

On the magnetic and spectroscopic properties of
high-valent Mn_3CaO_4 cubanes as structural units of
natural and artificial water oxidizing catalysts

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SUPPORTING INFORMATION

Methodological details

Comparison of functionals: Six different functionals (BP86,^{1,2} PBE,^{3,4} TPSS,⁵ B3LYP,^{6,7} PBE0,⁸ and TPSSh⁹) were tested for the optimization of the synthetic complexes **1** and **2**. A comparison of interatomic distances and angles of the XRD structures with fully relaxed structures is presented in Tables S1 and S2. Although all methods yield good results, TPSSh,⁹ PBE0⁸ and TPSS⁵ are consistently better compared to other functionals. The lowest mean absolute deviations (MAD) for bond lengths are obtained with TPSSh and PBE0 (both 0.025 Å for **1** and 0.031 Å for **2**), while TPSS is second best with a MAD of 0.028 Å for **1** and 0.032 Å for **2**. This is consistent with previous studies of transition metal systems.^{10,11} In the following, TPSS-optimized structures are used in order to benefit from the reduced cost of the non-hybrid functional, but all properties are computed with TPSSh, as it is more reliable for magnetic and spectroscopic properties.¹¹⁻¹³ Selected distances of the XRD and optimized structures are presented in Table 1. We note that if dispersion corrections are omitted, slightly longer Mn–Mn and Mn–Ca distances are obtained for both compounds (Table S3), but these effects are marginal (maximum differences of 0.01 Å).

Construction of broken-symmetry guesses: Initial wave functions for BS-DFT calculations were set up by reading the high-spin (ferromagnetic) optimized single-determinant SCF solution, which is the unique $S = 9/2$, $M_S = 9/2$ state for a Mn(IV) trimer, and “flipping” successively each of the localized Mn ion spins using the “flipspin” feature of ORCA.¹⁴ The three resulting wave functions, all of which are characterized by a value of 3/2 for the total M_S , were subsequently converged as usual, with a shift of 0.2–0.5 a.u. applied in the initial SCF steps to facilitate convergence. Attainment of the correct BS solution was confirmed by the spin populations of the Mn ions, which are close to +3 for two of them and –3 for the “flipped” center.

Calculation of EPR parameters: Isotropic ^{55}Mn HFCs A_{iso} are of particular interest because of their utility as probes of the electronic structure. Given the detailed treatment of the subject elsewhere,¹² we only mention here that the extraction of experimentally comparable HFCs from BS-DFT calculations is possible by defining a transformation of the “raw” value $A_{\text{iso,BS}}^{(K)}$ obtained from the BS-DFT calculation for nucleus K to the final projected value $A_{\text{iso}}^{(K)}$ according to:

$$A_{\text{iso}}^{(K)} = \pm A_{\text{iso,BS}}^{(K)} \left(\frac{\langle S_z \rangle_{\text{BS}}}{S_A} \right) \left(\frac{\langle S_z^{(A)} \rangle}{S_T} \right) \quad (6)$$

In the above equation S_T is the total spin and $\langle S_z \rangle_{\text{BS}}$ is the total M_S of the BS wave function. The crucial quantity for the projection is the on-site spin expectation value $\langle S_z^{(A)} \rangle$ that is obtained as

$$\langle S_z^{(A)} \rangle = \sum_{S_A M_{S_A} \dots S_N M_{S_N}} \left| C_I^{S_A M_{S_A} \dots S_N M_{S_N}} \right|^2 M_{S_A} \quad (7)$$

where the coefficient C_I represents the weight of the basis state $I = |S_A M_{S_A} \dots S_N M_{S_N}\rangle$ in the ground-state eigenfunction of the HDvV Hamiltonian $|S_A S_B \dots S_N, S M_S\rangle$ with $S = M_S$.

All approximate DFT functionals are known to underestimate core spin polarization, resulting in diminished hyperfine values. For this reason, and in order to facilitate comparisons with experiment, the BS-DFT derived values are typically scaled by a factor that depends on the functional and basis set combination used for a particular element. In the present case, using a standard test set of Mn complexes,¹⁵ a value of 1.78 was obtained for the ^{55}Mn scaling factor.

Table S1. Selected interatomic distances (in Å) and angles (in degrees) from the crystal structure of **1** and its optimized geometries using various density functionals with dispersion corrections.

	XRD	BP86	PBE	TPSS	B3LYP	PBE0	TPSSH
Mn1-Mn2	2.757	2.785	2.787	2.773	2.782	2.763	2.763
Mn1-Mn3	2.730	2.739	2.737	2.726	2.740	2.718	2.718
Mn2-Mn3	2.857	2.860	2.860	2.845	2.859	2.836	2.836
Mn1-Ca1	3.394	3.484	3.491	3.477	3.489	3.464	3.464
Mn2-Ca1	3.454	3.457	3.482	3.446	3.479	3.436	3.436
Mn3-Ca1	3.418	3.437	3.452	3.435	3.450	3.429	3.429
Mn1-O1	1.899	1.927	1.927	1.920	1.918	1.909	1.909
Mn1-O2	1.844	1.855	1.856	1.849	1.844	1.840	1.840
Mn1-O3	1.820	1.830	1.831	1.827	1.822	1.818	1.818
Mn2-O1	1.891	1.905	1.909	1.902	1.895	1.891	1.891
Mn2-O2	1.862	1.879	1.881	1.873	1.866	1.863	1.863
Mn2-O4	1.866	1.888	1.889	1.883	1.881	1.873	1.873
Mn3-O1	1.892	1.892	1.890	1.884	1.881	1.875	1.875
Mn3-O3	1.830	1.830	1.828	1.826	1.822	1.817	1.817
Mn3-O4	1.889	1.886	1.886	1.880	1.878	1.870	1.870
Ca1-O2	2.452	2.521	2.537	2.515	2.544	2.507	2.507
Ca1-O3	2.470	2.564	2.565	2.557	2.563	2.552	2.552
Ca1-O4	2.660	2.609	2.631	2.603	2.629	2.599	2.599
Ca2-O4	2.361	2.461	2.458	2.449	2.449	2.435	2.435
Mn1-O1-Mn2	93.3	93.2	93.2	93.0	93.7	93.3	93.3
Mn1-O1-Mn3	92.1	91.7	91.7	91.6	92.3	91.8	91.8
Mn1-O2-Mn2	96.2	96.5	96.4	96.3	97.1	96.5	96.5
Mn1-O3-Mn3	96.8	96.9	96.8	96.6	97.5	96.8	96.8
Mn2-O1-Mn3	98.1	97.8	97.7	97.5	98.4	97.7	97.7
Mn2-O4-Mn3	99.1	98.5	98.5	98.2	99.0	98.5	98.5
Ca1-O2-Mn1	103.5	104.5	104.2	104.6	104.2	104.6	104.6
Ca1-O2-Mn2	105.6	102.6	103.0	102.5	103.1	102.7	102.7
Ca1-O3-Mn1	103.6	103.7	103.9	103.7	104.2	103.6	103.6
Ca1-O3-Mn3	104.3	101.6	102.3	101.9	102.4	102.1	102.1
Ca1-O4-Mn2	97.9	99.2	99.5	99.1	99.6	99.1	99.1
Ca1-O4-Mn3	95.9	98.5	98.3	98.7	98.5	98.9	98.9
Ca2-O4-Mn2	119.9	121.0	121.1	121.7	121.2	121.9	121.9
Ca2-O4-Mn3	125.2	126.3	125.1	124.9	125.2	124.6	124.6
Ca2-O4-Ca1	113.3	108.2	109.5	109.2	108.4	109.0	109.0

Table S2. Selected interatomic distances (in Å) and angles (in degrees) from the crystal structure of **2** and its optimized geometries using various density functionals with dispersion corrections.

	XRD	BP86	PBE	TPSS	B3LYP	PBE0	TPSSh
Mn1-Mn2	2.839	2.829	2.837	2.820	2.830	2.808	2.811
Mn1-Mn3	2.833	2.828	2.837	2.820	2.835	2.812	2.811
Mn2-Mn3	2.830	2.825	2.834	2.817	2.830	2.806	2.807
Mn1-Ca1	3.231	3.330	3.332	3.315	3.316	3.286	3.304
Mn2-Ca1	3.224	3.330	3.329	3.314	3.331	3.299	3.302
Mn3-Ca1	3.238	3.330	3.333	3.318	3.316	3.287	3.307
Mn1-O1	1.916	1.929	1.933	1.923	1.919	1.904	1.914
Mn1-O2	1.842	1.840	1.841	1.837	1.829	1.818	1.828
Mn1-O3	1.862	1.876	1.876	1.871	1.871	1.854	1.862
Mn2-O1	1.912	1.922	1.926	1.917	1.918	1.903	1.908
Mn2-O2	1.871	1.875	1.875	1.871	1.867	1.851	1.861
Mn2-O4	1.825	1.841	1.842	1.836	1.828	1.817	1.827
Mn3-O1	1.923	1.923	1.927	1.918	1.920	1.904	1.909
Mn3-O3	1.829	1.838	1.839	1.834	1.832	1.821	1.826
Mn3-O4	1.864	1.877	1.877	1.872	1.867	1.850	1.862
Ca1-O2	2.391	2.505	2.505	2.489	2.506	2.483	2.483
Ca1-O3	2.432	2.506	2.511	2.497	2.485	2.465	2.490
Ca1-O4	2.430	2.502	2.502	2.490	2.508	2.485	2.484
Mn1-O1-Mn2	95.7	94.5	94.7	94.5	95.1	95.1	94.7
Mn1-O1-Mn3	95.1	94.5	94.6	94.5	95.2	95.2	94.7
Mn1-O2-Mn2	99.7	99.2	99.5	99.1	99.9	99.9	99.3
Mn1-O3-Mn3	100.2	99.2	99.6	99.1	99.9	99.8	99.3
Mn2-O1-Mn3	95.1	94.6	94.7	94.6	95.0	95.0	94.7
Mn2-O4-Mn3	100.2	98.9	99.3	98.9	100.0	99.8	99.1
Ca1-O2-Mn1	98.7	98.9	99.0	99.0	98.6	98.4	99.0
Ca1-O2-Mn2	97.6	98.0	97.9	97.9	98.2	98.1	97.9
Ca1-O3-Mn1	96.7	97.9	97.8	97.7	98.2	98.1	97.8
Ca1-O3-Mn3	97.9	98.9	98.8	98.9	99.2	99.0	98.9
Ca1-O4-Mn2	97.5	99.0	98.9	98.8	99.2	99.0	98.9
Ca1-O4-Mn3	97.0	98.0	98.1	98.0	97.5	97.5	98.1

Table S3. Selected interatomic distances (in Å) and angles (in degrees) from optimized structures of **1** and **2** with the TPSS and TPSSh functionals without dispersion corrections.

	1		2	
	TPSS	TPSSh	TPSS	TPSSh
Mn1-Mn2	2.778	2.769	2.839	2.828
Mn1-Mn3	2.735	2.725	2.839	2.828
Mn2-Mn3	2.853	2.845	2.837	2.826
Mn1-Ca1	3.488	3.475	3.332	3.321
Mn2-Ca1	3.553	3.533	3.324	3.312
Mn3-Ca1	3.480	3.475	3.326	3.317
Mn1-O1	1.918	1.907	1.931	1.920
Mn1-O2	1.857	1.847	1.837	1.828
Mn1-O3	1.829	1.820	1.872	1.862
Mn2-O1	1.901	1.892	1.926	1.915
Mn2-O2	1.875	1.866	1.870	1.861
Mn2-O4	1.892	1.882	1.838	1.829
Mn3-O1	1.884	1.875	1.925	1.916
Mn3-O3	1.824	1.815	1.836	1.827
Mn3-O4	1.886	1.875	1.873	1.863
Ca1-O2	2.560	2.545	2.505	2.496
Ca1-O3	2.543	2.543	2.505	2.502
Ca1-O4	2.722	2.715	2.493	2.487
Ca2-O4	2.509	2.500		
Mn1-O1-Mn2	93.4	93.6	94.8	95.0
Mn1-O1-Mn3	92.0	92.2	94.8	95.0
Mn1-O2-Mn2	96.2	96.5	99.9	100.1
Mn1-O3-Mn3	96.9	97.1	99.9	100.1
Mn2-O1-Mn3	97.8	98.1	94.9	95.0
Mn2-O4-Mn3	98.1	98.4	99.7	99.9
Ca1-O2-Mn1	103.1	103.4	99.1	99.2
Ca1-O2-Mn2	105.4	105.4	97.8	97.9
Ca1-O3-Mn1	104.6	104.4	98.1	98.0
Ca1-O3-Mn3	104.4	104.5	98.8	98.8
Ca1-O4-Mn2	99.1	98.9	99.1	99.1
Ca1-O4-Mn3	96.4	96.7	98.2	98.3
Ca2-O4-Mn2	119.8	119.9		
Ca2-O4-Mn3	124.4	124.0		
Ca2-O4-Ca1	114.0	113.9		

Table S4. Total charges, relative energies (kcal mol⁻¹), calculated J couplings (cm⁻¹), ground state spin and energetic separations between the ground and first excited states (cm⁻¹) for proton-optimized idealized cubanes where all heavy atom positions are kept fixed at the geometry of model **3**.

Model	Charge	E_{rel}	J_{12}	J_{13}	J_{23}	$S_{\text{T}}(\text{GS})$	ΔE
3	-1	0.0	22.0	20.7	23.2	9/2	191.2
3-H[1]	0	14.1	28.7	32.5	41.2	9/2	273.7
3-H[2]	0	5.1	2.0	10.1	19.0	9/2	49.2
3-H[3]	0	4.0	16.1	-1.4	18.0	9/2	42.5
3-H[4]	0	0.0	13.9	17.3	12.5	9/2	118.0
3-H[1,2]	+1	17.3	-15.5	22.6	35.3	7/2	10.4
3-H[1,3]	+1	15.5	9.1	-8.3	40.9	7/2	2.9
3-H[1,4]	+1	12.9	19.5	30.4	8.8	9/2	119.7
3-H[2,3]	+1	9.1	13.4	-1.3	19.6	9/2	39.2
3-H[2,4]	+1	2.1	4.0	11.9	13.5	9/2	61.8
3-H[3,4]	+1	0.0	7.0	7.7	15.0	9/2	65.7
3-H[1,2,3]	+2	17.8	-18.3	-1.7	30.8	3/2	46.4
3-H[1,2,4]	+2	12.4	-17.9	26.6	14.8	5/2	10.4
3-H[1,3,4]	+2	10.4	13.0	-1.1	14.3	9/2	34.0
3-H[2,3,4]	+2	0.0	5.7	8.8	15.7	9/2	64.2
3-H[1,2,3,4]	+3	0.0	-20.5	-2.1	16.0	3/2	50.0

Table S5. Calculated effective ^{55}Mn hyperfine coupling constants (MHz) for cubane **3** and its fully optimized protonated derivatives.

	Mn1	Mn2	Mn3
3	-212	-211	-213
3-H[1]	-192	-182	-183
3-H[2]	-183	-168	-160
3-H[3]	-180	-156	-166
3-H[4]	-161	-182	-182
3-H[1,2]	-200	-187	-182
3-H[1,3]	-196	-182	-183
3-H[1,4]	-187	-199	-198
3-H[2,3]	-189	-169	-167
3-H[2,4]	-184	-189	-186
3-H[3,4]	-184	-184	-185
3-H[1,2,3]	-193	-186	-181
3-H[1,2,4]	-198	-201	-200
3-H[1,3,4]	-198	-200	-192
3-H[2,3,4]	-192	-193	-191
3-H[1,2,3,4]	-196	-203	-199

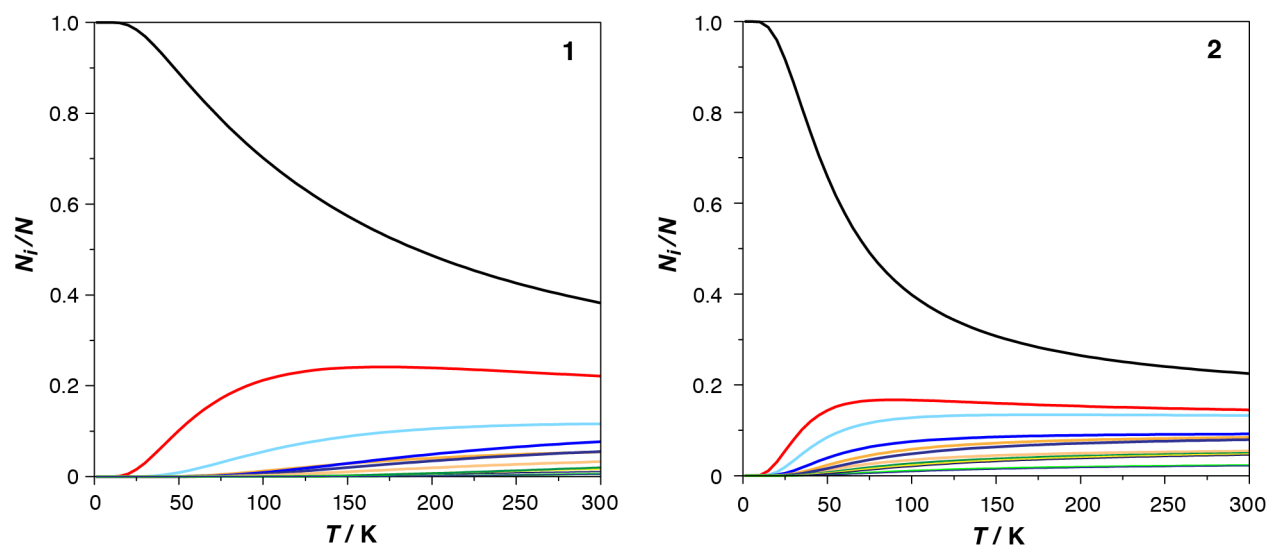


Figure S1. Boltzmann population analysis for cubanes **1** (left) and **2** (right), based on energy levels computed at the XRD structures.

