	2.92367100	-1.67830600
H	-3.53754400	3.60706500	-2.17929900
H	-5.09909300	3.64392200	-2.99603800
H	-5.31015800	0.33142900	-2.05115100
H	-5.73463700	1.58671300	-3.21196000
C	-3.61485200	1.07521600	-3.15251200
H	-3.29600600	1.94975700	-3.72625400
H	-2.84334200	0.82289300	-2.41895600
H	-3.70246300	0.24275700	-3.85897800
C	-5.00955100	4.93148400	-1.27603400
H	-4.50861300	5.76526400	-1.78011800
H	-6.08278000	5.12786900	-1.32634200
H	-4.70297400	4.94242300	-0.22850900
C	-7.17457900	1.23752400	-0.34846200
H	-7.28294000	0.45728000	-1.10720700
H	-6.72083900	0.81650100	0.54932300
H	-8.18534800	1.56659500	-0.08352100
C	-1.16295200	-3.47547000	-3.19653600
H	-2.05376100	-3.16808200	-3.75099100
H	-0.92344300	-2.71402000	-2.44817100
H	-0.33784600	-3.52272500	-3.91527000
C	-4.94638500	-4.99450300	-1.27721800
H	-5.80003700	-4.49625900	-1.74967200
H	-5.12524900	-6.06953200	-1.34987600
H	-4.93848700	-4.71348900	-0.22248900
C	-1.19401200	-7.12304400	-0.50422100
H	-0.43055300	-7.18741400	-1.28462300
H	-0.76041200	-6.69447800	0.39995100
H	-1.49754900	-8.14919100	-0.26974400
C	3.68572500	-1.10885100	-3.24383200
H	3.38119800	-1.98464300	-3.82311800
H	2.89280200	-0.85228700	-2.53585200
H	3.79755200	-0.27908100	-3.94975100
C	7.16880600	-1.27980900	-0.35045300
H	7.30868100	-0.51069900	-1.11537400
H	6.69401400	-0.84187600	0.52821800
H	8.16749900	-1.61685200	-0.05188500

C	5.00032900	-4.96118900	-1.31357900
H	4.50074300	-5.79169400	-1.82437000
H	6.07311200	-5.16216000	-1.35385900
H	4.68362200	-4.97309600	-0.26922400
C	1.07806000	3.75754400	-3.21708800
H	1.95022400	3.45816100	-3.80450000
H	0.81981000	2.95440500	-2.52138100
H	0.24645100	3.88521300	-3.91817500
C	1.27358500	7.18427800	-0.25913500
H	0.49781300	7.34022200	-1.01417100
H	0.84370500	6.69067600	0.61310900
H	1.61284400	8.17652800	0.05784300
C	4.94793300	5.03957900	-1.29498200
H	5.77456500	4.54826600	-1.81990600
H	5.14728500	6.11307500	-1.32173400
H	4.96898200	4.70829100	-0.25535400



Charge=2 S=5/2

SCF energy: -4867.68352587 Ha

O	-0.10640700	1.94126700	3.48053200
O	-1.90950700	-0.09333100	3.45267100
O	1.91777100	0.11737400	3.50245500
O	0.10758900	-1.91467600	3.49053300
O	0.18331200	0.27619100	5.74309200
O	-0.18679700	0.12344300	1.15177900
Mn	-0.00146400	-0.00520600	3.41820600
C	-0.15385700	2.63261200	2.37187800
C	-2.67327500	-0.13939500	2.39883000
C	2.67733400	0.15094900	2.43851900
C	0.15496700	-2.61137100	2.38454800
H	-0.01114500	1.21844600	5.85642700
H	1.12648200	0.15766100	5.92770400
O	0.56728800	-0.30356700	0.15264600
C	1.03821600	3.09144900	1.74847100
C	-1.39797100	2.95452600	1.76267400
C	-3.19595700	1.05323700	1.83071700
C	-3.04186200	-1.38232900	1.81652500
C	3.19387500	-1.04737300	1.87811500
C	3.03525600	1.38585200	1.83494900
C	-1.03451500	-3.07191200	1.75869000
C	1.40208400	-2.94646500	1.79262400
C	0.95616400	3.96426900	0.66430500
C	2.40362600	2.69458400	2.31933100

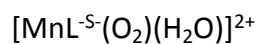
C	-1.42089000	3.82219600	0.67574100
C	-2.70791100	2.41039800	2.34017500
C	-4.22301500	0.96986800	0.89348500
C	-4.06272200	-1.40842600	0.86852200
C	-2.40365000	-2.67861300	2.32189200
C	4.20990500	-0.97358200	0.92834300
C	2.70496800	-2.40399100	2.38732500
C	4.04111100	1.40134800	0.86967900
C	-0.94568400	-3.95121400	0.68079100
C	1.43226000	-3.82323500	0.71313400
H	1.90335000	4.29719200	0.28465800
C	-0.26545800	4.41120500	0.12295200
H	3.10929100	3.51009700	2.11309500
H	2.29417200	2.62212300	3.40648600
H	-2.39500400	4.02729600	0.27852400
H	-3.49727600	3.15084400	2.15495900
H	-2.57957600	2.32884900	3.42450000
H	-4.61392000	1.91614600	0.57007200
C	-4.75338100	-0.25563900	0.43794400
H	-4.31868200	-2.38174800	0.49775600
H	-3.10233700	-3.50285900	2.12716700
H	-2.29543000	-2.58704100	3.40808500
H	4.59871900	-1.92271900	0.61174400
C	4.72719300	0.24539300	0.44527800
H	3.49725200	-3.14303400	2.20954700
H	2.56283900	-2.32581300	3.47012900
H	4.28585400	2.36975500	0.47970200
H	-1.89060900	-4.28555400	0.29749000
C	0.27831700	-4.40647300	0.15269400
H	2.40908800	-4.03559600	0.32675700
N	-0.36621300	5.36960300	-1.07941600
N	-5.93993800	-0.35493900	-0.54172800
N	5.88845500	0.33042000	-0.56557600
N	0.37941100	-5.36698600	-1.04833700
C	-1.43718400	6.65846700	-0.70730500
C	1.17945800	6.03129200	-1.41009100
C	-0.91960000	4.41912100	-2.38892500
C	-7.11269700	-1.45740300	0.07968200
C	-6.68501400	1.19102500	-0.69216800
C	-5.29218300	-0.86548900	-2.02279200
C	7.06670900	1.44994400	-0.00177100
C	6.63951900	-1.21368100	-0.70209800
C	5.19543100	0.80416300	-2.04116000
C	1.44255700	-6.65900100	-0.67292300

C	-1.16892600	-6.02313100	-1.38432400
C	0.93923300	-4.41766900	-2.35415300
C	0.28913300	-3.01670800	-2.29855200
H	-0.78963100	-3.01787700	-2.41604300
H	0.53562600	-2.45566700	-1.39566700
H	0.69506200	-2.45987000	-3.15067100
C	-1.88756300	-6.54502300	-0.08969400
H	-2.87736100	-6.08789400	-0.00936500
H	-2.04640400	-7.62358500	-0.15595300
H	-1.37483400	-6.34057100	0.84223400
C	2.75816400	-6.27110200	0.05319800
H	3.38051800	-5.54637700	-0.46325700
H	2.59333000	-5.95187400	1.08073200
H	3.33956700	-7.19797100	0.09618800
C	3.82510000	0.11198100	-2.21734800
H	3.87321000	-0.97033500	-2.28072300
H	3.11241000	0.37683400	-1.43527300
H	3.42181400	0.46618400	-3.17253100
C	6.91242500	-1.86614800	0.69883200
H	6.47631800	-2.86813800	0.72548500
H	7.98653800	-1.98606600	0.85552100
H	6.50820200	-1.32999000	1.54844100
C	6.52707900	2.78884600	0.56977700
H	5.89223100	3.36434400	-0.09735500
H	6.03825600	2.66988000	1.53503400
H	7.42133900	3.39764500	0.73886800
C	-0.26269300	3.02138500	-2.33529400
H	0.81402900	3.02510300	-2.46888300
H	-0.49284000	2.47043400	-1.42315800
H	-0.68008400	2.45552600	-3.17551000
C	-2.75236200	6.26443000	0.01607900
H	-3.37156400	5.53811600	-0.50203200
H	-2.58805700	5.94402400	1.04335000
H	-3.33737400	7.18899000	0.05963700
C	1.89177800	6.55772600	-0.11364900
H	2.88235600	6.10330600	-0.02834900
H	2.04823400	7.63651500	-0.18190600
H	1.37566800	6.35431100	0.81655700
C	-3.92024500	-0.19072700	-2.24421100
H	-3.95006500	0.89329900	-2.27720500
H	-3.18556700	-0.48937900	-1.49598700
H	-3.56078900	-0.52903000	-3.22239600
C	-6.56297500	-2.78560400	0.66387200
H	-5.95195800	-3.37917000	-0.00971500

