

Supporting Information

Ca K-edge XAS as a probe of calcium centers in complex systems

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Section S1

Description of the X-ray structure of **8ⁱ**

The structure of $[\text{Ca}_2(\text{bzida})_2(\text{OH}_2)_6]_n$ (**8ⁱ**) consists of dimeric $[\text{Ca}_2(\text{bzida})_2(\text{OH}_2)_6]$ units, in which two $[\text{Ca}(\text{bzida})(\text{OH}_2)_2]$ moieties are bridged by two aqua ligands. These dimeric units form a three-dimensional coordination polymer through binding of one uncoordinated carboxylate O atom of each bzida^{2-} ligand to a neighbouring Ca^{+2} ion. Each Ca^{+2} ion is 8-coordinate, being bonded to the N and two O atoms from a bzida^{2-} ligand, two O atoms from terminal aqua ligands, two O atoms from bridging aqua ligands, and a carboxylate O atom from a bzida^{2-} ligand of a neighboring dimeric $[\text{Ca}_2(\text{bzida})_2(\text{OH}_2)_6]$ unit. The geometry about each Ca^{+2} ion can be approximated as distorted square antiprismatic, similar to that found in **8^h**, O4', O11, O12 and O13 are approximately coplanar, as O1, O3, O12' and N1, and the two planes lie above and below the Ca^{+2} ion, with the donor atoms in a staggered conformation. Ca-O distances lie in the range 2.3702(11) Å to 2.6410(12) Å, with those to the carboxylate O atoms being the shortest, and those to the bridging aqua ligands being the longest. The Ca-N distance (2.6935(13) Å) is the longest metal-ligand bond. Charge considerations and similarity between C2-O1, C2-O2, C4-O3 and C4-O4 distances (mean distance 1.258(5)) require the deprotonation of both ligand carboxylic acid moieties, resulting in dianionic bzida^{2-} , and this is supported by the relatively short Ca-O distances involving the carboxylate O atoms. Six really short hydrogen bond interactions (O – O distances range 2.687(2) – 2.887(2)) can be detected, creating a two dimensional network of water molecules.

Table S1.1. Crystallographic data for the structure of complex **8^{bzida}**.

	$\{[\text{Ca}_2(\text{bzida})_2(\text{OH}_2)_6]\}_n$
Empirical formula	$\text{C}_{22}\text{H}_{34}\text{Ca}_2\text{N}_2\text{O}_{14}$
Formula weight	630.67
Color, shape	Colorless, long block
Crystal size, mm	0.88x0.31x0.23
Crystal system	Monoclinic
Space group	$P 2_1/c$
a , Å	16.8494(6)
b , Å	9.8491(4)
c , Å	8.3210(4)
α , deg.	90.00
β , deg.	92.118(4)
γ , deg.	90.00
V , Å ³	1379.93(10)
Z	2
T , K	150(2)
ρ (calc), Mg/m ³	1.518
μ , mm ⁻¹	0.485
θ range, deg.	3.40 to 28.28
No. of rflcn/obsv	6154/3395
GooF	1.036
$R1$	0.0350
$wR2$	0.0757

Table S1.2. Selected bond lengths (Å) and angles (deg) for complex **8^{bzida}**.

Ca(1)-O(1)	2.3702(11)	Ca(1)-O(13)	2.4842(12)
Ca(1)-O(3)	2.3919(11)	Ca(1)-O(12)	2.5833(13)
Ca(1)-O(11)	2.4405(13)	Ca(1)-O(12')	2.6410(12)
Ca(1)-O(4')	2.4471(11)	Ca(1)-N(1)	2.6935(13)
O(3)-Ca(1)-O(1)	105.46(4)	O(12)-Ca(1)-O(13)	73.95(4)
O(11)-Ca(1)-O(1)	79.22(4)	O(12')-Ca(1)-O(1)	74.05(4)
O(11)-Ca(1)-O(3)	137.26(4)	O(12')-Ca(1)-O(3)	149.13(4)
O(4')-Ca(1)-O(1)	143.29(4)	O(12')-Ca(1)-O(11)	73.54(4)
O(4')-Ca(1)-O(3)	79.68(4)	O(12')-Ca(1)-O(4')	119.72(4)
O(4')-Ca(1)-O(11)	73.71(4)	O(12')-Ca(1)-O(13)	80.42(4)
O(13)-Ca(1)-O(1)	140.30(4)	O(12')-Ca(1)-O(12)	71.02(4)
O(13)-Ca(1)-O(3)	81.83(4)	N(1)-Ca(1)-O(1)	65.12(4)
O(13)-Ca(1)-O(11)	121.92(4)	N(1)-Ca(1)-O(3)	63.83(4)
O(13)-Ca(1)-O(4')	76.11(4)	N(1)-Ca(1)-O(11)	81.50(4)
O(12)-Ca(1)-O(1)	69.28(4)	N(1)-Ca(1)-O(4')	86.48(4)
O(12)-Ca(1)-O(3)	79.90(4)	N(1)-Ca(1)-O(13)	143.86(4)
O(12)-Ca(1)-O(11)	137.58(4)	N(1)-Ca(1)-O(12)	108.52(4)
O(12)-Ca(1)-O(4')	145.71(4)	N(1)-Ca(1)-O(12')	135.30(4)

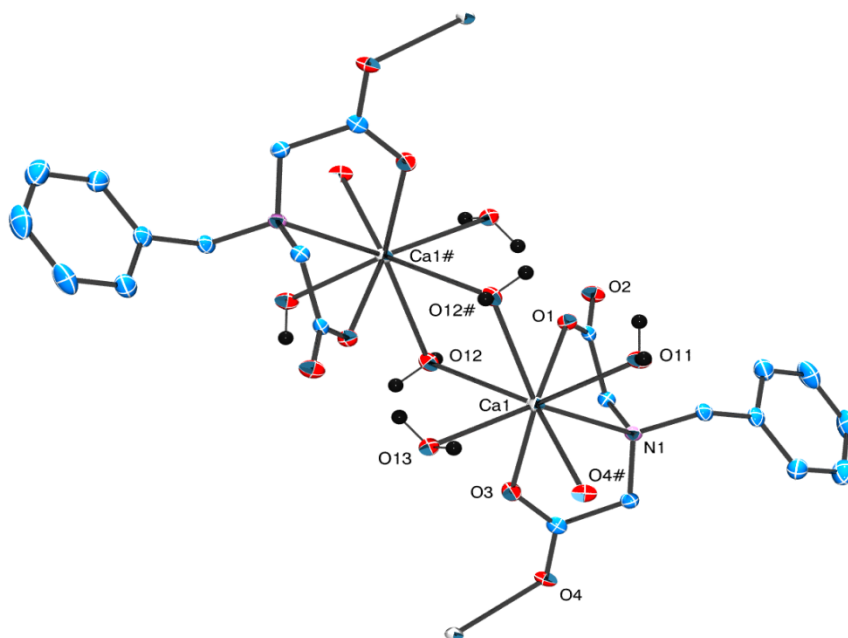


Figure S1.3: ORTEP-type drawings of complex **8ⁱ** with thermal ellipsoids at 50% probability. Only relevant hydrogen atoms are shown for clarity.

Section S2

Description of 8^i theoretical model

The 8^i polymer was truncated to a $[\text{Ca}_2(\text{bzida})_2(\text{OH}_2)_6]$ repeating unit (monomer). Each calcium center from one monomer is linked to a Ca center from a neighboring monomer via an acetyl ($-\text{CH}_2\text{COO}^-$) "linker" subunit. Each Ca center has two such interactions. Furthermore, the neighboring monomer calcium centers are separated by four bonds $\text{Ca}-\text{O}=\text{C}=\text{O}-\text{Ca}$, as such it is expected that Ca centers on neighboring monomers should at most exert only a small electronegative effect on the bonding interactions of their neighbor. Therefore the $[\text{Ca}_2(\text{bzida})_2(\text{OH}_2)_6]$ repeating unit (monomer) was constructed by first isolating the full coordination sphere of the monomer, the acetyl "linkers" and neighboring Ca^{+2} atoms from the neighboring repeating unit. In turn this was followed by replacement of the Ca^{+2} atoms and capping the "linker" carboxyl groups with protons, which serves to compensate for the excess negative charge resulting from the removal of neighboring monomer Ca^{+2} atoms.

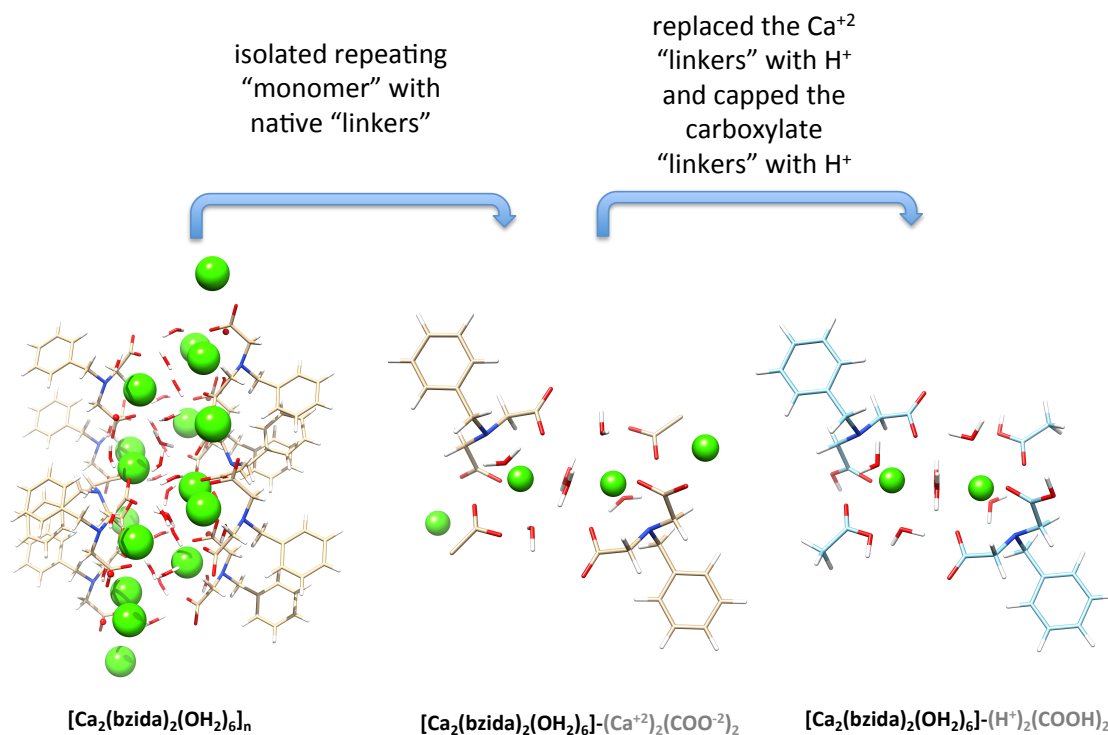


Figure S2.1: Schematic for the construction of the 8^i model used for properties calculations.

Description of 6^d theoretical model

The 6^d complex was geometry optimized using the TPSS functional, a def2-TZVP basis set and a dense integration grid (Grid 6) on the Ca and Mn centers. The first coordination sphere of calcium was isolated, consisting of the Ca⁺² center and acetate ligands. The acetate ligands were protonated and oxygen-hydrogen bond distances were optimized.

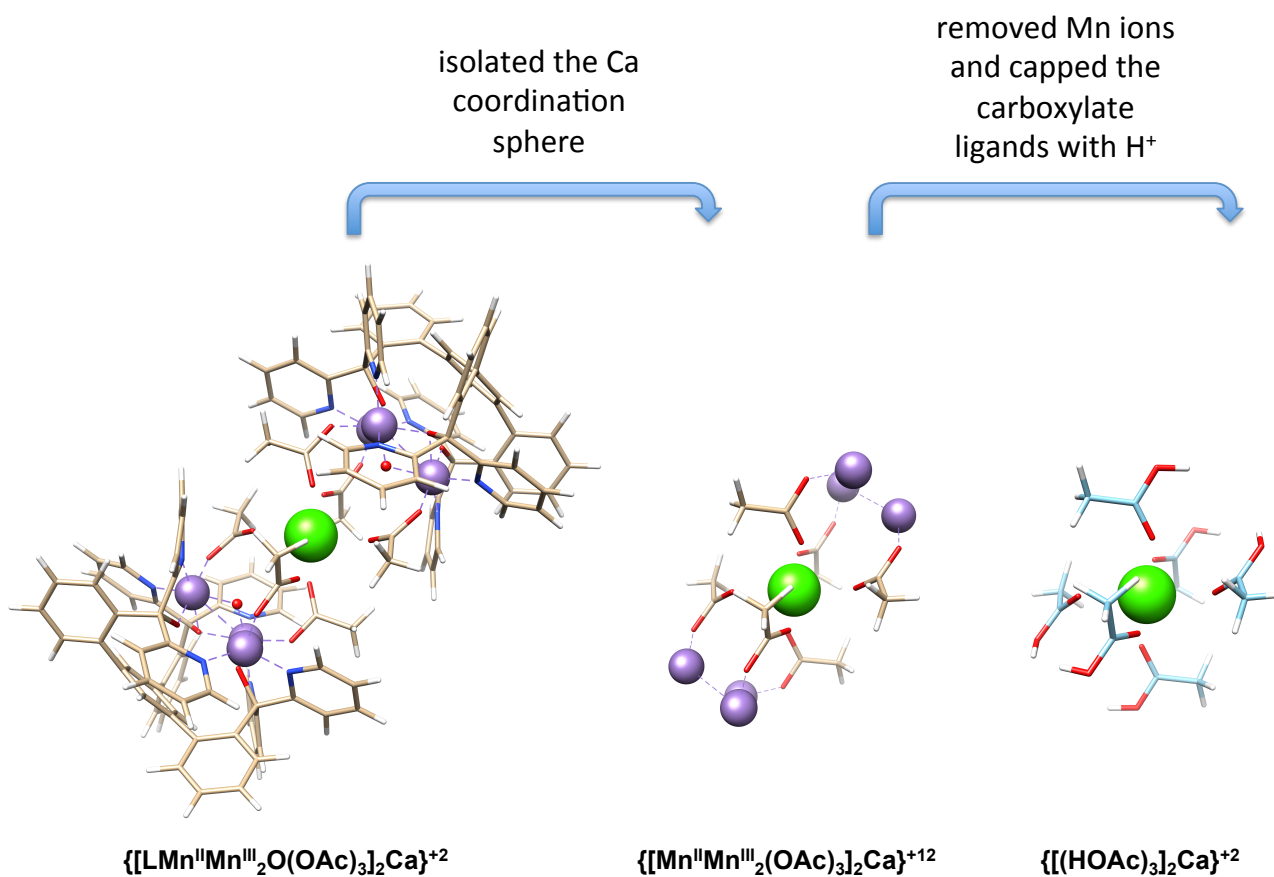


Figure S2.2: Schematic for the construction of the 6^d model used for properties calculations.

Section S3

Functional correlation study

The impact of functional on the calculated Ca K-edge was explored. Similar to previous studies (Inorg Chem 2012, 51, 680; Phys Chem Chem Phys 2013, 15, 2091) a dependence on the amount of Hartree-Fock exchange was found. Five functionals were tested (BP86, PBE, TPSSh, B3LYP and BHLYP) however only the BHLYP functional gave results comparable to experiment. Below the quadrupole intensity is used to help visually track transitions to the d orbitals. The BHLYP functional calculations resolved the Ca K- pre-edge, is the only functional that offers a picture where the pre-edge of the six coordinate complex is lower in intensity than that of the eight coordinate complex, as expected from experiment and predicts a ligand field splitting and relative pre-edge intensities for the six coordinate $\text{Ca}(\text{OH})_2$ ($6^{\text{D}_{2\text{h}}}$) that match experimentally observed values.