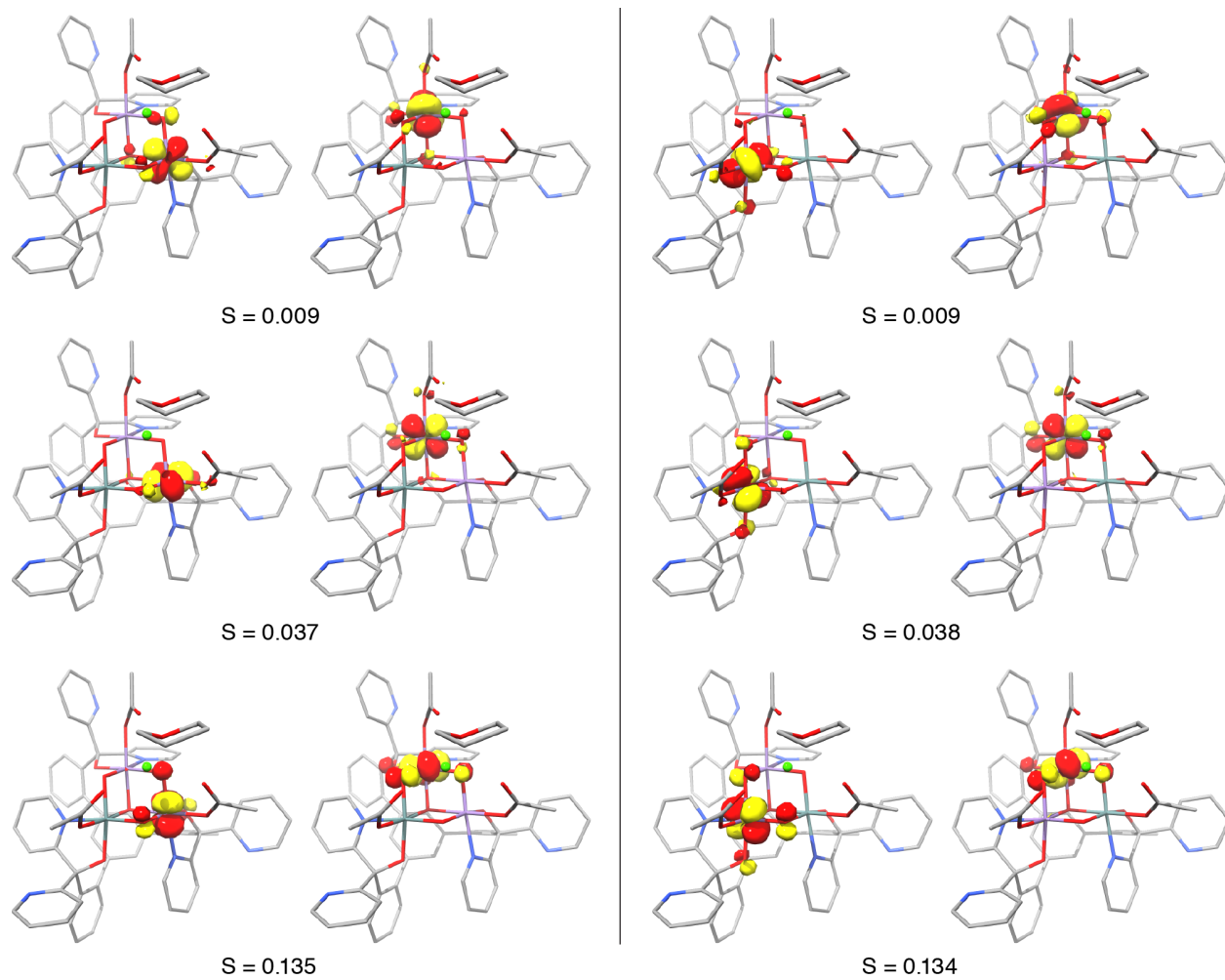


Figure S2. Magnetic orbital pairs and overlap integrals obtained with the corresponding orbital transformation for cubane **2** with Mn2 (left) and Mn3 (right) substituted by Ge^{4+} .

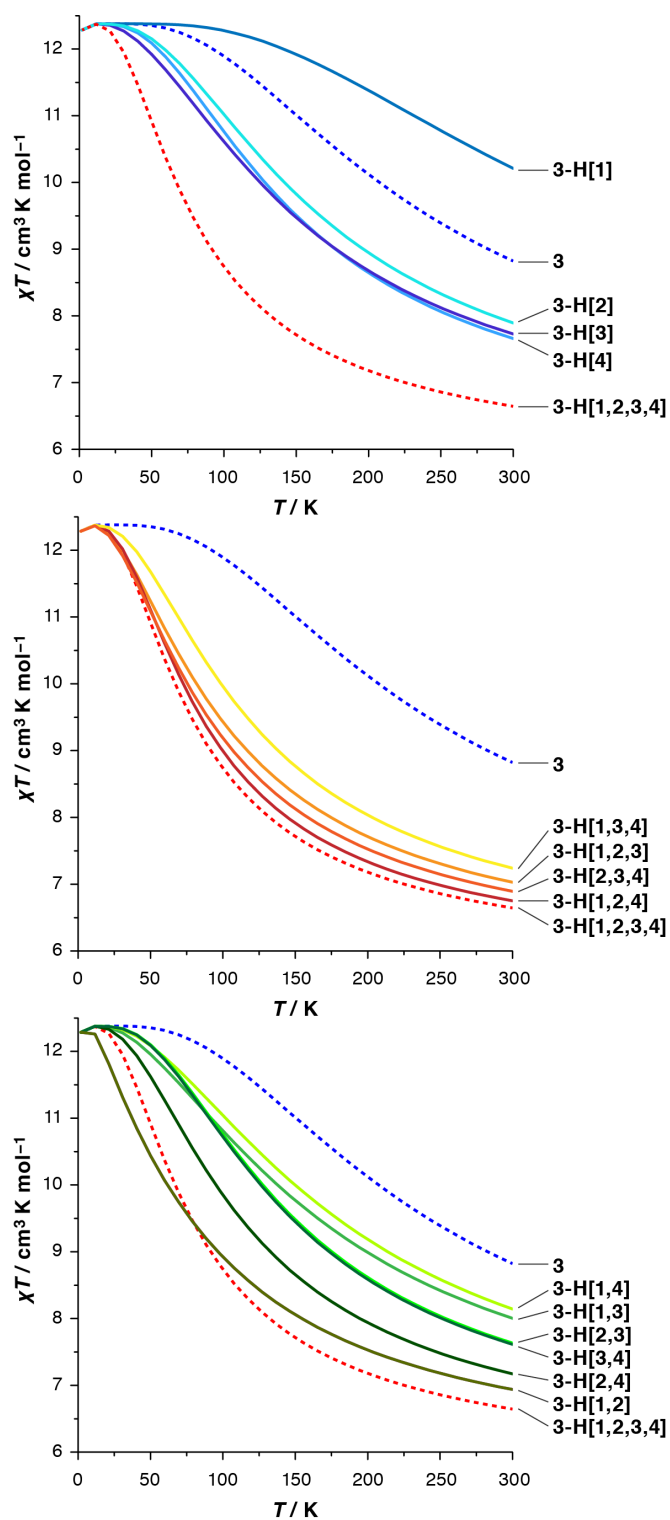


Figure S3. Plots of χT vs. T for the unprotonated cubane **3** and all its protonated derivatives.

Alternative carboxylate bridge coordination in the simplified cubane models

To address the question of alternative coordination modes for the carboxylate bridges in model **3** and its protonated derivatives, further calculations were performed. The possible coordination motifs for a carboxylate bridge above a Mn_2O_2 plane as it is found on the faces of the Mn_3CaO_4 cubane are: bridging bidentate (1), bridging monodentate (2), terminal (3), one-center bidentate and bridging monodentate at the same time (4) (see Figure S4). For coordination modes (2) and (3) the non-coordinating oxygen atom of the acetate bridge can be protonated or not. Coordination mode (4) is the only one where no Mn-OAc bonds are broken, although the possible protonation of the terminal acetate oxygen atom in (2) and (3) can partially compensate for the energy loss associated with a Mn-O bond cleavage.

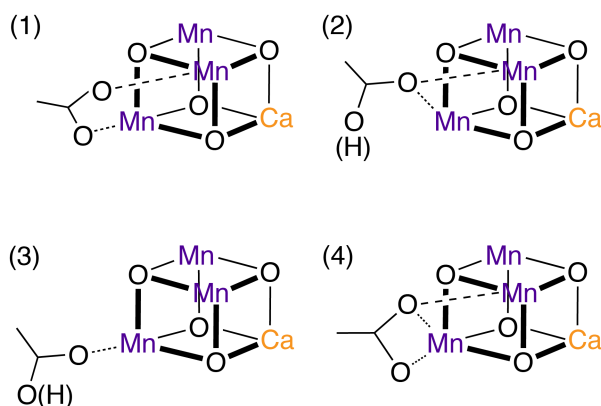


Figure S4. Coordination modes of acetate ligands, bridging bidentate (1), bridging monodentate (2), terminal (3), one-center bidentate and bridging monodentate at the same time (4)

The coordination mode (1) was followed for the models presented in the main text. Models following all three alternative coordination modes were also constructed as protonation isomers of the singly or doubly protonated variants of **3** to have more than one energetic reference point. During the optimization, only motif (3) in protonated and unprotonated variants was found to be a viable alternative. Starting from (2), a terminal acetate results which can form hydrogen bonds

with an oxo bridge or an OH^- ligand if it is protonated. Terminal acetate coordination, motif (3), as the starting geometry is preserved during the geometry optimization. If the models are singly protonated derivatives of **3**, the resulting geometries are within 3.7–9.1 kcal mol⁻¹ of **3-H[1]**, but at least 17 kcal mol⁻¹ higher in energy than **3-H[2]**, **3-H[3]** or **3-H[4]**. Protonation of O1 is excluded based on the results presented in the main text. Acetate coordination isomers of doubly protonated derivatives of **3** are energetically comparable to models where O1 is protonated, but clearly disfavored with respect to the preferred O2, O3 or O4 protonation. With an initial structure modeling coordination mode (4), the acetate bridging motif (1) results.

Table S6. Relative energies in kcal mol⁻¹ for optimized structures with terminal acetates. For all models, the Mn1–Mn3 bridge was modified (see Figure 8). The models are: terminal OAc with O2 protonated (**A**), terminal HOAc with H-bond to O1 (**B**), terminal HOAc with H-bond to O3 and protonated O2 (**C**), terminal HOAc with H-bond to an OH^- ligand and protonated O2 (**D**).

	ΔE (kcal mol ⁻¹) relative to									
	H[1]	H[2]	H[3]	H[4]	H[1,2]	H[1,3]	H[1,4]	H[2,3]	H[2,4]	H[3,4]
A	5.5	18.8	20.9	23.1						
B	3.7	17.1	19.2	21.4						
C					-1.0	1.0	3.5	10.7	15.3	17.5
D					6.5	8.5	11.0	18.1	22.7	24.9

In conclusion, coordination motifs other than bridging bidentate over Mn_2O_2 faces are not plausible for the acetate ligands in our present models (model **3** and its derivatives). This is mostly due to the lack of energetic compensation for the Mn–O bond cleavage and the resulting open coordination site on one Mn ion. It is possible that in real, hydrated systems, a water molecule could potentially saturate this coordination site, but a comparison of such hydrated alternatives is beyond the scope of the present work.

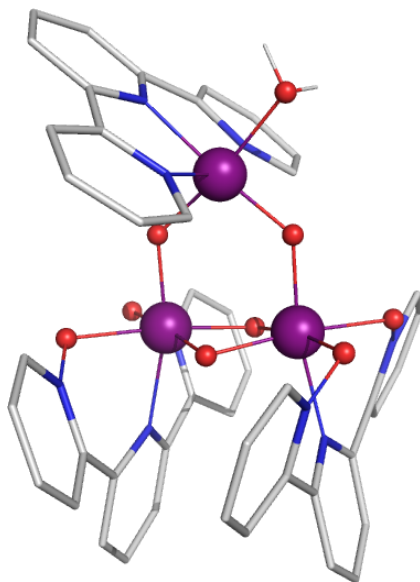


Figure S5. The $[\text{Mn}_3\text{O}_4(\text{terpy})(\text{terpyO}_2)_2(\text{H}_2\text{O})]^{2+}$ complex: it features a type of $\text{Mn(IV)}_3\text{O}_4$ core that allows antiferromagnetic interactions between the Mn ions, leading to a $S = 1/2$ ground state.

Cartesian Coordinates of all optimized models

with final single point energies (in E_h) including van der Waals corrections

1				C	2.500775	9.522218	3.231182
1 - TPSSh				H	3.533245	9.879983	3.215404
-9320.554839681				H	2.358336	8.918474	4.128696
Mn	3.564077	4.939427	3.178825	H	1.838369	10.391260	3.279550
Mn	5.958520	3.562757	3.105321	C	5.126800	4.837054	5.578737
Mn	3.695114	2.715820	1.621969	C	5.395892	5.289496	7.014858
Ca	5.361262	5.380386	0.250870	C	4.183189	4.919255	7.885450
Ca	6.993787	1.626042	0.033544	H	3.271358	5.367516	7.489003
O	4.139953	3.132436	3.395598	H	4.343654	5.281900	8.904455
O	5.322224	5.277957	2.755632	H	4.047633	3.835028	7.925227
O	3.292236	4.478416	1.441663	C	6.669921	4.637413	7.559680
O	5.519441	3.036312	1.362012	H	6.582914	3.548862	7.565091
O	2.952554	6.704452	2.991620	H	6.840844	4.978833	8.584472
O	3.864489	7.246635	1.003646	H	7.537596	4.900994	6.952838
O	4.021490	5.213125	5.069418	C	5.557475	6.823374	6.961816
O	6.025921	4.156720	5.000835	H	4.650028	7.291796	6.576789
O	1.759141	4.292623	3.594573	H	6.393466	7.107269	6.317134
O	1.828108	2.476661	2.239101	H	5.752422	7.201409	7.969244
O	3.176501	2.357506	-0.192283	C	1.249081	3.261319	3.049404
O	3.870301	4.148740	-1.343937	C	-0.205391	2.958907	3.415676
O	5.225631	6.837883	-1.721242	C	-1.051294	4.165986	2.965577
C	4.534449	8.260788	-3.552253	H	-0.986209	4.307793	1.883228
C	3.143672	8.924436	-3.532008	H	-0.710000	5.079138	3.455305
H	2.380041	8.243966	-3.911932	H	-2.098851	3.992947	3.226701
H	3.162150	9.818025	-4.161540	C	-0.684749	1.680514	2.722305
H	2.869813	9.226442	-2.518435	H	-0.076215	0.822750	3.014868
O	3.595683	6.110752	-3.070994	H	-0.627765	1.776345	1.636341
H	3.660045	5.306472	-2.459536	H	-1.723562	1.484825	3.002416
C	4.490762	7.010869	-2.686980	C	-0.286554	2.805746	4.945800
C	4.889343	7.844092	-4.993555	H	0.318031	1.960823	5.286101
H	4.140991	7.160268	-5.397322	H	-1.324632	2.624627	5.237795
H	5.865051	7.353577	-5.030734	H	0.069382	3.709074	5.443036
H	4.929303	8.734624	-5.626347	C	3.228618	3.073369	-1.249821
C	5.592145	9.218482	-2.995046	C	2.416354	2.555912	-2.441912
H	6.581139	8.756448	-3.001787	C	1.139072	3.420689	-2.507383
H	5.361277	9.496773	-1.965030	H	1.380318	4.475576	-2.655295
H	5.622903	10.123927	-3.606676	H	0.555693	3.321008	-1.588428
O	6.960268	7.081018	0.994635	H	0.521202	3.088658	-3.346303
O	6.581238	7.465280	3.171772	C	2.038366	1.083257	-2.245363
H	6.098798	6.564610	3.096303	H	2.929214	0.457954	-2.170873
O	7.713453	4.242126	2.823111	H	1.447040	0.743901	-3.100582
O	8.624379	2.670525	1.506339	H	1.453172	0.944821	-1.335727
O	6.618923	1.918590	3.766962	C	3.235307	2.721653	-3.732856
O	6.951841	0.367682	2.165358	H	3.422762	3.769727	-3.966574
O	3.861896	0.791559	1.900303	H	2.682068	2.283144	-4.568030
O	4.979910	0.167439	0.071633	H	4.198643	2.216671	-3.646087
O	7.081313	4.141666	-0.896781	C	7.059624	7.797472	1.988552
O	8.641061	2.723411	-1.517172	C	7.695589	9.181394	1.933132
O	6.239003	1.140080	-2.336639	C	8.497838	9.322707	0.635699
O	5.325602	-0.905579	-2.248370	H	9.317905	8.602203	0.601956
H	5.139767	-0.601705	-1.296964	H	8.919326	10.329773	0.575736
O	8.555112	-0.126988	-0.671305	H	7.864618	9.150327	-0.235454
O	10.263468	0.762387	-1.830013	C	8.591884	9.424420	3.157297
H	9.689023	1.596197	-1.803303	H	8.029223	9.309167	4.084577
C	3.094030	7.465846	1.942107	H	8.994253	10.440350	3.114878
C	2.182248	8.699830	1.969535	H	9.431542	8.726002	3.173748
C	0.724094	8.204732	2.031215	C	6.524617	10.188533	1.938320
H	0.480855	7.594887	1.156526	H	5.951851	10.110168	2.864277
H	0.045975	9.062807	2.050586	H	5.854092	10.006552	1.095162
H	0.561113	7.602909	2.926356	H	6.919556	11.204764	1.855853
C	2.403657	9.537756	0.708447	C	8.713954	3.214824	2.214941
H	3.439474	9.873464	0.635202	C	10.068806	4.348660	2.467693
H	1.751505	10.415502	0.729870	C	11.089071	3.838436	1.445108
H	2.177469	8.955366	-0.186784	H	10.772083	4.072182	0.426397