H	-6.04481800	-2.64893000	1.61129300
H	-7.45485400	-3.38548400	0.87293100
C	-6.92255600	1.87418700	0.70028000
H	-6.47706700	2.87250300	0.69747700
H	-7.99209100	2.00746700	0.87633600
H	-6.50605300	1.35102100	1.55191200
C	-7.82450500	-0.82408900	1.28754400
H	-8.48789600	0.00254100	1.05254700
H	-8.45003400	-1.60659400	1.72761400
H	-7.11369200	-0.52068300	2.05788800
C	-8.14351300	-1.88847400	-0.98846800
H	-7.75451400	-2.65908700	-1.65496700
H	-8.97852400	-2.34319900	-0.44519100
H	-8.56463500	-1.09572300	-1.59171600
C	-8.07137400	1.16137200	-1.37655600
H	-8.84538200	0.68181300	-0.78190000
H	-8.36958300	2.21152000	-1.46457600
H	-8.08225300	0.75124400	-2.38283700
C	-5.84364400	2.16960900	-1.55290000
H	-5.80980800	1.91301500	-2.60836400
H	-6.35586500	3.13445000	-1.48712100
H	-4.82750400	2.32073700	-1.20210900
C	-5.00257800	-2.38255000	-2.06037500
H	-5.89243000	-3.00735100	-2.02794900
H	-4.52927300	-2.57183800	-3.02900400
H	-4.29268300	-2.70441800	-1.30386900
C	-6.20089400	-0.60686600	-3.24502200
H	-6.37359200	0.43965800	-3.47830200
H	-5.67784600	-1.02656700	-4.11025100
H	-7.15944500	-1.11864100	-3.18645500
C	-2.44062400	4.15266400	-2.33439400
H	-2.65998500	3.51280000	-3.19477300
H	-2.74612300	3.59582900	-1.45293900
H	-3.05624300	5.04195000	-2.44896300
C	-0.67218100	5.04804200	-3.77726300
H	0.37310400	5.13640600	-4.05864700
H	-1.12279800	4.36710900	-4.50630400
H	-1.15916400	6.01177000	-3.91201900
C	-1.88743600	7.44077300	-1.96215400
H	-2.65632700	6.91709800	-2.53084400
H	-2.35033100	8.36396600	-1.59864700
H	-1.10208900	7.74017900	-2.64407900
C	-0.77388800	7.61612300	0.30015800
H	0.06178900	8.18954800	-0.08820400

H	-1.53904300	8.34200900	0.59064600
H	-0.47275000	7.09553600	1.21075400
C	2.12677600	4.99944800	-2.07477500
H	1.87038300	4.76709500	-3.10539500
H	3.11064100	5.47787100	-2.10488800
H	2.23366700	4.06854700	-1.52713400
C	1.16146700	7.23276800	-2.38368000
H	0.71343400	8.13151500	-1.96610400
H	2.21500100	7.47576700	-2.55887600
H	0.72396600	7.02992000	-3.35711900
C	0.69428400	-5.04526400	-3.74371600
H	-0.35009600	-5.12746100	-4.03047200
H	1.15277100	-4.36715900	-4.47043100
H	1.17598900	-6.01201400	-3.87602600
C	2.46062300	-4.15843200	-2.29426500
H	3.07302400	-5.04909200	-2.41707100
H	2.68369200	-3.50973800	-3.14703900
H	2.76501600	-3.61204300	-1.40632400
C	-1.15082000	-7.22601000	-2.35622700
H	-2.20430800	-7.46790200	-2.53312300
H	-0.71128000	-7.02435400	-3.32907300
H	-0.70477100	-8.12485800	-1.93685300
C	-2.11177300	-4.99068500	-2.05563500
H	-3.09447000	-5.47100100	-2.09423900
H	-2.22535300	-4.06047900	-1.50806600
H	-1.84723300	-4.75621500	-3.08361200
C	1.89351300	-7.44389900	-1.92613500
H	2.67101400	-6.92617900	-2.48868400
H	2.34541700	-8.37201900	-1.56128300
H	1.11025500	-7.73446300	-2.61411100
C	0.77287500	-7.61294000	0.33396900
H	-0.06346500	-8.18431800	-0.05601400
H	1.53464500	-8.34085600	0.62825600
H	0.47049700	-7.08982500	1.24270300
C	6.07623500	0.53022600	-3.28009200
H	6.25731700	-0.51905400	-3.49351600
H	5.52415400	0.92190500	-4.14048100
H	7.02854600	1.05638900	-3.25942900
C	4.89192800	2.31755700	-2.09755100
H	4.39724500	2.48689600	-3.05903300
H	4.19457700	2.64378400	-1.33141900
H	5.77657300	2.95045300	-2.09342900
C	8.00886800	-1.19055300	-1.41958200
H	8.31159000	-2.24066900	-1.49136800

H	7.99225900	-0.80330700	-2.43499800
H	8.79417900	-0.69271000	-0.85565700
C	5.78480400	-2.21387800	-1.52350400
H	6.29849500	-3.17672500	-1.44182500
H	4.77423600	-2.35497300	-1.15393900
H	5.73520000	-1.98373500	-2.58447300
C	8.06723000	1.86511900	-1.10468900
H	7.65756800	2.62257700	-1.77390000
H	8.91451600	2.33305100	-0.59248200
H	8.47575100	1.06371900	-1.70512700
C	7.81478400	0.84834500	1.20131700
H	8.47846700	0.02144100	0.96809500
H	8.44496400	1.64473900	1.60849500
H	7.12582400	0.55599800	1.99544000



Charge=2 S=5/2

SCF energy: -4888.48110846 Ha

Mn	-0.01988900	-0.00958700	-2.14149400
O	-0.24467300	-0.17156400	-0.06886600
O	0.60973800	0.38615100	0.73149300
O	-0.43385100	-2.06407500	-2.27156800
O	-1.91049600	0.36997500	-2.19968600
O	1.83806800	-0.41185700	-2.12190200
O	0.38471800	1.97784800	-2.19051700
O	-0.13000200	-0.25060800	-4.30854100
C	-0.57999100	-2.80797300	-1.25416900
C	-2.72436000	0.53570000	-1.21525700
C	2.68757200	-0.56230200	-1.16994500
C	0.54752300	2.77153700	-1.21594200
H	-0.89176100	0.20736700	-4.69313300
H	-0.26496400	-1.20440400	-4.43169000
C	0.52994500	-3.49091600	-0.63155400
C	-1.88002100	-3.01746900	-0.65222200
C	-3.46437700	-0.56610800	-0.66679600
C	-2.97330900	1.84059700	-0.65908800
C	3.43902100	0.54284500	-0.64651700
C	2.96832900	-1.86970400	-0.63839200
C	-0.55558000	3.49415100	-0.63300000
C	1.85374400	3.01071900	-0.64349900
C	0.32047000	-4.43167300	0.37508700
C	-2.05780200	-3.96211600	0.34843700
C	-4.47974600	-0.34826100	0.26693200
C	-3.99268400	2.02292200	0.27128100

C	4.48533600	0.32307700	0.25150900
C	4.01944000	-2.05484500	0.25486200
C	-0.34075700	4.48379800	0.32483600
C	2.03806700	4.00306900	0.30751900
H	1.18877300	-4.95710600	0.75222300
C	-0.96874900	-4.69029800	0.84958500
H	-3.06731500	-4.12814400	0.71247600
H	-5.04112800	-1.21185600	0.59870900
C	-4.75951400	0.94172900	0.71818600
H	-4.18319600	3.03528400	0.61268000
H	5.05096400	1.18773800	0.57274300
C	4.79026000	-0.96865800	0.68304400
H	4.23112400	-3.06851900	0.57970700
H	-1.20485000	5.03287900	0.67733900
C	0.95241500	4.75869900	0.77812400
H	3.04947200	4.18400800	0.65868300
N	-1.24445500	-5.79036200	1.85018300
N	-5.91857500	1.22335300	1.64987000
N	5.98283200	-1.24452800	1.57354800
N	1.23699000	5.89837400	1.73043900
C	-2.13442500	-6.84291200	1.21826800
C	0.01126500	-6.48147100	2.31212900
C	-1.92702000	-5.22565300	3.07502500
C	-6.91965400	2.12679800	0.95556100
C	-6.65008900	-0.02779900	2.06099600
C	-5.42305600	1.89581700	2.91069500
C	6.96801600	-2.13490000	0.84099100
C	6.71663000	0.01118400	1.96645500
C	5.53623600	-1.92757500	2.84674300
C	2.13430000	6.91674900	1.05435600
C	-0.01284400	6.61773800	2.16292600
C	1.91655100	5.38048900	2.97795600
H	-1.62133800	-7.23770500	0.34133300
H	-3.07186700	-6.38051200	0.91484600
H	-2.32190400	-7.63551600	1.94621300
H	0.50651000	-6.93821700	1.45609600
H	0.66630800	-5.75156000	2.78679500
H	-0.27175300	-7.25170300	3.03065000
H	-1.27107900	-4.47219800	3.51141900
H	-2.86839500	-4.76672700	2.77955900
H	-2.11412500	-6.03467600	3.78445000
H	-7.26337600	1.62151300	0.05287700
H	-6.43122400	3.06182900	0.68769200
H	-7.75444800	2.31710700	1.63351200