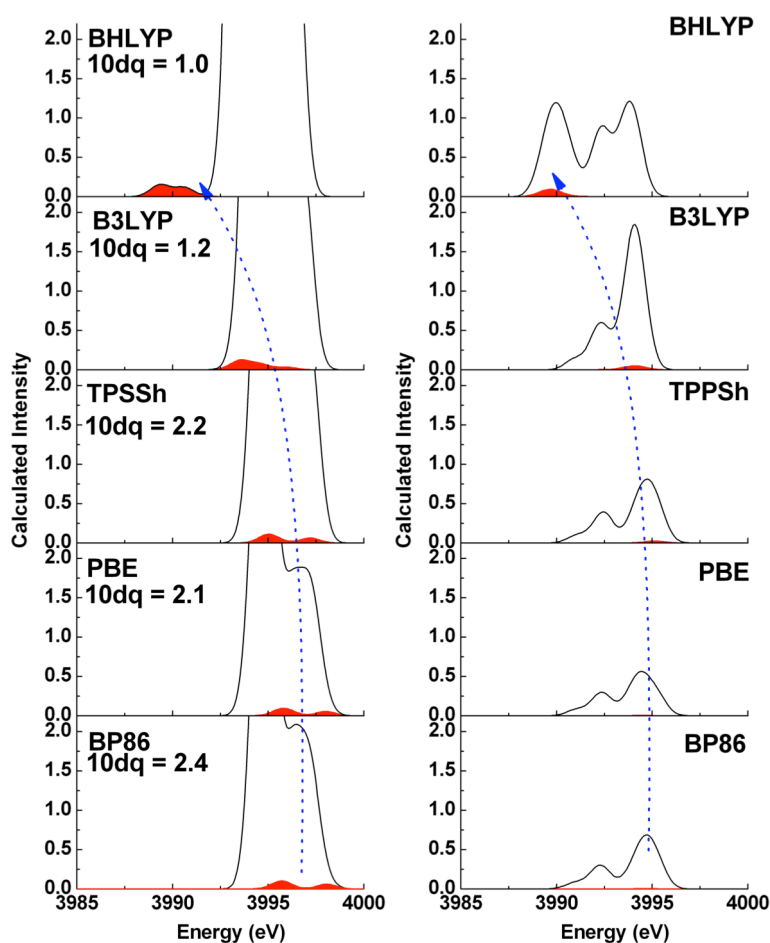


Figure S3.1 Study on the impact of the functional used on calculated Ca K- pre-edges. Study on the $\text{Ca}(\text{OH})_2$ ($6^{\text{D}_{2\text{h}}}$) (left); study on $[\text{Ca}(\text{Htpaa})(\text{H}_2\text{O})]$ (8^{f}) (right). Total calculated intensity (black), quadrupole intensity (red); Blue arrow shows the dependency of the pre-edge on functional. Calculated spectra were aligned with respect to the Ca 1s core orbital energies using the BHLYP calculation as the standard (energy shift is in eV):

($6^{\text{D}_{2\text{h}}}$): BP86 = 67.47; PBE = 69.44; TPSSh = 46.40; B3LYP = 41.23; BHLYP = 0;
 (8^{f}): BP86 = 67.67; PBE = 69.58; TPSSh = 46.56; B3LYP = 41.31; BHLYP = 0;

Section S4

Fitted Experimental and Calculated Ca K- pre-edge XAS spectra

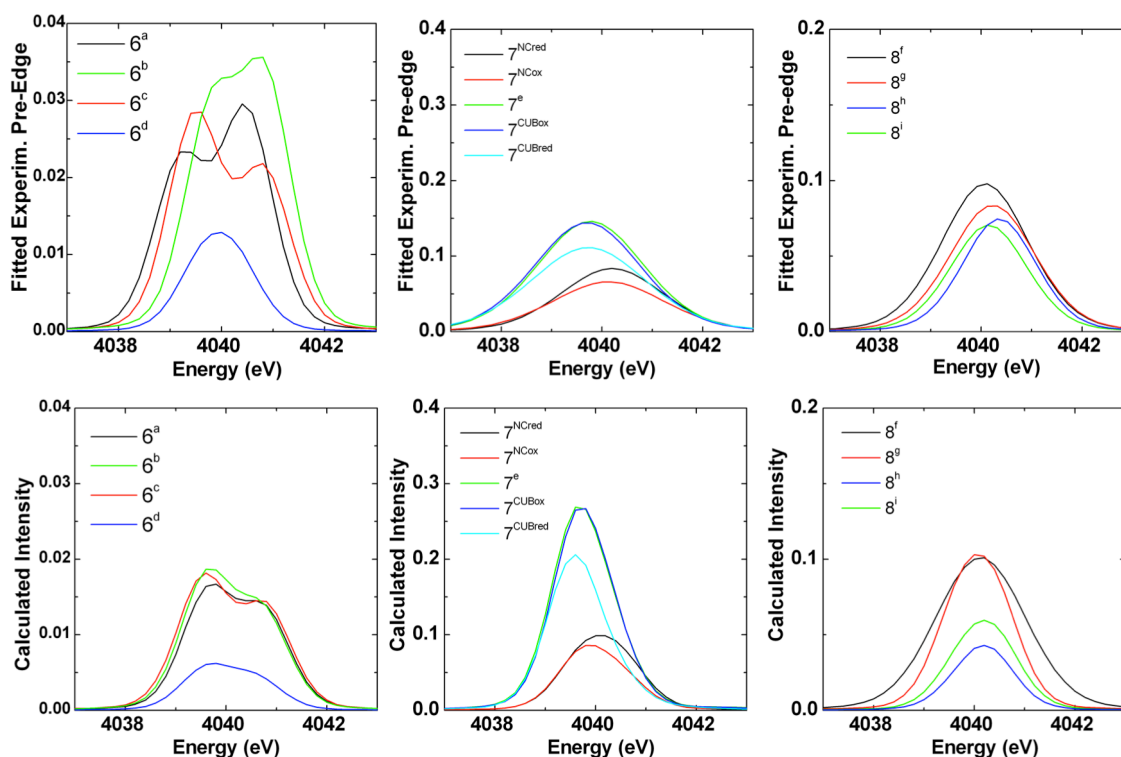


FIGURE S4.1: Fitted experimental Ca *K*- pre-edges of six, seven and eight coordinate species. The rising edge background has been subtracted for clarity. (top). Calculated Ca *K*-pre-edges for six, seven and eight coordinate species. The transitions were approximated as Gaussian-Lorentzian sum peaks with 75% Gaussian character. The transition energies were shifted by 50.17 eV and the intensities multiplied by a factor of 3500 units.

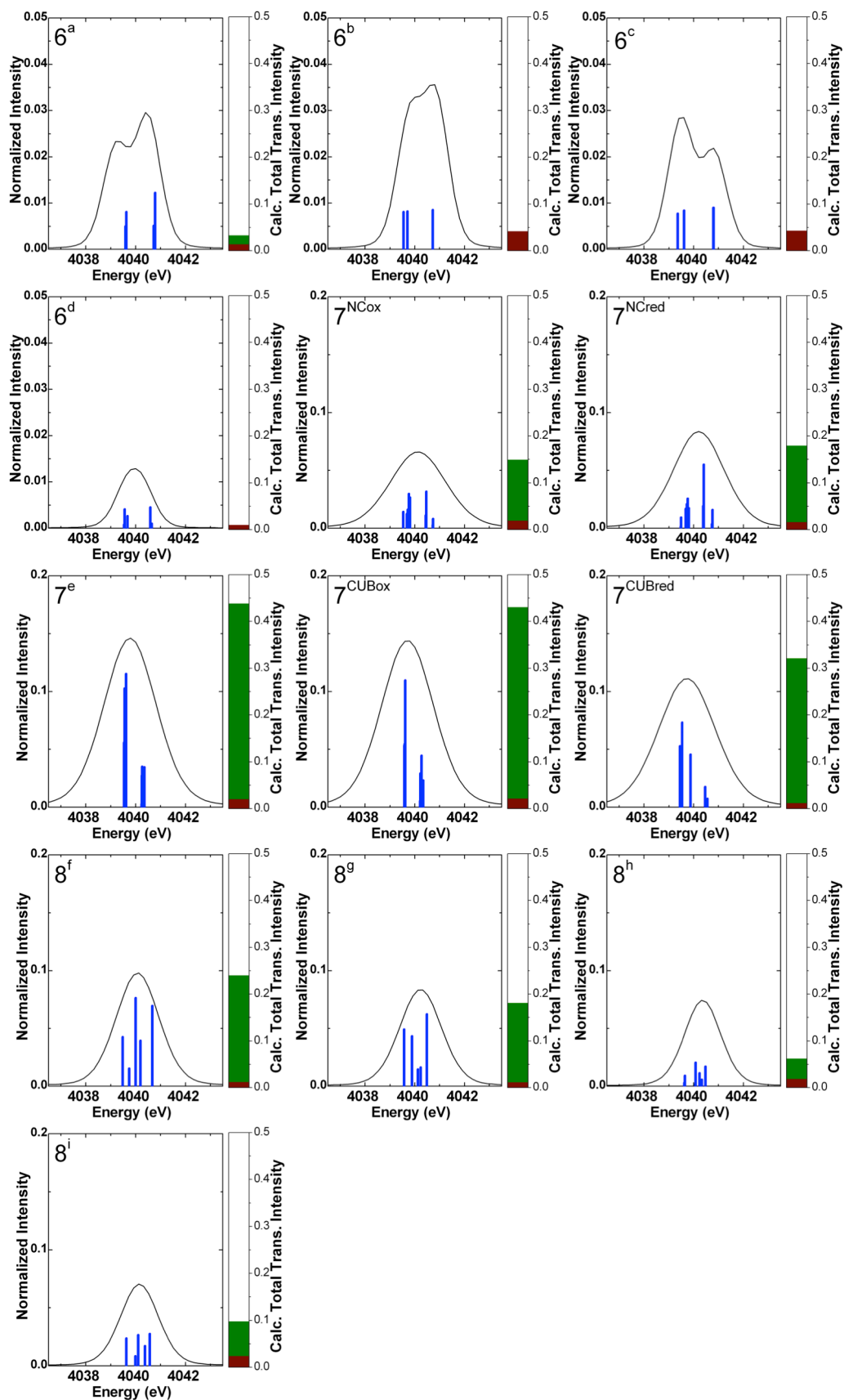


FIGURE S4.2: Fitted experimental Ca K- pre-edges (black line) overlaid with calculated transition intensities (blue bars). Contribution to the total calculated Ca K- pre-edge intensities from dipole (green) and quadrupole (red) is shown as a bar-graph for each complex. The calculated transitions were shifted by 50.17 eV and the intensity multiplied by a factor of 3500.

TABLE S4.3: Break down of calculated transitions contributing to the Ca K- pre-edge for the compounds under study. The energy for the calculated transitions were shifted by 50.17 eV and the total, dipole and quadrupole intensities were multiplied by a factor of 3500.

Compound	Label	Coordination	Local Symmetry*	Transition	Calculated			
					Energy(eV)	Total Intensity	Dipole Intensity	Quadrupole Intensity
CaO	6 ^a	6	O _h	1	4039.59	0.0050	0.0001	0.0031
				2	4039.63	0.0080	0.0032	0.0030
				3	4039.63	0.0081	0.0031	0.0031
				4	4040.72	0.0051	0.0004	0.0040
				5	4040.78	0.0122	0.0120	0.0001
				Total		0.0385	0.0188	0.0134
CaCO ₃	6 ^a	6	O _h /D _{4h}	1	4039.55	0.0081	0.0000	0.0081
				2	4039.55	0.0081	0.0000	0.0081
				3	4039.7	0.0082	0.0000	0.0082
				4	4040.73	0.0085	0.0000	0.0085
				5	4040.73	0.0085	0.0000	0.0085
				Total		0.0414	0.0000	0.0414
Ca(OH) ₂	6 ^c	6	O _h /D _{4h}	1	4039.36	0.0077	0.0000	0.0077
				2	4039.61	0.0084	0.0000	0.0084
				3	4039.61	0.0083	0.0000	0.0083
				4	4040.79	0.0090	0.0000	0.0090
				5	4040.8	0.0090	0.0000	0.0090
				Total		0.0425	0.0000	0.0425
{[LMn ^{II} Mn ^{III} O(OAc) ₃] ₂ Ca} ⁺²	6 ^d	6	O _h /D _{4h}	1	4039.53	0.0008	0.0000	0.0007
				2	4039.56	0.0041	0.0000	0.0026
				3	4039.67	0.0026	0.0000	0.0017
				4	4040.59	0.0045	0.0000	0.0039
				5	4040.64	0.0010	0.0000	0.0006
				Total		0.0130	0.0000	0.0095

Compound	Label	Coordination	Local Symmetry*	Transition	Calculated			
					Energy(eV)	Total Intensity	Dipole Intensity	Quadrupole Intensity
[LMn ^{IV} Mn ^{III} ₂ CaO ₃ (OAc) ₂ (DME)(OTf)] ⁺²	7 ^{NCox}	7	C _{2v} /C _{3v}	1	4039.53	0.0023	0.0013	0.0008
				2	4039.54	0.0142	0.0089	0.0046
				3	4039.68	0.0125	0.0116	0.0007
				4	4039.72	0.0160	0.0146	0.0010
				5	4039.76	0.0297	0.0273	0.0017
				6	4039.81	0.0266	0.0240	0.0017
				7	4040.44	0.0112	0.0098	0.0009
				8	4040.46	0.0315	0.0280	0.0023
				9	4040.73	0.0028	0.0014	0.0011
				10	4040.74	0.0080	0.0037	0.0038
				Total				
[LMn ^{III} ₃ CaO ₂ (OAc) ₂ (DME)(OTf)] ⁺¹	7 ^{NCred}	7	C _{2v} /C _{3v}	1	4039.48	0.0018	0.0009	0.0007
				2	4039.49	0.0092	0.0050	0.0035
				3	4039.68	0.0167	0.0146	0.0013
				4	4039.73	0.0210	0.0193	0.0011
				5	4039.76	0.0256	0.0229	0.0021
				6	4039.81	0.0172	0.0140	0.0025
				7	4040.39	0.0193	0.0180	0.0008
				8	4040.41	0.0548	0.0512	0.0023
				9	4040.74	0.0037	0.0031	0.0004
				10	4040.76	0.0157	0.0141	0.0011
				Total				
LMn ^{IV} ₃ CaO ₄ (OAc) ₃ (THF)	7 ^e	7	C _{3v}	1	4039.53	0.0559	0.0543	0.0010
				2	4039.56	0.1026	0.0995	0.0020
				3	4039.58	0.0551	0.0542	0.0006
				4	4039.61	0.1152	0.1132	0.0014
				5	4040.24	0.0030	0.0023	0.0005
				6	4040.25	0.0274	0.0226	0.0033
				7	4040.25	0.0058	0.0049	0.0006
				8	4040.26	0.0350	0.0306	0.0031
				9	4040.34	0.0094	0.0073	0.0020
				10	4040.35	0.0346	0.0287	0.0056
				Total				
LMn ^{IV} ₃ CaO ₄ (OAc) ₃ (DMF)	7 ^{CUBox}	7	C _{3v}	1	4039.58	0.0534	0.0519	0.0010
				2	4039.59	0.0546	0.0534	0.0008
				3	4039.61	0.1033	0.1001	0.0020
				4	4039.62	0.1096	0.1071	0.0018
				5	4040.21	0.0055	0.0046	0.0008
				6	4040.23	0.0292	0.0245	0.0040
				7	4040.26	0.0091	0.0083	0.0006
				8	4040.27	0.0444	0.0407	0.0029
				9	4040.33	0.0026	0.0016	0.0010
				10	4040.34	0.0232	0.0169	0.0059
				Total				
[LMn ^{IV} ₂ Mn ^{III} CaO ₄ (OAc) ₃ (DMF)] ⁻	7 ^{CUBred}	7	-	1	4039.44	0.0528	0.0507	0.0013
				2	4039.49	0.0513	0.0500	0.0009
				3	4039.53	0.0731	0.0713	0.0013
				4	4039.53	0.0647	0.0627	0.0015
				5	4039.87	0.0033	0.0033	0.0000
				6	4039.88	0.0455	0.0453	0.0002
				7	4040.46	0.0056	0.0047	0.0006
				8	4040.47	0.0175	0.0139	0.0023
				9	4040.54	0.0052	0.0035	0.0012
				10	4040.55	0.0074	0.0040	0.0025
				Total				