H	11.203537	2.755543	1.513447	H	12.133730	-0.340370	-0.060965
H	12.059197	4.309893	1.627377	H	12.106096	-2.068961	0.342558
C	10.503181	3.967097	3.897063	H	10.921774	-0.969905	1.074525
H	9.754569	4.288313	4.624629	C	8.782919	6.253387	-1.906306
H	11.453690	4.455026	4.131854	H	9.512497	6.197491	-1.093991
H	10.639643	2.887473	3.990704	H	7.837521	6.599097	-1.491379
C	9.920396	5.873638	2.371568	H	9.137770	6.995539	-2.628162
H	9.218745	6.236353	3.123231	C	7.402532	-1.392928	-4.248539
H	9.550401	6.171685	1.388508	H	6.993714	-2.277842	-3.758057
H	10.892972	6.347059	2.535868	H	8.291138	-1.068322	-3.702256
C	6.986318	0.752111	3.337171	H	7.704498	-1.660166	-5.264725
C	7.549248	-0.138779	4.457168	1 - TPSS			
C	7.775627	-1.561217	3.940306	-9321.170179348			
H	6.831813	-2.033131	3.660034	Mn	3.552080	4.939717	3.189603
H	8.241657	-2.166951	4.723036	Mn	5.964436	3.573192	3.146749
H	8.422929	-1.558957	3.061596	Mn	3.712961	2.701888	1.640926
C	6.587661	-0.139642	5.656303	Ca	5.381315	5.370663	0.264541
H	6.431834	0.875926	6.022126	Ca	7.062608	1.613529	0.090464
H	7.005134	-0.750229	6.462459	O	4.136941	3.126813	3.426495
H	5.615044	-0.556019	5.381224	O	5.319804	5.292382	2.777900
C	8.893670	0.489159	4.877535	O	3.298364	4.468764	1.442714
H	8.741098	1.504914	5.246024	O	5.547555	3.030280	1.392595
H	9.586913	0.524480	4.032444	O	2.932215	6.708228	2.985303
H	9.347838	-0.110911	5.671471	O	3.867869	7.247708	0.994615
C	4.295202	-0.095000	1.094025	O	3.989867	5.232920	5.088653
C	3.899378	-1.541787	1.396452	O	6.011830	4.183698	5.048112
C	3.568692	-1.708597	2.884238	O	1.739090	4.286038	3.592111
H	2.759817	-1.041293	3.183175	O	1.831275	2.452931	2.241371
H	4.439086	-1.479501	3.501807	O	3.203249	2.330728	-0.183876
H	3.269185	-2.742339	3.078756	O	3.890615	4.134123	-1.340998
C	2.641995	-1.828977	0.547757	O	5.246885	6.830028	-1.715427
H	1.828944	-1.149611	0.815721	C	4.534009	8.267576	-3.538106
H	2.311056	-2.855962	0.726341	C	3.129013	8.912478	-3.534616
H	2.853003	-1.717364	-0.518583	H	2.379875	8.222374	-3.932377
C	5.040486	-2.486934	0.990387	H	3.144146	9.813222	-4.158402
H	5.206964	-2.478183	-0.087837	H	2.834748	9.202959	-2.520913
H	4.788224	-3.509218	1.285707	O	3.602937	6.101222	-3.067521
H	5.973289	-2.197404	1.477543	H	3.675345	5.289575	-2.454504
C	8.097464	3.861154	-1.602692	C	4.500805	7.007519	-2.679136
C	8.629099	4.892158	-2.601600	C	4.916712	7.864096	-4.981739
C	9.969854	4.437805	-3.185703	H	4.184951	7.167055	-5.399754
H	9.871721	3.480711	-3.701793	H	5.904120	7.391519	-5.008342
H	10.721350	4.321275	-2.400972	H	4.947792	8.760861	-5.610599
H	10.332146	5.181677	-3.901482	C	5.572645	9.241442	-2.959836
C	7.574076	4.997875	-3.720937	H	6.570760	8.793499	-2.955029
H	7.449355	4.040621	-4.232623	H	5.322531	9.512101	-1.929642
H	7.890469	5.744742	-4.455341	H	5.598043	10.152271	-3.568212
H	6.611860	5.295977	-3.304879	O	6.975210	7.083551	1.014780
C	5.965702	0.071407	-2.874941	O	6.556175	7.497368	3.191412
C	6.355088	-0.261246	-4.308747	H	6.076188	6.585617	3.115595
C	5.114583	-0.740505	-5.083674	O	7.725419	4.265378	2.882572
H	4.351869	0.041213	-5.124312	O	8.671254	2.690077	1.574807
H	4.678880	-1.624306	-4.615687	O	6.628036	1.930994	3.828783
H	5.401868	-0.990345	-6.108552	O	6.997404	0.364764	2.234080
C	6.962969	0.979532	-4.969358	O	3.882528	0.769100	1.926649
H	6.237623	1.794577	-5.016110	O	5.041851	0.158322	0.106409
H	7.276440	0.735022	-5.987633	O	7.118800	4.137847	-0.873854
H	7.828531	1.334445	-4.407532	O	8.705115	2.722304	-1.464943
C	9.674410	-0.219326	-1.169874	O	6.326807	1.119374	-2.311557
C	10.524301	-1.473934	-1.016451	O	5.343029	-0.907371	-2.224615
C	11.334349	-1.756959	-2.290110	H	5.185083	-0.602618	-1.259994
H	10.674765	-1.947000	-3.141078	O	8.620736	-0.143869	-0.641784
H	11.952581	-2.645490	-2.135720	O	10.200562	0.709763	-2.014077
H	11.983465	-0.917340	-2.540134	H	9.657479	1.567483	-1.902438
C	9.617002	-2.661384	-0.673529	C	3.087761	7.472317	1.931572
H	8.916278	-2.866648	-1.486490	C	2.178567	8.714820	1.953098
H	9.035270	-2.460996	0.227006	C	0.712705	8.225298	2.001807
H	10.228933	-3.552715	-0.511406	H	0.474574	7.614850	1.123171
C	11.483196	-1.188605	0.162503				

H	0.037179	9.088701	2.014471	H	10.830266	4.113931	0.523822
H	0.538124	7.623486	2.897706	H	11.259228	2.798947	1.621261
C	2.415507	9.555483	0.690896	H	12.101133	4.364347	1.745822
H	3.455527	9.887772	0.626564	C	10.510421	4.007332	4.000673
H	1.765473	10.438077	0.707784	H	9.747858	4.325830	4.718542
H	2.193398	8.973867	-0.208731	H	11.457212	4.501078	4.249492
C	2.491008	9.537462	3.222147	H	10.650720	2.925896	4.096563
H	3.527550	9.890915	3.215134	C	9.935649	5.915519	2.459455
H	2.337547	8.932594	4.120021	H	9.215021	6.275520	3.197865
H	1.830676	10.411578	3.265450	H	9.582732	6.209199	1.466122
C	5.102153	4.873669	5.611046	H	10.903534	6.397248	2.642765
C	5.366143	5.363210	7.041322	C	7.002328	0.755113	3.410837
C	4.153872	4.998974	7.923514	C	7.534294	-0.134701	4.553570
H	3.235075	5.428796	7.516091	C	7.760322	-1.567426	4.051109
H	4.310805	5.388361	8.935873	H	6.816581	-2.034720	3.753694
H	4.030321	3.912167	7.988779	H	8.204708	-2.171929	4.850644
C	6.651645	4.736762	7.602440	H	8.428534	-1.578213	3.185035
H	6.578023	3.645163	7.632291	C	6.543461	-0.118492	5.734905
H	6.818006	5.103826	8.621752	H	6.390446	0.902867	6.093171
H	7.518505	4.998507	6.989114	H	6.937291	-0.730739	6.554983
C	5.511547	6.902446	6.952823	H	5.570607	-0.526418	5.439137
H	4.595276	7.353333	6.560910	C	8.878974	0.487183	5.000258
H	6.343096	7.180920	6.296188	H	8.726874	1.509437	5.358138
H	5.707496	7.305524	7.953016	H	9.592528	0.509376	4.168719
C	1.236972	3.245051	3.043102	H	9.310610	-0.111929	5.810766
C	-0.227569	2.942722	3.389953	C	4.336961	-0.115099	1.120908
C	-1.070900	4.142522	2.899114	C	3.947157	-1.570912	1.410299
H	-0.986065	4.262720	1.813129	C	3.573953	-1.745289	2.892024
H	-0.739966	5.068273	3.377667	H	2.746048	-1.087719	3.168778
H	-2.124935	3.971263	3.145394	H	4.424702	-1.505900	3.537045
C	-0.691768	1.646400	2.709194	H	3.281170	-2.785447	3.076190
H	-0.086242	0.793648	3.030647	C	2.714840	-1.873472	0.521509
H	-0.614044	1.722034	1.620461	H	1.884195	-1.203101	0.766926
H	-1.737797	1.453122	2.973384	H	2.391073	-2.907059	0.689720
C	-0.339109	2.817350	4.925577	H	2.956378	-1.757237	-0.540208
H	0.264643	1.980632	5.294012	C	5.115621	-2.503763	1.034676
H	-1.384246	2.635297	5.200601	H	5.309386	-2.494551	-0.041499
H	0.002645	3.733847	5.413929	H	4.869807	-3.531079	1.327078
C	3.247756	3.051576	-1.245174	H	6.033288	-2.198678	1.545649
C	2.427360	2.532231	-2.437081	C	8.141353	3.855450	-1.579860
C	1.142098	3.394966	-2.493627	C	8.662659	4.877641	-2.600324
H	1.379150	4.453592	-2.639296	C	9.999018	4.414394	-3.199608
H	0.562781	3.289265	-1.569887	H	9.890964	3.454730	-3.714522
H	0.520234	3.062258	-3.332516	H	10.760306	4.295780	-2.421499
C	2.053713	1.053261	-2.241291	H	10.357071	5.156168	-3.923479
H	2.948001	0.427438	-2.177445	C	7.591841	4.981048	-3.711358
H	1.454033	0.714957	-3.094309	H	7.460536	4.019898	-4.218967
H	1.475447	0.910290	-1.324985	H	7.901725	5.726225	-4.453956
C	3.240613	2.704314	-3.736328	H	6.632554	5.282603	-3.284969
H	3.418200	3.756014	-3.972865	C	5.997745	0.064657	-2.859563
H	2.686715	2.258377	-4.570215	C	6.330751	-0.261543	-4.314664
H	4.210965	2.207168	-3.652940	C	5.058882	-0.735238	-5.050487
C	7.056606	7.816260	2.005942	H	4.293522	0.047877	-5.056537
C	7.693754	9.204660	1.942349	H	4.639221	-1.625003	-4.573818
C	8.530061	9.325103	0.658454	H	5.309618	-0.976663	-6.089593
H	9.350779	8.600941	0.655015	C	6.923343	0.982355	-4.994064
H	8.956178	10.332613	0.593494	H	6.201228	1.804604	-5.010145
H	7.916112	9.141072	-0.227087	H	7.196518	0.739973	-6.027054
C	8.561556	9.473201	3.187615	H	7.815102	1.328379	-4.463898
H	7.974300	9.375603	4.104445	C	9.669576	-0.263708	-1.282595
H	8.965871	10.490592	3.135405	C	10.498222	-1.546880	-1.231423
H	9.402135	8.773854	3.238973	C	11.290000	-1.769953	-2.532501
C	6.518393	10.213928	1.899198	H	10.617421	-1.886322	-3.389203
H	5.921607	10.152799	2.814013	H	11.885670	-2.685343	-2.441296
H	5.867647	10.014155	1.041648	H	11.962255	-0.932994	-2.736780
H	6.916028	11.230895	1.806534	C	9.568000	-2.739562	-0.946271
C	8.743359	3.700447	2.286543	H	8.855587	-2.886206	-1.764996
C	10.093561	4.387064	2.560109	H	8.998544	-2.578857	-0.027247
C	11.135791	3.883054	1.549448	H	10.165582	-3.651918	-0.841587

C	11.480282	-1.356597	-0.044843	H	0.605202	7.787973	0.972556
H	12.144376	-0.503888	-0.219823	H	0.156676	9.245393	1.895774
H	12.092524	-2.258715	0.065754	H	0.550457	7.725422	2.751953
H	10.931690	-1.190785	0.888287	C	2.639763	9.660199	0.740075
C	8.829808	6.247378	-1.912129	H	3.691265	9.974739	0.769169
H	9.566290	6.192055	-1.102669	H	2.006135	10.559760	0.724678
H	7.886692	6.600841	-1.491701	H	2.484517	9.105005	-0.195343
H	9.183922	6.984652	-2.643052	C	2.547541	9.569953	3.265336
C	7.379009	-1.401038	-4.299222	H	3.602976	9.870175	3.344336
H	6.986266	-2.287635	-3.793337	H	2.300581	8.953025	4.139077
H	8.292191	-1.078429	-3.789089	H	1.930396	10.481061	3.287989
H	7.639139	-1.668054	-5.329633	C	5.023364	4.890505	5.651898
				C	5.324891	5.469513	7.043401
				C	4.081381	5.330215	7.940672
1 - BP				H	3.209479	5.814698	7.483173
-9321.228367326				H	4.277533	5.800944	8.915688
Mn	3.492440	4.953093	3.206666	H	3.836646	4.271915	8.114809
Mn	5.888282	3.532923	3.208611	C	6.532699	4.766004	7.677933
Mn	3.640301	2.707832	1.644123	H	6.344578	3.690770	7.805721
Ca	5.388519	5.349879	0.310654	H	6.732930	5.203977	8.667279
Ca	7.057582	1.599948	0.157709	H	7.430528	4.877136	7.056356
O	4.043445	3.121729	3.445222	C	5.642893	6.965382	6.799222
O	5.280773	5.269716	2.827648	H	4.776608	7.480880	6.363099
O	3.260723	4.488106	1.451567	H	6.493906	7.083789	6.112457
O	5.492673	3.000209	1.440860	H	5.897325	7.445593	7.756182
O	2.920878	6.742739	2.989533	C	1.147373	3.287771	3.024284
O	3.956131	7.275893	1.043682	C	-0.324903	3.001685	3.366965
O	3.913529	5.245943	5.119889	C	-1.150110	4.220449	2.898379
O	5.917416	4.155980	5.117289	H	-1.069375	4.357691	1.809833
O	1.656792	4.324746	3.577991	H	-0.803605	5.139145	3.389595
O	1.737694	2.486785	2.226189	H	-2.210502	4.063352	3.146564
O	3.166656	2.355578	-0.205487	C	-0.810060	1.725260	2.666641
O	3.957717	4.142636	-1.326928	H	-0.217272	0.853128	2.973628
O	5.260937	6.858276	-1.608508	H	-0.731547	1.814548	1.574779
C	4.480832	8.375401	-3.328342	H	-1.863176	1.542563	2.928013
C	3.038693	8.811399	-3.648617	C	-0.432096	2.849218	4.899318
H	2.512887	8.052362	-4.241708	H	0.165196	1.996161	5.253691
H	3.058313	9.751483	-4.219611	H	-1.481808	2.672190	5.177814
H	2.465663	8.985683	-2.726110	H	-0.078173	3.754952	5.408572
O	3.621353	6.147821	-2.978515	C	3.320190	3.050426	-1.272287
H	3.732477	5.303167	-2.405452	C	2.646361	2.497529	-2.540271
C	4.483692	7.066419	-2.543505	C	1.325835	3.285053	-2.712605
C	5.258150	8.100825	-4.638777	H	1.511062	4.362807	-2.824564
H	4.768369	7.317312	-5.233520	H	0.661841	3.130873	-1.849710
H	6.288452	7.783156	-4.422653	H	0.805972	2.931548	-3.615850
H	5.299283	9.021898	-5.239064	C	2.347736	0.997666	-2.386962
C	5.200650	9.453094	-2.502300	H	3.270449	0.423944	-2.233373
H	6.230334	9.151452	-2.269936	H	1.855710	0.624915	-3.297891
H	4.680970	9.626954	-1.549838	H	1.690731	0.808047	-1.528748
H	5.225358	10.396946	-3.066270	C	3.571118	2.735095	-3.749998
O	7.024818	6.972184	1.060417	H	3.701309	3.801940	-3.970311
O	6.551460	7.423179	3.221856	H	3.135946	2.259387	-4.641531
H	6.047248	6.508408	3.148721	H	4.565553	2.306826	-3.568378
O	7.673729	4.202445	2.968946	C	7.081294	7.719213	2.045785
O	8.626800	2.581883	1.720375	C	7.712520	9.110022	1.956187
O	6.515554	1.872128	3.894847	C	8.748611	9.131797	0.821313
O	6.880192	0.328963	2.274809	H	9.590406	8.460831	1.042405
O	3.804688	0.761726	1.908142	H	9.143060	10.151539	0.700362
O	5.001858	0.215105	0.089005	H	8.299965	8.808365	-0.126748
O	7.103266	4.050282	-0.768352	C	8.355193	9.526075	3.289442
O	8.758237	2.721086	-1.383288	H	7.619839	9.529637	4.104040
O	6.399194	1.157803	-2.279467	H	8.779813	10.536826	3.195333
O	5.456471	-0.891358	-2.169870	H	9.167824	8.838222	3.565424
H	5.253897	-0.568619	-1.208055	C	6.537432	10.056774	1.605618
O	8.539140	-0.188094	-0.597809	H	5.779311	10.053313	2.401343
O	9.962725	0.598917	-2.170085	H	6.058305	9.743823	0.666878
H	9.483625	1.489847	-1.984464	H	6.912766	11.084076	1.485502
C	3.149906	7.516396	1.956031	C	8.690924	3.629185	2.381944
C	2.287614	8.795442	1.957181	C	10.034704	4.356449	2.585299
C	0.807522	8.357713	1.891944				

C	11.075420	3.770071	1.620418	H	9.913153	-3.763974	-1.046328
H	10.747534	3.875745	0.576390	C	11.253718	-1.532690	-0.134053
H	11.229013	2.699186	1.807788	H	11.942211	-0.682770	-0.247884
H	12.035644	4.292856	1.747185	H	11.851430	-2.452364	-0.047526
C	10.462225	4.130033	4.051817	H	10.680273	-1.399003	0.793810
H	9.696222	4.509369	4.742531	C	8.638838	6.173380	-2.067279
H	11.407364	4.659100	4.248460	H	9.483329	6.171786	-1.361518
H	10.618429	3.061467	4.258490	H	7.749507	6.529786	-1.533569
C	9.848774	5.861364	2.322048	H	8.869195	6.890639	-2.870451
H	9.140285	6.295735	3.039279	C	7.428855	-1.409936	-4.266179
H	9.456775	6.041443	1.311451	H	7.020277	-2.288900	-3.750553
H	10.815430	6.378433	2.422439	H	8.360925	-1.107185	-3.768751
C	6.938754	0.723348	3.451065	H	7.673567	-1.690519	-5.301426
C	7.623361	-0.123787	4.545450				
C	7.895486	-1.541300	4.026494	1 - PBE			
H	6.958416	-2.071380	3.805304	-9313.832508836			
H	8.443444	-2.117368	4.787587	Mn	3.557310	4.939068	3.196942
H	8.490573	-1.516522	3.103777	Mn	5.977107	3.557916	3.156292
C	6.750602	-0.164448	5.8113043	Mn	3.711950	2.693753	1.638826
H	6.546896	0.850508	6.177639	Ca	5.376449	5.380344	0.250216
H	7.266342	-0.731239	6.603386	Ca	7.081516	1.592236	0.101179
H	5.786494	-0.656330	5.614618	O	4.139798	3.117420	3.429919
C	8.957991	0.598108	4.847735	O	5.333735	5.286177	2.785282
H	8.768949	1.609637	5.232025	O	3.300480	4.464573	1.447027
H	9.570702	0.682811	3.937588	O	5.554018	3.018405	1.395621
H	9.527087	0.032600	5.601403	O	2.936391	6.716790	2.988761
C	4.339788	-0.096830	1.125661	O	3.859311	7.255388	0.990790
C	4.112143	-1.577485	1.464193	O	3.999259	5.233036	5.107303
C	3.829289	-1.743151	2.965537	O	6.018386	4.176302	5.072779
H	2.947970	-1.165861	3.271722	O	1.731440	4.283719	3.600493
H	4.683881	-1.390341	3.559538	O	1.814882	2.451040	2.247051
H	3.659041	-2.805182	3.197527	O	3.201859	2.325780	-0.202013
C	2.882381	-2.018801	0.635396	O	3.870586	4.141083	-1.353174
H	1.991507	-1.437088	0.913260	O	5.214972	6.858927	-1.717200
H	2.675745	-3.083624	0.821506	C	4.459722	8.302683	-3.519782
H	3.063204	-1.887468	-0.441745	C	3.032918	8.886483	-3.558377
C	5.352800	-2.397383	1.061289	H	2.321012	8.170729	-3.989783
H	5.500445	-2.412232	-0.026518	H	3.027580	9.799415	-4.172380
H	5.229391	-3.437641	1.397969	H	2.687935	9.154325	-2.548900
H	6.257295	-1.977128	1.520785	O	3.575268	6.111831	-3.067006
C	8.087488	3.790870	-1.538496	H	3.661155	5.293090	-2.457122
C	8.418279	4.771238	-2.671883	C	4.455993	7.030977	-2.673254
C	9.667270	4.315748	-3.437463	C	4.910058	7.924244	-4.947610
H	9.518924	3.323564	-3.886599	H	4.222759	7.197272	-5.400799
H	10.540889	4.255487	-2.773338	H	5.920895	7.490592	-4.942578