H	-7.05756600	-0.51424600	1.17551500
H	-5.95878700	-0.69268000	2.57782400
H	-7.46080700	0.26042200	2.73104000
H	-4.94096700	2.83586600	2.64976700
H	-4.70231500	1.23234800	3.38913500
H	-6.27294500	2.08356300	3.57012600
H	7.27653000	-1.62153800	-0.06983400
H	6.47950500	-3.07294300	0.58400800
H	7.82686500	-2.32132000	1.48937600
H	7.08953500	0.50527100	1.07010100
H	6.03722600	0.66738400	2.50946100
H	7.55198200	-0.27326600	2.60717100
H	4.82495200	-1.27355300	3.35162000
H	5.05546800	-2.87138500	2.59709400
H	6.40935100	-2.10950500	3.47691700
H	1.62300600	7.27852400	0.16226600
H	3.06775100	6.43504800	0.76935100
H	2.32877300	7.73723300	1.74877400
H	-0.50523000	7.04097200	1.28818100
H	-0.67290100	5.91363700	2.66856700
H	0.27589400	7.41579900	2.84793300
H	2.85452200	4.90290600	2.70183300
H	1.25596400	4.64988900	3.44510900
H	2.10924800	6.21705800	3.65316300
S	2.19151400	-3.35383300	-1.31477500
S	-3.34193000	-2.23338700	-1.35393600
S	-2.20819400	3.33502700	-1.32968900
S	3.30981700	2.20898000	-1.33439000

[MnL(O₂)(H₂O)]²⁺ (in water)

Charge=2 S=5/2

SCF energy: -3453.14138349 Ha

O	1.59099600	-1.15091200	2.66865600
O	1.15169400	1.55638400	2.69235100
O	-1.12357800	-1.58036200	2.64687200
O	-1.54980600	1.11512300	2.66436400
O	0.02319000	-0.29362100	4.97928000
O	0.29132500	0.03035800	0.31816100
Mn	0.01261500	-0.01230000	2.57081200
C	2.17505400	-1.56322400	1.55695700
C	1.57999200	2.14689100	1.59022400
C	-1.54770900	-2.15045800	1.53081800
C	-2.13550700	1.55035100	1.56124100
H	0.88005400	-0.70259300	5.17321900

H	-0.64226900	-0.98222900	5.12863700
O	-0.54281700	-0.08599400	-0.70197400
C	1.76588700	-2.77566500	0.93820200
C	3.21910500	-0.78899700	0.97117600
C	2.81058600	1.75097100	0.99674700
C	0.81054500	3.18612400	0.99067500
C	-2.77787000	-1.74877700	0.94441200
C	-0.77943400	-3.18566300	0.92449400
C	-1.73548300	2.78377900	0.98003200
C	-3.18709300	0.79551000	0.96637300
C	2.44779500	-3.23355300	-0.19278400
C	0.58565400	-3.57243500	1.49206300
C	3.87823900	-1.27817900	-0.15323000
C	3.59893700	0.56900900	1.55916300
C	3.28871700	2.44068000	-0.11959200
C	1.31708800	3.84859100	-0.12550400
C	-0.55653300	3.56610200	1.55695800
C	-3.26784100	-2.44304900	-0.16434500
C	-3.56750300	-0.57556300	1.52239400
C	-1.29501600	-3.85020200	-0.18629600
C	-2.43977800	3.28491100	-0.11840400
C	-3.87283400	1.33024300	-0.12124200
H	2.13262600	-4.17283700	-0.62993300
C	3.50165600	-2.49608800	-0.73073900
H	0.75709000	-4.63501900	1.28394200
H	0.55810100	-3.44191200	2.57714600
H	4.68880100	-0.68859600	-0.57067600
H	4.66497300	0.74202700	1.37104500
H	3.44804000	0.53361100	2.64115500
H	4.24040400	2.13526100	-0.53634600
C	2.55111400	3.48668200	-0.67482900
H	0.72931000	4.65488700	-0.55365300
H	-0.72394900	4.63298200	1.36872300
H	-0.53677000	3.41373200	2.63944800
H	-4.22433000	-2.13974000	-0.57168300
C	-2.53597200	-3.49088800	-0.72255200
H	-4.63246000	-0.74450500	1.32498400
H	-3.42398600	-0.56142000	2.60636900
H	-0.71212000	-4.65839700	-0.61745500
H	-2.13581200	4.24216200	-0.52324400
C	-3.50724700	2.56872700	-0.65963100
H	-4.69589700	0.75916800	-0.54015000
N	4.27635600	-2.98766300	-1.93075100
N	3.06130000	4.26765100	-1.86299800

N	-3.05774000	-4.27559000	-1.90355900
N	-4.30854200	3.10721800	-1.82160500
C	5.73075700	-3.18517100	-1.55539600
C	3.76322300	-4.30321400	-2.46017300
C	4.17871900	-1.97828600	-3.05582200
C	3.23292500	5.72422200	-1.48323700
C	4.39474300	3.77027100	-2.36195800
C	2.07989800	4.15844600	-3.01149200
C	-3.21493100	-5.73328700	-1.52212800
C	-4.40143000	-3.78727700	-2.38353500
C	-2.09270900	-4.15900800	-3.06503200
C	-5.75351900	3.29137700	-1.40535400
C	-3.80563500	4.44177800	-2.31161700
C	-4.23814500	2.14269300	-2.98739600
H	5.77617100	-3.91467300	-0.74738800
H	6.14815300	-2.23580200	-1.22700200
H	6.26936900	-3.54775700	-2.43171500
H	3.85762700	-5.06358800	-1.68662000
H	2.72449300	-4.18721600	-2.76535300
H	4.37424300	-4.57349300	-3.32062900
H	3.12650300	-1.85407000	-3.30985300
H	4.59890500	-1.03064800	-2.72673100
H	4.73901800	-2.35743700	-3.91124200
H	3.93964100	5.77779400	-0.65569400
H	2.27058000	6.13153900	-1.18093200
H	3.61345800	6.26631500	-2.34974400
H	5.13610900	3.87357800	-1.57127000
H	4.29810400	2.73034500	-2.66971700
H	4.67728600	4.38467200	-3.21605500
H	1.11960500	4.56656400	-2.70478500
H	1.97480800	3.10494800	-3.26891500
H	2.47226700	4.72401000	-3.85743300
H	-3.91107400	-5.79160300	-0.68597000
H	-2.24655600	-6.13500000	-1.23194800
H	-3.60265600	-6.27768300	-2.38398900
H	-5.12992200	-3.89309900	-1.58130400
H	-4.31563300	-2.74754300	-2.69500900
H	-4.69297600	-4.40515800	-3.23207200
H	-1.99902000	-3.10464200	-3.32343900
H	-1.12537700	-4.55970100	-2.77072900
H	-2.49175200	-4.72725700	-3.90606800
H	-5.77872200	3.98754900	-0.56755700
H	-6.16568100	2.33013000	-1.10622200
H	-6.31101100	3.69010800	-2.25370000

H	-3.88067100	5.17174300	-1.50731600
H	-2.77444100	4.33641300	-2.64472400
H	-4.43565100	4.74513300	-3.14701400
H	-4.64724300	1.18145100	-2.68514200
H	-3.19250800	2.03206600	-3.27311600
H	-4.82096100	2.55356400	-3.81257800

[MnL(O₂)(H₂O)]²⁺ (in methanol)

Charge=2 S=5/2

SCF energy: -3453.13645368 Ha

O	1.74985400	-0.86920700	2.65814000
O	0.86154800	1.72192700	2.70685000
O	-0.84662200	-1.76314300	2.64240600
O	-1.72009000	0.82511200	2.65570500
O	-0.10668500	-0.51676500	4.96112600
O	0.27828900	0.07877100	0.31754700
Mn	0.01044900	-0.01356200	2.55986200
C	2.40828100	-1.16906300	1.55263600
C	1.18529500	2.38290600	1.60795100
C	-1.15973000	-2.39069100	1.51908400
C	-2.37273000	1.15763500	1.55454500
H	0.77950000	-0.70979000	5.29923100
H	-0.51125800	-1.37484300	4.74736400
O	-0.53540500	-0.14687400	-0.70025200
C	2.21939300	-2.43157700	0.92800500
C	3.31076600	-0.22482300	0.98204300
C	2.46734500	2.20587400	1.01794000
C	0.24981000	3.27527200	1.00798800
C	-2.43663500	-2.19937900	0.92678700
C	-0.22042200	-3.26989600	0.90796800
C	-2.19096400	2.44430100	0.98058400
C	-3.27872800	0.23567300	0.95667500
C	2.98065300	-2.76108900	-0.19672400
C	1.19079700	-3.42086600	1.47472400
C	4.05558600	-0.58946200	-0.13620000
C	3.44623400	1.17514700	1.57893400
C	2.82357900	2.97181100	-0.09428000
C	0.63920900	4.01945700	-0.10384000
C	-1.16547000	3.41409400	1.56645600
C	-2.79429000	-2.95654900	-0.19132100
C	-3.41834000	-1.18262200	1.50693300
C	-0.60893800	-4.00310000	-0.21164000
C	-2.97104700	2.82228300	-0.11577900
C	-4.04497400	0.64900800	-0.12994700