Compound	Label	Coordination	Local Symmetry*	Transition	Calculated			
					Energy(eV)	Total Intensity	Dipole Intensity	Quadrupole Intensity
[Ca(Htpaa)(H ₂ O)]	8 ^f	8	D _{2d}	1	4039.48	0.0425	0.0365	0.0053
				2	4039.74	0.0152	0.0112	0.0028
				3	4040	0.0764	0.0707	0.0045
				4	4040.19	0.0393	0.0352	0.0039
				5	4040.67	0.0695	0.0691	0.0003
				Total		0.2429	0.2227	0.0169
[Ca(dpaa)(H ₂ O)(MeOH)] ₂	8 ^e	8	D _{2d}	1	4039.57	0.0491	0.0459	0.0027
				2	4039.89	0.0433	0.0405	0.0020
				3	4040.13	0.0145	0.0092	0.0034
				4	4040.24	0.0162	0.0142	0.0018
				5	4040.49	0.0622	0.0604	0.0011
				Total		0.1853	0.1702	0.0111
[Mn ₂ (tpaa) ₂ Ca ₂ (H ₂ O) ₁₂]	8 ^b	8	D _{4d} /D _{2d}	1	4039.63	0.0029	0.0013	0.0014
				2	4039.65	0.0091	0.0043	0.0042
				3	4040.07	0.0020	0.0015	0.0003
				4	4040.08	0.0203	0.0161	0.0028
				5	4040.24	0.0001	0.0001	0.0001
				6	4040.24	0.0112	0.0060	0.0034
				7	4040.33	0.0001	0.0000	0.0000
				8	4040.33	0.0057	0.0005	0.0036
				9	4040.47	0.0003	0.0002	0.0000
				10	4040.48	0.0169	0.0140	0.0021
Total		0.0686	0.0441	0.0179				
{[Ca ₂ (bzida) ₂ (H ₂ O) ₆]} _n	8 ⁱ	8	D _{4d} /D _{2d}	1	4039.63	0.0236	0.0195	0.0028
				2	4039.99	0.0082	0.0030	0.0039
				3	4040.1	0.0264	0.0189	0.0074
				4	4040.37	0.0171	0.0101	0.0062
				5	4040.57	0.0274	0.0225	0.0032
				Total		0.1026	0.0739	0.0235

Section S5

Ca *K*-edge calculated XAS pre-edge of Pantazis *et al.* truncated model of 7^{CUBred}

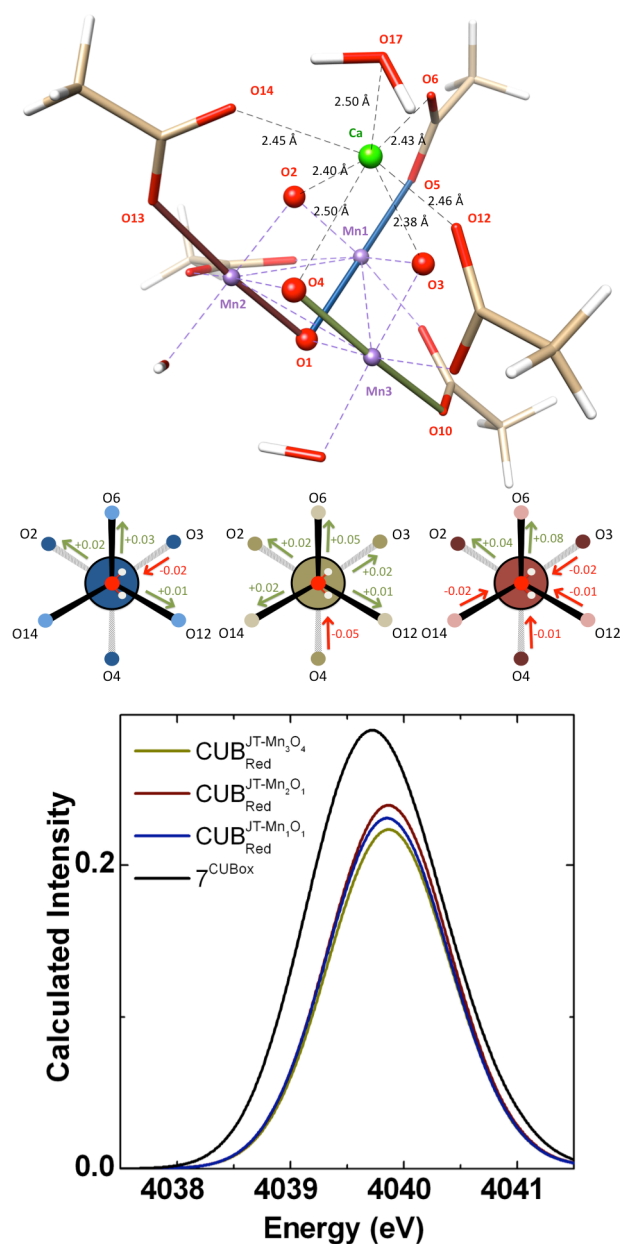


FIGURE S5.1: Model study of the reduced "cubane-like" 7^{CUBred} cluster using the models from Pantazis *et al.* (Krewald, V.; Neese, F.; Pantazis, D. A. *J. Am. Chem. Soc.* 2013, 135, p.5726). (top) Structural parameters of the starting (oxidized) geometry with the JT distortion axes upon reduction highlighted (blue, yellow, red). (middle) Bond distance changes associated with one electron reduction for the three different JT distortion models. (bottom) Calculated Ca *K*-edge pre-edges.

Section S6

Selected bond distances and XYZ coordinates of models used

Table S6.1. Selected experimental vs. calculated bond lengths.

Compound	Label	Coordination	Local Symmetry*	Bond	Average Bond Distances	
					Crystal Str. Distance (Å)	Geom. Opt. Distance (Å)
CaO	6 ^a	6	O _h	Ca-O _{oxo}	2.41	-
CaCO ₃	6 ^b	6	O _h /D _{4h}	Ca-O _{COO}	2.36	-
Ca(OH) ₂	6 ^c	6	O _h /D _{4h}	Ca-O _{OH}	2.36	-
{[LMn ^{III} Mn ^{III} ₂ O(OAc) ₃] ₂ Ca} ⁺²	6 ^d	6	O _h /D _{4h}	Ca-O _{COO}	2.29	2.31
[LMn ^{IV} Mn ^{III} ₂ CaO ₂ (OAc) ₂ (DME)(OTf)] ⁺²	7 ^{NCox}	7	C _{2v} /C _{3v}	Mn-X	2.16	1.92
				Ca-O _{oxo}	2.41	2.39
				Ca-O _x	2.39	2.36
[LMn ^{III} ₃ CaO ₂ (OAc) ₂ (DME)(OTf)] ⁺¹	7 ^{NCred}	7	C _{2v} /C _{3v}	Mn-X	2.06	1.82
				Ca-O _{oxo}	2.39	2.6
				Ca-O _x	2.41	2.38
LMn ^{IV} ₃ CaO ₄ (OAc) ₃ (THF)	7 ^e	7	C _{3v}	Mn-X	2.11	1.87
				Ca-O _{oxo}	2.42	2.43
				Ca-O _x	2.35	2.35
LMn ^{IV} ₃ CaO ₄ (OAc) ₃ (DMF)	7 ^{CUBox}	7	C _{3v}	Mn-X	1.93	1.81
				Ca-O _{oxo}	2.44	2.44
				Ca-O _x	2.31	2.35
[LMn ^{IV} ₂ Mn ^{III} CaO ₄ (OAc) ₃ (DMF)] ⁻	7 ^{CUBred}	7	-	Mn-X	1.92	1.81
				Ca-O _{oxo}	-	2.29
				Ca-O _x	-	2.44
[Ca(Htpaa)(H ₂ O)]	8 ^f	8	D _{2d}	Mn-X	-	1.95
				Ca-O _x	2.43	2.42
				Ca-N _x	2.59	2.66
[Ca(dpaea)(H ₂ O)(MeOH)] ₂	8 ^g	8	D _{2d}	Ca-O _x	2.52	2.44
				Ca-N _x	2.66	2.63
				Ca-O _{H₂O}	2.48	2.48
[Mn ₂ (tpaa) ₂ Ca ₂ (H ₂ O) ₁₂]	8 ^h	8	D _{4d} /D _{2d}	Ca-O _{H₂O}	2.48	2.48
				Ca-O _{COO}	2.43	2.46
				Mn-X	2.33	2.00
{[Ca ₂ (bzida) ₂ (H ₂ O) ₆] _n }	8 ⁱ	8	D _{4d} /D _{2d}	Ca-O _{H₂O}	2.52	2.48
				Ca-O _{COO}	2.40	2.40
				Ca-N _x	2.69	2.72

* X = coordinating ligands

List S6.2. XYZ coordinates for models used

Inorganic Lattice - Quantum Cluster

CaO (6^a)

Ca	0.00000	0.00000	0.00000
O	-1.46376	0.53094	-1.83618
O	1.91139	0.39852	-1.40849
O	-0.00668	-2.31416	-0.66383
O	0.00668	2.31416	0.66383
O	-1.91139	-0.39852	1.40849
O	1.46376	-0.53094	1.83618

CaCO₃ (6^b)

Ca	0.00000	0.00000	0.00000
C	-2.12905	-0.19428	-2.39813
C	1.93552	2.35206	-1.02137
C	1.80533	-2.60932	-0.50385
C	-1.80533	2.60932	0.50385
C	-1.93552	-2.35206	1.02137
C	2.12905	0.19428	2.39814
O	-3.14333	0.42832	-2.88648
O	-2.16261	-1.47332	-2.26472
O	-1.08120	0.46217	-2.04320
O	0.92124	2.97466	-1.50971
O	0.79105	-1.98672	-0.99219
O	1.90196	1.07302	-0.88795
O	2.98337	3.00851	-0.66643
O	1.77177	-3.88836	-0.37043
O	2.85318	-1.95287	-0.14892
O	-2.85318	1.95287	0.14892
O	-1.77177	3.88837	0.37043
O	-2.98337	-3.00851	0.66643
O	-1.90196	-1.07302	0.88795
O	-0.79105	1.98672	0.99220
O	-0.92124	-2.97466	1.50971
O	1.08120	-0.46217	2.04320
O	2.16261	1.47332	2.26472
O	3.14333	-0.42832	2.88648

Ca(OH)₂ (6^c)

Ca	0.00000	0.00000	0.00000
O	0.12011	1.21440	-2.02063
O	-1.50794	-1.28429	-1.28410
O	1.43625	-1.78597	-0.56538
O	-1.43625	1.78598	0.56537
O	1.50794	1.28429	1.28410
O	-0.12011	-1.21440	2.02063
H	1.01441	1.42240	-2.40060
H	2.33055	-1.57797	-0.94534
H	-2.40224	-1.49229	-0.90414
H	2.40224	1.49229	0.90414
H	-2.33055	1.57798	0.94534
H	-1.01441	-1.42240	2.40059

Geometry Optimized Structures of Molecular Complexes

{[LMn^{II}Mn^{III}2O(OAc)₃]₂Ca}⁺² (6^d)

Mn	-1.35472550587577	10.19431571761198	35.21507943530560
Mn	-1.71304017496507	13.26084440035536	34.22973765263434
Mn	-3.66977686860157	10.17869065340813	33.59497935896952
Ca	-4.87420969532092	12.14357550374976	37.99929564345436
O	-0.72980834907827	11.72706587091692	34.25847302732831
O	-2.83352844671272	11.21140379002777	32.50554286333667
O	-1.98890445096990	9.31955049972182	33.72555665552876
O	-2.92844353216623	10.93592650879102	34.98490010359417
O	-1.03781386962843	11.06703063122428	36.71880254551294
O	-2.91822758401827	10.90639241136805	37.95149609859806
O	-3.02153575138714	14.34473991946150	34.62147409134815
O	-3.70020050723021	13.60414473719413	36.63242736989037
O	-4.64129185168576	9.22263108982281	34.79011683020920
O	-5.41568966510393	10.75582624194931	36.25463948278863
N	0.41675005727314	9.72037792352112	35.13586629476868
N	-0.55333694969479	13.80131506285450	35.50539844565962
N	-1.78915577361234	13.78841793934900	32.49164006515173
N	-5.12651850369190	11.24325840646350	33.21260983119932
N	-4.03168637647713	8.77930960990893	32.51144222793871
N	-1.87856610565528	8.62651074386258	36.02912115283764
C	0.94002491923528	8.45071351144456	35.36137475956721
H	0.21571971709332	7.68939205934029	35.63592909508316
C	2.28698894490516	8.16599272212403	35.28132042435028
H	2.60983097294631	7.14056808123805	35.47817594746292
C	3.21969528930679	9.18316871966168	34.96429073902722
H	4.28939144464510	8.97449757806312	34.89067301133787
C	2.71371538258264	10.47477519918802	34.73797752869201
H	3.37136522744506	11.30144505073769	34.45355484522831
C	1.35310037007031	10.72318753846609	34.82982868385275
C	0.73783029360757	12.05101683559338	34.52992029792573
C	0.59913103984416	13.00510820709581	35.69684568028461
C	1.50353063252217	13.23719876032591	36.70827196438031
H	2.36713152438110	12.57099017428512	36.79959485134161
C	1.33736545704262	14.35065708626650	37.56408851929805
H	2.05086743233453	14.55662811504499	38.36537771540078
C	0.23832583065141	15.21089313735766	37.32050878449471
H	0.09697184962468	16.11864009907344	37.91465903257048
C	-0.67402219518860	14.93149318587949	36.32337424819308
H	-1.52298819771760	15.58068632679331	36.10074176006759
C	1.35523859331309	12.78436980461798	33.31559598645467
C	2.15079371236778	13.92148173456422	33.57775638662156
H	2.29288898912011	14.24930905360018	34.60952742621195
C	2.75562622866579	14.65926083248455	32.55420096591703
H	3.36833903793507	15.53093133108635	32.80383893229830
C	2.56278010634408	14.27685358117168	31.22209939515581
H	3.02124454337390	14.84337541468461	30.40552301200279
C	1.78618324199565	13.14888050465410	30.94315275064321
H	1.63953854808216	12.83238522829109	29.90572577480636
C	1.19229677541439	12.37091835369819	31.95926034491832
C	-0.93903980606738	14.86344365215517	32.19681783163600
H	-0.19118870191744	15.08066799581008	32.96428425749665
C	-1.03795493242012	15.61230390830131	31.04349075130697
H	-0.34086542169628	16.44140778150279	30.89647596368193
C	-2.02533166738297	15.29586214052171	30.08736591180624

H	-2.14280912303036	15.88275848033469	29.17319888370374
C	-2.83237823556184	14.17266772271855	30.33445267924415
H	-3.55999370644500	13.83768285237462	29.59182400232576
C	-2.69949713025291	13.42375122155745	31.50229790335412
C	-3.55164486695780	12.19009323037647	31.71522363672940
C	-4.79834156585083	12.43353583326883	32.52955695543893
C	-5.65049687387177	13.51536816921342	32.48989007048304
H	-5.32085359071927	14.42082945220386	31.96928847477083
C	-6.94929721582536	13.40749896835475	33.04147253856418
H	-7.64335518715466	14.25150736622312	33.02165968172284
C	-7.36187960715287	12.12088631941487	33.49999218365412
H	-8.40347794581867	11.93107139439593	33.77402038885251
C	-6.45833552544733	11.08294389142925	33.57383315288931
H	-6.74598848349642	10.08225733378662	33.90212433046472
C	-3.88535609360742	11.51024071936294	30.35704883517056
C	-5.15736700368921	11.66962643338436	29.78119471055052
H	-5.89962935011287	12.29450645073228	30.28638387115404
C	-5.49906846615088	11.02729743026141	28.58260244799310
H	-6.49605668923679	11.17073419162893	28.15415105133676
C	-4.56603411730123	10.19866688784580	27.94879173616769
H	-4.82269099453173	9.68602767296898	27.01634098739624
C	-3.29606263961919	10.02868403965911	28.51420004166184
H	-2.56008385515347	9.38231214228870	28.02507797355227
C	-2.92872614521700	10.68324723870745	29.70478635246545
C	-5.08993931050475	8.66873872469682	31.61413680456178
H	-5.63619716008552	9.59273216148763	31.42750853865792
C	-5.38902750449850	7.48392952755279	30.97218602615867
H	-6.21738460843952	7.47624302757611	30.25840792794979
C	-4.62768521515941	6.31855259982003	31.21830428486958
H	-4.84868009426442	5.37685785534953	30.71079388158129
C	-3.55648169370894	6.41620251508576	32.13106529662307
H	-2.91254355990424	5.55726299090916	32.34073602890494
C	-3.28073255671108	7.61429520214564	32.76283584813621
C	-2.15389478568201	7.82547351668243	33.75494765538738
C	-2.47553519489449	7.61535160657554	35.22069414198815
C	-3.12066966165429	6.52882200851372	35.77130657066925
H	-3.61026220129003	5.82006862221243	35.09567497545736
C	-3.10122436603139	6.31239848372050	37.16776166503677
H	-3.60474522883094	5.45194489576138	37.61433406196995
C	-2.31411252875632	7.20711150734144	37.95399600629113
H	-2.14527680697632	7.02020964395627	39.01828675406089
C	-1.73027877906948	8.31224400370973	37.38228474915160
H	-1.09215157051562	8.98584937624693	37.95503322000618
C	-0.88159728956623	7.07626180068948	33.31856710026420
C	-0.58235662930746	5.84519366629506	33.93592703492664
H	-1.22364098990613	5.47504136541852	34.73915676833457
C	0.53977079247934	5.09511337489403	33.56363855843851
H	0.74220191845350	4.14121936447914	34.06056434161746
C	1.39967520995880	5.57668372258034	32.56956055187634
H	2.28726790853206	5.00657350608428	32.27772567610823
C	1.11103937419209	6.79505232647218	31.94492302349083
H	1.77354767158142	7.18494187327393	31.16562085458477
C	-0.03136275396289	7.54363926909357	32.28486424269171
C	0.36792308469968	11.21381558787860	31.52556782978390
C	-0.70281575263032	11.43521577454018	30.64358469786335
H	-0.87475817575655	12.44030197401175	30.25609718904604
C	-1.60583118363616	10.40612514098990	30.33173856648998