-9313.832508836

C	0.722266	8.257550	1.998265	C	10.126492	4.358356	2.593339
H	0.482109	7.658663	1.106609	C	11.181538	3.833801	1.611296
H	0.047838	9.127262	2.017955	H	10.899000	4.052838	0.571400
H	0.531351	7.641571	2.887060	H	11.297481	2.745188	1.696674
C	2.441039	9.588154	0.719212	H	12.151753	4.310288	1.818770
H	3.486848	9.920348	0.666572	C	10.512497	3.996171	4.043282
H	1.792874	10.477345	0.738082	H	9.742815	4.338812	4.749328
H	2.227035	9.018842	-0.195893	H	11.467732	4.477254	4.304023
C	2.502005	9.540450	3.243460	H	10.633127	2.909586	4.162395
H	3.547269	9.883499	3.249272	C	9.983028	5.883664	2.462855
H	2.335839	8.930297	4.140997	H	9.249311	6.268211	3.182929
H	1.851961	10.427368	3.293145	H	9.649919	6.166226	1.453578
C	5.111931	4.875246	5.630169	H	10.953993	6.365742	2.655122
C	5.387366	5.387619	7.053843	C	7.011457	0.730163	3.430212
C	4.163314	5.093619	7.939314	C	7.526813	-0.171077	4.576329
H	3.255552	5.544812	7.518500	C	7.758452	-1.596983	4.064947
H	4.329843	5.505577	8.945980	H	6.817129	-2.062599	3.740438
H	3.996945	4.010416	8.037186	H	8.185628	-2.215717	4.868819
C	6.643879	4.729550	7.636548	H	8.446543	-1.604855	3.208682
H	6.532356	3.637619	7.695133	C	6.516769	-0.167727	5.737272
H	6.821715	5.115322	8.651617	H	6.352017	0.852643	6.107304
H	7.528572	4.941945	7.021641	H	6.894514	-0.790099	6.563085
C	5.594488	6.913776	6.922815	H	5.544717	-0.574763	5.420514
H	4.694763	7.396863	6.518031	C	8.862621	0.443515	5.047729
H	6.438533	7.144821	6.255722	H	8.710279	1.466775	5.417238
H	5.809974	7.340450	7.914084	H	9.593328	0.475080	4.225059
C	1.224147	3.246978	3.047815	H	9.286985	-0.165465	5.860749
C	-0.249254	2.957735	3.383661	C	4.326094	-0.145618	1.118361
C	-1.075385	4.145256	2.845445	C	3.903999	-1.597919	1.401009
H	-0.972096	4.237431	1.753686	C	3.530576	-1.773174	2.880141
H	-0.750070	5.088704	3.303830	H	2.723255	-1.088895	3.170550
H	-2.139701	3.988010	3.076333	H	4.392837	-1.569244	3.530717
C	-0.710157	1.648945	2.731255	H	3.202201	-2.808095	3.059097
H	-0.112667	0.795997	3.081837	C	2.663473	-1.861616	0.516636
H	-0.618736	1.692508	1.637375	H	1.846787	-1.168963	0.768003
H	-1.764441	1.464082	2.986371	H	2.308558	-2.890572	0.679926
C	-0.386025	2.871924	4.916170	H	2.900387	-1.747850	-0.551236
H	0.207373	2.038043	5.319772	C	5.043439	-2.558795	1.020864
H	-1.440006	2.701946	5.182761	H	5.250633	-2.545058	-0.057388
H	-0.045551	3.800037	5.393366	H	4.764996	-3.586758	1.297567
C	3.238298	3.050490	-1.260510	H	5.972244	-2.293160	1.544779
C	2.422879	2.527469	-2.458662	C	8.130465	3.860082	-1.600630
C	1.136605	3.382660	-2.518004	C	8.645765	4.874158	-2.637451
H	1.364292	4.447960	-2.664172	C	9.978018	4.410391	-3.238899
H	0.550136	3.274873	-1.593449	H	9.874475	3.441095	-3.746421
H	0.513674	3.047134	-3.360891	H	10.750230	4.302186	-2.463589
C	2.053815	1.049366	-2.269048	H	10.332099	5.147184	-3.976139
H	2.950995	0.418193	-2.211754	C	7.572260	4.964439	-3.742977
H	1.448896	0.710020	-3.123420	H	7.432389	3.992805	-4.239065
H	1.476904	0.896210	-1.347950	H	7.880590	5.698610	-4.503709
C	3.240701	2.702205	-3.751618	H	6.609190	5.277629	-3.320654
H	3.415983	3.757559	-3.995290	C	6.009335	0.045310	-2.851838
H	2.694472	2.249468	-4.592747	C	6.345591	-0.280678	-4.309231
H	4.218968	2.209595	-3.664848	C	5.078396	-0.753784	-5.046602
C	7.075083	7.806692	1.998730	H	4.308414	0.031543	-5.057849
C	7.709416	9.199552	1.939422	H	4.651581	-1.646167	-4.570835
C	8.578920	9.314786	0.680579	H	5.329659	-0.998190	-6.089580
H	9.412526	8.598521	0.706403	C	6.937309	0.960149	-4.988927
H	8.998522	10.329456	0.613100	H	6.213829	1.787496	-5.010168
H	7.992791	9.112904	-0.225551	H	7.214711	0.717724	-6.025317
C	8.540462	9.484306	3.201795	H	7.831844	1.312844	-4.457906
H	7.929277	9.399354	4.109553	C	9.715797	-0.240705	-1.280766
H	8.950573	10.504119	3.149926	C	10.564323	-1.514848	-1.248773
H	9.383222	8.783343	3.288655	C	11.331425	-1.723098	-2.563577
C	6.529347	10.195701	1.851870	H	10.642877	-1.850253	-3.412068
H	5.899949	10.140383	2.750965	H	11.946768	-2.632250	-2.489131
H	5.902353	9.983752	0.973346	H	11.989353	-0.873246	-2.784708
H	6.918812	11.220849	1.761404	C	9.659383	-2.720212	-0.952175
C	8.772513	3.677680	2.304253	H	8.931755	-2.879387	-1.761532

H	9.097903	-2.573104	-0.020515	C	2.182248	8.699830	1.969535
H	10.272382	-3.628753	-0.858770	C	0.724094	8.204732	2.031215
C	11.563444	-1.312764	-0.083233	H	0.480855	7.594887	1.156526
H	12.216061	-0.447046	-0.265997	H	0.045975	9.062807	2.050586
H	12.195304	-2.208146	0.016449	H	0.561113	7.602909	2.926356
H	11.031541	-1.156823	0.866577	C	2.403657	9.537756	0.708447
C	8.817679	6.247338	-1.962780	H	3.439474	9.873464	0.635202
H	9.556639	6.199629	-1.148351	H	1.751505	10.415502	0.729870
H	7.874127	6.614659	-1.541592	H	2.177469	8.955366	-0.186784
H	9.176614	6.981471	-2.701053	C	2.500775	9.522218	3.231182
C	7.394353	-1.415457	-4.288232	H	3.533245	9.879983	3.215404
H	7.004010	-2.308316	-3.781430	H	2.358336	8.918474	4.128696
H	8.310681	-1.091264	-3.773739	H	1.838369	10.391260	3.279550
H	7.662838	-1.686193	-5.320365	C	5.126800	4.837054	5.578737
1 - PBE0				C	5.395892	5.289496	7.014858
-9320.554839681				C	4.183189	4.919255	7.885450
Mn	3.564077	4.939427	3.178825	H	3.271358	5.367516	7.489003
Mn	5.958520	3.562757	3.105321	H	4.343654	5.281900	8.904455
Mn	3.695114	2.715820	1.621969	H	4.047633	3.835028	7.925227
Ca	5.361262	5.380386	0.250870	C	6.669921	4.637413	7.559680
Ca	6.993787	1.626042	0.033544	H	6.582914	3.548862	7.565091
O	4.139953	3.132436	3.395598	H	6.840844	4.978833	8.584472
O	5.322224	5.277957	2.755632	H	7.537596	4.900994	6.952838
O	3.292236	4.478416	1.441663	C	5.557475	6.823374	6.961816
O	5.519441	3.036312	1.362012	H	4.650028	7.291796	6.576789
O	2.952554	6.704452	2.991620	H	6.393466	7.107269	6.317134
O	3.864489	7.246635	1.003646	H	5.752422	7.201409	7.969244
O	4.021490	5.213125	5.069418	C	1.249081	3.261319	3.049404
O	6.025921	4.156720	5.000835	C	-0.205391	2.958907	3.415676
O	1.759141	4.292623	3.594573	H	-1.051294	4.165986	2.965577
O	1.828108	2.476661	2.239101	C	-0.986209	4.307793	1.883228
O	3.176501	2.357506	-0.192283	H	-0.710000	5.079138	3.455305
O	3.870301	4.148740	-1.343937	H	-2.098851	3.992947	3.226701
O	5.225631	6.837883	-1.721242	C	-0.684749	1.680514	2.722305
C	4.534449	8.260788	-3.552253	H	-0.076215	0.822750	3.014868
C	3.143672	8.924436	-3.532008	H	-0.627765	1.776345	1.636341
H	2.380041	8.243966	-3.911932	H	-1.723562	1.484825	3.002416
H	3.162150	9.818025	-4.161540	C	-0.286554	2.805746	4.945800
H	2.869813	9.226442	-2.518435	H	0.318031	1.960823	5.286101
O	3.595683	6.110752	-3.070994	H	-1.324632	2.624627	5.237795
H	3.660045	5.306472	-2.459536	H	0.069382	3.709074	5.443036
C	4.490762	7.010869	-2.686980	C	3.228618	3.073369	-1.249821
C	4.889343	7.844092	-4.993555	C	2.416354	2.555912	-2.441912
H	4.140991	7.160268	-5.397322	C	1.139072	3.420689	-2.507383
H	5.865051	7.353577	-5.030734	H	1.380318	4.475576	-2.655295
H	4.929303	8.734624	-5.626347	H	0.555693	3.321008	-1.588428
C	5.592145	9.218482	-2.995046	H	0.521202	3.088658	-3.346303
H	6.581139	8.756448	-3.001787	C	2.038366	1.083257	-2.245363
H	5.361277	9.496773	-1.965030	H	2.929214	0.457954	-2.170873
H	5.622903	10.123927	-3.606676	H	1.447040	0.743901	-3.100582
O	6.960268	7.081018	0.994635	H	1.453172	0.944821	-1.335727
O	6.581238	7.465280	3.171772	C	3.235307	2.721653	-3.732856
H	6.098798	6.564610	3.096303	H	3.422762	3.769727	-3.966574
O	7.713453	4.242126	2.823111	H	2.682068	2.283144	-4.568030
O	8.624379	2.670525	1.506339	H	4.198643	2.216671	-3.646087
O	6.618923	1.918590	3.766962	C	7.059624	7.797472	1.988552
O	6.951841	0.367682	2.165358	C	7.695589	9.181394	1.933132
O	3.861896	0.791559	1.900303	C	8.497838	9.322707	0.635699
O	4.979910	0.167439	0.071633	H	9.317905	8.602203	0.601956
O	7.081313	4.141666	-0.896781	H	8.919326	10.329773	0.575736
O	8.641061	2.723411	-1.517172	H	7.864618	9.150327	-0.235454
O	6.239003	1.140080	-2.336639	C	8.591884	9.424420	3.157297
O	5.325602	-0.905579	-2.248370	H	8.029223	9.309167	4.084577
H	5.139767	-0.601705	-1.296964	H	8.994253	10.440350	3.114878
O	8.555112	-0.126988	-0.671305	H	9.431542	8.726002	3.173748
O	10.263468	0.762387	-1.830013	C	6.524617	10.188533	1.938320
H	9.689023	1.596197	-1.803303	H	5.951851	10.110168	2.864277
C	3.094030	7.465846	1.942107	H	5.854092	10.006552	1.095162
				H	6.919556	11.204764	1.855853

C	8.713954	3.674824	2.214941	H	8.916278	-2.866648	-1.486490
C	10.068806	4.348660	2.467693	H	9.035270	-2.460996	0.227006
C	11.089071	3.838436	1.445108	H	10.228933	-3.552715	-0.511406
H	10.772083	4.072182	0.426397	C	11.483196	-1.188605	0.162503
H	11.203537	2.755543	1.513447	H	12.133730	-0.340370	-0.060965
H	12.059197	4.309893	1.627377	H	12.106096	-2.068961	0.342558
C	10.503181	3.967097	3.897063	H	10.921774	-0.969905	1.074525
H	9.754569	4.288313	4.624629	C	8.782919	6.253387	-1.906306
H	11.453690	4.455026	4.131854	H	9.512497	6.197491	-1.093991
H	10.639643	2.887473	3.990704	H	7.837521	6.599097	-1.491379
C	9.920396	5.873638	2.371568	H	9.137770	6.995539	-2.628162
H	9.218745	6.236353	3.123231	C	7.402532	-1.392928	-4.248539
H	9.550401	6.171685	1.388508	H	6.993714	-2.277842	-3.758057
H	10.892972	6.347059	2.535868	H	8.291138	-1.068322	-3.702256
C	6.986318	0.752111	3.337171	H	7.704498	-1.660166	-5.264725
C	7.549248	-0.138779	4.457168				
C	7.775627	-1.561217	3.940306	2			
H	6.831813	-2.033131	3.660034	2 - TPSSh			
H	8.241657	-2.166951	4.723036	-8145.116474031			
H	8.422929	-1.558957	3.061596	Mn	-1.053952	3.026833	0.738234
C	6.587661	-0.139642	5.656303	Mn	-0.784994	1.201156	2.858122
H	6.431834	0.875926	6.022126	Mn	1.502114	2.256729	1.618924
H	7.005134	-0.750229	6.462459	Ca	-0.118732	-0.017403	-0.143511
H	5.615044	-0.556019	5.381224	O	-1.658279	1.345126	1.261519
C	8.893670	0.489159	4.877535	O	0.509141	2.377086	0.049220
H	8.741098	1.504914	5.246024	O	0.802757	0.629891	2.070051
H	9.586913	0.524480	4.032444	O	-0.105983	2.924662	2.397805
H	9.347838	-0.110911	5.671471	O	-0.612951	4.831981	0.477687
C	4.295202	-0.095000	1.094025	O	-2.185583	1.913386	3.884541
C	3.899378	-1.541787	1.396452	O	2.481866	2.465992	3.206101
C	3.568692	-1.708597	2.884238	O	-2.028457	2.979351	-0.942767
H	2.759817	-1.041293	3.183175	O	-1.572040	0.941909	-1.799958
H	4.439086	-1.479501	3.501807	O	-1.397833	-0.614665	3.223706
H	3.269185	-2.742339	3.078756	O	-1.103997	-1.702737	1.270167
C	2.641995	-1.828977	0.547757	O	3.069858	1.526364	0.717303
H	1.828944	-1.149611	0.815721	O	2.246895	-0.094430	-0.616764
H	2.311056	-2.855962	0.726341	O	0.002045	-1.987089	-1.641851
H	2.853003	-1.717364	-0.518583	N	-2.777948	3.935488	1.421008
C	5.040486	-2.486934	0.990387	N	0.019131	1.036025	4.751715
H	5.206964	-2.478183	-0.087837	N	2.442936	4.052886	1.240115
H	4.788224	-3.509218	1.285707	N	-3.261197	6.465777	-1.330560
H	5.973289	-2.197404	1.477543	N	-2.966422	-0.363819	6.554747
C	8.097464	3.861154	-1.602692	N	5.909829	3.155704	2.374933
C	8.629099	4.892158	-2.601600	C	-3.786860	3.309742	2.038303
C	9.969854	4.437805	-3.185703	H	-3.636404	2.252214	2.189434
H	9.871721	3.480711	-3.701793	C	-4.908404	4.002282	2.463988
H	10.721350	4.321275	-2.400972	H	-5.695049	3.477650	2.991265
H	10.332146	5.181677	-3.901482	C	-4.988881	5.369855	2.211599
C	7.574076	4.997875	-3.720937	H	-5.853183	5.937612	2.537968
H	7.449355	4.040621	-4.232623	C	-3.953178	6.001509	1.535936
H	7.890469	5.744742	-4.455341	H	-3.976804	7.057008	1.304889
H	6.611860	5.295977	-3.304879	C	-2.848769	5.247667	1.157771
C	5.965702	0.071407	-2.874941	C	-1.637465	5.777503	0.404846
C	6.355088	-0.261246	-4.308747	C	-2.045038	5.976742	-1.075759
C	5.114583	-0.740505	-5.083674	C	-1.131070	5.665815	-2.082659
H	4.351869	0.041213	-5.124312	H	-0.176813	5.237743	-1.813359
H	4.678880	-1.624306	-4.615687	C	-1.494442	5.885301	-3.402710
H	5.401868	-0.990345	-6.108552	H	-0.805221	5.651797	-4.207165
C	6.962969	0.979532	-4.969358	C	-2.762507	6.393646	-3.679852
H	6.237623	1.794577	-5.016110	H	-3.090893	6.572423	-4.697138
H	7.276440	0.735022	-5.987633	C	-3.606635	6.660556	-2.609454
H	7.828531	1.334445	-4.407532	H	-4.607093	7.050689	-2.773979
C	9.674410	-0.219326	-1.169874	C	-1.117774	7.102322	1.005769
C	10.524301	-1.473934	-1.016451	C	-1.213280	8.288303	0.271666
C	11.334349	-1.756959	-2.290110	H	-1.713999	8.279858	-0.686722
H	10.674765	-1.947000	-3.141078	C	-0.673023	9.486256	0.729024
H	11.952581	-2.645490	-2.135720	H	-0.768479	10.384176	0.128180
H	11.983465	-0.917340	-2.540134	C	-0.007775	9.514358	1.946923
C	9.617002	-2.661384	-0.673529	H	0.427487	10.434674	2.321191