H	2.83642700	-3.73851300	-0.63976200
C	3.89829800	-1.85098100	-0.72110700
H	1.54091900	-4.43736500	1.26061100
H	1.14268600	-3.30372800	2.56056900
H	4.75918600	0.13092900	-0.54235300
H	4.46685000	1.53169100	1.39738100
H	3.29943600	1.10834300	2.66003900
H	3.81523000	2.83735400	-0.50787600
C	1.91911500	3.87810000	-0.64851600
H	-0.07694600	4.71435400	-0.53190500
H	-1.51142500	4.43739400	1.37976300
H	-1.12734100	3.26390100	2.64873000
H	-3.78623200	-2.81793000	-0.60287800
C	-1.89018000	-3.85774800	-0.75304700
H	-4.43759500	-1.53212800	1.30536600
H	-3.28259600	-1.14903100	2.59141700
H	0.10623600	-4.69553500	-0.64511600
H	-2.83697400	3.81943300	-0.51595200
C	-3.89970000	1.93528000	-0.66044200
H	-4.75556000	-0.05389900	-0.55420000
N	4.75980300	-2.19710500	-1.91264800
N	2.29184000	4.74236300	-1.82997500
N	-2.26539900	-4.71584300	-1.93855000
N	-4.78373000	2.33305200	-1.81936500
C	6.22131000	-2.15202500	-1.51624600
C	4.47939400	-3.57525300	-2.45692800
C	4.51172500	-1.20940400	-3.03398300
C	2.20764500	6.20446900	-1.44152700
C	3.69291100	4.48440300	-2.32452900
C	1.34855700	4.47312100	-2.98411400
C	-2.18699000	-6.17958400	-1.55500500
C	-3.66519400	-4.45046500	-2.43279300
C	-1.32089600	-4.44646100	-3.09152200
C	-6.23955400	2.24202700	-1.40951200
C	-4.53403600	3.74422500	-2.28886100
C	-4.53485900	1.41329100	-2.99669500
H	6.37656800	-2.86878600	-0.71047500
H	6.46904100	-1.14837600	-1.17756400
H	6.82552200	-2.41368200	-2.38568700
H	4.68924900	-4.31578700	-1.68698600
H	3.43945500	-3.63024600	-2.77475900
H	5.13707400	-3.73330900	-3.31091800
H	3.45715200	-1.25945000	-3.30330900
H	4.76497600	-0.20775000	-2.69414700

H	5.13878800	-1.48445500	-3.88282100
H	2.89097100	6.37502600	-0.61022200
H	1.18803700	6.43692500	-1.14200100
H	2.49179600	6.80951500	-2.30326300
H	4.40205900	4.70663900	-1.52883900
H	3.77614500	3.44549300	-2.63954100
H	3.87015200	5.14401900	-3.17327300
H	0.33109300	4.70698200	-2.67914300
H	1.42855200	3.41930300	-3.24893900
H	1.64034300	5.10428500	-3.82425300
H	-2.87106300	-6.35016000	-0.72429300
H	-1.16822300	-6.41684100	-1.25620600
H	-2.47343500	-6.78064900	-2.41876100
H	-4.37567600	-4.67557200	-1.63916300
H	-3.74476400	-3.40928300	-2.74127200
H	-3.84381200	-5.10424700	-3.28571900
H	-1.39767800	-3.39175900	-3.35379600
H	-0.30425000	-4.68418000	-2.78702500
H	-1.61425200	-5.07459500	-3.93343400
H	-6.39598100	2.90629700	-0.56023100
H	-6.46996500	1.21632600	-1.13020900
H	-6.85700900	2.54683700	-2.25519100
H	-4.73982200	4.43597700	-1.47361500
H	-3.50146600	3.83377700	-2.62213400
H	-5.20986600	3.94008000	-3.12068800
H	-4.76240600	0.38984200	-2.70718200
H	-3.48598800	1.49941500	-3.27897800
H	-5.18114400	1.72093000	-3.81952200

[MnL(O₂)(H₂O)]²⁺ (in chloroform)

Charge=2 S=5/2

SCF energy: -3453.08845379 Ha

O	1.60161800	-1.12673500	2.63074400
O	1.12593200	1.56621100	2.64687500
O	-1.10070700	-1.59371500	2.61438100
O	-1.56445700	1.08832200	2.62646100
O	0.02661800	-0.29263300	4.92311500
O	0.27777800	0.03949100	0.28427300
Mn	0.01135200	-0.01092400	2.54667300
C	2.19513100	-1.53130900	1.52641900
C	1.54741700	2.16591800	1.55281400
C	-1.51946000	-2.17176700	1.50546400
C	-2.15988400	1.51772600	1.53189800
H	0.88884200	-0.68808700	5.12085000

H	-0.63205600	-0.98613900	5.07985000
O	-0.57195900	-0.08624200	-0.72228700
C	1.80746600	-2.75371500	0.91113200
C	3.23484400	-0.74587500	0.94526700
C	2.78827000	1.79279800	0.96447800
C	0.76577100	3.20020200	0.95863400
C	-2.75962200	-1.79112900	0.92328000
C	-0.73831200	-3.19928300	0.90017600
C	-1.77982400	2.75833900	0.95102700
C	-3.20756500	0.75025900	0.94405300
C	2.51656000	-3.21731300	-0.19960200
C	0.63461400	-3.56219600	1.46486500
C	3.92121100	-1.24130600	-0.15918000
C	3.58953200	0.62060500	1.52919700
C	3.27082700	2.50994100	-0.13148200
C	1.27784300	3.89112300	-0.13664000
C	-0.60812400	3.55423400	1.52507900
C	-3.25060100	-2.50686800	-0.17020100
C	-3.56243900	-0.62688400	1.50178300
C	-1.25574200	-3.88521300	-0.19590800
C	-2.50779300	3.25821900	-0.13153800
C	-3.91753300	1.28466800	-0.12687100
H	2.22275500	-4.16731700	-0.62898300
C	3.57440100	-2.47423100	-0.72399400
H	0.82094500	-4.62363700	1.26229300
H	0.60571800	-3.42664100	2.54933900
H	4.73324800	-0.64683500	-0.56810800
H	4.65428300	0.80921300	1.34730700
H	3.43315100	0.58527900	2.61050700
H	4.23302000	2.22666900	-0.54033900
C	2.52630300	3.55920400	-0.67323600
H	0.68588900	4.69999300	-0.55527400
H	-0.79254500	4.61965500	1.34283200
H	-0.58389600	3.39686900	2.60686000
H	-4.21589200	-2.22286100	-0.57107800
C	-2.50917100	-3.55287900	-0.72084000
H	-4.62621700	-0.81282100	1.31176900
H	-3.41232500	-0.60844900	2.58477100
H	-0.66683200	-4.69291200	-0.62098600
H	-2.22272800	4.22275300	-0.53343900
C	-3.57784100	2.53400500	-0.65791800
H	-4.74192700	0.70768300	-0.53591500
N	4.39204000	-2.98026900	-1.89039300
N	3.04989500	4.38462700	-1.82647700