C	-1.34894087166254	9.10541300833405	30.79414806133947
H	-2.04608033779531	8.29911155055682	30.55274695620348
C	-0.25351881556806	8.86091331794685	31.63448207431108
C	0.60557484608371	9.91094330041390	31.98580069852967
H	1.45891080805022	9.70198404291945	32.63134522751364
C	-1.77390895349175	11.35640034477258	37.78324832405323
C	-1.10507610427716	12.26124377228911	38.77696364674966
H	-0.02125299250672	12.08205189013149	38.81791395334061
H	-1.57315027406411	12.13177646604736	39.76270903830932
H	-1.26391640678406	13.30371513624073	38.45017716434494
C	-3.85550095949108	14.36805737115696	35.65863024169717
C	-4.99964239516105	15.32858578034603	35.52070637793946
H	-5.29490909944333	15.71467519071500	36.50741413287129
H	-5.86459772177533	14.77694274684638	35.10343088189162
H	-4.75028283641192	16.14811954514499	34.83079642609453
C	-5.29167200039694	9.57902406603181	35.88186947265437
C	-5.91359019904480	8.41974492604018	36.61647622604026
H	-6.67259390064862	8.78631040703479	37.32140927672199
H	-5.12211340285537	7.88779318634494	37.17282280533077
H	-6.34379275605904	7.69996474032124	35.90244026926026
Mn	-8.38722526663147	14.10794205482609	40.77618864404970
Mn	-8.04151773455951	11.03583041819319	41.75311527554369
Mn	-6.07358748247877	14.11244328852748	42.39680891687490
O	-9.01769303375407	12.57558082333560	41.72993811934453
O	-6.91357592986270	13.07928499934025	43.48292799382771
O	-7.74969477425699	14.97769389447117	42.26681516788061
O	-6.81622465601347	13.35936010800685	41.00462637314907
O	-8.70895072398166	13.24155647123071	39.26976652913363
O	-6.82488106916226	13.39020433849210	38.04063614834030
O	-6.74514691187060	9.93659778467200	41.36140613171696
O	-6.04636355403968	10.68203369084964	39.35951186817672
O	-5.09996795818271	15.06890898557785	41.20364308116061
O	-4.32823491499075	13.53751016834350	39.73657171106765
N	-10.15700615712573	14.58878058748810	40.85757248325421
N	-9.20507585265061	10.50477873831388	40.47652572621660
N	-7.96651323428086	10.50523357425611	43.49124389803327
N	-4.62020589882724	13.04039844924984	42.77285483224736
N	-5.70610738548745	15.50767826374677	43.48316823447993
N	-7.85806450609666	15.67602543412777	39.96505994173173
C	-10.67559386883808	15.86073897880505	40.63520053127711
H	-9.94837944420962	16.61958769560389	40.36151221892557
C	-12.02131133937568	16.15060865785587	40.71746707382088
H	-12.34040083583075	17.17766592210531	40.52302626789829
C	-12.95765205752123	15.13654642766789	41.03350097375662
H	-14.02647707580632	15.34907961198164	41.10823350484137
C	-12.45631457062499	13.84253575754274	41.25662097664524
H	-13.11679620182111	13.01785377440611	41.54023324393599
C	-11.09659159064680	13.58936289062501	41.16295077662123
C	-10.48635707875789	12.25836002809180	41.45926618709289
C	-10.35388900120895	11.30729212670284	40.28929107927883
C	-11.26027755819947	11.08353049644677	39.27773699510763
H	-12.12061997388155	11.75431865427567	39.18929552436337
C	-11.10021720023753	9.97271151473406	38.41732095901293
H	-11.81536726391561	9.77321450808603	37.61587389729961
C	-10.00507534295205	9.10628353123731	38.65662014137077
H	-9.86861263561198	8.20036029940952	38.05854327771002
C	-9.09068533997455	9.37724524333076	39.65405244090122

H	-8.24488469636218	8.72295306894961	39.87361515324329
C	-11.10546988825746	11.52410975942154	42.67246034516887
C	-11.90481072825160	10.39028359702846	42.40804319830803
H	-12.04838770268353	10.06552643105783	41.37547716609845
C	-12.51153691640599	9.65189162273572	43.42996422809639
H	-13.12718763006507	8.78284196834392	43.17845465105578
C	-12.31662369591547	10.03033489212171	44.76300604547508
H	-12.77638703761971	9.46325344846501	45.57844188480137
C	-11.53594893716410	11.15492462179727	45.04421603405364
H	-11.38750034243903	11.46829621248113	46.08234296795538
C	-10.94023612611578	11.93352827046692	44.02970733839826
C	-8.81919773169584	9.43178399817874	43.78344745436419
H	-9.56747399524681	9.21791116378243	43.01549120531849
C	-8.72304327208641	8.68045375830132	44.93551594692944
H	-9.42279490192932	7.85338959224493	45.08077816050226
C	-7.73464728086046	8.99234003342507	45.89219235243034
H	-7.61883098995155	8.40354106126743	46.80537948656125
C	-6.92385791547743	10.11313829134141	45.64710985781721
H	-6.19476769583670	10.44392763087657	46.39019086415082
C	-7.05453190669480	10.86477298622244	44.48082461052741
C	-6.19784796631805	12.09514551840650	44.26911819708045
C	-4.95398147211190	11.84873000158813	43.45113660454015
C	-4.10665038628803	10.76281874988263	43.48583922321798
H	-4.44026229425988	9.85665161649060	44.00272154554298
C	-2.80753360722907	10.86743379429273	42.93471796465219
H	-2.11719096526934	10.02028483018855	42.95052099762006
C	-2.38877402583252	12.15450993267568	42.48271504705323
H	-1.34619442902954	12.34087323013233	42.21022384030822
C	-3.28781015694816	13.19678366941303	42.41330518334575
H	-2.99528764310424	14.19752309362125	42.08943261654713
C	-5.85860486459105	12.77066424401346	45.62797363749485
C	-4.58601870417761	12.60504990649351	46.20061388780043
H	-3.84756731768743	11.97794640112589	45.69257786833627
C	-4.23903056690519	13.24382522342643	47.39970257811462
H	-3.24176824703540	13.09550823929425	47.82583033299102
C	-5.16728897995023	14.07513948126629	48.03695644321392
H	-4.90649802895343	14.58495082404873	48.96981995456552
C	-6.43785407380506	14.25138288513480	47.47467239395505
H	-7.17013900171119	14.89972156247773	47.96672293197938
C	-6.81059911249997	13.60040824927910	46.28381935325522
C	-4.64797656603926	15.61212374237053	44.38100006358737
H	-4.10558751160761	14.68540970479929	44.56557769404520
C	-4.34417986894827	16.79437963000021	45.02554459133109
H	-3.51611654279484	16.79734195516640	45.73967270238711
C	-5.10075682747121	17.96317444622787	44.78154008608720
H	-4.87629964384610	18.90295559435551	45.29105813519144
C	-6.17176796563812	17.87175225336880	43.86779613267528
H	-6.81193449663168	18.73385363523002	43.65956959431697
C	-6.45222496593318	16.67611110062915	43.23355584710047
C	-7.58015830330493	16.47122886940615	42.24117063797393
C	-7.25877670714355	16.68414202002689	40.77570486598515
C	-6.61134632840562	17.77041333627555	40.22715457693382
H	-6.12015685916833	18.47664550551820	40.90429633598037
C	-6.63025450131939	17.98989896491952	38.83125914648239
H	-6.12500265558171	18.85031464330341	38.38654352898240
C	-7.41845493503741	17.09795525433499	38.04292315781213
H	-7.58634914711662	17.28701520974548	36.97887825686978

C	-8.00457291312432	15.99277129381108	38.61244435144407
H	-8.64303606145689	15.32109723984401	38.03782354570961
C	-8.84947502336776	17.22368113141430	42.68081865078549
C	-9.14578112290232	18.45681516691688	42.06614307509027
H	-8.50457411429260	18.82644485788213	41.26261097199132
C	-10.26479419148615	19.20986014076276	42.44174110861977
H	-10.46489061990344	20.16539912768981	41.94704323962116
C	-11.12474798941676	18.72907250777080	43.43615018318678
H	-12.01002251648169	19.30148378576857	43.73048575621526
C	-10.83924804567400	17.50845208098036	44.05780572025886
H	-11.50184317330141	17.11926268249680	44.83738129752024
C	-9.69967064690800	16.75694196992927	43.71487560063402
C	-10.11130650742957	13.08649839353068	44.46579825203244
C	-9.04108046287966	12.85926226991367	45.34703535712671
H	-8.87279567058976	11.85278109613485	45.73241184209864
C	-8.13363999629928	13.88414303275716	45.65999666778053
C	-8.38612896631602	15.18697382204295	45.20081457871888
H	-7.68594233773747	15.99016884988259	45.44365949555698
C	-9.48130792049269	15.43732721145988	44.36184493791611
C	-10.34442573397230	14.39125768423585	44.00877019581430
H	-11.19786535606627	14.60482711466650	43.36488983073912
C	-7.97326169009523	12.94944912717703	38.20556620151631
C	-8.64874564755043	12.05459687005259	37.20733524143508
H	-9.73195252737674	12.23825437766647	37.17165436834704
H	-8.18337660146159	12.18945324862687	36.22094456237535
H	-8.49294805208593	11.00887214542947	37.52523336703952
C	-5.90602897799429	9.90966125859250	40.32912503510189
C	-4.77397448089409	8.93468168991445	40.46571201643076
H	-4.48875144823903	8.54114187714643	39.47889753657953
H	-3.89959956377955	9.47710929427972	40.87527782900070
H	-5.03057499774186	8.12087692445475	41.15954685525270
C	-4.45144976587260	14.71384749698409	40.11053529607712
C	-3.83140913187751	15.87291246563060	39.37401566569596
H	-3.06273277656448	15.50695752466439	38.67921593541537
H	-4.62138768284431	16.39264141133992	38.80415135332499
H	-3.41475165160511	16.60237929389569	40.08604525145330

[LMn^{IV}Mn^{III}₂CaO₂(OAc)₂(DME)(OTf)]⁺² (⁷NCo_x)

Mn	11.46931464068301	4.03779389315528	3.10399634678821
Mn	9.70208484759364	6.10326656241942	4.12172175662350
Mn	8.56399513940377	3.81879348948845	2.60032358703388
Ca	8.34620649243197	2.65965141608898	5.90963594931100
S	10.71477037272242	1.28239597125349	7.73912345020050
O	9.88307998596512	4.26232853621849	3.98735275062881
O	11.63579904113929	2.32935318568504	3.52473103885449
O	11.21165357687061	5.84788436554158	3.03229778980848
N	12.60140335385889	3.65679104680259	1.71734630204197
N	12.70160227177515	4.51728587865045	4.37653554647724
O	6.47730062440915	3.07603045965593	7.38549265228461
N	7.28905595806314	4.18021159695536	1.41187666667966
O	9.32853826930859	4.52957634898685	6.79968281511680
O	7.61734240453403	3.52753853731714	3.86457723881180
O	8.67293417221333	5.69232583230287	2.66439193299400
C	5.66125141366495	3.67291150035128	-0.31317938292877
O	10.54943614604937	6.05951015115934	5.68745963522394
C	4.97071611007589	4.87077090543113	-0.08341690719703
C	9.47194341364065	8.97857132724840	4.13577340218268

C	6.78056341784111	3.35016294477728	0.41376460918094
C	11.62221117970941	8.00405473786064	3.83643854358949
C	15.66949573180580	7.42351837006283	1.67781472119151
N	8.05414613761395	6.40157309595565	4.88222194152768
C	8.92800073747545	6.35269835284535	-0.14535432891842
C	11.56901041592245	6.94199794508775	0.52440373125299
O	11.43388792864140	2.32731746345332	6.99742006318136
C	6.59698587236544	5.39094068266867	1.62252781130603
C	13.38680322056149	3.65571351751934	5.22037955390550
O	6.92238771447056	0.65375888380320	6.01434513815275
C	9.21218735582083	7.48430075007476	0.62043877514605
C	15.29039453394284	7.54378372475072	0.34392213078441
C	10.28276552497587	5.30667517165547	6.76443626245531
C	12.20223978085785	9.25188047591898	3.85414040338244
C	6.91420851307882	6.14023885929246	4.08291814037281
C	9.84452229919022	2.95910223990959	-0.61275576106001
C	13.35511923545507	6.98544057897529	2.31390851345838
C	10.02890961095222	10.23174078245357	4.16928661686505
C	11.20763800149975	5.52271646676462	7.91693075458374
C	8.13375151835493	8.29569410091214	1.22882437936587
O	9.23753674798467	1.48846323759268	7.70364522314384
C	13.94781050571790	3.93100258035742	1.64341568559063
C	13.76287078340761	6.36219563607335	5.55905134428294
C	6.79579959180887	3.32090913208873	8.77957363003428
C	10.17716679122154	0.29830260140306	1.35963761509896
C	6.55767805318160	6.71435210321696	6.74788155861493
C	7.76061287605807	1.11531643147203	2.43955537349369
C	8.55770756552582	3.11823221926065	-3.11758733998625
C	8.00645276678677	-0.22606176983356	2.27227682584748
C	8.93197180692404	4.27135821764481	-2.43588000889610
O	9.84033638869404	1.49218246278533	4.60586370208805
C	11.42283125096202	10.39691435121546	4.05028019151327
C	5.46911416728804	6.20797069100060	5.99669469920032
C	14.14679136699917	2.82388514931953	-0.48652249988828
C	5.66803679538376	5.97957750333254	4.62958021886398
N	10.23388873616578	7.83385906363732	4.00847028401905
O	10.19365931163756	3.91165972835199	1.75045731831271
C	14.22961997124246	4.09875515654808	6.20677726510939
C	9.45690068232595	1.80464311657907	-1.31077270496955
C	8.83500737014853	1.87516447671181	-2.55516152457558
C	9.59838564810400	4.21770095488360	-1.20405080364026
C	7.79975173661448	6.80951404172496	6.18625642946470
C	12.02489622949216	2.93295041861073	0.65684475503406
C	14.41988059273737	5.47551542831982	6.41808274749285
C	11.27217667489234	5.80772063065559	-0.22895172290811
C	9.95011249509469	5.49094769068287	-0.53978302932795
C	5.43499844138449	2.08946880676489	7.19779165930917
C	8.04102588750328	9.65596442450230	0.90901038078581
C	10.53870451174247	7.79490381230828	0.92098383956032
C	12.78141240820518	2.54297773119307	-0.43095532083075
C	7.60559191930893	-0.62346722779353	5.93574899757835
C	14.70935336623180	7.13529815056512	2.64552656818465
C	5.48491801427974	5.73461315187139	0.89469517153945
C	11.80442459853249	0.12213297343269	4.36456090318994
C	13.95048810652469	7.38952227296004	0.00004459647644
C	12.35446855604646	6.73712081471804	3.45376344612017
C	12.95904262766350	5.89147545661110	4.55104250482103