C	0.086980	8.345620	2.692572	H	1.839945	6.137285	3.135437
H	0.587452	8.359966	3.654747	C	-2.152243	2.041877	-1.815958
C	-0.463445	7.131592	2.257174	C	-3.128384	2.369593	-2.927212
C	1.280762	0.683388	5.024463	H	-2.980787	1.695481	-3.769517
H	1.894491	0.499031	4.156587	H	-3.019382	3.409982	-3.233531
C	1.736821	0.600531	6.329694	H	-4.143506	2.242555	-2.540228
H	2.771365	0.345720	6.521586	C	-1.455095	-1.647245	2.465017
C	0.847536	0.862524	7.369394	C	-2.039344	-2.880264	3.124922
H	1.179025	0.809803	8.400522	H	-3.091687	-2.954442	2.836644
C	-0.469495	1.189977	7.075313	H	-1.983833	-2.808732	4.209802
H	-1.198815	1.387860	7.848016	H	-1.524205	-3.770751	2.763546
C	-0.851485	1.275422	5.742067	C	3.178553	0.595212	-0.157848
C	-2.250293	1.610862	5.246181	C	4.599940	0.330021	-0.611637
C	-3.143718	0.362424	5.448625	H	4.602433	-0.040745	-1.636458
C	-4.111613	0.054829	4.491991	H	5.025872	-0.440345	0.037329
H	-4.182930	0.662413	3.601903	H	5.211522	1.226168	-0.516601
C	-4.929580	-1.044608	4.701492	C	-0.866370	-3.140895	-1.601183
H	-5.690841	-1.308222	3.974863	H	-1.608563	-3.044895	-2.401820
C	-4.749950	-1.812207	5.850972	H	-1.360892	-3.122824	-0.631910
H	-5.361159	-2.684717	6.050486	H	-0.355321	-5.014285	-2.598887
C	-3.753646	-1.431284	6.740463	H	0.159607	-4.950206	-0.913096
H	-3.571225	-1.999810	7.648095	C	1.405495	-3.743099	-2.254543
C	-2.848289	2.827601	5.986250	H	2.112252	-3.754118	-1.422765
C	-3.942852	2.658409	6.839476	H	1.859514	-4.264761	-3.098981
H	-4.319171	1.662170	7.028109	C	1.041928	-2.299069	-2.587951
C	-4.577385	3.735708	7.450142	H	1.842997	-1.580065	-2.428220
H	-5.424290	3.561234	8.104861	H	0.640850	-2.203399	-3.605771
C	-4.123980	5.024271	7.203500	C	0.052034	-4.361116	-1.824714
H	-4.607154	5.880486	7.661626				
C	-3.029636	5.207400	6.366922				
H	-2.653398	6.208155	6.183861	2 - TPSS			
C	-2.366031	4.134553	5.754717	-8145.707934161			
C	2.188334	4.851761	0.197123	Mn	-1.048093	3.028784	0.731334
H	1.407285	4.501594	-0.459343	Mn	-0.778449	1.197169	2.858751
C	2.872292	6.043447	0.021955	Mn	1.516612	2.260956	1.618241
H	2.623054	6.687352	-0.811883	Ca	-0.103815	-0.023708	-0.152129
C	3.861723	6.390810	0.938836	O	-1.654668	1.337155	1.253360
H	4.409429	7.320156	0.828523	O	0.522727	2.377532	0.037631
C	4.143521	5.535521	1.995927	O	0.818663	0.623280	2.068554
H	4.911119	5.755612	2.724279	O	-0.099088	2.931726	2.401201
C	3.402662	4.366700	2.121309	O	-0.605554	4.842878	0.474568
C	3.586104	3.320893	3.211139	O	-2.188129	1.912635	3.885951
C	4.862307	2.506145	2.887688	O	2.496171	2.473594	3.215086
C	4.884851	1.138750	3.164214	O	-2.023977	2.981500	-0.960700
H	3.993521	0.665264	3.548586	O	-1.565996	0.929891	-1.815439
C	6.044730	0.425546	2.904458	O	-1.393132	-0.627681	3.226137
H	6.091632	-0.638733	3.109634	O	-1.102563	-1.717064	1.258858
C	7.142677	1.093109	2.364240	O	3.096462	1.532087	0.713772
H	8.066243	0.573191	2.137477	O	2.271095	-0.109210	-0.613795
C	7.020696	2.453964	2.115417	O	0.013389	-2.000705	-1.655827
H	7.846468	3.017822	1.690602	N	-2.776388	3.934607	1.414687
C	3.695996	3.962925	4.611287	N	0.025814	1.036519	4.756601
C	4.902239	3.902932	5.315458	N	2.453339	4.064167	1.241354
H	5.771124	3.465277	4.842867	N	-3.271979	6.473823	-1.332846
C	5.021969	4.379511	6.617274	N	-2.951060	-0.380813	6.561741
H	5.975733	4.313416	7.129510	N	5.930394	3.189545	2.379290
C	3.912903	4.924679	7.249325	C	-3.789665	3.302832	2.029936
H	3.979688	5.295774	8.266289	H	-3.637933	2.241884	2.174588
C	2.709991	5.001535	6.557810	C	-4.915237	3.993956	2.459325
H	1.842252	5.444763	7.034439	H	-5.703349	3.463885	2.984213
C	2.572138	4.541980	5.240315	C	-4.998684	5.366325	2.213588
C	1.218164	4.737792	4.642390	H	-5.866295	5.932097	2.542714
C	0.112221	4.186746	5.296299	C	-3.960352	6.004685	1.540191
H	0.280562	3.547445	6.152554	H	-3.985721	7.063885	1.314639
C	-1.188598	4.515907	4.919821	C	-2.850242	5.253729	1.158778
C	-1.376193	5.424431	3.873966	C	-1.638214	5.791215	0.406112
H	-2.382861	5.739687	3.634476	C	-2.048092	5.988777	-1.079407
C	-0.293036	5.988550	3.202694	C	-1.132507	5.677113	-2.089647
C	1.000495	5.640348	3.603005	H	-0.173687	5.253132	-1.819625
				C	-1.500933	5.889008	-3.413538

H	-0.811410	5.653309	-4.220388	H	3.980292	5.289237	8.303654
C	-2.775289	6.391608	-3.690679	C	2.710353	5.003129	6.587282
H	-3.107586	6.563129	-4.710696	H	1.838920	5.441799	7.067038
C	-3.620939	6.661773	-2.617191	C	2.574722	4.552430	5.261977
H	-4.625764	7.047867	-2.781568	C	1.219692	4.750088	4.660943
C	-1.116384	7.118959	1.008608	C	0.107901	4.198590	5.313082
C	-1.209933	8.306670	0.269545	H	0.272919	3.557290	6.171427
H	-1.714214	8.296406	-0.689871	C	-1.195732	4.527836	4.930502
C	-0.663240	9.507162	0.723605	C	-1.379600	5.439693	3.881530
H	-0.757364	10.405865	0.119239	H	-2.387438	5.755154	3.636792
C	0.007099	9.536192	1.943175	C	-0.290873	6.005683	3.211891
H	0.447569	10.458071	2.314739	C	1.004639	5.656096	3.618375
C	0.098995	8.366415	2.694278	H	1.847928	6.153603	3.153011
H	0.601663	8.382157	3.658152	C	-2.146712	2.036708	-1.835180
C	-0.458239	7.149195	2.262802	C	-3.125472	2.357196	-2.952991
C	1.292862	0.686314	5.033102	H	-2.883242	1.771209	-3.841935
H	1.908634	0.498811	4.164080	H	-3.125003	3.426240	-3.174495
C	1.750034	0.609913	6.342334	H	-4.131362	2.080374	-2.615154
H	2.787837	0.358082	6.535031	C	-1.452512	-1.663081	2.460548
C	0.858490	0.873596	7.384620	C	-2.037401	-2.900720	3.122139
H	1.191028	0.825104	8.418174	H	-3.087290	-2.987670	2.819175
C	-0.462978	1.197646	7.088328	H	-1.996779	-2.822737	4.209667
H	-1.193892	1.397602	7.862486	H	-1.507870	-3.790815	2.772866
C	-0.847128	1.279467	5.751447	C	3.206045	0.589497	-0.157800
C	-2.250176	1.611001	5.255951	C	4.629964	0.320433	-0.617478
C	-3.140545	0.353938	5.456802	H	4.634420	0.077388	-1.683137
C	-4.113173	0.045566	4.499857	H	5.009367	-0.548872	-0.067975
H	-4.193260	0.661295	3.612927	H	5.278994	1.172136	-0.408230
C	-4.924040	-1.064734	4.704909	C	-0.926308	-3.112253	-1.650481
H	-5.688015	-1.329391	3.977855	H	-1.667232	-2.943648	-2.442779
C	-4.732543	-1.841898	5.850487	H	-1.412841	-3.095150	-0.674030
H	-5.337295	-2.723065	6.045679	H	-0.470735	-4.928255	-2.782153
C	-3.733104	-1.459449	6.741890	H	-0.093406	-5.061303	-1.059683
H	-3.541954	-2.034740	7.646520	C	1.344997	-3.840953	-2.192744
C	-2.856471	2.829844	5.993693	H	1.957680	-3.893616	-1.287588
C	-3.957355	2.655456	6.844154	H	1.857313	-4.385792	-2.991290
H	-4.328707	1.654614	7.033048	C	1.093709	-2.375773	-2.545285
C	-4.603091	3.733265	7.450545	H	1.923714	-1.700975	-2.331291
H	-5.454082	3.555230	8.103142	H	0.761554	-2.256195	-3.587996
C	-4.155022	5.027530	7.201788	C	-0.081605	-4.383000	-1.916788
H	-4.646819	5.883954	7.656325	2 - BP			
C	-3.054354	5.215987	6.368530	-8145.693279497			
H	-2.681787	6.220815	6.185503	Mn	-1.058703	3.031944	0.729082
C	-2.378250	4.142799	5.760906	Mn	-0.785288	1.193258	2.860857
C	2.197826	4.865284	0.193663	Mn	1.514590	2.253708	1.608523
H	1.421073	4.508421	-0.468608	Ca	-0.128452	-0.038636	-0.162707
C	2.875808	6.065210	0.022023	O	-1.669257	1.338193	1.255744
H	2.624347	6.708900	-0.814615	O	0.511865	2.375666	0.029156
C	3.862317	6.420665	0.944515	O	0.811154	0.614363	2.062041
H	4.405185	7.355928	0.836134	O	-0.100892	2.930543	2.400875
C	4.146763	5.564393	2.005196	O	-0.603129	4.846174	0.469374
H	4.911661	5.790650	2.738175	O	-2.198272	1.912587	3.886546
C	3.410929	4.387804	2.129782	O	2.498975	2.452708	3.208049
C	3.600077	3.341229	3.222206	O	-2.038971	2.988933	-0.966902
C	4.883263	2.529432	2.893526	O	-1.573559	0.939722	-1.833347
C	4.910166	1.156354	3.159621	O	-1.410341	-0.634888	3.231268
H	4.019116	0.677038	3.544880	O	-1.144313	-1.723630	1.256967
C	6.072866	0.445267	2.886147	O	3.092406	1.521678	0.689791
H	6.122519	-0.623270	3.081279	O	2.250657	-0.116355	-0.637213
C	7.169437	1.121238	2.344252	O	-0.006168	-2.020849	-1.645244
H	8.094250	0.603055	2.106541	N	-2.778066	3.954033	1.427406
C	7.044750	2.488108	2.107806	N	0.019857	1.042226	4.764782
H	7.869302	3.058586	1.682929	N	2.450703	4.067355	1.248640
C	3.705045	3.979680	4.628714	N	-3.267268	6.501143	-1.330905
C	4.914057	3.918750	5.335819	N	-2.972028	-0.382071	6.566363
H	5.786519	3.486750	4.858876	N	5.943867	3.189844	2.398887
C	5.031082	4.387438	6.644659	C	-3.783011	3.338655	2.072444
H	5.986814	4.321377	7.158446	H	-3.639207	2.272419	2.223253
C	3.915908	4.924711	7.281446				

C	-4.888530	4.047934	2.530718	C	6.067197	0.423051	2.796361
H	-5.668503	3.529155	3.087271	H	6.107963	-0.657754	2.945564
C	-4.964043	5.420354	2.272720	C	7.175968	1.116372	2.297649
H	-5.818588	6.002018	2.622849	H	8.105808	0.601873	2.050750
C	-3.935395	6.040987	1.564747	C	7.059283	2.494728	2.113473
H	-3.950366	7.103156	1.329776	H	7.896315	3.078805	1.719292
C	-2.841057	5.273216	1.165926	C	3.703162	3.938950	4.634675
C	-1.628331	5.796892	0.401769	C	4.906389	3.856985	5.352281
C	-2.051447	5.991841	-1.082771	H	5.782399	3.419400	4.876641
C	-1.151297	5.647482	-2.099123	C	5.016830	4.310480	6.668821
H	-0.198653	5.197317	-1.830226	H	5.970887	4.228039	7.192987
C	-1.526718	5.854016	-3.423649	C	3.900907	4.855367	7.301661
H	-0.847568	5.591491	-4.237191	H	3.961120	5.211310	8.332006
C	-2.793634	6.382919	-3.694979	C	2.700533	4.953485	6.597787
H	-3.133451	6.551476	-4.717889	H	1.826544	5.398793	7.077132
C	-3.624342	6.683177	-2.614610	C	2.569974	4.515086	5.265701
H	-4.626611	7.091079	-2.776542	C	1.219162	4.723234	4.658278
C	-1.093153	7.120189	1.001035	C	0.100286	4.176983	5.306128
C	-1.168546	8.309094	0.259205	H	0.260786	3.532099	6.168082
H	-1.671160	8.304151	-0.706378	C	-1.202459	4.515945	4.922072
C	-0.607837	9.504410	0.715150	C	-1.377277	5.431490	3.872611
H	-0.687466	10.407738	0.107334	H	-2.386751	5.755847	3.627094
C	0.056738	9.526172	1.940104	C	-0.282241	5.993581	3.205822
H	0.507698	10.447072	2.314965	C	1.011130	5.633326	3.615286
C	0.131433	8.354705	2.693763	H	1.861116	6.130606	3.151996
H	0.631606	8.366094	3.664138	C	-2.146131	2.052824	-1.853955
C	-0.437491	7.141607	2.259583	C	-3.094151	2.398149	-2.990112
C	1.293210	0.721229	5.048511	H	-2.879606	1.775442	-3.866238
H	1.918892	0.536300	4.179896	H	-3.028907	3.464796	-3.238093
C	1.751224	0.676178	6.361336	H	-4.122745	2.195033	-2.655282
H	2.799539	0.454095	6.558631	C	-1.493150	-1.665142	2.461412
C	0.849669	0.930504	7.399703	C	-2.075959	-2.904026	3.121907
H	1.182299	0.904366	8.438858	H	-2.958022	-3.229183	2.552320
C	-0.479917	1.220513	7.095460	H	-2.358597	-2.710520	4.162096
H	-1.222500	1.416970	7.865997	H	-1.335105	-3.714855	3.075509
C	-0.860284	1.282798	5.754853	C	3.189972	0.588929	-0.195095
C	-2.263957	1.607032	5.251268	C	4.597941	0.392729	-0.731257
C	-3.147053	0.341845	5.451125	H	4.717327	-0.622645	-1.127469
C	-4.096648	0.013239	4.474839	H	5.342465	0.600776	0.046719
H	-4.159233	0.620206	3.574678	H	4.756981	1.109692	-1.551133
C	-4.899058	-1.106597	4.671329	C	-0.904518	-3.165650	-1.583154
H	-5.644181	-1.389780	3.925266	H	-1.693435	-3.033909	-2.342508
C	-4.722630	-1.872382	5.829238	H	-1.349238	-3.150320	-0.580395
H	-5.321778	-2.764028	6.019532	H	-0.396858	-4.940323	-2.765237
C	-3.745329	-1.469091	6.739818	H	-0.045087	-5.123944	-1.036236
H	-3.566255	-2.038788	7.656642	C	1.383677	-3.834652	-2.114092
C	-2.874075	2.825631	5.985037	H	1.969840	-3.840115	-1.184081
C	-3.982013	2.655549	6.829344	H	1.944840	-4.384966	-2.881619
H	-4.359115	1.651892	7.018578	C	1.092126	-2.390548	-2.512772
C	-4.628767	3.738075	7.430240	H	1.904830	-1.681814	-2.312599
H	-5.488315	3.564115	8.080369	H	0.769062	-2.313708	-3.568409
C	-4.173183	5.031887	7.182416	C	-0.032098	-4.413002	-1.872519
H	-4.666522	5.894163	7.635217				
C	-3.065572	5.216084	6.354471	2 - PBE			
H	-2.686919	6.223789	6.172493	-8139.249158681			
C	-2.389265	4.138566	5.750354	Mn	-1.053594	3.022120	0.716272
C	2.180038	4.892559	0.223593	Mn	-0.789085	1.181786	2.859231
H	1.399113	4.543643	-0.446098	Mn	1.523495	2.245558	1.613036
C	2.839718	6.109234	0.082439	Ca	-0.108876	-0.050410	-0.161479
H	2.568848	6.776825	-0.734969	O	-1.662779	1.329511	1.247694
C	3.831595	6.450382	1.007296	O	0.524395	2.365893	0.031111
H	4.363104	7.399822	0.922317	O	0.813898	0.608217	2.068818
C	4.134818	5.566527	2.042416	O	-0.101094	2.921274	2.395408
H	4.903667	5.779991	2.782006	O	-0.610590	4.850675	0.467778
C	3.408205	4.379917	2.142106	O	-2.198163	1.912168	3.899005
C	3.599771	3.317372	3.220692	O	2.505761	2.472140	3.221055
C	4.886652	2.514718	2.873722	O	-2.017842	2.961577	-0.997497
C	4.902348	1.129551	3.081935	O	-1.554531	0.904363	-1.843941
H	3.996394	0.638030	3.428687	O	-1.419671	-0.656060	3.212680