N	-3.03949200	-4.37239500	-1.87543100
N	-4.41767200	3.08020500	-1.79028700
C	5.83757600	-3.14711000	-1.46917300
C	3.91594800	-4.31548400	-2.40244200
C	4.31242500	-1.99929400	-3.04061000
C	3.19191400	5.83100300	-1.39877700
C	4.40113600	3.92332600	-2.30898800
C	2.09660800	4.29707100	-2.99914700
C	-3.16609900	-5.82348600	-1.45940700
C	-4.39926300	-3.91681300	-2.33919000
C	-2.09981800	-4.26699400	-3.05754600
C	-5.85353400	3.23699800	-1.33370600
C	-3.94731800	4.42982200	-2.26844300
C	-4.36476900	2.13757200	-2.97359100
H	5.87058000	-3.85784600	-0.64390400
H	6.22993700	-2.18516000	-1.14707100
H	6.40830400	-3.51951400	-2.32111000
H	3.99622100	-5.05431000	-1.60662000
H	2.88508700	-4.22300500	-2.74073700
H	4.55671700	-4.59903600	-3.23709300
H	3.26577900	-1.89490900	-3.32530400
H	4.70898200	-1.03838400	-2.72038400
H	4.90202400	-2.38787300	-3.87226700
H	3.88194500	5.86949400	-0.55633300
H	2.21837100	6.21275900	-1.09942000
H	3.57921800	6.40727000	-2.24033100
H	5.12111000	4.00935900	-1.49670100
H	4.32666600	2.89228000	-2.65111400
H	4.69697000	4.56869700	-3.13579000
H	1.12425200	4.68277300	-2.70109500
H	2.00987100	3.25000700	-3.28819900
H	2.49820000	4.89252100	-3.82038200
H	-3.84747600	-5.87501900	-0.61063300
H	-2.18673500	-6.20050100	-1.17326300
H	-3.55730900	-6.39524400	-2.30222200
H	-5.10977100	-4.01565400	-1.52005300
H	-4.33596600	-2.88215600	-2.67252000
H	-4.69906300	-4.55691000	-3.16865800
H	-2.02341200	-3.21659500	-3.33734500
H	-1.12165900	-4.64888200	-2.77389600
H	-2.50654200	-4.85727200	-3.87999600
H	-5.86714200	3.92122600	-0.48573400
H	-6.24150200	2.26595600	-1.03420900
H	-6.44083500	3.63776800	-2.16122300

H	-4.00785900	5.14272100	-1.44760500
H	-2.92415600	4.34472000	-2.63115000
H	-4.60448000	4.74286400	-3.07947500
H	-4.75871000	1.16768600	-2.67832800
H	-3.32428500	2.03916200	-3.28209100
H	-4.96902700	2.55564600	-3.78001800

[MnL(O₂)(H₂O)]²⁺ (in benzene)

Charge=2 S=5/2

SCF energy: -3453.03186319 Ha

O	1.74312000	-0.88279400	2.59294600
O	0.89154000	1.70811200	2.60323300
O	-0.86009700	-1.73221500	2.58672500
O	-1.70156400	0.85444800	2.59093000
O	0.06827200	-0.26516700	4.87289800
O	0.26343800	0.05730800	0.26148200
Mn	0.01122000	-0.00575600	2.52132100
C	2.38848400	-1.20309400	1.49611800
C	1.22027800	2.36243900	1.51528900
C	-1.19359300	-2.36624900	1.48519600
C	-2.35470200	1.19553000	1.50447600
H	0.97346900	-0.53097800	5.09260600
H	-0.49747100	-1.02886900	5.06078600
O	-0.58484600	-0.17199600	-0.72784700
C	2.18593000	-2.47546100	0.89008900
C	3.30968700	-0.28039800	0.91311700
C	2.50430400	2.17581500	0.92722800
C	0.29954300	3.28177200	0.92804400
C	-2.47765500	-2.16861000	0.90369400
C	-0.27564600	-3.27754100	0.88293700
C	-2.16139100	2.48116300	0.92651700
C	-3.28669700	0.28678200	0.92049100
C	2.97529000	-2.84801600	-0.19956000
C	1.13641300	-3.43757700	1.44561500
C	4.07957900	-0.68843200	-0.17068600
C	3.46230200	1.12642500	1.48963900
C	2.88780700	2.97733800	-0.14826500
C	0.71673000	4.06007900	-0.14752300
C	-1.11022100	3.43194000	1.49807200
C	-2.86801600	-2.96146100	-0.17595800
C	-3.43611500	-1.12707500	1.47915800
C	-0.69797500	-4.04493300	-0.19877900
C	-2.97130600	2.87930200	-0.13915600
C	-4.08119500	0.72140500	-0.13456600

H	2.83046200	-3.83794400	-0.61563700
C	3.92695000	-1.96840500	-0.71734200
H	1.47087700	-4.46354800	1.24868900
H	1.08902900	-3.30304400	2.52980200
H	4.80666200	0.01049300	-0.57537200
H	4.48999100	1.46403200	1.30806400
H	3.31286700	1.07227800	2.57155600
H	3.88527400	2.84459700	-0.55013500
C	2.00572400	3.92364000	-0.67451400
H	0.01913700	4.78675800	-0.55516300
H	-1.44483500	4.46172600	1.32307400
H	-1.05937300	3.27423600	2.57924800
H	-3.86673200	-2.82245300	-0.57221500
C	-1.98993000	-3.90221500	-0.71630800
H	-4.46325700	-1.46406300	1.29353900
H	-3.28796400	-1.08431600	2.56199800
H	-0.00320400	-4.76821300	-0.61704000
H	-2.83597500	3.87944200	-0.53328600
C	-3.93568700	2.01259100	-0.65520100
H	-4.81987200	0.03420000	-0.53803900
N	4.84221100	-2.37258000	-1.85199100
N	2.41919400	4.85210700	-1.79525900
N	-2.40948200	-4.81558500	-1.84728100
N	-4.87295300	2.44326000	-1.76226600
C	6.28531000	-2.30959800	-1.39561000
C	4.58538600	-3.77542000	-2.33723400
C	4.64647200	-1.44277300	-3.02917200
C	2.33877300	6.29050200	-1.32680400
C	3.83080900	4.61005100	-2.26212400
C	1.50816300	4.66013300	-2.98754300
C	-2.33009200	-6.25980800	-1.39767300
C	-3.82229900	-4.56461800	-2.30617300
C	-1.50248900	-4.60935800	-3.04026800
C	-6.30635200	2.37411900	-1.27764500
C	-4.62200700	3.85535100	-2.22290800
C	-4.70334200	1.53769700	-2.96220200
H	6.40411000	-2.98777700	-0.55097000
H	6.51846800	-1.29264600	-1.08794800
H	6.92930100	-2.60891100	-2.22439200
H	4.74938600	-4.47378200	-1.51787400
H	3.56186900	-3.84523300	-2.70264100
H	5.28471200	-3.98280100	-3.14730900
H	3.60371100	-1.50413500	-3.34019100
H	4.88210900	-0.42570200	-2.72345100

H	5.31069800	-1.75372300	-3.83750300
H	3.00272800	6.40606900	-0.47050800
H	1.31544600	6.51351200	-1.03307500
H	2.64643600	6.94424300	-2.14485900
H	4.51618600	4.77389700	-1.43184100
H	3.91404700	3.58968300	-2.63349500
H	4.04407600	5.31673600	-3.06425800
H	0.48465200	4.88349100	-2.69443900
H	1.58312200	3.62117100	-3.30811800
H	1.82485800	5.33519400	-3.78459900
H	-2.99183100	-6.38534900	-0.54103700
H	-1.30623500	-6.48833000	-1.10998100
H	-2.64139300	-6.90249100	-2.22304600
H	-4.50517000	-4.73767300	-1.47570100
H	-3.90444900	-3.53939900	-2.66413300
H	-4.03963200	-5.26069700	-3.11646500
H	-1.57460700	-3.56533100	-3.34464400
H	-0.47874500	-4.84123700	-2.75471300
H	-1.82525300	-5.27136900	-3.84577000
H	-6.40586000	3.03501500	-0.41694800
H	-6.53586400	1.35158900	-0.98621700
H	-6.96648700	2.69202400	-2.08657500
H	-4.76864400	4.53691100	-1.38628400
H	-3.60548300	3.93046700	-2.60628500
H	-5.33626100	4.08121700	-3.01484000
H	-4.93645800	0.51520400	-2.67319500
H	-3.66636500	1.60174000	-3.29147100
H	-5.38180400	1.86781400	-3.75091200

[MnL(O₂)(H₂O)]²⁺-8H₂O (in water)

Charge=2 S=5/2

SCF energy: -4064.84015966 Ha

O	1.83648500	-0.10060000	-3.23716600
O	-0.07076200	-2.04149900	-3.15648200
O	-1.99187700	-0.12041500	-3.13672100
O	-0.05305200	-0.05008200	-5.49316600
O	0.17422600	-0.19240600	-0.78285200
Mn	-0.08515400	-0.11253300	-3.16926200
C	2.63773700	-0.08833900	-2.18950100
C	-0.02845200	-2.70865600	-2.01514400
C	-0.07716600	2.52601200	-2.10182000
C	-2.73956600	-0.09484000	-2.04922400
H	-0.31690300	0.82147700	-5.82430600
H	0.84539200	-0.20479200	-5.82208100