C	10.99035773468845	1.36324514408208	4.18689195272836
C	14.72459083608758	3.53803085760650	0.58378669230078
O	11.13278469156665	-0.08618861923270	7.50646925914121
N	8.72080248237389	2.07281246090792	2.13164967435215
C	6.28928709136167	8.59783940288505	2.77173231990012
C	7.25440512996672	7.75854967051350	2.19534838486076
C	7.07430314068651	10.47643901932233	1.48305884376813
F	12.44057396054516	1.60483089734359	9.71864992338741
F	10.53043582769978	0.73716073366698	10.33291659220096
C	10.54483817006292	2.77452614197624	0.74270161966516
C	9.25242147888432	-0.67021769893940	1.79694501967855
C	12.96806283211185	7.13987623875273	0.96618629323940
C	6.01871361266012	0.69358939468076	7.14027877489821
C	7.25407426987617	6.29098007862566	2.62908249498469
C	9.88609102689255	1.63035398985148	1.48431761901298
C	6.18905256690113	9.94127316795883	2.41581263680961
C	11.11100436859804	1.63432323762041	9.52553572079919
F	10.66325093824573	2.86784781921188	9.86831863384317
H	5.33210750610804	2.97394284821864	-1.07453175553198
H	4.08612105144932	5.13276356009094	-0.65093847891513
H	8.40826738555940	8.82002529084354	4.23083400442509
H	7.33572243293452	2.44358636018442	0.23437609053885
H	16.70756918495094	7.54333041461634	1.97113563674469
H	7.90129254780707	6.11316179627242	-0.39702826953776
H	13.19430683792946	2.60736088155114	5.06888400115952
H	16.02844352969345	7.75741753107568	-0.42283957933768
H	13.26948245105322	9.33018105683497	3.67361900773100
H	9.37148312293399	11.08493209982187	4.29212684227005
H	11.85138656591342	4.64078325031606	7.99370036396860
H	11.81308310246356	6.41837967171213	7.78563384359991
H	10.62460886326812	5.57535686976352	8.83917401774720
H	14.35973459986284	4.46687564536341	2.48572063396186
H	13.88100776872453	7.43613199060281	5.66631804745526
H	7.59002976520252	4.06648399996126	8.78098946885145
H	5.90638690010708	3.70670692034485	9.28821874833153
H	7.15422164650709	2.40796090535556	9.26353793002168
H	11.10586154865110	0.01094867705785	0.87497516798718
H	6.42253908178727	7.04206043336489	7.77264859954265
H	6.84282439046915	1.50599591837345	2.85815921238656
H	8.06108851289988	3.19092783636212	-4.08006910899897
H	7.22842500660455	-0.93340758551777	2.53767966765964
H	8.73201316783481	5.24787123867535	-2.86709557798644
H	11.87673372303060	11.38040881967233	4.07162510227087
H	4.49365297866296	6.07357541319542	6.44846622716766
H	14.74316103533354	2.50416348797574	-1.33285766130267
H	4.84106299576932	5.72655260249336	3.97236139853684
H	14.71881455547894	3.36037616568376	6.83155902096419
H	9.63200756477750	0.82843926449888	-0.87543020156986
H	8.56433633262261	0.95991711150621	-3.07183031348649
H	8.64986428506389	7.20210674527643	6.72907200345711
H	15.05615876342765	5.84064277754523	7.21576384095906
H	12.07647524391554	5.15302425496056	-0.54293447876375
H	4.95395772437995	2.34223454530473	6.24792502812064
H	4.69778960700766	2.16942324531878	8.00435791975533
H	8.73600823975683	10.06131537978552	0.17934109764564
H	10.76098108920173	8.68147109944999	1.50470580523505
H	12.28586618368447	2.02411138358283	-1.24466078612570

H	8.17827618360355	-0.79709653463855	6.85134425604295
H	6.86974098093128	-1.41993033378731	5.78047671988585
H	8.28292449450636	-0.55608929528832	5.08573773155555
H	15.03162506722693	7.00919237982262	3.67197516811966
H	5.02719824523856	6.69966759295498	1.08577395282192
H	12.21123315652570	0.12796369433608	5.38335324169968
H	11.15753903633559	-0.75357882536231	4.29440521802945
H	12.61607641532086	0.07105376381473	3.63846987834937
H	13.63981815622680	7.47970223781081	-1.03675148337616
H	15.78091970029938	3.78006561691825	0.59486661011954
H	5.61412481804684	8.19902420819790	3.52075584529583
H	7.01233900382428	11.52301465075338	1.20158185920143
H	9.47992996919505	-1.72707384657553	1.72212448267130
H	6.57609663522409	0.45075723624753	8.05427325818027
H	5.22171495323883	-0.04852871182654	6.99880705973442
H	5.42496642345737	10.56246655207057	2.87220167875194

[LMn^{III}₃CaO₂(OAc)₂(DME)(OTf)]⁺¹ (7^{NCred})

Mn	10.81662293833674	3.88263809030237	4.27987653098100
Mn	8.07809932629681	5.26865942310246	5.54370136014120
Mn	10.69249524588139	5.49299627563441	6.73373497470247
Ca	9.81320350354271	1.54862581417950	6.66860732892292
O	9.62053183716523	4.29894610138681	5.77463876226207
O	11.63514034488091	5.30485480431139	5.17506492413970
O	7.97496561456925	1.97805060132313	5.36102331526480
N	9.80201532581439	2.82577152128168	3.22950876091139
O	9.94115608391121	-0.66062935757487	5.58602254097190
O	6.90765346948286	3.96102411644761	5.36077133302643
O	11.22764586485930	0.02960459395407	7.99814590371628
C	11.61957412959791	9.68518797016551	8.54717296343518
C	7.84293765165857	7.05077334294880	7.62167798324737
C	10.17160869424786	8.09571403665324	7.45537990626506
C	12.46046529035722	3.40700387540047	2.00894450531454
O	9.74639139019792	5.25994697062703	8.22986497914487
C	13.14684215302291	5.03755055818393	5.27653178027289
C	8.89114631966443	9.19657146959285	4.63133967435948
N	7.41308479743537	6.04966539512922	4.01050259261915
N	7.29831481177980	5.89939051382208	7.02811081174357
C	8.98560321844609	0.70212225189033	2.45103751987136
N	11.18587818249843	7.11426656935528	7.42421963318693
C	9.70965827253697	5.22065138489396	1.13062624425805
C	6.21812689570533	5.31814454273349	7.69331892800397
C	14.39508835095055	8.67816265986108	5.11303739338447
N	12.29125849392227	3.90441292337132	3.30219601324269
C	9.95669847520250	1.45743489947243	3.06599662213151
N	12.15500167235807	4.57593728303261	7.40744876707881
C	12.40637157507321	7.47563584080311	7.96660233240563
C	8.71167963638896	3.43958887736605	2.60992446502723
C	7.17103481151953	9.46933108045631	6.31493537341549
C	9.89760429421304	7.92896710148159	2.76934958812560
C	7.77725648748066	5.78782471506240	2.68957368488048
C	10.20948195809928	4.61151028710565	-1.17341773057650
C	10.38362425649777	9.34614334471171	7.98512101651784
C	12.35134220758907	7.72879759197544	4.07055512098451
C	13.43860734009985	4.42782105400650	3.93579918408249
C	13.92929309966339	6.33274104169699	5.48694067924898
C	13.14587988804797	4.15078044982880	6.48619859939575

C	8.25941117005620	10.20977721408891	3.89461474100375
C	10.06742335414640	8.54309242665492	4.01166560081504
C	8.90559115972152	7.69189736004072	6.75413644966995
O	9.77770684835968	3.01893196855610	8.40362078863967
C	6.27227564845699	6.84253145435754	4.18204243338093
C	8.31440693678760	8.79608044201946	5.86127035714655
C	15.53907091415104	8.60111468006803	5.90303696265912
C	10.91803867365061	7.16283960466941	2.20470513875654
C	14.66446406276656	4.43962035859102	3.31950591747421
C	7.40390595633338	7.53494383493819	8.82710812476779
C	12.15980585821402	7.09519284377183	2.84069013784936
C	13.68160823838415	3.39820723493415	1.38846466901383
C	6.93538084200777	2.64057920821164	5.24221915905402
C	6.32181976511825	6.93163299770427	9.48561974783425
C	9.50753131813974	4.40493427764952	0.01430016321341
C	5.52838801325020	7.33480478349177	3.14325048429173
C	10.64147964917274	6.28195418498332	1.04233926291111
C	12.37976183098652	4.22205763744681	8.73615088509098
C	11.31377644016575	8.47267546418258	4.63580936830664
C	7.70263030097738	2.70666037799815	2.03970863346507
C	6.58130855182709	10.49808802662604	5.58519227478637
C	15.88738910845436	7.38499502908023	6.48535174244402
C	5.89220971805954	7.04466919207519	1.81626737775161
C	8.67749750987268	-1.36026706088189	5.46728217528320
C	13.59018301088804	7.55764623580272	4.87079556480181
C	14.13316471728733	2.67754708661920	8.10812821643756
C	12.63849095535946	8.70659583790810	8.52020261619134
C	11.35594171337838	6.45999257602625	-0.14721492088794
C	15.08142752541645	6.26743268505322	6.28183624963554
C	14.06369876889076	3.18601417739324	6.79986307848148
C	7.12371713440732	10.86547855296022	4.35748232236530
C	11.14589339242106	5.63819087880261	-1.25222764895637
C	7.80283610998158	1.30194196186774	1.98575074127059
C	14.82745808279691	3.90370027618291	2.03100357326902
C	8.66363535533880	4.27084356691509	10.11352124922944
C	7.04218953476440	6.26533623481739	1.62382215056146
C	13.32187609237542	3.29957031675305	9.09419884798139
C	10.98473065862172	-1.35406023373069	7.67813780263461
C	5.73071240414467	5.81744602085650	8.87665873444103
C	10.98743197073634	-1.46605989718860	6.16753978007034
C	5.60425021770719	2.01645725271042	4.95822967686367
C	9.42934370739657	4.11811695663639	8.83881097400109
C	8.98903773317367	4.92172808578151	2.47183869897383
O	9.35713861341166	6.52580274382500	5.92478419065330
O	9.93232451063710	5.17852031016334	3.52930928994431
O	11.23169985013937	2.65819515031672	5.25858278788154
C	11.23098548323090	0.25123573065637	9.42553181916618
O	8.28041132119790	0.38677473282417	8.00421598862863
S	6.87792678535425	0.79553107798223	8.28885776336393
O	5.87863715438884	-0.02069835278434	7.62293409075862
O	6.67992010567558	2.24574356009540	8.25027343278851
C	6.73463082918668	0.36259501548129	10.09811852013060
F	5.51681993569071	0.68035812898701	10.57027595980746
F	6.94464224553585	-0.95300191322733	10.29847761525920
F	7.65692741552599	1.04461358652372	10.82461166535196
H	11.78943684230976	10.66719694162484	8.97164726249549
H	11.56139289550161	3.05076124629198	1.52869247271751

H	9.14241319362985	-0.36667271675678	2.35611811557630
H	5.82643361391612	4.42321893582774	7.23644644448491
H	14.11045071596447	9.62210156822282	4.65723766020101
H	10.85959471911760	1.04305850972054	3.49234785749735
H	13.16745260852051	6.71255352506547	7.93749937425094
H	6.71150581552667	9.17085394849901	7.24913901771763
H	8.93198266035656	7.97970132616101	2.28093456712238
H	10.02852171210506	3.96292806009198	-2.02521918382022
H	9.57785216046337	10.07133221491991	7.92519557861895
H	8.69661550404845	10.48995928953824	2.94069483927815
H	6.0099030871941	7.05264790871018	5.20981364681978
H	16.15168964944855	9.48374974137747	6.06005303451028
H	15.49848384635724	4.89022301197406	3.84767216616594
H	7.91035592766989	8.39619799822754	9.25167004087572
H	12.94962267934747	6.48856469967049	2.41122416783033
H	13.73715325690470	2.99927375482484	0.38104357254882
H	5.95881931372746	7.31710051531004	10.43128253950141
H	8.80696354999851	3.57908897803955	0.07412978633240
H	4.66465661869010	7.94925355826801	3.37317957957180
H	11.76598725806543	4.73123440652216	9.46876016300995
H	11.47941942675762	8.97182750996225	5.58236105592066
H	6.86416531772453	3.23255860790540	1.59244724624338
H	5.69747070428054	10.99447733835417	5.97360675007417
H	16.77647363813333	7.30205987046008	7.10295079077643
H	5.31644236982307	7.41206069461444	0.97523265140203
H	7.97077085531906	-0.63795782492111	5.06113672190863
H	8.80168372495423	-2.20860184118275	4.78445384505965
H	8.32283322716129	-1.69554633067748	6.44508164080495
H	14.84100811078011	1.90084332284333	8.37126279678912
H	13.62117861071476	8.90666141041842	8.93208280984230
H	12.07802399713780	7.26993045678138	-0.19923925398446
H	15.33860491769395	5.32975432044672	6.76290431149507
H	14.76372774062851	2.87013395964177	6.03143032144711
H	6.67244970451743	11.65631794831806	3.76610951327757
H	11.70832245098080	5.80183478480239	-2.16649374996512
H	7.00810089258242	0.70587706170795	1.55173637095253
H	15.79546504021234	3.90204467413625	1.54543347307916
H	7.70464278508271	3.75922160632115	9.99314930482004
H	9.20667193184234	3.75421929486267	10.91112604787964
H	8.51303314144144	5.31746855916780	10.37227030103381
H	7.39796507166016	6.04019087246593	0.62435137122974
H	13.45095708386804	3.07035124289019	10.14686610579801
H	10.02059734696182	-1.65854907665022	8.10579270745917
H	11.78399030732944	-1.97472824035604	8.10681393003306
H	4.89486073895698	5.30290112675933	9.33846446693491
H	11.92717260038329	-1.07557165656801	5.76465682002503
H	10.87054433869897	-2.51105913418127	5.85714311538044
H	5.31973218206115	1.39246133098048	5.81260080464399
H	4.84230877758022	2.77262773444178	4.76955216279803
H	5.70421835031622	1.35667902693980	4.09115977424842
H	10.25704789275470	-0.01715908291985	9.84733843871988
H	12.02779481551934	-0.34423516945871	9.88605341813182
H	11.42142794263572	1.31351027931691	9.57161043961792

LMn^{IV}₃CaO₄(OAc)₃(THF) (7^e)

Mn	-1.03616615130431	2.91738693799153	0.90107615110809
Mn	-0.60302494386206	1.19154412120708	3.09404529139134

Mn	1.59774603249412	2.33215733514379	1.74211809781211
Ca	0.05856513959413	-0.05554411243552	0.17272101920171
O	-1.46194132425916	1.27644887586227	1.51943327299312
O	0.53915817079018	2.32404429389379	0.27970210835256
O	0.94414252248038	0.74618059044411	2.27307703677440
O	-0.03502899999782	2.87062824748880	2.48565098645998
O	-0.58066640678987	4.60245212503644	0.59793713963542
O	-1.97792961048078	1.91535451512992	3.94582571604758
O	2.43712092576228	2.56695067240539	3.28519663264617
O	-1.80182316722178	2.74053421910655	-0.70016770839235
O	-1.19842881800523	0.74992650703326	-1.60919876997962
O	-1.18477637426029	-0.47129643149631	3.38009527383452
O	-0.98824828913862	-1.67497226811106	1.46506649731432
O	3.01918663968579	1.55358896780805	0.99028269442588
O	2.33083208589588	-0.20748545840487	-0.26564894595424
O	0.03582736601295	-1.93996675420239	-1.39140709083814
N	-2.60806626088416	3.65675601450385	1.46450201971973
N	0.13387593360031	1.12076920283021	4.76212388322560
N	2.36703310052203	3.93111633314985	1.31240048461909
N	-3.20509160050990	5.88596040738871	-1.48564842730756
N	-2.75947781383208	-0.44194459496092	6.53052951549664
N	5.86576232420403	3.10417500651615	2.37407273575271
C	-3.65705179890376	2.98524335581720	2.04318205834295
H	-3.46889965811613	1.93500429322525	2.19892265221412
C	-4.83835647894320	3.60850992822794	2.37348921537959
H	-5.62404578648631	3.02166496333434	2.83904286769265
C	-5.01732560717198	4.97431850941453	2.10525257539598
H	-5.93904943881710	5.48218619246797	2.36877388364959
C	-3.98353504293201	5.65317332310195	1.45423946279794
H	-4.07274033120297	6.69780682037686	1.17873070391482
C	-2.81692265616174	4.99087558123891	1.14122292834092
C	-1.63655181696954	5.55488116077227	0.39624925220779
C	-1.94570686725970	5.62153892466390	-1.11810954630839
C	-0.90730839016432	5.45341414877727	-2.03939752441000
H	0.08955194456549	5.23268762006853	-1.68066844042180
C	-1.18736323825210	5.57567268126859	-3.39490599791202
H	-0.39802036210365	5.46034959650364	-4.13326452754950
C	-2.50057739017684	5.84466918895878	-3.79029487966303
H	-2.76764043691924	5.94052021451520	-4.83869272674672
C	-3.46740415484865	5.98612931877172	-2.79996068871875
H	-4.50459979466458	6.19168548466688	-3.06030188474846
C	-1.16618179297221	6.92433316786071	0.90611202147256
C	-1.33043788376999	8.06174376847464	0.10497335468823
H	-1.84628920841952	7.97384550017363	-0.84471337430312
C	-0.83737756726661	9.30839939555075	0.48585424842683
H	-0.98482339674266	10.16851510312765	-0.16159402263153
C	-0.14551436025623	9.43250973266787	1.68696725533755
H	0.26089084591647	10.39145868235711	1.99727780635968
C	0.01047753866524	8.31349032804884	2.50025983083589
H	0.52716151876213	8.40432356002270	3.45217763199396
C	-0.50339344382980	7.05476340392013	2.14739069987499
C	1.41441966651680	0.72709198671661	5.06456987913245
H	2.01293049708961	0.48999821329926	4.19949968970231
C	1.87067653621345	0.63736317029301	6.35985350534344
H	2.89846818489994	0.33212763588880	6.52980490857762
C	1.01683933308147	0.93216213313193	7.43281389641329
H	1.36474333567706	0.87593222313446	8.45886710684829