O	-1.128330	-1.746531	1.242785	H	1.456702	4.480586	-0.502969
O	3.105696	1.491743	0.702731	C	2.914713	6.041209	-0.010252
O	2.271442	-0.142704	-0.633132	H	2.675074	6.677151	-0.862642
O	0.012757	-2.035106	-1.661799	C	3.888487	6.407181	0.923076
N	-2.795136	3.933346	1.392750	H	4.437062	7.344468	0.811321
N	0.016627	1.010014	4.767510	C	4.155342	5.562824	1.998882
N	2.473375	4.052815	1.227227	H	4.912947	5.800057	2.743575
N	-3.290713	6.451205	-1.338671	C	3.418243	4.384706	2.125851
N	-2.938366	-0.406509	6.551129	C	3.601025	3.343589	3.227323
N	5.926601	3.179457	2.346763	C	4.892867	2.534944	2.905016
C	-3.817055	3.299205	1.990624	C	4.936092	1.171217	3.223384
H	-3.670615	2.229919	2.128029	H	4.054199	0.700061	3.652667
C	-4.947811	3.988700	2.413912	C	6.097960	0.455802	2.951890
H	-5.748704	3.452215	2.923081	H	6.159379	-0.608465	3.189945
C	-5.021505	5.365736	2.186244	C	7.178392	1.116911	2.359290
H	-5.894404	5.934280	2.512950	H	8.105330	0.593560	2.118935
C	-3.970306	6.007995	1.535182	C	7.038838	2.474988	2.076411
H	-3.988888	7.075681	1.324513	H	7.856130	3.035692	1.611714
C	-2.858606	5.255799	1.152911	C	3.709740	3.999205	4.628335
C	-1.640241	5.796310	0.408694	C	4.925328	3.949557	5.328912
C	-2.053669	6.005508	-1.078793	H	5.798604	3.507848	4.850947
C	-1.119080	5.739481	-2.087636	C	5.055551	4.439163	6.629629
H	-0.140508	5.350719	-1.813681	H	6.020395	4.379864	7.137363
C	-1.485244	5.952186	-3.413274	C	3.946465	4.988382	7.268555
H	-0.777166	5.751939	-4.220349	H	4.020595	5.370779	8.288679
C	-2.776394	6.409725	3.695245	C	2.734520	5.056962	6.583165
H	-3.109982	6.580209	-4.720194	H	1.864079	5.506754	7.065548
C	-3.637997	6.639047	-2.623021	C	2.585040	4.585611	5.264940
H	-4.659534	6.993618	-2.793106	C	1.224304	4.780807	4.677461
C	-1.131091	7.127861	1.020053	C	0.117166	4.225053	5.337090
C	-1.235956	8.318489	0.283453	H	0.290407	3.578432	6.196566
H	-1.735837	8.304896	-0.683852	C	-1.191634	4.548506	4.961610
C	-0.710878	9.527541	0.742667	C	-1.385229	5.460217	3.912239
H	-0.815453	10.429295	0.135910	H	-2.400922	5.769898	3.669069
C	-0.049258	9.565415	1.967632	C	-0.301864	6.030760	3.234598
H	0.376571	10.497215	2.345521	C	0.998638	5.686514	3.634839
C	0.054832	8.394982	2.717470	H	1.841583	6.186544	3.159333
H	0.552347	8.416975	3.689395	C	-2.127736	2.016449	-1.873502
C	-0.481295	7.168257	2.281280	C	-3.076047	2.348555	-3.012377
C	1.277683	0.639691	5.044384	H	-2.918836	1.661042	-3.851075
H	1.895565	0.441748	4.171076	H	-2.947710	3.390989	-3.330472
C	1.734715	0.552824	6.354621	H	-4.109776	2.240685	-2.650247
H	2.772011	0.278680	6.547857	C	-1.485372	-1.688648	2.443899
C	0.848059	0.835615	7.397361	H	-2.091655	-2.917631	3.099306
H	1.180402	0.781245	8.435880	C	-3.168930	-2.933883	2.873487
C	-0.467189	1.186283	7.099775	H	-1.976186	-2.884692	4.188848
H	-1.196081	1.403201	7.878566	H	-1.640979	-3.827095	2.683310
C	-0.852285	1.270790	5.761119	C	3.209938	0.548927	-0.169449
C	-2.254255	1.616268	5.265978	C	4.634035	0.267149	-0.616729
C	-3.154066	0.362086	5.474950	H	4.641312	-0.081260	-1.656831
C	-4.166112	0.091877	4.544382	H	5.043414	-0.534404	0.017069
H	-4.274602	0.740585	3.677533	H	5.270423	1.151278	-0.494464
C	-4.983047	-1.016153	4.745016	C	-0.895261	-3.164563	-1.648876
H	-5.780424	-1.249914	4.036030	C	-1.644665	-3.024117	-2.447606
C	-4.759206	-1.830556	5.859613	H	-1.391384	-3.153843	-0.670405
H	-5.368317	-2.715499	6.051222	H	-0.438529	-5.016720	-2.725818
C	-3.724614	-1.482365	6.726882	H	0.037895	-5.056180	-1.018362
H	-3.509445	-2.089464	7.612000	C	1.368076	-3.835888	-2.277931
C	-2.847436	2.836006	6.017781	H	2.052063	-3.890641	-1.419298
C	-3.939306	2.658423	6.882303	H	1.836252	-4.358668	-3.123191
H	-4.315729	1.653154	7.066479	C	1.065022	-2.371974	-2.590968
C	-4.572991	3.731185	7.511637	H	1.893858	-1.679373	-2.399379
H	-5.419479	3.546923	8.176266	H	0.693889	-2.243187	-3.625693
C	-4.122771	5.027565	7.273506	C	-0.021456	-4.414065	-1.907006
H	-4.606970	5.884132	7.747018				
C	-3.031572	5.221264	6.427933	2 - PBEO			
H	-2.654866	6.231181	6.252348	-8145.116474031			
C	-2.366286	4.152737	5.797149	Mn	-1.053952	3.026833	0.738234
C	2.231332	4.843691	0.168893	Mn	-0.784994	1.201156	2.858122

Mn	1.502114	2.256729	1.618924	H	-3.571225	-1.999810	7.648095
Ca	-0.118732	-0.017403	-0.143511	C	-2.848289	2.827601	5.986250
O	-1.658279	1.345126	1.261519	C	-3.942852	2.658409	6.839476
O	0.509141	2.377086	0.049220	H	-4.319171	1.662170	7.028109
O	0.802757	0.629891	2.070051	C	-4.577385	3.735708	7.450142
O	-0.105983	2.924662	2.397805	H	-5.424290	3.561234	8.104861
O	-0.612951	4.831981	0.477687	C	-4.123980	5.024271	7.203500
O	-2.185583	1.913386	3.884541	H	-4.607154	5.880486	7.661626
O	2.481866	2.465992	3.206101	C	-3.029636	5.207400	6.366922
O	-2.028457	2.979351	-0.942767	H	-2.653398	6.208155	6.183861
O	-1.572040	0.941909	-1.799958	C	-2.366031	4.134553	5.754717
O	-1.397833	-0.614665	3.223706	C	2.188334	4.851761	0.197123
O	-1.103997	-1.702737	1.270167	H	1.407285	4.501594	-0.459343
O	3.069858	1.526364	0.717303	C	2.872292	6.043447	0.021955
O	2.246895	-0.094430	-0.616764	H	2.623054	6.687352	-0.811883
O	0.002045	-1.987089	-1.641851	C	3.861723	6.390810	0.938836
N	-2.777948	3.935488	1.421008	H	4.409429	7.320156	0.88523
N	0.019131	1.036025	4.751715	C	4.143521	5.535521	1.995927
N	2.442936	4.052886	1.240115	H	4.911119	5.755612	2.724279
N	-3.261197	6.465777	-1.330560	C	3.402662	4.366700	2.121309
N	-2.966422	-0.363819	6.554747	C	3.586104	3.320893	3.211139
N	5.909829	3.155704	2.374933	C	4.862307	2.506145	2.887688
C	-3.786860	3.309742	2.038303	C	4.884851	1.138750	3.164214
H	-3.636404	2.252214	2.189434	H	3.993521	0.665264	3.548586
C	-4.908404	4.002282	2.463988	C	6.044730	0.425546	2.904458
H	-5.695049	3.477650	2.991265	H	6.091632	-0.638733	3.109634
C	-4.988881	5.369855	2.211599	C	7.142677	1.093109	2.364240
H	-5.853183	5.937612	2.537968	H	8.066243	0.573191	2.137477
C	-3.953178	6.001509	1.535936	C	7.020696	2.453964	2.115417
H	-3.976804	7.057008	1.304889	H	7.846468	3.017822	1.690602
C	-2.848769	5.247667	1.157771	C	3.695996	3.962925	4.611287
C	-1.637465	5.777503	0.404846	C	4.902239	3.902932	5.315458
C	-2.045038	5.976742	-1.075759	H	5.771124	3.465277	4.842867
C	-1.131070	5.665815	-2.082659	C	5.021969	4.379511	6.617274
H	-0.176813	5.237743	-1.813359	H	5.975733	4.313416	7.129510
C	-1.494442	5.885301	-3.402710	C	3.912903	4.924679	7.249325
H	-0.805221	5.651797	-4.207165	H	3.979688	5.295774	8.266289
C	-2.762507	6.393646	-3.679852	C	2.709991	5.001535	6.557810
H	-3.090893	6.572423	-4.697138	H	1.842252	5.444763	7.034439
C	-3.606635	6.660556	-2.609454	C	2.572138	4.541980	5.240315
H	-4.607093	7.050689	-2.773979	C	1.218164	4.737792	4.642390
C	-1.117774	7.102322	1.005769	C	0.112221	4.186746	5.296299
C	-1.213280	8.288303	0.271666	H	0.280562	3.547445	6.152554
H	-1.713999	8.279858	-0.686722	C	-1.188598	4.515907	4.919821
C	-0.673023	9.486256	0.729024	C	-1.376193	5.424431	3.873966
H	-0.768479	10.384176	0.128180	H	-2.382861	5.739687	3.634476
C	-0.007775	9.514358	1.946923	C	-0.293036	5.988550	3.202694
H	0.427487	10.434674	2.321191	C	1.000495	5.640348	3.603005
C	0.086980	8.345620	2.692572	H	1.839945	6.137285	3.135437
H	0.587452	8.359966	3.654747	C	-2.152243	2.041877	-1.815958
C	-0.463445	7.131592	2.257174	C	-3.128384	2.369593	-2.927212
C	1.280762	0.683388	5.024463	H	-2.980787	1.695481	-3.769517
H	1.894491	0.499031	4.156587	H	-3.019382	3.409982	-3.233531
C	1.736821	0.600531	6.329694	H	-4.143506	2.242555	-2.540228
H	2.771365	0.345720	6.521586	C	-1.455095	-1.647245	2.465017
C	0.847536	0.862524	7.369394	C	-2.039344	-2.880264	3.124922
H	1.179025	0.809803	8.400522	H	-3.091687	-2.954442	2.836644
C	-0.469495	1.189977	7.075313	H	-1.983833	-2.808732	4.209802
H	-1.198815	1.387860	7.848016	H	-1.524205	-3.770751	2.763546
C	-0.851485	1.275422	5.742067	C	3.178553	0.595212	-0.157848
C	-2.250293	1.610862	5.246181	C	4.599940	0.330021	-0.611637
C	-3.143718	0.362424	5.448625	H	4.602433	-0.040745	-1.636458
C	-4.111613	0.054829	4.491991	H	5.025872	-0.440345	0.037329
H	-4.182930	0.662413	3.601903	H	5.211522	1.226168	-0.516601
C	-4.929580	-1.044608	4.701492	C	-0.866370	-3.140895	-1.601183
H	-5.690841	-1.308222	3.974863	H	-1.608563	-3.044895	-2.401820
C	-4.749950	-1.812207	5.850972	H	-1.360892	-3.122824	-0.631910
H	-5.361159	-2.684717	6.050486	H	-0.355321	-5.014285	-2.598887
C	-3.753646	-1.431284	6.740463	H	0.159607	-4.950206	-0.913096

C	1.405495	-3.743099	-2.254543	O	5.184049	5.207358	2.771783
H	2.112252	-3.754118	-1.422765	O	3.071244	4.489669	1.505466
H	1.859514	-4.264761	-3.098981	O	5.289085	3.019208	1.256056
C	1.041928	-2.299069	-2.587951	O	2.904248	6.708742	3.121466
H	1.842997	-1.580065	-2.428220	O	3.865233	7.359161	1.166610
H	0.640850	-2.203399	-3.605771	O	4.042006	5.046531	5.141280
C	0.052034	-4.361116	-1.824714	O	6.029754	3.929353	4.914566
				O	1.636084	4.228539	3.699843
				O	1.622884	2.440471	2.267647
				O	2.943516	2.341875	-0.257076
3				O	3.968372	4.016162	-1.387102
-5845.909570257911				O	7.647230	4.002887	2.574306
Mn	3.423539	4.939071	3.236546	O	7.402475	5.273041	0.707918
Mn	5.785823	3.541906	2.976482	O	6.367039	1.728357	3.337007
Mn	3.482039	2.698133	1.621919	O	3.801627	0.858688	1.858161
Ca	4.904575	5.463302	0.421358	C	3.175423	7.575352	2.177852
O	3.985658	3.136132	3.389998	C	2.530102	8.925738	2.412938
O	5.149753	5.321222	2.801990	H	1.463502	8.847159	2.173925
O	2.994442	4.559213	1.520806	H	2.990505	9.673443	1.765922
O	5.264090	3.134750	1.250028	H	2.615756	9.211571	3.464012
O	2.830260	6.793325	3.150215	C	5.177417	4.638399	5.558098
O	3.752315	7.465935	1.177822	C	5.565387	5.038040	6.964991
O	3.993009	5.108326	5.172192	H	4.674531	5.151586	7.585488
O	5.987802	4.002923	4.932509	H	6.255648	4.309894	7.394579
O	1.601135	4.273191	3.757570	H	6.073443	6.008120	6.909361
O	1.588237	2.485396	2.322889	C	1.078026	3.246453	3.092542
O	2.953601	2.386509	-0.248769	C	-0.389175	3.023900	3.386528
O	4.029627	4.038194	-1.380442	H	-0.968090	3.642484	2.690467
O	7.622866	4.095081	2.490650	H	-0.654483	1.977648	3.226567
O	7.339208	5.282693	0.571255	H	-0.624037	3.341053	4.404412
O	6.370784	1.797916	3.285211	C	3.225305	3.007175	-1.327800
O	3.821580	0.924149	1.897621	C	2.604379	2.443880	-2.589786
C	3.069119	7.648126	2.213730	H	2.415103	3.249554	-3.302430
C	2.397579	8.999904	2.425699	H	1.686696	1.899526	-2.362033
H	1.371307	8.937681	2.044073	H	3.318620	1.742573	-3.037201
H	2.930863	9.775130	1.870908	C	8.089380	4.764827	1.616411
H	2.348801	9.243586	3.489741	C	9.590142	4.974511	1.663449
C	5.116186	4.665843	5.584623	H	9.867936	5.820559	1.033203
C	5.471669	4.988981	7.027156	H	10.079482	4.068211	1.289152
H	4.564135	5.091489	7.626240	H	9.920752	5.130813	2.693008
H	6.127085	4.217320	7.436675	H	6.876237	1.699477	4.166146
H	6.007995	5.945491	7.040600	H	4.762996	0.742031	2.006305
C	1.065478	3.267761	3.177166	O	5.611515	6.028536	-1.991713
C	-0.383071	2.990076	3.546298	H	6.493287	6.081704	-2.387138
H	-1.022129	3.643906	2.940805	H	5.127666	5.309454	-2.446674
H	-0.636931	1.949966	3.332967	H	3.816460	2.333655	4.060003
H	-0.553091	3.226403	4.599595				
C	3.314342	2.999704	-1.311288				
C	2.837353	2.361984	-2.610243	3-H2			
H	2.664550	3.132423	-3.366212	-5846.426126894607			
H	1.936219	1.768740	-2.443027	Mn	3.424191	4.979638	3.202643
H	3.628047	1.693615	-2.972517	Mn	5.895331	3.527125	3.016630
C	8.040554	4.769515	1.485500	Mn	3.610436	2.705325	1.632146
C	9.554433	4.929210	1.402023	Ca	5.077008	5.464865	0.285969
H	9.799332	5.965859	1.152275	O	4.073608	3.214618	3.406025
H	9.926990	4.292087	0.591023	O	5.283491	5.442732	2.722753
H	10.033085	4.634785	2.337470	O	3.146967	4.599234	1.492645
H	6.683289	1.488224	2.415877	O	5.395924	3.176650	1.296747
H	4.589533	0.899973	2.510959	O	2.887524	6.815224	3.073806
O	6.051169	5.838141	-1.863363	O	3.872583	7.421799	1.115550
H	6.910984	5.525349	-1.521454	O	4.033569	5.222068	5.108937
H	5.591588	5.050515	-2.221003	O	6.034550	4.129928	4.942481
				O	1.690622	4.343748	3.681533
3-H1				O	1.711046	2.520690	2.300574
-5846.404890068929				O	3.053794	2.340034	-0.182694
Mn	3.446919	4.923193	3.214724	O	4.038141	3.996918	-1.365667
Mn	5.877672	3.462793	2.956051	O	7.711064	4.020562	2.590961
Mn	3.493658	2.620775	1.537687	O	7.451519	5.328107	0.748251
Ca	5.021983	5.381607	0.351351	O	6.363951	1.814691	3.411250
O	4.003751	3.017830	3.394415	O	3.970052	0.971008	1.958178