O	-0.22279800	0.04682700	0.45454600
C	3.07122300	1.15131900	-1.63583600
C	3.10581900	-1.31264300	-1.63754000
C	1.22928000	-3.08452800	-1.45865900
C	-1.23390300	-3.07386400	-1.35556900
C	-1.30591500	2.93491100	-1.50467000
C	1.16158500	2.93133900	-1.52951200
C	-3.15499200	-1.31575200	-1.44314900
C	-3.19122600	1.14696900	-1.52519100
C	4.09087500	1.14110700	-0.68364200
C	2.48889200	2.47237600	-2.14160000
C	4.13366400	-1.28349000	-0.68896000
C	2.53575800	-2.64452600	-2.12192700
C	1.25233000	-3.89165300	-0.32377500
C	-1.16984500	-3.88134500	-0.21415100
C	-2.59089300	-2.65247300	-1.92401800
C	-1.27172300	3.83605500	-0.44155800
C	-2.64467900	2.46321300	-2.07775000
C	1.15267100	3.83840500	-0.46246700
C	-4.15906100	-1.27514500	-0.47666700
C	-4.21220400	1.14634900	-0.56745000
H	4.45853900	2.09379400	-0.31564200
C	4.64655300	-0.06355000	-0.23740600
H	3.23145300	3.25901300	-1.96852500
H	2.34193300	2.38368900	-3.22231200
H	4.53306900	-2.22882200	-0.34275800
H	3.28669400	-3.42412500	-1.95221900
H	2.36196900	-2.57309800	-3.19927800
H	2.21685900	-4.20833200	0.06047500
C	0.06294100	-4.29865400	0.29154900
H	-2.10254900	-4.19191700	0.24033200
H	-3.31887800	-3.43497200	-1.68295900
H	-2.49746600	-2.60796700	-3.01323000
H	-2.21646100	4.19045900	-0.04166800
C	-0.05486100	4.29953700	0.06986900
H	-3.38840400	3.24685600	-1.89661900
H	-2.52714000	2.35657500	-3.16039100
H	2.10701200	4.20372200	-0.10142800
H	-4.52077800	-2.21604400	-0.07409000
C	-4.71927900	-0.05751500	-0.07360600
H	-4.61320900	2.10213400	-0.25196800
N	5.84412200	-0.00507200	0.68214000
N	0.15374700	-5.25817500	1.45522400
N	-0.09038500	5.38228200	1.12464000

N	-5.92439500	-0.09436800	0.83798500
C	5.49221300	0.70438000	1.97304700
C	6.36889400	-1.37174000	1.04746200
C	6.96956800	0.74068000	-0.00893100
C	-1.19000700	-5.56392900	2.06994600
C	0.74542900	-6.57024800	0.97662300
C	1.03231000	-4.68564300	2.54872000
C	1.27540200	5.71545600	1.67245400
C	-0.65765600	6.65006400	0.51384300
C	-0.95816300	4.96557400	2.29523200
C	-6.46733100	1.27778400	1.15322600
C	-7.03801500	-0.86990200	0.15939000
C	-5.58171600	-0.76329700	2.15236000
H	4.73573600	0.11604400	2.49055000
H	5.10001100	1.69329900	1.74987200
H	6.39524000	0.78092100	2.57968700
H	5.59196700	-1.93014500	1.56707700
H	6.68146500	-1.89090600	0.14303900
H	7.22355200	-1.22902300	1.70767800
H	7.19163900	0.22913100	-0.94487600
H	6.65475400	1.76329100	-0.20494100
H	7.84060700	0.73673300	0.64711600
H	-1.82437000	-6.04607000	1.32850200
H	-1.64337600	-4.64079700	2.42790900
H	-1.02249200	-6.24151100	2.90604300
H	0.09986100	-6.96799200	0.19426400
H	1.74311000	-6.38747500	0.58276000
H	0.79439400	-7.25792400	1.82174100
H	0.60401300	-3.73905100	2.87517600
H	2.03646400	-4.52928000	2.16195300
H	1.06087600	-5.39837100	3.37341300
H	1.90529100	6.09425500	0.87001800
H	1.71179900	4.82570500	2.12345300
H	1.14755800	6.48703700	2.43041600
H	-0.01579400	6.94384800	-0.31617200
H	-1.66563200	6.45055400	0.15566700
H	-0.67564800	7.42625600	1.27997600
H	-1.98000100	4.81694400	1.95488200
H	-0.56214800	4.03932000	2.70906300
H	-0.93198300	5.76172000	3.03951700
H	-6.76397400	1.76885400	0.22800600
H	-5.70968500	1.85976200	1.67449400
H	-7.33584700	1.14663900	1.79756200
H	-7.26018500	-0.38448800	-0.79034700

H	-6.71112600	-1.89329100	-0.00971200
H	-7.91246600	-0.85984300	0.81073500
H	-4.81780300	-0.16929700	2.65077500
H	-5.20686700	-1.76565100	1.96014400
H	-6.48571700	-0.80928100	2.76057600
O	1.87954900	-0.68853700	1.84605500
H	2.47910600	-1.11202100	1.21390600
H	1.02351800	-0.49722100	1.34623500
O	-2.11119300	-1.57764600	2.55402800
H	-1.60140600	-1.88739000	1.79063200
H	-2.23202000	-0.61456900	2.40579400
O	-1.96368100	1.18561600	2.08671900
H	-2.68204800	1.75986400	1.79284600
H	-1.40157700	0.97972900	1.29417800
O	2.34927800	1.98275700	2.29786700
H	1.89189200	2.41521700	1.56263700
H	2.28878200	1.01497600	2.11284200
O	-0.09201300	1.81458100	-3.21499800
O	-1.22892400	1.35532500	4.80704600
H	-1.21518300	0.39128100	5.02046800
H	-1.46650500	1.40866000	3.85806600
O	1.76208400	-0.97057500	4.62617800
H	1.85209600	-1.01789500	3.65016600
H	1.77400300	-0.00742800	4.84157500
O	1.49222000	1.79503400	4.92812300
H	0.50516100	1.76189500	4.91915800
H	1.77198600	2.04240500	4.01946100
O	-0.93208200	-1.40085700	5.06958900
H	0.04748700	-1.37406300	4.94558800
H	-1.32103900	-1.62930700	4.19659700

[MnL(O₂)(H₂O)]²⁺-8H₂O (in methanol)

Charge=2 S=5/2

SCF energy: -4064.83522846 Ha

O	1.85101100	-0.11107000	-3.21937900
O	-0.08451000	-2.01854700	-3.16100800
O	-1.97710700	-0.06724000	-3.14855800
O	-0.01155500	-0.03507400	-5.49092500
O	0.17319100	-0.18494600	-0.78277100
Mn	-0.07044400	-0.08982600	-3.17076100
C	2.64791400	-0.11121200	-2.16926100
C	-0.06126000	-2.69062100	-2.02248900
C	-0.02600000	2.54163500	-2.09506400
C	-2.73095000	-0.03671900	-2.06596900

H	-0.19205400	0.85419200	-5.83119300
H	0.87097200	-0.27509000	-5.81134300
O	-0.21644700	0.05763300	0.45653500
C	3.10204200	1.12196400	-1.61813200
C	3.09405300	-1.34245500	-1.61411300
C	1.18582800	-3.08711900	-1.45566000
C	-1.27798700	-3.04236500	-1.37619400
C	-1.25075900	2.96432800	-1.49873000
C	1.21639900	2.92405100	-1.51462400
C	-3.16923500	-1.25457000	-1.46981600
C	-3.16622700	1.20891300	-1.53686600
C	4.12343600	1.09674500	-0.66842200
C	2.53929300	2.45066400	-2.12509800
C	4.12088000	-1.32855400	-0.66375300
C	2.50569500	-2.66467100	-2.10382900
C	1.18586500	-3.90269900	-0.32656300
C	-1.23678900	-3.85860900	-0.24001800
C	-2.62274100	-2.59691000	-1.95482200
C	-1.20668700	3.85410300	-0.42643700
C	-2.59529000	2.51875800	-2.07970000
C	1.21726900	3.81926700	-0.43775700
C	-4.17741300	-1.20403800	-0.50826400
C	-4.19232000	1.21858200	-0.58457100
H	4.51257700	2.04412600	-0.30909100
C	4.65499000	-0.11621000	-0.21566000
H	3.29121400	3.22773800	-1.94883500
H	2.39376500	2.36527100	-3.20618900
H	4.50366200	-2.27967900	-0.31411600
H	3.24262200	-3.45634200	-1.92863700
H	2.34388700	-2.58880300	-3.18284600
H	2.14203700	-4.23625100	0.06433600
C	-0.01503900	-4.29739600	0.27428300
H	-2.17819700	-4.15925500	0.20316700
H	-3.36517100	-3.36926600	-1.72529900
H	-2.51830400	-2.54709700	-3.04277500
H	-2.14736000	4.21966100	-0.02690100
C	0.01499800	4.29277000	0.09531100
H	-3.32610100	3.31414800	-1.89693600
H	-2.47550000	2.41616700	-3.16247100
H	2.17584000	4.16487700	-0.06867000
H	-4.55536700	-2.14163700	-0.11306000
C	-4.72041100	0.01970500	-0.10028100
H	-4.58069800	2.17857600	-0.26570900
N	5.86569300	-0.07568900	0.68802200