C	-0.30827964863688	1.26674965174087	7.14085802494196
H	-1.03208194810174	1.46377601797672	7.92345248290936
C	-0.72382136455876	1.34503373157023	5.82984602037407
C	-2.12032852893438	1.63241294780387	5.34662148900036
C	-3.00621727108238	0.37363434120144	5.49875424184855
C	-4.05390807366521	0.16038298742725	4.59741756565480
H	-4.19853875339663	0.85327502688068	3.77888422491461
C	-4.88453924248943	-0.93824626916696	4.78319576499121
H	-5.71409335997165	-1.12292193476968	4.10553627689637
C	-4.63206441883412	-1.80062407906844	5.85375586567802
H	-5.25014886676514	-2.67539691114065	6.03371166934370
C	-3.55937301565543	-1.51045127539673	6.69075369181754
H	-3.32143152835132	-2.15621733524187	7.53462800080225
C	-2.78618664538980	2.83558538305433	6.02911931158064
C	-3.86658989392042	2.63497135960012	6.89820570052267
H	-4.18412843205551	1.62402835157463	7.12823837858566
C	-4.55970094485526	3.70030701973522	7.46991522426434
H	-5.39229604810395	3.50555915917373	8.14043234623670
C	-4.18607705014824	5.00463168975927	7.16009023356521
H	-4.72198077324176	5.85092161135246	7.58159702901410
C	-3.10334096172361	5.21799607388834	6.31154745208780
H	-2.78625297892877	6.23230362236325	6.08345749998789
C	-2.37382457258969	4.15768223754498	5.74889056888699
C	2.14361868979228	4.65484312513760	0.16679114900534
H	1.40263824529066	4.22083285613569	-0.48507816765285
C	2.82231389440961	5.81849392311606	-0.11348931337072
H	2.58802258382439	6.34941710457288	-1.03090513578809
C	3.79864788282464	6.29888250396100	0.77209990214510
H	4.33572345420563	7.21954832019632	0.56990761009508
C	4.08321474021709	5.53564915125652	1.90782624558893
H	4.85442870387340	5.82728452920625	2.61155252523760
C	3.37867688137347	4.37713396774875	2.15133629754073
C	3.59258125483652	3.41971311373200	3.29365524405770
C	4.84242261002761	2.54694294153761	3.03250454006438
C	4.88247081320023	1.24008802539118	3.52821813614766
H	4.01981564695381	0.84346799024983	4.04730980065463
C	6.03439767689895	0.48635570723112	3.33935084763057
H	6.09749498530353	-0.52903040939025	3.72210725173548
C	7.10630056053139	1.05562578098376	2.64640563045318
H	8.02333576783286	0.50156252041791	2.46843746312808
C	6.96905381278657	2.36059527636508	2.18408040740846
H	7.77612886696243	2.84438385770030	1.63598814783580
C	3.69343358806392	4.10023474524547	4.66609451661596
C	4.91243223797638	4.10364449281545	5.35640252595820
H	5.79051870128893	3.67324362884770	4.88795411082707
C	5.03082235041706	4.63469190605300	6.63948678253802
H	5.99341825222157	4.62044706551886	7.14341229941625
C	3.90712992485261	5.16361510658108	7.26736963934243
H	3.97250746416098	5.56999322834752	8.27317451889737
C	2.69282255094313	5.17983233160852	6.58672137231204
H	1.81385065704222	5.61155595519029	7.05833548543467
C	2.55938307375757	4.67450659166991	5.28294670716312
C	1.20789553837840	4.81811360465935	4.66850041456262
C	0.10527967379628	4.26464065739659	5.32882941367421
H	0.27467003075857	3.65961748882120	6.21192855168712
C	-1.19906882162035	4.54834057664431	4.91792104903119
C	-1.39385244070524	5.40729446408784	3.83056624239486

H	-2.40543725982425	5.68311992270738	3.55651196098500
C	-0.31014989856544	5.97062466380902	3.15302513646537
C	0.98707146008991	5.67202737379692	3.58547524590214
H	1.82459303681674	6.16526471137176	3.10600150246822
C	-1.82371345963742	1.83218282283669	-1.64517934402082
C	-2.65333990168685	2.21734498224234	-2.84065407729831
H	-1.99557937424696	2.64493522173503	-3.60733358546695
H	-3.39775602925733	2.96929445538305	-2.57529007844955
H	-3.12841165675274	1.32740844000690	-3.26063731582484
C	-1.30827882853529	-1.56664622773186	2.66774318729071
C	-1.92427740585080	-2.71449410776832	3.42228756912898
H	-2.99857035778403	-2.74730099697191	3.20297001621590
H	-1.80224785178552	-2.58623687710106	4.49870309667314
H	-1.48096346130370	-3.65501793063667	3.08669652168397
C	3.22517984328271	0.53972009865463	0.18446789212392
C	4.67813731359864	0.30517012172676	-0.13270944774208
H	4.77458199472625	-0.10626796230918	-1.13994050254066
H	5.08090971275331	-0.42876187015667	0.57598725156573
H	5.25446410740261	1.22568523854445	-0.02800543714914
C	-1.23646325979975	-2.58771766293551	-1.66163142362913
H	-1.98030268792719	-1.81169874165861	-1.88344467388785
H	-1.51498947123209	-3.10800943318491	-0.74447439755569
H	-1.73109437446672	-3.31147419552054	-3.66201912939443
H	-1.05843867674711	-4.56325826777185	-2.61256137393457
C	0.43916320190997	-3.13477373721021	-3.35687950771836
H	1.16492444867797	-3.87232575183717	-3.00157018786316
H	0.51792432850510	-3.07162329752276	-4.44594680721396
C	0.69338650450500	-1.79329654526752	-2.67262757627155
H	1.73978188641282	-1.56668830610504	-2.46254042546573
H	0.23254207666153	-0.95663652144988	-3.21814308477281
C	-0.99013246954917	-3.50614022074346	-2.88140271584963

LMn^{IV}₃CaO₄(OAc)₃(DMF) (7^{CUBox})

Mn	1.86952886544987	10.04080270449516	4.17794172459843
Mn	0.68591156776727	10.82786962116233	1.74409165982426
Mn	2.17893591298198	12.68345458267295	3.25084773868461
Ca	-0.76579122062989	11.94646561726873	4.44199621185824
O	2.34283386936982	10.93522677296593	2.60655681198644
O	0.29496852325575	10.05118564234678	3.32394388361067
O	1.65574969627573	11.75380091616046	4.69305476132674
O	0.56987078933293	12.46298667547711	2.46715457989577
O	1.36680950360459	11.48624572188913	0.24870272730648
N	0.82690242346975	9.23359701372453	0.86708397574272
O	3.85862059990786	12.69039314880080	3.80858877941812
O	-0.97939440645696	10.91488097510667	1.11516138875101
O	1.15956910975170	9.28341696674820	5.62463440244374
O	1.83025600605690	14.24047368081232	4.04491284637552
N	2.84799838312501	13.65723562640451	1.86065983442484
O	2.29010431182110	8.47471171661050	3.47066173327782
C	1.06625868171795	9.29751572559446	-0.49864807346531
N	3.48624253387086	9.87104238099317	5.01029160011019
C	4.07249534219728	8.61302976115126	4.96904010567220
C	0.57525166896784	7.99359066457610	1.39919814878797
O	-0.18261469160532	14.09973403905462	5.07441070137233
C	4.11260236590003	10.57945905736121	0.00720181952818
C	2.18200287683062	11.30366585367882	-3.22127650055844
C	1.13718171878008	8.17236812412239	-1.28905225547906

O	-2.75897816489554	12.50151329458557	5.69862373153847
C	4.75566096699351	11.34257827728254	-2.23251583659362
C	2.39082447111037	10.98278323586938	-1.87442654544948
C	5.44247643171524	11.08660442586679	1.98187281711277
O	-2.33381123683019	11.71055265274383	2.74836926420261
C	6.42370333961561	11.95723280863071	2.68657092432858
C	4.53698523885546	7.39794697948562	1.99574529781026
C	4.86150796823770	11.47875273292352	0.77407246191069
C	4.53279755646235	8.85088321628445	1.66869124471411
C	5.27550275428663	9.76705173220925	2.41645400550396
C	4.13053687914023	14.16274295104190	2.01990747698562
N	3.00441115702494	6.37972909226293	6.28829127145730
C	5.13927139338702	6.55846503785034	1.04477247493970
C	-0.48409501184804	12.53578820904176	-1.55953633385315
C	0.63994307028351	6.84374127858011	0.64625598045542
C	4.01226879136042	6.81436694253626	3.16939899842116
O	-0.81680707127153	10.28633446707020	6.09134920760024
C	0.94937654775565	6.90924354136132	-0.72056792217133
C	6.14559374304633	13.21779852284834	3.25856840901705
C	3.96043765249873	9.26789958432725	0.46182498192462
N	-0.80951879097669	10.28446256361995	-2.33116401361441
C	5.26726542292443	5.18682703177161	1.24415581070401
C	3.71000870768526	10.97292498015567	-1.37140790364746
C	4.16157835696350	5.43603513375261	3.36579048653988
C	4.73207902863177	14.96124994850971	1.07312918661534
C	4.53334413278276	11.67605107513265	-3.56558177447700
C	5.91435090585680	9.32985538004917	6.33334149766694
C	1.18540228139581	6.23608674680176	4.72575904092215
C	4.78942806513195	4.62348372634483	2.42375762285690
C	-2.36251210884035	12.01616774525447	-2.95981359759678
C	7.73820086569346	11.46849463928997	2.75506141989869
C	8.77163195180315	12.20342218155983	3.32918238495068
C	1.19269220691008	10.72532593217496	-0.95479274224652
C	5.29269135360912	10.58428863194272	6.43236170085107
C	2.43044162347025	6.72661024980092	5.13036318325877
C	8.50137903272151	13.46610606306656	3.84847568067721
C	-0.11159127114676	11.19064068814901	-1.63698028419233
C	2.34107786658559	5.52602631177259	7.08788797918940
C	4.03936157733978	15.30069445572664	-0.09251321223886
C	0.84469731145933	14.73009895431697	4.75990811089083
C	-2.14502311022125	11.28105538887598	1.59393111075501
C	-3.26764062593545	11.17846970254728	0.59685374601084
C	4.10179167884463	10.82168115455119	5.78580916791415
C	-1.91764814378481	10.69856881975920	-2.96940593058987
C	2.15381621839490	14.05541193252410	0.74549383549824
C	3.23626851144058	11.63868177296953	-4.06873505284467
C	1.10545558826485	4.97474458461929	6.76621841504499
C	0.51764609564582	5.33881080212032	5.55150265309917
C	7.19679968263426	13.95491544869436	3.81732981250218
C	1.07533183376114	16.14412652546497	5.22022904606290
C	5.26142880982715	8.33203439678319	5.60345625797584
C	2.71866149228898	14.84825952756185	-0.22709070651332
C	0.06874251965204	9.43624214455583	6.33104955060479
C	-0.06621503050101	8.45983803773000	7.46773215479429
C	-1.62129003371165	12.95633599997442	-2.23865310690840
C	4.71045029666826	13.74727685303622	3.34419654421620
C	3.22478102546162	7.65090049479208	4.18311223366288

C	4.63178632475248	14.91077654087100	4.35544095809795
C	4.49643581286251	14.62687126175834	5.71763259937184
N	4.75609726572461	16.15648944180568	3.88374573377278
C	4.50027689212594	15.67962379996196	6.62489660926378
C	4.62043005790492	16.98571228652503	6.14204123171837
C	4.74010256293321	17.16834305215512	4.76862618180458
C	-5.17861903446613	13.44970443271351	6.73382520101838
C	-3.32965484224993	11.86191296718427	6.58921839606630
C	-5.11382156302161	11.42637173664061	8.20051091317496
N	-4.49678522721824	12.23173118442984	7.15754070108429
H	0.31426506003286	8.01257048704855	2.44485354824921
H	1.17280052697526	11.30319187106221	-3.61715499160240
H	1.33556915256903	8.29607948710034	-2.34736315233449
H	5.76666154120482	11.34311641897729	-1.83431412348831
H	5.04191340280150	12.47347841894539	0.38479100548815
H	5.78758986146612	9.44369913095348	3.31467634100226
H	5.53087686669198	7.01415047251199	0.13942012874528
H	0.11788300334073	13.22174162800342	-0.97838341783308
H	0.44273432876526	5.89250794788106	1.13026510732907
H	1.01332077172940	6.01080256856105	-1.32483225419555
H	3.44802282986519	8.53808365305555	-0.15329844635297
H	5.74579682835677	4.56977599839756	0.48863658338286
H	3.77008843304864	4.98250538143270	4.26924861976619
H	5.73950379266014	15.31475114166410	1.25961122777644
H	5.36857224958997	11.95012254900263	-4.20419891957610
H	6.85807180718306	9.13064675053116	6.82943123086044
H	0.76952258204245	6.55683008539545	3.77979110039458
H	4.88929682104130	3.55790551561811	2.61028087357109
H	-3.26198696381752	12.29800285650254	-3.49905366223667
H	7.94136294105716	10.49244445026849	2.32293135377341
H	9.77833189755690	11.79562403416908	3.35761492113959
H	5.73401548662683	11.38265172724801	7.02042608661927
H	9.29263282731492	14.06591060268282	4.28935245273255
H	2.83474501538188	5.27675432672590	8.02575397669803
H	4.50087326869801	15.91861346246725	-0.85516437555176
H	-3.05388976067466	10.41826901813561	-0.15600131662961
H	-4.20299995289285	10.96334818957847	1.11770039842922
H	-3.37585065264246	12.14146341012125	0.08335954222052
H	3.56150577546408	11.75237455148192	5.84654113694809
H	-2.46441582246452	9.93033159981407	-3.51374711682935
H	1.13650970366358	13.70053102236008	0.71457546520899
H	3.03720584301865	11.88121576456922	-5.10881584984737
H	0.61787548540986	4.28154695900390	7.44530348635766
H	-0.44419080969789	4.92856341173017	5.25548657065827
H	6.99251069780309	14.92837459736276	4.24852852661872
H	1.55296502198209	16.12346254911314	6.20718569951166
H	1.74078162433390	16.67354447804136	4.53656114530135
H	0.11770000873057	16.66013496127766	5.31436354571074
H	5.66598432882043	7.32979237162089	5.52241061538434
H	2.12059926675736	15.11686439527676	-1.09203443299162
H	0.90602135928275	8.05912292005311	7.75690754838934
H	-0.55275141728373	8.94678844974338	8.31671993892699
H	-0.69765457096900	7.62189925265751	7.14741305366717
H	-1.92827949855338	13.99830227503130	-2.20647443369897
H	4.39540309844406	13.59879546107131	6.03945127756591
H	4.40888390275328	15.48850579103902	7.69078565393902
H	4.62017296669410	17.83926242965759	6.81340255939722

H	4.83173058153662	18.16744165659166	4.34579138937168
H	-4.57612641611225	13.91850265186040	5.95580832744441
H	-6.17273866662694	13.20687345295623	6.34146777291406
H	-5.28966366316611	14.13316135835840	7.58337427806155
H	-2.90736287239782	10.92641373802991	6.98584694529322
H	-6.10711900135636	11.08521442898175	7.88540990070404
H	-4.48462993502410	10.55533344519250	8.39786190681651
H	-5.21894744376473	12.00836174130464	9.12378990178373

[LMn^{IV}₂Mn^{III}CaO₄(OAc)₃(DMF)]⁻ (7^{CUBred})