C	3.120556	7.638295	2.088699	C	3.346945	2.937610	-1.377389
C	2.365315	8.948305	2.197678	C	2.900638	2.276791	-2.666532
H	1.345137	8.785008	1.830839	H	2.801565	3.019985	-3.460589
H	2.844946	9.710304	1.581274	H	1.964786	1.734760	-2.519253
H	2.297701	9.269804	3.239422	H	3.669268	1.551200	-2.958230
C	5.098601	4.705420	5.596718	C	8.069247	4.712336	1.674208
C	5.263118	4.774992	7.097182	C	9.579255	4.839717	1.730885
H	4.729204	5.636982	7.500986	H	9.915199	5.634075	1.063171
H	4.824025	3.863753	7.520395	H	10.026412	3.888496	1.421203
H	6.321259	4.800813	7.363468	H	9.900099	5.035443	2.757464
C	1.162249	3.298517	3.128789	H	7.011975	1.544915	2.922223
C	-0.264990	3.018092	3.536664	H	4.728752	0.954205	2.415423
H	-0.913968	3.761463	3.060589	O	5.492767	6.052683	-2.095919
H	-0.556357	2.017759	3.215921	H	6.253332	6.246691	-2.659984
H	-0.367716	3.126087	4.619280	H	5.022736	5.274649	-2.469567
C	3.319443	2.965088	-1.272113	H	2.074475	4.772993	1.118445
C	2.726172	2.353489	-2.525614				
H	2.475094	3.139155	-3.242221	3-H4			
H	1.849530	1.750110	-2.285948	-5846.433053739564			
H	3.482481	1.701522	-2.978582	Mn	3.498206	4.903487	3.113681
C	8.151843	4.748221	1.605197	Mn	5.861872	3.502373	3.016134
C	9.664638	4.837614	1.540599	Mn	3.460622	2.633654	1.558359
H	9.963627	5.719988	0.972261	Ca	5.098365	5.403958	0.258481
H	10.039758	3.943996	1.027841	O	4.028707	3.085662	3.300710
H	10.094308	4.852680	2.544524	O	5.251192	5.221807	2.697757
H	7.048361	1.540859	2.773288	O	3.132887	4.494311	1.389400
H	4.758285	0.938151	2.549603	O	5.382188	3.056779	1.131960
O	5.465547	6.060944	-2.096238	O	2.958884	6.732498	3.022693
H	6.208911	6.253640	-2.683007	O	3.970736	7.375108	1.093840
H	4.979751	5.287891	-2.459822	O	4.041619	5.078678	5.057170
H	5.682715	6.047158	3.369290	O	6.003873	3.913308	4.889227
				O	1.664361	4.282030	3.600092
3-H3				O	1.661576	2.449742	2.230581
-5846.429533604041				O	2.921528	2.304227	-0.270782
Mn	3.422616	5.003689	3.201940	O	3.991761	3.939942	-1.414420
Mn	5.734798	3.519065	2.960517	O	7.684267	4.016565	2.656965
Mn	3.508720	2.646646	1.532525	O	7.454128	5.260222	0.770170
Ca	5.076236	5.474929	0.284753	O	6.336630	1.716019	3.191258
O	3.909242	3.182743	3.309837	O	3.925860	0.891553	1.781647
O	5.113352	5.319849	2.722004	C	3.273585	7.600252	2.105218
O	3.018895	4.654700	1.308864	C	2.719590	8.987528	2.366455
O	5.241672	3.150399	1.204121	H	1.654406	8.925423	2.605697
O	2.855445	6.826625	3.044140	H	2.882895	9.627279	1.498299
O	3.912270	7.448975	1.128421	H	3.228508	9.412436	3.238571
O	3.887415	5.166441	5.052803	C	5.116043	4.604295	5.525880
O	5.880714	4.052920	4.907111	C	5.438114	4.869587	6.978373
O	1.567432	4.348752	3.565906	H	4.543017	5.199389	7.506630
O	1.591155	2.529004	2.181440	H	5.856108	3.971736	7.439450
O	2.991700	2.318941	-0.305000	H	6.197136	5.658762	7.023593
O	4.027767	3.996493	-1.420895	C	1.122064	3.265766	3.063920
O	7.574149	3.939815	2.594404	C	-0.318212	2.976639	3.417019
O	7.416455	5.304484	0.788524	H	-0.955609	3.494893	2.691148
O	6.155053	1.753551	3.333774	H	-0.516694	1.905607	3.351860
O	3.881730	0.948669	1.888934	H	-0.541517	3.360238	4.413925
C	3.232380	7.695440	2.146121	C	3.211657	2.954130	-1.343070
C	2.779481	9.111911	2.440275	C	2.560059	2.431640	-2.609047
H	1.791810	9.113834	2.906530	H	2.154859	3.270745	-3.181881
H	2.783342	9.704047	1.523701	H	1.775891	1.709896	-2.379352
H	3.487100	9.554539	3.151244	H	3.329194	1.946467	-3.220774
C	5.000121	4.711107	5.530139	C	8.126496	4.796793	1.716088
C	5.248304	5.030818	6.985766	C	9.597647	5.143059	1.847779
H	4.320308	4.930504	7.553147	H	9.993517	5.467406	0.883972
H	6.024118	4.377020	7.385309	H	10.162573	4.293516	2.237649
H	5.579175	6.073161	7.057356	H	9.691100	5.967327	2.564712
C	1.076320	3.262853	3.087976	H	7.000851	1.571504	3.884874
C	-0.242535	2.808423	3.668985	H	4.599664	0.823473	2.495458
H	-0.819526	3.663419	4.025927	O	5.360053	6.030317	-2.110091
H	-0.802046	2.229412	2.932274	H	5.818040	6.507139	-2.813023
H	-0.020856	2.157527	4.523035	H	4.842043	5.293836	-2.501570

H	5.817236	2.204402	0.941229	O	3.917913	5.152493	5.063323
				O	5.921735	4.058393	4.907244
3-H1H2				O	1.573546	4.316503	3.573326
-5846.799731119234				O	1.590738	2.503081	2.175967
Mn	3.392827	4.971314	3.220746	O	3.013907	2.265351	-0.282889
Mn	5.948406	3.441752	3.013434	O	4.047717	3.954194	-1.385197
Mn	3.563675	2.631572	1.569916	O	7.582441	3.869954	2.642278
Ca	5.102969	5.415849	0.242827	O	7.415044	5.199913	0.819561
O	4.040842	3.099970	3.442269	O	6.136753	1.721520	3.401416
O	5.266490	5.333723	2.727107	O	3.832738	0.880202	1.902428
O	3.170105	4.538476	1.519410	C	3.262340	7.649870	2.152676
O	5.363739	3.067455	1.323790	C	2.782875	9.049022	2.446737
O	2.886615	6.741978	3.085691	H	1.779752	9.033077	2.877722
O	3.895643	7.340132	1.140837	H	2.811853	9.646881	1.535215
O	4.061007	5.153832	5.115597	H	3.458425	9.491762	3.188120
O	6.055888	4.046147	4.930552	C	5.064522	4.756888	5.527365
O	1.665851	4.312119	3.661130	C	5.372812	5.181737	6.937775
O	1.675887	2.503761	2.259165	H	4.456542	5.226527	7.529234
O	3.036417	2.318042	-0.194637	H	6.101844	4.504708	7.384101
O	4.024034	3.986834	-1.357892	H	5.802669	6.189815	6.896457
O	7.707235	3.934250	2.644777	C	1.046704	3.262852	3.049038
O	7.437848	5.207301	0.789568	C	-0.330651	2.885852	3.529473
O	6.351994	1.744426	3.439999	H	-0.883714	3.774925	3.836217
O	3.860232	0.899088	1.932443	H	-0.861164	2.330152	2.755045
C	3.142534	7.583400	2.094071	H	-0.216119	2.232699	4.403175
C	2.409040	8.893773	2.230928	C	3.364890	2.910005	-1.367375
H	1.382573	8.747393	1.874458	C	2.880878	2.255351	-2.637762
H	2.894638	9.653373	1.617436	H	2.818579	2.992739	-3.439538
H	2.357371	9.203082	3.276804	H	1.919738	1.762932	-2.480200
C	5.157400	4.689365	5.589414	H	3.609762	1.485853	-2.918867
C	5.439708	4.948734	7.047171	C	8.089003	4.625692	1.688718
H	4.504379	5.003510	7.606434	C	9.593595	4.713090	1.728595
H	6.100337	4.179998	7.450122	H	9.930044	5.554623	1.122508
H	5.945119	5.918498	7.130500	H	10.004987	3.784641	1.315757
C	1.108342	3.299888	3.062315	H	9.946013	4.805088	2.758309
C	-0.346860	3.084496	3.377703	H	7.074854	1.531915	3.576929
H	-0.931997	3.715392	2.697674	H	4.775711	0.798880	2.189057
H	-0.615540	2.041125	3.209370	O	5.415977	6.282380	-2.027292
H	-0.564373	3.393053	4.401736	H	5.851928	6.988026	-2.526194
C	3.295630	2.974390	-1.290865	H	5.025898	5.665832	-2.671168
C	2.662171	2.374812	-2.522549	H	2.104300	4.714677	1.118720
H	2.520123	3.146898	-3.280620	H	3.704180	2.442533	4.076432
H	1.717616	1.887318	-2.276472				
H	3.344360	1.613083	-2.918284	3-H1H4			
C	8.158649	4.641337	1.627251	-5846.806886713503			
C	9.663851	4.690564	1.551915	Mn	3.483547	4.896858	3.159168
H	9.976924	5.557463	0.968832	Mn	5.942400	3.475197	3.052078
H	10.005951	3.780008	1.045566	Mn	3.428023	2.571164	1.514365
H	10.105451	4.704798	2.550193	Ca	5.104012	5.378410	0.246260
H	7.084989	1.698145	4.082061	O	4.038863	2.980173	3.361887
H	4.815704	0.712024	2.037997	O	5.241552	5.151558	2.720601
O	5.426139	6.265849	-2.029570	O	3.153020	4.436318	1.442530
H	5.865556	6.954683	-2.548010	O	5.368920	3.007660	1.178713
H	4.986302	5.661950	-2.653687	O	2.955546	6.660764	3.057359
H	5.702000	5.954003	3.337084	O	3.954154	7.304871	1.127885
H	3.835067	2.445049	4.134561	O	4.061685	5.049549	5.079134
				O	6.052672	3.934851	4.907947
3-H1H3				O	1.671833	4.228220	3.620520
-5846.802952042104				O	1.644133	2.423861	2.214236
Mn	3.409220	5.010611	3.229091	O	2.900508	2.294189	-0.247128
Mn	5.802727	3.470949	2.980422	O	3.960536	3.952396	-1.369863
Mn	3.496760	2.571660	1.492662	O	7.700391	3.950223	2.687580
Ca	5.105191	5.427739	0.245440	O	7.439970	5.216022	0.825662
O	3.906970	3.085297	3.371424	O	6.323046	1.685346	3.270081
O	5.101337	5.236251	2.717569	O	3.861465	0.835334	1.780858
O	3.041246	4.589165	1.348566	C	3.249103	7.542625	2.119512
O	5.232907	3.069874	1.246208	C	2.617698	8.891202	2.359108
O	2.881910	6.771736	3.070683	H	1.543168	8.814174	2.158798
O	3.943873	7.375756	1.155555	H	3.061138	9.628787	1.689964

H	2.738770	9.187417	3.403818	H	1.944488	1.746190	-2.420882
C	5.178252	4.657921	5.537101	H	3.637879	1.466738	-2.841008
C	5.553327	5.050645	6.940673	C	8.139041	4.624770	1.641871
H	4.653792	5.211170	7.536494	C	9.645858	4.606721	1.577251
H	6.201176	4.297355	7.391347	H	10.005445	5.472666	1.020201
H	6.108019	5.995141	6.883570	H	9.952780	3.695786	1.049177
C	1.095343	3.252668	3.036149	H	10.077875	4.573975	2.579357
C	-0.364515	3.023794	3.320680	H	7.077441	1.553728	3.138177
H	-0.939846	3.600323	2.586140	H	4.740485	0.954856	2.485125
H	-0.615253	1.968372	3.206213	O	5.461203	6.196593	-2.154311
H	-0.612717	3.388005	4.318701	H	5.907482	6.825125	-2.739196
C	3.179653	2.982467	-1.327099	H	5.016068	5.532665	-2.712153
C	2.465433	2.468366	-2.553412	H	5.669916	6.094103	3.234900
H	2.744571	3.059991	-3.425486	H	2.180964	4.865268	1.059967
H	1.384534	2.520926	-2.390816				
H	2.720752	1.416120	-2.710295				
C	8.143551	4.747975	1.732740	3-H2H4			
C	9.616475	5.051634	1.848927	-5846.825618925596			
H	9.989686	5.432038	0.897614	Mn	3.447886	4.957220	3.152743
H	10.171916	4.165360	2.162751	Mn	5.929248	3.524911	3.066648
H	9.747821	5.819446	2.620338	Mn	3.523410	2.681913	1.580269
H	7.143465	1.482995	3.751289	Ca	5.116640	5.485810	0.170418
H	4.668798	0.722206	2.330234	O	4.101569	3.173119	3.336954
O	5.483222	6.193820	-2.031914	O	5.310855	5.380827	2.666909
H	5.937444	6.898387	-2.515974	O	3.195274	4.562757	1.434516
H	5.011538	5.648409	-2.684535	O	5.438086	3.141496	1.177756
H	5.834661	2.185537	0.933791	O	2.929944	6.763926	3.040143
H	3.824261	2.369576	4.090217	O	3.927545	7.378531	1.099794
				O	4.060086	5.177715	5.057599
				O	6.055467	4.077015	4.900853
3-H2H3				O	1.715112	4.329684	3.624714
-5846.818317311472				O	1.725402	2.495758	2.264859
Mn	3.396310	5.053521	3.220570	O	2.985811	2.350087	-0.202959
Mn	5.823359	3.519734	2.986615	O	4.013547	3.987055	-1.376361
Mn	3.563624	2.684954	1.558880	O	7.723154	4.008493	2.669961
Ca	5.158956	5.488762	0.162450	O	7.452108	5.273036	0.806642
O	3.971789	3.280301	3.337164	O	6.382366	1.811916	3.359447
O	5.227739	5.440986	2.665202	O	3.978584	0.953319	1.806876
O	3.099210	4.703489	1.337127	C	3.163709	7.606175	2.057119
O	5.307251	3.196531	1.253180	C	2.406634	8.905596	2.174439
O	2.897834	6.866848	3.023832	H	1.385821	8.738387	1.810686
O	3.950813	7.429893	1.091317	H	2.881761	9.670584	1.559333
O	3.942947	5.264006	5.030993	H	2.339432	9.222030	3.217374
O	5.930638	4.145373	4.917697	C	5.116545	4.684249	5.558347
O	1.641978	4.441541	3.584488	C	5.327522	4.791822	7.043238
O	1.644156	2.599181	2.233494	H	4.784088	5.651292	7.437835
O	3.036524	2.327870	-0.228558	H	4.924065	3.880475	7.501153
O	4.047848	3.987891	-1.384741	H	6.391886	4.849532	7.276740
O	7.636810	3.914827	2.626788	C	1.172328	3.288822	3.095840
O	7.458232	5.255454	0.810753	C	-0.248630	2.997723	3.490047
O	6.173667	1.799147	3.410879	H	-0.905727	3.591189	2.843233
O	3.905270	0.999557	1.950314	H	-0.469325	1.939861	3.344721
C	3.222076	7.710149	2.060304	H	-0.418609	3.301712	4.524415
C	2.615403	9.080314	2.236459	C	3.248802	2.997732	-1.300627
H	1.523856	8.996091	2.236261	C	2.572047	2.429644	-2.524602
H	2.942372	9.739616	1.432558	H	2.650579	3.127292	-3.359110
H	2.906837	9.488881	3.208856	H	1.525952	2.203390	-2.305105
C	5.010262	4.731620	5.556595	H	3.062899	1.486480	-2.789575
C	5.118770	4.842184	7.051449	C	8.171537	4.744598	1.673333
H	4.623467	3.963006	7.481714	C	9.674388	4.882207	1.648909
H	6.167518	4.829359	7.351371	H	9.960502	5.714742	1.005473
H	4.608568	5.736874	7.411261	H	10.101762	3.956316	1.246322
C	1.126019	3.334451	3.116917	H	10.065670	5.014775	2.660098
C	-0.197141	2.943677	3.713039	H	7.331813	1.712500	3.559858
H	-0.762042	3.826869	4.015370	H	4.515161	0.804017	2.612052
H	-0.756697	2.331045	3.004946	O	5.461609	6.191769	-2.143991
H	0.009975	2.342172	4.606658	H	5.881945	6.851551	-2.713548
C	3.374000	2.931130	-1.329968	H	4.982330	5.566485	-2.717061
C	2.903453	2.240328	-2.586600	H	5.869401	2.307604	0.910902
H	2.841298	2.952348	-3.411115	H	5.717697	6.050174	3.243813