N	0.05033600	-5.26914900	1.42950700
N	-0.00807700	5.36291100	1.16337800
N	-5.92994400	-0.00444600	0.80611700
C	5.57632100	0.72444900	1.94080300
C	6.31875600	-1.44749900	1.12499300
C	7.01773400	0.56660900	-0.06124000
C	-1.30299900	-5.55582000	2.03218800
C	0.62178100	-6.58729700	0.94322300
C	0.93080300	-4.72292800	2.53474300
C	1.35995900	5.66438300	1.72391900
C	-0.54939400	6.64798600	0.56557600
C	-0.89010200	4.94595300	2.32317500
C	-6.45207500	1.37386800	1.12917600
C	-7.05336700	-0.75692100	0.11755300
C	-5.60359100	-0.68850200	2.11696800
H	4.78595400	0.22034100	2.49444700
H	5.25354000	1.72561800	1.66772600
H	6.48892200	0.77263000	2.53573300
H	5.51356800	-1.93749900	1.67049100
H	6.60480900	-2.02842800	0.24990200
H	7.18055800	-1.31660200	1.77856700
H	7.19447200	-0.00827100	-0.96980300
H	6.75203500	1.59169500	-0.31152500
H	7.90015500	0.55248000	0.57936900
H	-1.94138000	-6.01803000	1.28160800
H	-1.74080800	-4.62771300	2.39674400
H	-1.15415500	-6.24516300	2.86222400
H	-0.02635000	-6.96806600	0.15454900
H	1.62436500	-6.41861100	0.55554700
H	0.65459500	-7.28231600	1.78312800
H	0.51765100	-3.77137600	2.86632700
H	1.94078100	-4.58233100	2.15719400
H	0.93943900	-5.44311900	3.35336100
H	2.00302600	6.03713800	0.92917200
H	1.77511200	4.76221400	2.17043200
H	1.24231200	6.43203900	2.48754500
H	0.10541100	6.94414800	-0.25345000
H	-1.55630700	6.46864300	0.19388100
H	-0.56387000	7.41314600	1.34285700
H	-1.91306400	4.82365500	1.97564200
H	-0.51451300	4.00550900	2.72390100
H	-0.85189100	5.72946600	3.08027000
H	-6.73511600	1.87692000	0.20612400
H	-5.68812700	1.93905900	1.65976500

H	-7.32653400	1.25237100	1.76740400
H	-7.26584700	-0.25962200	-0.82825700
H	-6.74160900	-1.78357900	-0.06015800
H	-7.92943200	-0.73936000	0.76662000
H	-4.83127400	-0.11178600	2.62282500
H	-5.24453800	-1.69551800	1.91921500
H	-6.51057000	-0.72383300	2.72149400
O	1.85185600	-0.74409800	1.86120400
H	2.45301200	-1.17058900	1.23267400
H	1.00747700	-0.52811200	1.35140400
O	-2.16776900	-1.56825400	2.52747700
H	-1.66553300	-1.88812700	1.76335000
H	-2.26340400	-0.60149900	2.38458800
O	-1.96014900	1.19559200	2.08247600
H	-2.66986200	1.77738900	1.78262100
H	-1.38967400	0.98951300	1.29539000
O	2.36271000	1.91324300	2.33672400
H	1.93133600	2.35674900	1.59252800
H	2.28808500	0.94743800	2.14572100
O	-0.04702400	1.83788400	-3.21314600
O	-1.24449500	1.33310300	4.80969100
H	-1.25227300	0.36754400	5.01635500
H	-1.47092300	1.39753100	3.85873400
O	1.70168800	-1.04909100	4.63777200
H	1.80134400	-1.08547200	3.66236400
H	1.73153300	-0.08947700	4.86630000
O	1.48311600	1.71947900	4.96263500
H	0.49568200	1.70445700	4.94506700
H	1.77447200	1.97027600	4.05915600
O	-1.00493600	-1.43061200	5.05301300
H	-0.02382900	-1.42239400	4.93954000
H	-1.38847900	-1.64588800	4.17437500

[MnL(O₂)(H₂O)]²⁺-8H₂O (in chloroform)

Charge=2 S=5/2

SCF energy: -4064.78694571 Ha

O	1.85626000	-0.10006200	-3.20947000
O	-0.06921700	-2.01644500	-3.14635000
O	-1.96844500	-0.07488000	-3.11966100
O	-0.04039900	-0.01473600	-5.45918100
O	0.18948600	-0.18164000	-0.76973600
Mn	-0.06360500	-0.09209900	-3.17101600
C	2.65472300	-0.09838300	-2.16407200
C	-0.03906200	-2.68574200	-2.00925000

C	-0.03980200	2.53837600	-2.08754400
C	-2.72593000	-0.04826200	-2.04502300
H	-0.16577300	0.89060700	-5.78154100
H	0.78948000	-0.33355200	-5.84367300
O	-0.16937000	0.04280200	0.48205200
C	3.10072300	1.13695200	-1.60979000
C	3.11226300	-1.32854000	-1.61404500
C	1.21178300	-3.07814400	-1.44628600
C	-1.25273400	-3.04138100	-1.35794200
C	-1.26670000	2.95534100	-1.48906700
C	1.20133900	2.92560700	-1.50551700
C	-3.15928900	-1.26895300	-1.44981900
C	-3.17664800	1.19598100	-1.52247800
C	4.12113500	1.11674500	-0.65951200
C	2.52630500	2.46033000	-2.11777400
C	4.14285500	-1.30922600	-0.66791900
C	2.52612100	-2.65164700	-2.10365800
C	1.21858300	-3.89008200	-0.31468100
C	-1.20432500	-3.85477100	-0.22047700
C	-2.60005500	-2.60482400	-1.93757000
C	-1.22592200	3.83973600	-0.41209600
C	-2.60908200	2.50467200	-2.07156600
C	1.19785400	3.81601600	-0.42523700
C	-4.17452900	-1.22413100	-0.49613600
C	-4.21133100	1.19961000	-0.57888200
H	4.49670400	2.06559300	-0.28947800
C	4.66596100	-0.09332600	-0.21407500
H	3.27285600	3.24400600	-1.94731600
H	2.37764400	2.36921900	-3.19792500
H	4.53654100	-2.25869900	-0.32530000
H	3.26670400	-3.44214400	-1.93769600
H	2.35449600	-2.57240400	-3.18083700
H	2.17738500	-4.22048200	0.07311400
C	0.02105200	-4.28597700	0.29292300
H	-2.14346500	-4.15916900	0.22507200
H	-3.33674600	-3.38495200	-1.71540100
H	-2.49152600	-2.54725600	-3.02478100
H	-2.16831100	4.20001900	-0.01114000
C	-0.00625800	4.27972600	0.11345700
H	-3.34260200	3.30007100	-1.89841500
H	-2.48448700	2.39305900	-3.15285900
H	2.15477500	4.16246900	-0.05285300
H	-4.54846400	-2.16402700	-0.10231000
C	-4.72977100	-0.00420800	-0.09226700

H	-4.61606800	2.15743400	-0.27220400
N	5.86009100	-0.04356500	0.71172600
N	0.09214900	-5.25262400	1.45322600
N	-0.03038700	5.33809200	1.19364600
N	-5.94395700	-0.04006500	0.80855700
C	5.50774100	0.67402300	1.99906900
C	6.36929000	-1.41349300	1.08540800
C	6.99705100	0.68696100	0.02303800
C	-1.25874900	-5.53312400	2.06470700
C	0.65958800	-6.57354500	0.97035600
C	0.97773400	-4.70249800	2.55273700
C	1.33868700	5.63185000	1.75718800
C	-0.57390000	6.62866100	0.61037500
C	-0.90867700	4.90713300	2.35138700
C	-6.46382000	1.33404500	1.15069000
C	-7.06518200	-0.77948000	0.10211200
C	-5.62561400	-0.74571200	2.11076900
H	4.74470500	0.09349600	2.51629400
H	5.12253100	1.66465500	1.77056100
H	6.40862600	0.74804100	2.60956700
H	5.58447500	-1.96129500	1.60483200
H	6.67975500	-1.94053100	0.18460700
H	7.22309200	-1.27798300	1.74865400
H	7.21950700	0.16745400	-0.90866900
H	6.69291000	1.71089100	-0.18302400
H	7.86501800	0.67979700	0.68359800
H	-1.89983600	-6.00442700	1.32185900
H	-1.69491400	-4.60026200	2.41953300
H	-1.10701800	-6.21292600	2.90236500
H	0.00975400	-6.95557500	0.18356200
H	1.66145300	-6.40795100	0.57902200
H	0.69363800	-7.26684100	1.81195700
H	0.56558300	-3.75124600	2.88653700
H	1.98511900	-4.56004600	2.16896400
H	0.99311900	-5.42092600	3.37311700
H	1.97805500	6.02314500	0.96812400
H	1.75705100	4.72035200	2.18259300
H	1.22109200	6.38361600	2.53685700
H	0.07555300	6.93080900	-0.21090700
H	-1.58303600	6.45340500	0.24231600
H	-0.58353900	7.38862300	1.39313100
H	-1.92953100	4.77280400	2.00211900
H	-0.52273400	3.97062000	2.75184800
H	-0.88077300	5.68856200	3.11133400