Mn	6.63435285771953	12.77858270035963	1.92182850447732
Mn	5.68047514238720	10.23681727329151	3.06122581552854
Mn	8.16920514195080	11.50344430795789	3.91918451377437
Ca	8.09060274715210	10.22313435524739	1.15369157324360
O	8.40506612411283	12.23071573327534	2.19264736534560
O	6.40367537253169	12.16282304930612	3.65587446717307
O	5.98736680720748	11.10277542727757	1.36262414894294
O	7.50396340121776	9.86025197769243	3.35406498904795
O	6.92066612927151	13.41521123504193	0.06560140463582
O	10.07341119844036	10.85067567451035	4.07765925186338
O	8.08564315931829	11.66128986228634	-0.76509715857554
O	10.23600920954658	9.81013210502769	2.06954957690525
O	5.12520862043269	8.28055987225848	2.41327076085429
O	6.78220541427527	8.18352230441327	0.87425284801507
O	7.04898964063884	14.46650288064743	2.59570346837496
O	7.79275588710581	11.01844197399615	5.68679654543139
O	3.93025218175777	10.84752713171519	3.06750351748133
O	9.11531717806176	8.81623177107589	-0.69442611248949
C	5.79929291256521	7.70853704212580	1.47363627981899
C	7.53805669908239	12.77470324732136	-0.87679086497910
C	10.70103002124989	10.17498691084734	3.16292520828009
C	7.52551551177482	13.49718185093391	-2.20849577030590
H	8.41370297891830	13.22855984531528	-2.78445780505050
H	7.46632573190162	14.57736667023261	-2.06523482857844
H	6.63955136424819	13.17623416797783	-2.77050449830911
C	5.25829490361979	6.34070075418565	1.09266924972132
H	4.74964094171511	5.87435559644702	1.93833522339407
H	6.06806863154911	5.70563231042252	0.72624879338523
H	4.52209240389972	6.47147303684618	0.29050797466524
C	12.12012831647453	9.80880996639869	3.55118968002818
H	12.12268893446132	8.77810877084335	3.92402783514125
H	12.49225466341200	10.46172685023059	4.34235042781297
H	12.76466567947510	9.85221600471619	2.67003667134037
N	8.94256892125265	13.13631487860536	4.88836426174016
N	5.03619568950281	9.43896198875653	4.88282461447110
N	4.81209630291491	13.71995212181788	1.64460862969383
C	6.27999739541468	15.56038386069851	2.15746275360645
C	4.27170531877717	14.12757200838687	4.58200544124193
H	3.66359804010198	14.66929831490426	3.86703325090600
C	4.51704864657597	12.28038149644938	6.10792168511205
H	4.11724554397904	11.39286451346305	6.58438241881837
C	5.72850485237234	12.80812961609617	6.57394285687366
C	5.47872437582500	14.67541532715627	5.02594879891131
C	5.89848071066125	16.05856589918256	4.65301883933843
C	8.57675707401988	11.59547142564032	6.70875458784787
C	7.65979810754867	11.73410816442401	7.94057713535680
C	1.40570710064449	13.49441015473699	5.02093273100817

H	1.74076828304900	14.46672166441623	5.37190442729157
C	3.78081805663586	12.92451011444607	5.11040066007948
C	5.49836202238188	12.18900695381192	8.92888224767283
H	4.48188506650273	12.55517341383064	8.81189370422008
C	1.95813997221581	11.24196553293709	4.32379711790988
C	2.38452197919518	12.51239997669691	4.78979689482661
C	6.33806628455246	12.22337831113829	7.80349473907868
C	2.97284831316658	10.17558023205839	3.86946746451807
C	6.19523465354966	14.00739120931772	6.02732256959772
H	7.09287095387829	14.46836338937367	6.42353270564299
C	5.98457551939978	16.96338324058990	5.72477849554279
H	5.76529368187441	16.58814642412494	6.72074420215896
C	0.58530174615437	11.00704310077461	4.17353888601344
H	0.25621354616186	10.0363304430452	3.82912743577763
C	6.50621172742733	17.88952800377883	3.18480210724261
H	6.72333790870330	18.25864412377878	2.18956007080641
C	6.56356637195919	18.77419126687364	4.26026988923516
H	6.81618876955784	19.81755949716101	4.08852456257143
C	6.19315713502343	16.53580801140039	3.35238486116808
C	-0.36823252313123	11.98869726430991	4.43273025810075
H	-1.42357768009614	11.76598548990725	4.29626333377826
C	6.31523354802851	18.30351091288556	5.54632446891676
H	6.36765870233415	18.96978937919030	6.40377113688331
C	5.93191185916305	11.72960232363325	10.16965722158774
H	5.25049466135983	11.72430815442477	11.01671205501411
C	0.04674809741686	13.25366798485937	4.84453194387024
H	-0.67590339258433	14.04186899228446	5.04037707926319
C	8.08998033959597	11.29545543587765	9.19904389015912
H	9.10500000281882	10.93279527484934	9.30979133145720
C	7.24721312489004	11.29445832812427	10.30854848284423
H	7.61717622828242	10.93970830846310	11.26739202057473
C	4.90129681697054	15.07463083757964	1.73505462296616
C	9.09832450827780	12.94103067836284	6.23155242467088
C	3.68037435849597	9.50403580414885	5.03535709279377
C	3.80254688057495	15.88192790211995	1.50613131712149
H	3.91767022592670	16.95541888397254	1.59080174622521
C	5.81055794490217	8.89354447624921	5.85265115251359
H	6.87103622383864	8.91731003103098	5.65439015794467
C	2.49866469212420	13.89382889144530	1.10537950223642
H	1.56347509842021	13.38946964249323	0.88443465670373
C	9.32978723993764	14.30723878992295	4.32463601652399
H	9.15553294489795	14.37915104467057	3.26244225025297
C	5.25502572993415	8.39700137784170	7.01043282231301
H	5.90749382457934	7.99327965207905	7.77762425012997
C	3.63102002359510	13.13530490720446	1.32384915679588
H	3.64884334537306	12.05675539975594	1.29792999353525
C	9.87088577638446	15.32201275447984	5.08435544541262
H	10.14933411277196	16.25161236771826	4.59883658887094
C	3.07090480665857	9.00788737320796	6.17237118735380
H	1.99287686178422	9.07591258780338	6.25715559000960
C	3.85529607425035	8.44615384715792	7.18770075273030
H	3.39530803306281	8.06014455564511	8.09169212005190
C	2.57088922236256	15.29249754528768	1.19085304116251
H	1.69143797830775	15.90647130877394	1.02375679902918
C	9.64219524476043	13.92475113242141	7.03699983927689
H	9.74168470927073	13.73129131758050	8.09833474634646
C	10.03353601432844	15.14242316468236	6.47091341691606

H	10.45059367390814	15.93088428813781	7.08948521660741
C	9.76864354419856	10.65802889885357	7.00502930549969
C	6.99312738119758	16.21556443181074	0.95486363355228
C	2.29915499926482	9.09678764146456	2.99359911233643
C	11.89259381379241	9.01833076952083	7.55499362397606
H	12.76010554747832	8.40695839090414	7.78888119273893
C	2.38518687665830	9.18400969072857	1.60372415307911
H	2.94479925168940	9.99483372760057	1.15536508723885
C	9.72632145489066	9.33234449640238	6.56727697892572
H	8.87889958088172	8.99412571272454	5.98603459155782
C	8.33448226752537	15.91840495648857	0.71098702113150
H	8.83823435759652	15.19341001897947	1.33688406615559
C	8.24509857273713	17.41944558711506	-1.16290294120278
H	8.69882942500676	17.91599165669194	-2.01660193083042
C	1.11490686627847	7.14837833531455	1.47819273420225
H	0.63790792234950	6.34754873889512	0.91879907312875
C	11.84517216872814	10.35394866907385	7.94555197409796
H	12.67195445099524	10.80336251208696	8.49447989750231
C	8.97413310086106	16.53598751782720	-0.36235258072350
H	10.01560192434169	16.31608478864431	-0.58172444132459
C	1.78234172333498	8.18952243546938	0.83109751866807
H	1.84799126537596	8.21986466387321	-0.25376422223049
C	1.07093767922043	7.15628188932858	2.86946811784940
H	0.55147386373183	6.36878392099578	3.41416217328876
C	10.80411203115640	8.49880314628559	6.85311609719788
H	10.80339687561458	7.46565248926148	6.51479422618142
C	6.91010211576788	17.64718889839444	-0.84420660422556
H	6.30386489050376	18.32690303169174	-1.44206817447914
N	10.80665031385765	11.16661367855451	7.68329374925131
N	6.28352101578289	17.06542878524941	0.19550558007970
N	1.65077576612354	8.10786720893147	3.62664383027097
C	8.65438844106847	7.84466593974994	-1.28886803983279
H	9.12540225725590	6.84562413400291	-1.22741657096578
C	7.01351681791699	6.61267522393067	-2.60340578236162
H	6.05390556343339	6.39230677520818	-2.11847070075253
H	7.70869128316246	5.79510366778827	-2.39393330539728
H	6.85333875289299	6.67710999727234	-3.68648645511993
C	6.77507289326916	9.06828508266737	-2.25456271246922
H	5.89406798000895	9.03257747460407	-1.60332469105187
H	6.45571422503455	9.15349827487400	-3.29910156025567
H	7.38613313975286	9.92878081573343	-1.97684121600904
N	7.57085628703074	7.85419757306711	-2.09882704029795

[Ca(Htpaa)(H₂O)] (8ⁿ)

Ca	3.88653480747588	7.59973054182657	2.96564016393308
O	3.28750473415354	8.95054277607140	1.13564036272256
O	2.74884918624207	9.10311605030514	-1.06749127947380
N	2.71608926072521	5.06075800958574	3.67049001882565
N	2.48775113105709	6.36720075951994	1.18009758832461
C	2.40898798034160	4.29183252833372	2.45732493833854
H	3.34209545988205	3.79915162623318	2.15198284871567
H	1.67555207160204	3.48915985254409	2.65336730522547
C	1.94362998124279	5.14317795269855	1.29490983844115
C	1.05266266050267	4.63315420249442	0.35091105999486
H	0.60813910393425	3.65215817762599	0.49616276553270
C	0.75584044027939	5.39910067807941	-0.77668866930236
H	0.06888089044159	5.02183263717453	-1.52977892403172

C	1.34835126583956	6.64892726528624	-0.91661597659042
H	1.17440255439079	7.29177543535348	-1.77252841531455
C	2.19202838241021	7.11299820550683	0.09560691143279
C	2.80033986683730	8.52094134379730	0.01760366948685
O	5.03105072989068	8.74893841887577	4.57847462257652
O	5.31612212940549	9.44139337624505	6.72850177275885
N	2.98092263227469	7.21801466912163	5.27155005117284
C	1.51129521669981	5.53166142326848	4.38585474414438
H	0.91571535354022	6.10949666445649	3.66815337355501
H	0.88843661544507	4.69694980863525	4.75308454902940
C	1.92833375658345	6.42742345839569	5.53591749036438
C	1.31248512112535	6.42507280652417	6.78493375640239
H	0.46430948551011	5.77452608162916	6.98015681848671
C	1.82161766068803	7.26698110048306	7.77989879675352
H	1.35907310556609	7.28525331875226	8.76347561098237
C	2.93365851103209	8.05824966936785	7.50721305657607
H	3.39199291827802	8.70607315469276	8.24682024578217
C	3.49289090684003	8.00952217665497	6.22647289873423
C	4.73627208029922	8.82483296256742	5.82714505247564
O	6.12564153973849	7.60734608882071	1.85472289541517
O	8.29929285228293	7.00405893068274	1.93530601394914
N	5.42905343268929	5.47432674920945	3.38405223392612
C	3.62504772269054	4.30808254900876	4.54061430313333
H	3.58631955188416	4.75150657834784	5.54182051228665
H	3.32723636340007	3.25014107830525	4.65024164127315
C	5.06347437550992	4.38605574712725	4.07179907838707
H	8.37494176208322	7.84232435217034	1.43770935490311
C	5.98313072503568	3.38004086367552	4.40256805521583
H	5.64757290486839	2.50159630761481	4.94681419497792
C	7.31504659096133	3.52384335463870	4.03446803673094
H	8.04400488558413	2.76023587927981	4.28913299116286
C	7.70105566625007	4.66223795524207	3.32664548279777
H	8.72668545607822	4.82091284179216	3.01520315124326
C	6.71793909803066	5.59930490323491	3.01709257174415
C	6.99337034633070	6.83552630572034	2.22264198245695
O	1.63832357365389	8.82770078417932	3.18633672744921
H	1.98081989191564	9.18837580805555	2.32657832014683
H	1.63560526047630	9.57229979078790	3.80698940674499

[Ca(dpaea)(H₂O)(MeOH)]₂ (8g)

Ca	11.19765589739197	1.06468553256320	4.54826767819057
O	10.95477349044539	-1.20530521563486	3.95002344494526
O	10.36497020774520	-2.89128854681954	2.55341546982369
O	13.06257788625045	0.05646131293704	5.76236417760971
O	15.27395576551803	-0.11344341633242	6.20501646080870
O	8.96016656028617	2.14794443600605	4.68498548333944
H	8.48234532225531	1.37031982977972	5.13470765830616
H	8.94597225714839	2.84127392483734	5.36288626514241
O	11.63884819891666	2.74939268270730	6.31953701069613
H	11.99607910972872	2.15570791964162	7.06636028798515
N	11.31247837326996	3.13643527634758	2.69338802078649
N	10.23113745124722	0.64534883020316	2.21644647326669
N	13.53131446040934	1.73138540791394	3.72446950988691
C	10.08958977250148	3.04433192193465	1.87675723441577
H	10.09501446415344	3.73767272448272	1.01909529013632
H	9.25119621519375	3.31280448255002	2.52989530053631
C	9.86470299641593	1.63082107259982	1.38115824557358

C	9.28155588451382	1.36394381718454	0.14157186883673
H	9.00381330434099	2.18283938271486	-0.51644564012759
C	9.06812819843162	0.03671897893658	-0.23183161349852
H	8.61387720673156	-0.19490900341874	-1.19166270152759
C	9.45273674022725	-0.98223827168353	0.63460453054132
H	9.32325577483447	-2.03372860606598	0.40257313906853
C	10.03498398557116	-0.63529567345092	1.85423562805086
C	10.48211521765075	-1.69812706703275	2.85341103708212
C	12.51846655707311	2.91627690218931	1.87623137570300
H	12.73209650223808	3.75706177702317	1.19702294462255
H	12.32317321206091	2.03769446987285	1.24921749706596
C	13.72591880907753	2.61775993945335	2.73369639450217
C	14.97475733486932	3.19198114191083	2.49252743566224
H	15.09187569691297	3.92049033990328	1.69525496254364
C	16.05640620132031	2.81655824959426	3.28886092928005
H	17.03755717658393	3.25320489379265	3.12362405512682
C	15.85911123255126	1.88009010896577	4.29843652542062
H	16.65849268921996	1.54062153265140	4.94721185144694
C	14.57516459908995	1.36648266983618	4.48795888455079
C	14.28957998989329	0.35343953959496	5.58021046700338
C	11.37101584571140	4.37999796280108	3.49822196987274
H	12.20688951131219	4.26981665708366	4.19662180767989
H	10.45588353475845	4.38896591597466	4.09772808667283
C	11.49248233709077	5.70098411257203	2.72588069662660
H	11.49300723153900	6.53455665171085	3.43616558861346
H	10.65526341541195	5.85027766282539	2.03599242974342
H	12.42443144768043	5.75817498529828	2.15388563005068
C	10.84011305449808	3.72203442415713	7.00426321022945
H	11.34844168349211	4.04640189207357	7.91871624497136
H	9.85841580792169	3.30580286725938	7.28480574402123
H	10.69450727846589	4.58235531273741	6.34336518021063
Ca	12.08340242851350	-1.06478428326986	7.69104132631519
O	12.32634162473552	1.20520910821356	8.28934134697500
O	12.91625490351829	2.89109405379070	9.68602035228483
O	10.21846205217951	-0.05651365042042	6.47698755787999
O	8.00706355631302	0.11338036084225	6.03436845262863
O	14.32086327397999	-2.14809197244524	7.55421918141021
H	14.79894638911074	-1.37000596252610	7.10557253564619
H	14.33522540109876	-2.84073444728250	6.87562752028073
O	11.64221837637218	-2.74943038001816	5.91976986988365
H	11.28414754692958	-2.15583937469010	5.17326176576912
N	11.96855755757187	-3.13657236761891	9.54589471902361
N	13.05007078917528	-0.64555808841835	10.02278238303659
N	9.74976789587047	-1.73132806982800	8.51497558174264
C	13.19152096616337	-3.04456175682027	10.36242658355042
H	13.18610875613126	-3.73789984638692	11.22008589852186
H	14.02983724860208	-3.31308920580303	9.70921335692927
C	13.41655640987888	-1.63107304436656	10.85800034818079
C	13.99988858317373	-1.36425864904208	12.09750969013510
H	14.27767691894816	-2.18319054819073	12.75546295285636
C	14.21345998150181	-0.03705597620107	12.47091403781611
H	14.66786678950559	0.19451879589382	13.43068329353088
C	13.82878267347667	0.98194883718764	11.60455637796980
H	13.95835989335492	2.03342726712545	11.83658462454987
C	13.24635773778938	0.63506694304988	10.38500032902670
C	12.79923193752972	1.69795640792475	9.38589680487365
C	10.76265351301351	-2.91628411488468	10.36314780204787