3-H3H4				O	5.985759	4.114963	4.898688
-5846.829131268722				O	1.638330	4.388091	3.624262
Mn	3.478346	4.982432	3.145114	O	1.615621	2.563209	2.245641
Mn	5.805029	3.507198	2.989696	O	3.019758	2.263965	-0.219380
Mn	3.426566	2.614146	1.512935	O	4.008284	3.954086	-1.346576
Ca	5.153493	5.469170	0.157358	O	7.642747	3.856497	2.619763
O	3.950152	3.145309	3.243993	O	7.424612	5.159182	0.788615
O	5.181277	5.248164	2.637516	O	6.202665	1.741379	3.428950
O	3.088141	4.603428	1.260811	O	3.817383	0.910054	1.962370
O	5.314106	3.092638	1.093257	C	3.206825	7.656619	2.085853
O	2.934419	6.777375	2.994999	C	2.590675	9.010722	2.288726
O	3.979124	7.379819	1.076134	H	1.499705	8.919398	2.246508
O	3.966006	5.135249	4.990875	H	2.941089	9.692224	1.513719
O	5.926142	3.971649	4.854178	H	2.844058	9.390074	3.283283
O	1.623899	4.349730	3.519381	C	5.104219	4.752034	5.551218
O	1.620595	2.503141	2.173485	C	5.305673	4.994382	7.017500
O	2.911965	2.314755	-0.290323	H	4.801881	4.186354	7.563950
O	3.992918	3.957256	-1.417615	H	6.369509	4.965081	7.256897
O	7.615197	3.945372	2.661208	H	4.849887	5.940022	7.316287
O	7.445248	5.226387	0.803216	C	1.076637	3.316958	3.102725
O	6.180371	1.724046	3.203745	C	-0.314400	3.032432	3.585470
O	3.873974	0.921222	1.787643	H	-0.991403	3.785974	3.165309
C	3.312093	7.656125	2.090506	H	-0.622053	2.038246	3.261626
C	2.868494	9.066108	2.390550	H	-0.356561	3.126052	4.674053
H	1.860761	9.071720	2.811619	C	3.338677	2.905355	-1.329475
H	2.921536	9.674553	1.487200	C	2.832770	2.234718	-2.574908
H	3.545508	9.484179	3.144866	H	2.762811	2.959999	-3.386534
C	5.046270	4.653227	5.487106	H	1.873297	1.746549	-2.394296
C	5.310007	4.933454	6.940083	H	3.554279	1.456259	-2.853302
H	4.366268	4.998815	7.484022	C	8.140147	4.562495	1.604690
H	5.958538	4.164363	7.360991	C	9.639333	4.554232	1.544268
H	5.818145	5.902636	7.009682	H	9.989209	5.396857	0.947102
C	1.101248	3.279612	3.064643	H	9.953930	3.619994	1.062138
C	-0.238379	2.860058	3.603401	H	10.071073	4.571849	2.547184
H	-0.792786	3.730936	3.955676	H	7.124607	1.547469	3.686370
H	-0.797427	2.306487	2.847420	H	4.767921	0.713329	2.124506
H	-0.057193	2.191452	4.453843	O	5.522716	6.470287	-2.080736
C	3.254881	2.946919	-1.380933	H	5.991958	7.253765	-2.409584
C	2.697168	2.333359	-2.642726	H	5.187995	6.009906	-2.868902
H	2.729418	3.054428	-3.460653	H	5.674204	6.001178	3.201980
H	1.679333	1.974023	-2.477571	H	3.749417	2.525822	4.116845
H	3.314526	1.466135	-2.904890	H	2.187614	4.786114	1.090678
C	8.108407	4.733707	1.735774	3-H1H3H4			
C	9.582277	5.015707	1.892529	-5847.075147368253			
H	9.990769	5.393370	0.954709	Mn	3.407890	4.949947	3.182245
H	10.114614	4.120243	2.220314	Mn	5.999410	3.474170	3.088991
H	9.704179	5.778959	2.670111	Mn	3.455552	2.598851	1.543256
H	7.025050	1.525962	3.642943	Ca	5.114399	5.457832	0.126588
H	4.542473	0.851929	2.513874	O	4.074495	3.062408	3.402126
O	5.452832	6.166036	-2.163843	O	5.291443	5.296850	2.686119
H	5.889936	6.819062	-2.728826	O	3.210759	4.491773	1.477370
H	4.986706	5.536224	-2.742277	O	5.401616	3.063390	1.229991
H	2.167129	4.799554	1.016967	O	2.899957	6.697588	3.054609
H	5.784778	2.273674	0.846518	O	3.905666	7.302701	1.119801
3-H5H6H7				O	4.077464	5.134067	5.079389
-5847.068329526440				O	6.081791	4.044001	4.910939
Mn	3.368824	5.043724	3.263568	O	1.685598	4.295021	3.628920
Mn	5.892660	3.442181	2.980350	O	1.663667	2.479783	2.241719
Mn	3.528775	2.589450	1.521247	O	2.912746	2.315262	-0.186893
Ca	5.150887	5.461973	0.106388	O	3.972117	3.948564	-1.332540
O	3.965655	3.157801	3.403041	O	7.723450	3.953925	2.691736
O	5.200421	5.342008	2.661458	O	7.435858	5.191594	0.815971
O	3.100341	4.622763	1.392340	O	6.351442	1.745375	3.388424
O	5.271175	3.099967	1.277929	O	3.863965	0.875860	1.811959
O	2.887469	6.793585	3.068217	C	3.140842	7.555990	2.058082
O	3.923288	7.354177	1.127622	C	2.387460	8.847038	2.195626
O	3.989457	5.221774	5.049949	H	1.370213	8.686516	1.816846
				H	2.871922	9.619873	1.597886

H	2.307959	9.144346	3.243226	H	2.713738	3.027740	-3.435790
C	5.167056	4.704146	5.570494	H	1.612872	1.996289	-2.451466
C	5.478777	4.974640	7.013091	H	3.228891	1.419314	-2.858823
H	4.556573	5.176172	7.559435	C	8.105508	4.691217	1.702272
H	6.029203	4.138261	7.448132	C	9.578661	4.950425	1.831733
H	6.120514	5.863623	7.062624	H	9.972831	5.304738	0.878731
C	1.103218	3.292434	3.054242	H	10.105206	4.055353	2.169281
C	-0.341299	3.067234	3.380860	H	9.722374	5.728347	2.591906
H	-0.935357	3.671992	2.683272	H	7.024511	1.408704	3.654823
H	-0.600589	2.016830	3.242175	H	4.630454	0.755318	2.362629
H	-0.555621	3.405265	4.396327	O	5.557553	6.434304	-2.074302
C	3.186465	2.986734	-1.292702	H	6.055811	7.214464	-2.367315
C	2.481555	2.442263	-2.503206	H	5.215483	6.019560	-2.883799
H	2.580545	3.140805	-3.334288	H	3.720646	2.431504	4.061239
H	1.430125	2.249945	-2.275695	H	5.770721	2.241252	0.826854
H	2.938233	1.482609	-2.772006	H	2.155261	4.728741	1.066266
C	8.177682	4.688115	1.665589				
C	9.674108	4.811599	1.650905				
H	9.965290	5.646204	1.012330				
H	10.092487	3.883855	1.241052				
H	10.065117	4.931543	2.663661				
H	7.239282	1.541990	3.741068				
H	4.630559	0.693612	2.395287				
O	5.588522	6.382546	-2.079385				
H	6.095750	7.137169	-2.418881				
H	5.200555	5.949387	-2.858426				
H	5.711493	5.983421	3.236634				
H	3.848716	2.482131	4.154513				
H	5.872984	2.272470	0.902552				
3-H1H3H4							
-5847.078979865117							
Mn	3.452815	4.969428	3.201891				
Mn	5.877438	3.467080	3.013918				
Mn	3.378299	2.526649	1.480968				
Ca	5.128486	5.455210	0.119270				
O	3.947568	3.031495	3.324456				
O	5.148681	5.159283	2.645179				
O	3.072733	4.528528	1.328958				
O	5.275916	3.025124	1.137202				
O	2.934786	6.711420	3.061000				
O	3.954523	7.313932	1.132501				
O	4.005940	5.107817	5.025448				
O	5.989671	3.985137	4.858184				
O	1.619298	4.282966	3.571805				
O	1.592408	2.457898	2.191420				
O	2.864497	2.263173	-0.261584				
O	3.953488	3.919268	-1.357685				
O	7.622327	3.895287	2.656209				
O	7.401887	5.169601	0.803974				
O	6.175539	1.683569	3.263411				
O	3.819007	0.846333	1.801978				
C	3.298982	7.609315	2.137811				
C	2.831640	9.000337	2.453843				
H	1.830292	8.984680	2.889690				
H	2.861896	9.611039	1.551015				
H	3.511700	9.426976	3.201539				
C	5.132697	4.699456	5.496916				
C	5.467747	5.083165	6.905601				
H	4.554740	5.178735	7.496096				
H	6.156617	4.359986	7.344007				
H	5.960816	6.063527	6.872307				
C	1.055819	3.253207	3.064637				
C	-0.348997	2.926247	3.477583				
H	-1.030432	3.328646	2.717145				
H	-0.488670	1.843941	3.513111				
H	-0.575484	3.393791	4.436449				
C	3.216162	2.921434	-1.363163				
C	2.645112	2.314966	-2.613504				
3-H2H3H4							
-5847.093958962161							
Mn	3.417442	5.032811	3.178103				
Mn	5.867954	3.510975	3.019555				
Mn	3.447362	2.649494	1.541228				
Ca	5.177596	5.508951	0.023568				
O	4.002194	3.239714	3.265422				
O	5.245555	5.373300	2.595336				
O	3.121285	4.646943	1.301900				
O	5.343028	3.128212	1.135386				
O	2.930839	6.817721	2.992324				
O	3.963297	7.367497	1.054250				
O	3.992318	5.221520	4.986503				
O	5.963537	4.075904	4.861487				
O	1.670206	4.418752	3.569464				
O	1.645055	2.555840	2.249429				
O	2.915483	2.327180	-0.216843				
O	3.972711	3.955796	-1.373313				
O	7.649278	3.942786	2.662731				
O	7.436479	5.205089	0.799883				
O	6.214973	1.791390	3.342231				
O	3.856568	0.958935	1.837306				
C	3.244175	7.673907	2.019320				
C	2.640430	9.036425	2.201818				
H	1.548349	8.953378	2.174006				
H	2.986237	9.704998	1.413822				
H	2.905644	9.430539	3.187724				
C	5.048842	4.697543	5.511318				
C	5.213878	4.830367	6.993211				
H	4.730577	3.959541	7.455830				
H	6.272271	4.818986	7.258336				
H	4.716528	5.732891	7.351978				
C	1.129907	3.324625	3.128414				
C	-0.199196	2.948708	3.705354				
H	-0.752085	3.840728	4.004383				
H	-0.760419	2.343733	2.991531				
H	-0.008313	2.341867	4.600396				
C	3.249292	2.939802	-1.337048				
C	2.694800	2.288781	-2.572369				
H	2.770247	2.967591	-3.422124				
H	1.661246	1.974655	-2.408895				
H	3.280049	1.383931	-2.776991				
C	8.146071	4.670782	1.669401				
C	9.644541	4.772543	1.679371				
H	9.964821	5.593642	1.037637				
H	10.058155	3.833052	1.292319				
H	10.016567	4.898643	2.698761				
H	7.130685	1.600536	3.624411				
H	4.390533	0.819674	2.651399				
O	5.623977	6.369391	-2.210612				
H	6.148152	7.101719	-2.573185				
H	5.237248	5.913067	-2.977048				

H	5.806482	2.328101	0.819689	O	5.238836	5.194441	2.766713
H	2.228200	4.870032	0.981424	O	3.083564	4.418550	1.456616
H	5.701590	6.080426	3.087233	O	5.337645	2.968486	1.279911
3-H1H2H3H4				O	2.879079	7.102045	2.920807
-5847.219980988147				O	3.973174	7.408671	0.959824
Mn	3.367465	4.993252	3.222924	O	4.003085	5.130511	5.151652
Mn	5.945090	3.456485	3.022216	O	5.951104	3.937670	4.995920
Mn	3.386731	2.508455	1.525088	O	1.593359	4.275234	3.689940
Ca	5.123782	5.507369	-0.073766	O	1.630360	2.402726	2.374136
O	3.997003	3.096090	3.356214	O	2.933530	2.235681	-0.202851
O	5.192729	5.276573	2.581096	O	4.008357	3.849690	-1.379429
O	3.091088	4.518580	1.371670	O	7.678548	3.983972	2.629312
O	5.288695	3.017157	1.184418	O	7.465804	5.170484	0.705069
O	2.871075	6.718303	3.024825	O	6.484608	1.680449	3.403970
O	3.805142	7.255075	1.035275	O	3.857130	0.747235	1.859760
O	4.029864	5.180383	5.005519	C	3.264707	7.815499	1.929850
O	6.032010	4.087378	4.840273	C	2.806030	9.270412	1.905935
O	1.650122	4.317735	3.628926	H	1.984756	9.365981	1.185026
O	1.597588	2.469211	2.283043	H	3.620965	9.917071	1.567409
O	2.834854	2.221648	-0.182713	H	2.450470	9.593841	2.886785
O	3.871461	3.887092	-1.295016	C	5.094394	4.655915	5.618671
O	7.652096	3.915403	2.613261	C	5.421357	5.000886	7.058975
O	7.366956	5.103918	0.715650	H	4.505918	5.063415	7.652196
O	6.248054	1.739991	3.373107	H	6.107476	4.268442	7.488779
O	3.778891	0.831524	1.869392	H	5.905753	5.984981	7.074804
C	3.125293	7.584872	2.009556	C	1.068488	3.230732	3.168656
C	2.486724	8.921187	2.212655	C	-0.383103	2.961115	3.515860
H	1.416148	8.832846	1.983490	H	-1.012350	3.579970	2.864473
H	2.940872	9.648168	1.537633	H	-0.635278	1.911777	3.351504
H	2.569422	9.237815	3.255708	H	-0.584827	3.246144	4.551389
C	5.146321	4.751532	5.501609	C	3.230272	2.865040	-1.289444
C	5.433262	5.068958	6.933189	C	2.594258	2.313018	-2.555256
H	4.501294	5.109597	7.502101	H	2.369319	3.129002	-3.246675
H	6.132906	4.342686	7.350691	H	1.690916	1.741758	-2.331220
H	5.897378	6.065053	6.971124	H	3.316487	1.646119	-3.041946
C	1.067627	3.256089	3.141533	C	8.137145	4.704993	1.662149
C	-0.319437	2.968892	3.616840	C	9.636202	4.959610	1.698180
H	-1.018348	3.514033	2.966165	H	9.850253	5.974183	1.351715
H	-0.529240	1.900672	3.532733	H	10.122790	4.258267	1.009460
H	-0.453587	3.332277	4.638183	H	10.043780	4.805035	2.699324
C	3.148401	2.880639	-1.308451	H	6.953903	1.415170	2.594192
C	2.561901	2.264778	-2.538385	H	4.648605	0.756254	2.439632
H	2.561501	2.994390	-3.349615	O	5.527633	6.183482	-1.911946
H	1.558352	1.879077	-2.343389	H	6.313389	6.623159	-2.273046
H	3.189814	1.409474	-2.822980	H	5.251213	5.538938	-2.586389
C	8.124850	4.619770	1.563194	3-R2			
C	9.616572	4.720587	1.542348	-5846.151854462942			
H	9.918046	5.562729	0.917384	Mn	3.511769	4.804901	3.207644
H	10.016761	3.793952	1.108305	Mn	5.995695	3.435108	3.009754
H	10.019714	4.810361	2.553750	Mn	3.490351	2.588195	1.646044
H	7.124109	1.484949	3.728885	Ca	5.080359	5.186011	0.345057
H	4.566256	0.653224	2.433112	O	3.880001	3.005809	3.414959
O	6.066104	6.832609	-1.880066	O	5.253813	5.155394	2.783576
H	7.014099	6.974341	-2.048715	O	3.089462	4.437684	1.477287
H	5.615901	7.308277	-2.600148	O	5.254498	2.871508	1.252344
H	5.658634	5.996451	3.049343	O	2.976093	6.709029	3.104972
H	2.200069	4.735203	1.034421	O	3.935508	7.281977	1.129713
H	3.778910	2.525127	4.121179	O	3.988374	5.035415	5.159428
H	5.787259	2.265591	0.804571	O	5.969210	3.899354	5.089814
3-R1				O	1.584905	4.315331	3.672084
-5846.147396019414				O	1.503844	2.481706	2.305554
Mn	3.430603	5.005298	3.190645	O	2.886979	2.224344	-0.213692
Mn	5.795106	3.429794	3.020300	O	3.942263	3.862702	-1.378549
Mn	3.543107	2.605477	1.660340	O	7.950877	4.196185	2.549964
Ca	5.045352	5.278010	0.354973	O	7.496510	5.222967	0.585336
O	4.073725	2.880887	3.413083	O	6.653848	1.694055	3.353750
				O	3.696755	0.741572	1.965617
				C	3.253309	7.540725	2.151641

C	2.648517	8.925213	2.315229	O	3.908143	7.152170	1.031742
H	1.642317	8.915214	1.878275	O	4.070582	5.065818	5.144146
H	3.248285	9.665589	1.781409	O	6.028721	3.899989	5.001502
H	2.558079	9.193360	3.370512	O	1.670161	4.352625	3.903831
C	5.075325	4.584010	5.677859	O	1.296216	2.444996	2.724270
C	5.308646	4.942139	7.134529	O	2.677293	2.095720	-0.214830
H	4.359587	5.029655	7.668495	O	3.834428	3.679487	-1.345961
H	5.951106	4.200439	7.613935	O	7.711289	3.969169	2.676274
H	5.814042	5.915067	7.172512	O	7.449126	5.202113	0.782397
C	0.994483	3.317765	3.121113	O	6.462435	1.611793	3.474472
C	-0.473684	3.142219	3.463214	O	3.664126	0.627617	1.968556
H	-1.061344	3.791022	2.802231	C	3.242133	7.447969	2.054213
H	-0.786673	2.108249	3.304340	C	2.650485	8.842894	2.177657
H	-0.664988	3.446035	4.495282	H	1.678118	8.849813	1.669793
C	3.185795	2.861175	-1.297119	H	3.298015	9.571100	1.683442
C	2.575044	2.293907	-2.568821	H	2.493984	9.117101	3.223235
H	2.368933	3.099067	-3.278370	C	5.176417	4.617794	5.616045
H	1.664489	1.729966	-2.355277	C	5.498878	5.014931	7.044621
H	3.304039	1.614462	-3.027464	H	4.584523	5.083514	7.638958
C	8.277893	4.892376	1.528636	H	6.195741	4.305002	7.494780
C	9.730382	5.342711	1.430470	H	5.970206	6.005300	7.028872
H	9.768363	6.420313	1.240891	C	0.937611	3.364152	3.506218
H	10.200090	4.841467	0.576208	C	-0.487413	3.368615	4.038607
H	10.287508	5.104527	2.338725	H	-1.083317	4.056603	3.426304
H	6.684678	1.259531	2.483381	H	-0.926668	2.371067	3.971410
H	4.522996	0.700399	2.484163	H	-0.513963	3.728076	5.070674
O	5.218342	7.009469	-1.353769	C	2.995273	2.743033	-1.285472
H	5.101885	6.975828	-2.316399	C	2.311714	2.280646	-2.561394
H	4.640137	7.728633	-1.041902	H	2.223832	3.110893	-3.265944
				H	1.329559	1.851738	-2.350047
				H	2.933082	1.503655	-3.023724
				C	8.131960	4.752490	1.737981
				C	9.591015	5.166046	1.856600
				H	9.629958	6.146984	2.346285
				H	10.034674	5.266737	0.862809
				H	10.160560	4.455417	2.459239
				H	6.569657	1.173462	2.611709
				H	4.419074	0.639758	2.588681
				O	5.396967	5.984606	-1.926108
				O	5.612100	6.865257	-2.270769
				H	4.819934	5.568868	-2.589368

3-R3							
-5846.152948571307							
Mn	3.506690	4.760473	3.212646				
Mn	5.854971	3.342504	2.990363				
Mn	3.349102	2.455852	1.642287				
Ca	5.033030	5.054058	0.331907				
O	4.035768	2.976044	3.432496				
O	5.221939	5.115159	2.743517				
O	3.012414	4.321895	1.510399				
O	5.518096	2.865158	1.315064				
O	2.968185	6.653335	3.040941				

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