H	-6.75218700	1.84797000	0.23518900
H	-5.69556900	1.89291700	1.68245700
H	-7.33467700	1.20708800	1.79323300
H	-7.26957000	-0.26845200	-0.83825000
H	-6.75333500	-1.80381300	-0.08941500
H	-7.94636900	-0.76991600	0.74486700
H	-4.85279700	-0.18142700	2.63044700
H	-5.26895400	-1.75085900	1.89973400
H	-6.53516400	-0.78808300	2.71109700
O	1.94038300	-0.73551100	1.83422700
H	2.53674900	-1.11505700	1.17092100
H	1.07660400	-0.53338200	1.35283500
O	-2.10054600	-1.63399900	2.42066700
H	-1.56992800	-1.89312000	1.65200400
H	-2.25507700	-0.67150900	2.30247500
O	-2.02670000	1.13513500	1.97880100
H	-2.75107700	1.62593400	1.56983400
H	-1.38280500	0.91362600	1.25046600
O	2.28949300	1.97405900	2.20423400
H	1.78018300	2.31306100	1.45271800
H	2.29668700	0.99472600	2.08389900
O	-0.05635800	1.83655700	-3.20389600
O	-1.30567300	1.35740900	4.71594000
H	-1.30314200	0.39839400	4.95095000
H	-1.55485600	1.39502400	3.77059900
O	1.70268300	-1.01348800	4.62290000
H	1.83503200	-1.06029800	3.65377500
H	1.71783700	-0.05080300	4.84022400
O	1.42632100	1.75986700	4.86826100
H	0.43980500	1.73457700	4.85671800
H	1.71001100	2.01442700	3.96567200
O	-1.02071000	-1.40419800	5.00300900
H	-0.03710900	-1.38711800	4.92093800
H	-1.37235600	-1.65519700	4.12315500

[MnL(O₂)(H₂O)]²⁺-8H₂O (in benzene)

Charge=2 S=5/2

SCF energy: -4064.73033495 Ha

O	1.86005400	-0.10633700	-3.20801900
O	-0.14431100	-1.92836100	-3.18403100
O	-1.95513900	0.09573500	-3.11105000
O	-0.04042200	0.11070200	-5.46244900
O	0.19488100	-0.15742600	-0.75406600
Mn	-0.05454900	-0.01139100	-3.19979000

C	2.66211900	-0.15397600	-2.17085000
C	-0.15369900	-2.61141100	-2.05830500
C	0.08211300	2.58340300	-2.03887700
C	-2.72337200	0.13019600	-2.05135100
H	-0.09453200	1.02278700	-5.78417000
H	0.72654400	-0.29714500	-5.89136400
O	-0.09474100	0.01157100	0.52520500
C	3.16775900	1.05430600	-1.60727600
C	3.06757300	-1.40977200	-1.63531400
C	1.07373300	-3.06133600	-1.48286300
C	-1.38930900	-2.92660900	-1.42642200
C	-1.12107500	3.03101400	-1.41192700
C	1.34390600	2.90394800	-1.45948800
C	-3.22144700	-1.08493200	-1.49331500
C	-3.12635100	1.38093600	-1.50135400
C	4.18573400	0.98014700	-0.65824500
C	2.64310100	2.40430300	-2.09699800
C	4.10437200	-1.44471200	-0.69549900
C	2.41313800	-2.69869900	-2.13066900
C	1.03165100	-3.87273100	-0.35137400
C	-1.38856300	-3.74748200	-0.29442800
C	-2.71121200	-2.42818100	-2.01287700
C	-1.03223400	3.85739700	-0.29276200
C	-2.48702300	2.67357400	-2.00631800
C	1.38825800	3.74689900	-0.34414800
C	-4.23982000	-1.01902700	-0.54503300
C	-4.17312900	1.40703000	-0.57054900
H	4.59569700	1.90833600	-0.27249400
C	4.67957300	-0.25665200	-0.22721800
H	3.42004800	3.15763100	-1.92403700
H	2.48034400	2.33286000	-3.17633500
H	4.45935700	-2.41444200	-0.36609900
H	3.11073200	-3.52788000	-1.96543300
H	2.25105500	-2.60793700	-3.20861700
H	1.97107300	-4.24156200	0.04998200
C	-0.18871500	-4.22028700	0.24176200
H	-2.34479100	-4.01253500	0.13913600
H	-3.47972400	-3.18500300	-1.81924600
H	-2.58765100	-2.34588200	-3.09683700
H	-1.95506200	4.23050500	0.14163800
C	0.21012200	4.22364300	0.23807100
H	-3.17571300	3.50261700	-1.80690700
H	-2.36830300	2.59138300	-3.09100200
H	2.36196600	4.03259400	0.03519500

H	-4.65136300	-1.95136900	-0.17103100
C	-4.74586300	0.21375000	-0.11416500
H	-4.54097800	2.37437000	-0.24657200
N	5.85225300	-0.26536400	0.72863800
N	-0.17429700	-5.17150700	1.41761100
N	0.24157700	5.20789600	1.38650800
N	-5.94759000	0.20666700	0.80546700
C	5.47237700	0.40032000	2.03766000
C	6.33351700	-1.65777700	1.05259700
C	7.01987500	0.47742000	0.10777600
C	-1.54638500	-5.39002200	2.01008400
C	0.35333000	-6.51954200	0.96903400
C	0.70685300	-4.63141900	2.52602400
C	1.63465500	5.43997600	1.92235000
C	-0.29776300	6.54458300	0.91578700
C	-0.60128600	4.70514400	2.54229500
C	-6.43562700	1.59287100	1.14652600
C	-7.09825900	-0.51497000	0.12818400
C	-5.61413600	-0.49574800	2.10708200
H	4.67965800	-0.18488700	2.50312900
H	5.11501600	1.40877200	1.84159800
H	6.35374200	0.42776500	2.68027800
H	5.53439100	-2.21339000	1.54125000
H	6.64475700	-2.15387900	0.13416300
H	7.18152000	-1.56575400	1.73085700
H	7.26897800	-0.00769100	-0.83585800
H	6.73583800	1.51265100	-0.06862800
H	7.86430400	0.43494800	0.79745700
H	-2.19053200	-5.85018200	1.26241200
H	-1.95210100	-4.43399800	2.34172100
H	-1.43479300	-6.06207200	2.86089200
H	-0.29537400	-6.89321000	0.17699200
H	1.36718600	-6.39796700	0.59248400
H	0.34829800	-7.19911500	1.82300500
H	0.31179600	-3.66722400	2.84235900
H	1.72276200	-4.51568900	2.15675900
H	0.69194700	-5.33940800	3.35585000
H	2.25385900	5.87411300	1.13857500
H	2.05026100	4.49436500	2.27087000
H	1.55605200	6.13938300	2.75459400
H	0.32523700	6.89130000	0.09102800
H	-1.32465500	6.41556800	0.57795000
H	-0.26072900	7.24946200	1.74796900
H	-1.63141600	4.58756300	2.21489600

H	-0.20201500	3.74624500	2.87147400
H	-0.55102700	5.43666100	3.35007900
H	-6.71543100	2.11062200	0.23010900
H	-5.65369400	2.13737200	1.67386000
H	-7.30566900	1.48771800	1.79409600
H	-7.31388600	-0.00491000	-0.81038000
H	-6.81235200	-1.54635300	-0.06559400
H	-7.96459200	-0.48576000	0.79071300
H	-4.81595000	0.05518600	2.60365300
H	-5.28323300	-1.50982800	1.89476200
H	-6.50925000	-0.51482600	2.73075600
O	2.02418300	-0.85143100	1.78253600
H	2.59321300	-1.20622900	1.08415400
H	1.15192500	-0.62272800	1.33124900
O	-2.07584300	-1.80462000	2.23456300
H	-1.52749700	-1.96667900	1.45185900
H	-2.26096000	-0.84142900	2.20064400
O	-2.10019500	0.97820700	1.89069800
H	-2.81991700	1.33573200	1.35360200
H	-1.35871200	0.77650000	1.24815900
O	2.28061000	1.87674600	2.14011500
H	1.72582100	2.14386000	1.39150500
H	2.34622800	0.89693700	2.05731900
O	0.02784800	1.91407100	-3.17084800
O	-1.37720200	1.19632500	4.62433500
H	-1.36418400	0.23555900	4.85437600
H	-1.67097200	1.24103200	3.69457300
O	1.69218900	-1.16148300	4.56459600
H	1.87515400	-1.19429500	3.60485000
H	1.69198500	-0.20175500	4.79729300
O	1.35878800	1.59816300	4.80181500
H	0.37210600	1.57411800	4.78818200
H	1.64959700	1.87161600	3.91013100
O	-1.03560700	-1.56055500	4.86524100
H	-0.04918500	-1.53760900	4.82382300
H	-1.35375000	-1.82049700	3.97877400