H	10.54899300111732	-3.75703163004581	11.04238837832327
H	10.95808204573454	-2.03771267998490	10.99013457167551
C	9.55516451780601	-2.61764581522176	9.50579727197817
C	8.30627662664441	-3.19169855777020	9.74712987295552
H	8.18915398295334	-3.92015467457909	10.54444871039550
C	7.22460088448764	-2.81619363291426	8.95088089706836
H	6.24341602879273	-3.25272068283689	9.11623569166970
C	7.42189604643655	-1.87980471070498	7.94123996746484
H	6.62249351801023	-1.54029440660367	7.29251200965164
C	8.70588036032906	-1.36634673728529	7.75157561648544
C	8.99145668962856	-0.35341758129533	6.65921700475712
C	11.90984511277148	-4.38017025679573	8.74113314299133
H	11.07393238502984	-4.26994157126192	8.04278509526457
H	12.82493769696866	-4.38925391269683	8.14157028820493
C	11.78830332010790	-5.70110707797191	9.51354595722416
H	11.78765159188673	-6.53472222966981	8.80331443820037
H	12.62555072982810	-5.85044263515053	10.20338889555097
H	10.85638452149626	-5.75817341193936	10.08560236671256
C	12.44103527593670	-3.72155612166697	5.23440693519194
H	11.93238480160810	-4.04590612282119	4.32012123935431
H	13.42241775942003	-3.30482572874214	4.95346695928667
H	12.58734800861634	-4.58199060003939	5.89501082523243

[Mn₂(tpaa)₂Ca₂(H₂O)₁₂] (8^h)

Mn	5.79489415476730	4.50431144069647	9.88150147608260
O	5.71084547580117	3.03216162881419	8.82699171510304
O	5.93543623919275	2.48075312113977	6.62909060311141
O	4.94917957447851	5.38344547168923	8.56865271730241
O	3.50268958579162	7.06171514897015	8.14868641067058
O	4.15685167455258	4.04452304344407	10.42163423176646
O	2.87884265037898	2.50938782748934	11.51997078347907
N	8.14254022082319	5.28810044434475	11.42919169270454
N	7.41368148306686	4.83877561064840	8.90376877140250
N	5.66032415408103	6.09395020724003	10.81597406652944
N	6.36818017015987	3.31837723893131	11.26414444363851
C	8.62063517143085	6.25462174665284	10.48803050183359
H	9.67475136177819	6.53528110071106	10.63394454296096
H	8.03006148121588	7.17111572874213	10.60816879873175
C	8.44883730268795	5.69748441570797	9.09797543141226
C	9.32778568530302	6.00331813267605	8.07090774560629
H	10.14901704971207	6.68004991561059	8.27839880429138
C	9.15082750316880	5.43767204598177	6.77222973593790
H	9.81872532000832	5.70531937553114	5.96066175974512
C	8.14472676416738	4.52212315360414	6.58524636652219
H	7.98523137055928	4.02546652537237	5.63446236517616
C	7.30828528653910	4.19284594460072	7.65093811398510
C	6.31977781590244	3.18656830797572	7.60204587252619
C	7.37908685149333	5.74278933104448	12.55408771045212
H	7.94485202961074	6.38511782398855	13.24614737269190
H	7.05301861077419	4.86769065591983	13.12747401935358
C	6.19023765870707	6.52172709509811	12.02841565755552
C	5.71175043976501	7.65220239154625	12.66332042530183
H	6.17180228845452	7.93925523597773	13.60360812390817
C	4.68013889997050	8.43085895787041	12.10725304991169
H	4.30818543399503	9.30903851417922	12.62266345682016
C	4.19659694937694	8.07027782110124	10.86056584819801
H	3.44309097136104	8.64703058466891	10.33493046715523

C	4.69583337618334	6.93910286113256	10.24236721241297
C	4.30745069951050	6.51422319938895	8.90591102834906
C	8.71350462234176	3.97499840289743	11.43072976241741
H	9.14906396269793	3.79722438644405	10.44061200030738
H	9.52038944349870	3.84141036378626	12.16691657809889
C	7.61175150316084	2.98717135615873	11.72975965857056
C	7.81763506288935	1.89469674395670	12.55072790888252
H	8.82046584719431	1.70960939878418	12.91983226970820
C	6.72804075197750	1.06709866133781	12.95105795725770
H	6.89478935057496	0.20593413366768	13.58875933280429
C	5.46240970374303	1.42983137059309	12.56834293722672
H	4.57861542205517	0.88832342391496	12.88852837226201
C	5.28056280530780	2.54942371688672	11.75041137733329
C	4.01066452243314	2.98519627135654	11.29255237248597
Ca	4.10853878741445	0.85724436572166	6.36527792257429
O	6.23739483599336	0.05041013124842	5.37834508926134
H	6.73516715877665	0.84243934546877	5.66359069653662
H	6.68812335910337	-0.70386315374947	5.79086749931852
O	3.49429210864097	-0.81321447599663	4.79596864751669
H	2.60116459303185	-0.67782652192159	4.39064741556573
H	4.10871578576252	-0.91875419012281	4.05302673824148
O	5.32705970769703	-0.06783064155429	8.31459066716063
H	5.73036225531343	0.50667838323267	8.98597007998973
H	4.61150504670581	-0.56483747937257	8.75435013269997
O	3.99504577440470	2.16746570802927	4.21960959404842
H	3.47105983317939	1.73004163508099	3.47638959599104
H	4.72290753978543	2.65859444034058	3.81072284441079
O	2.66563975931488	-0.59641227952862	7.78309075201167
H	2.31548798439404	-1.45854702900844	7.38544896973966
H	1.89856344308796	-0.21554936273829	8.24125100019510
O	1.86160143845143	2.05937485718662	5.83124391081266
H	1.03249372585637	1.60424479080226	5.50099880734928
H	2.27440349798499	2.49485156306772	5.05847161587703
Mn	-0.59173870831938	-0.52745679115755	4.44058768529649
O	-0.50889409239830	1.09129173720604	5.24708566835662
O	-0.81402946227314	2.02861222303229	7.29510223857430
O	0.23875430528538	-1.17923837713713	5.88869261679043
O	1.69283593763146	-2.76123997341890	6.57439247007407
O	1.04547336673097	-0.16512845968198	3.83984786650321
O	2.32136186149077	1.11574745082164	2.45335658722920
N	-2.94563651041130	-1.58693866188364	3.01932283974958
N	-2.22433357744611	-0.70557278018905	5.44002442696893
N	-0.46415204969303	-2.26261897728342	3.77471650912344
N	-1.17118050749497	0.38980536136065	2.87441973536834
C	-3.41423111398021	-2.38363142033620	4.11098652709091
H	-4.46485173793241	-2.69739379863150	4.01504941507582
H	-2.81328682702969	-3.30030726394480	4.15012445260438
C	-3.25482135400479	-1.59019417664192	5.38581633612977
C	-4.15608036480319	-1.71513638812807	6.42772722703555
H	-4.97111614218705	-2.42222777472977	6.32232131519459
C	-4.01587033282847	-0.92451755008148	7.60816722002643
H	-4.70425596388588	-1.04684385144264	8.43733575272814
C	-3.01793229391233	0.01918256805410	7.64991192929914
H	-2.88665637585691	0.68207648928615	8.49827326748251
C	-2.15217286614689	0.15778678186483	6.56131497255003
C	-1.16294288999113	1.15674616918209	6.45056001968256
C	-2.16970200955772	-2.21309591457903	1.99613541486977

H	-2.72461528107743	-2.96257312889800	1.41106592241040
H	-1.83872580701990	-1.44207191395677	1.29119121814024
C	-0.98747214275834	-2.89007018854316	2.65436253376593
C	-0.50153204965854	-4.11423047607448	2.22944130268602
H	-0.95480856035572	-4.56188878293858	1.35066213913559
C	0.53088875128964	-4.78287471575964	2.92168148764239
H	0.90700946732445	-5.73712145224451	2.57078794134227
C	1.00543018280205	-4.20827840218318	4.08528981576265
H	1.75714678634523	-4.68073403819013	4.70846160510861
C	0.50060309234827	-2.98829686414202	4.49218430695599
C	0.88497355083358	-2.34504446081567	5.73919107248470
C	-3.51455737286727	-0.29082186544174	2.80670449617308
H	-3.95237380763091	0.04390657106159	3.75410386317402
H	-4.31995990668065	-0.27629607429955	2.05687668263923
C	-2.41243181735825	0.63541930221995	2.35255381719256
C	-2.60991878139366	1.56893011193769	1.34982876666712
H	-3.61061469137055	1.68767672381251	0.94871803776548
C	-1.51619942691060	2.30706419297369	0.81163104225595
H	-1.67684361602880	3.04074466007899	0.02930633357874
C	-0.25506954987047	2.00991632358533	1.25577822049951
H	0.63346118436238	2.47859780918180	0.84646632504291
C	-0.08329755401486	1.05552270010981	2.25949063120433
C	1.18963869444173	0.70400866600853	2.78080527286796
Ca	1.06551422254184	3.48855762974955	7.70907077924372
O	-1.04079775278400	4.25904568152711	8.78652158864553
H	-1.56077423033372	3.53210164343269	8.38721334113288
H	-1.46595335258059	5.08290041492449	8.50012891981053
O	1.70609731428256	4.85871086529654	9.54811016044163
H	2.58405737147701	4.63475480444054	9.94519657683101
H	1.07224021242073	4.87195133358257	10.28166303743133
O	0.01464034287912	4.80238126103751	5.91689771274806
H	-0.52106735892148	4.49658005446259	5.16993506057390
H	0.77919193312654	5.28985053175815	5.55598243733696
O	1.08362309731823	1.85367619603690	9.66127849559585
H	1.61622622805482	2.13718480029797	10.46640815921539
H	0.28751640951899	1.40331367522029	9.98054202795079
O	2.62299318346307	5.08807396073714	6.57867433911568
H	2.92640679215140	5.88572502360116	7.12188734904037
H	3.44500704307665	4.74860465157177	6.19132545682572
O	3.28216925451379	2.31174477540889	8.17777132086896
H	4.12764311110214	2.71799772684947	8.52564083014530
H	2.91315220541307	1.78918628658049	8.91438624946104

{{Ca₂(bzida)₂(H₂O)₆}}_n (8ⁱ)

Ca	6.41301079845073	5.64708357499786	3.63951275486474
O	6.50589353192802	3.31348463806478	3.62438954264638
O	6.36883367892898	1.39776123510056	2.44532241494026
O	6.21202227639080	6.30900682777768	1.28536967728057
O	4.82452287872593	6.93888096893199	-0.37355325237739
N	4.44138196380414	4.43427234914851	2.21830493668594
C	5.19947501359909	3.31810310714884	1.60571694753496
H	4.54705189360098	2.61044774713380	1.08286549101262
H	5.88534732307482	3.73975799133591	0.86047428640129
C	6.06617797586156	2.57038436059932	2.63028164268376
C	3.98175632087443	5.36366867098352	1.17842762608324
H	3.51770715550409	4.87527506082361	0.31053086099931
H	3.22267637205116	6.03312696148642	1.60159714218077

C	5.12372725383440	6.23903412631118	0.71903084520222
C	3.28512250930087	3.89890378668240	3.01646529029591
H	2.86724420036813	4.75041698616927	3.56407811039620
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C	2.20052324035854	3.21075009860609	2.22241890528026
C	2.26979584762208	1.83758938863768	1.95213955452280
H	3.09059543860739	1.24670191381684	2.35283719625869
C	1.28275751271746	1.21723687828004	1.18690959344657
H	1.34453115461679	0.15199246476099	0.98724761204743
C	0.21217445270019	1.96101284818660	0.68999766994294
H	-0.55912842372622	1.47658238549612	0.09947766301357
C	0.12331822573925	3.32532841596742	0.96959654246881
H	-0.71943581216017	3.90326019314756	0.60290186750755
C	1.11123873307985	3.94357474489940	1.73352785937155
H	1.02324382294635	5.00301574041403	1.96721726636515
O	4.87287532756984	5.10567136190414	5.53196324418052
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H	4.15623908118473	5.63442753956826	5.91398970284324
O	8.66696955210391	4.83811025008707	2.75302357476791
H	8.51195219598955	4.06978567337849	2.17607996015015
H	9.16403202404191	5.48615957007812	2.22284708224156
O	7.86247564897875	7.54186673881946	3.69495274565523
H	8.77416831214153	7.31787021277078	4.08412892208048
H	7.90384502819475	8.46479810168832	3.41166079891448
Ca	10.14323547992023	4.18504761445408	4.70563730805036
O	10.05031647199392	6.51171317830180	4.72382439054848
O	10.18697492328738	8.43028850422930	5.89756807570498
O	10.35166045474693	3.52070291914486	7.05716715651005
O	11.74281324008061	2.89117683509037	8.71336202465820
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C	11.36331938734904	6.51269180942827	6.73723573829445
H	12.01783769283290	7.22121465253772	7.25626721342543
H	10.68094643268981	6.09181958518986	7.48613345747593
C	10.49184571951759	7.25787599028646	5.71465590061395
C	12.58146729905896	4.46659891659642	7.16013497428112
H	13.04757609141934	4.95448348740819	8.02720687153434
H	13.33961467411777	3.79726055469350	6.73502858562688
C	11.44123629601543	3.59068192479788	7.62179052132203
C	13.27277975890534	5.93110950314789	5.31939527852005
H	13.68575321856307	5.08014354381795	4.76735542038371
H	12.83285831719295	6.63894888144374	4.60733136293987
C	14.36251623610272	6.61445410688547	6.11054589765930
C	14.29747835537277	7.98673950332209	6.38629435068734
H	13.47651396106399	8.58105111531301	5.99104383808311
C	15.28916680998338	8.60201697427144	7.14962149354564
H	15.23065529081568	9.66664097627806	7.35354526631645
C	16.36021573458276	7.85400501911217	7.63910694553731
H	17.13508470323782	8.33447573842860	8.22819777561670
C	16.44497106370256	6.49062390419555	7.35374205333339
H	17.28810674612505	5.90947187386712	7.71442029423694
C	15.45244020064116	5.87743550382884	6.59171473177911
H	15.53729768583073	4.81880940578177	6.35329282005936
O	11.67985846840227	4.72988338922930	2.80576827374196
H	12.06263822468684	5.61750863663848	2.90247878981691
H	12.35591993078459	4.19272620510873	2.36599896143071
O	7.88662120507862	4.99453483683308	5.60239372289399
H	8.05163026504810	5.77034617970225	6.16681048180036

H	7.39537654197803	4.35520962862495	6.14752129754615
O	8.69380360341635	2.28997274320365	4.65252189280719
H	7.77936727378483	2.50618289702307	4.26393746756202
H	8.62297027795665	1.42368486973442	5.07521351540450
O	11.66513899850994	2.28911427201415	4.49105648394447
O	4.90737761386971	7.52276689619468	3.84472138175765
O	10.62957832907386	1.75591755859526	2.51584529964423
C	11.43167165379892	1.48884532781115	3.57083950267655
O	5.95220082805712	8.25837296775978	5.74544852286784
C	4.33972820253673	9.70429673222394	4.53464168785652
H	4.13156205782942	9.86220947135828	3.47741619384744
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C	5.11720243260475	8.41360779124583	4.69010365728781
H	5.58750593244198	7.50319402512600	-0.61304982666113
H	10.98203848435912	2.32448651861764	8.95404053495055
H	4.85451459528634	10.57444137489624	4.95386565425406
C	11.95971918980435	0.07488580090846	3.70124831416504
H	12.79013518653136	0.06332891267712	4.40494155556647
H	11.15029302170296	-0.55091869135654	4.09854433502376
H	12.27206335323030	-0.35350282212176	2.74328669719459
H	10.53498594611436	0.96159424241015	1.95889104381744
H	6.00270114294712	9.08646767072333	6.25785631354081