Electronic Supplementary Information for Dalton Transactions

Tuning the thermodynamic stability of oxothiomolybdenum wheels: crystal structures, studies in solution and DFT calculations

Jean-François Lemonnier,[a] Ali Kachmar,[b] Sébastien Floquet,*[,a] Jérôme Marrot,[a]

Marie-Madeleine Rohmer,*[,b] Marc Bénard,[b] and Emmanuel Cadot[a]

a - Institut Lavoisier de Versailles, UMR 8180, University of Versailles, 45 avenue des Etats-Unis, 78035 Versailles, France. E-mail : sebastien.floquet@chimie.uvsq.fr.

b - Laboratoire de Chimie Quantique, Institut de Chimie-UMR 7177, CNRS-ULP, 4 rue Blaise Pascal, 67000 Strasbourg, France. E-mail : mmrohmer@quantix.u-strasbg.fr.

Supporting Information

Table S1 Final proportions of molybdenum complexes in mixtures Mo_{12}:$L1^{n-}$:$L2^{n-}$ in 1:1:1 ratio. The uncertainties are estimated to be about ±0.02 excepted for mixture 7 (±0.05) due to the strong overlap between the NMR signals of the free ligand and of the host-guest complex.

Mixtures	$L1^{n-}$	$L2^{n-}$	% $[Mo_{12}L1]^{n-}$	% $[Mo_{12}L2]^{n-}$
1	$Adip^{2-}$	Sub^{2-}	0.95(2)	0.05(2)
2	$Adip^{2-}$	Pim^{2-}	0.95(2)	0.05(2)
3	$Adip^{2-}$	$Muco^{2-}$	0.20(2)	0.80(2)
4	$Adip^{2-}$	$TerP^{2-}$	0.52(2)	0.48(2)
5	$Adip^{2-}$	TMT^{2-}	0.10(2)	0.90(2)
6	$Adip^{2-}$	$Trim^{3-}$	0.00(2)	1.00(2)
7	Pim^{2-}	Sub^{2-}	0.85(5)	0.15(5)
8	Pim^{2-}	$TerP^{2-}$	0.13(2)	0.87(2)
9	Pim^{2-}	$Trim^{3-}$	0.00(2)	1.00(2)
10	Sub^{2-}	$TerP^{2-}$	0.05(2)	0.95(2)
11	Sub^{2-}	$Trim^{3-}$	0.00(2)	1.00(2)
12	$Muco^{2-}$	$TerP^{2-}$	0.78(2)	0.22(2)
13	$Muco^{2-}$	TMT^{2-}	0.20(2)	0.80(2)
14	$Muco^{2-}$	$Trim^{3-}$	0.00(2)	1.00(2)
15	$TerP^{2-}$	TMT^{2-}	0.00(2)	1.00(2)
16	$TerP^{2-}$	$Trim^{3-}$	0.00(2)	1.00(2)
17	TMT^{2-}	$Trim^{3-}$	0.00(2)	1.00(2)

Bond energies and optimized geometries computed for host-guest complexes (without solvent)

$(Adipate)^{2-}@[Mo_{12}O_{12}S_{12}(OH)_{12}]$ (C_2 symmetry, Figure 7a)

78 atoms; Bond energy: -519.6581 eV

Mo	6.565597	0.053557	0.026212
Mo	0.198067	5.560235	0.007811
Mo	-0.198067	-5.560235	0.007811
Mo	2.987826	5.035511	0.012418
Mo	-2.987826	-5.035511	0.012418
Mo	5.526637	2.671035	0.023157
Mo	-5.526637	-2.671035	0.023157
Mo	-6.565597	-0.053557	0.026212
Mo	5.502047	-3.158923	0.018302
Mo	-5.502047	3.158923	0.018302
Mo	3.181516	-4.786154	0.011033
Mo	-3.181516	4.786154	0.011033
S	1.505454	4.924812	1.836946
S	5.937492	1.327627	1.908109
S	4.095922	-3.667419	1.845259
S	1.509953	4.913657	-1.814802
S	5.943362	1.325390	-1.858509
S	4.097618	-3.653874	-1.813780
S	-1.505454	-4.924812	1.836946
S	-5.937492	-1.327627	1.908109
S	-4.095922	3.667419	1.845259
S	-1.509953	-4.913657	-1.814802
S	-5.943362	-1.325390	-1.858509
S	-4.097618	3.653874	-1.813780
O	0.120170	7.258635	0.003411
O	3.652931	6.599169	0.009894
O	6.877202	3.717988	0.025044
O	8.271907	0.183434	0.028754
O	6.686755	-4.376290	0.015293
O	3.828504	-6.358949	0.005419
O	-0.120170	-7.258635	0.003411
O	-3.652931	-6.599169	0.009894
O	-6.877202	-3.717988	0.025044
O	-8.271907	-0.183434	0.028754
O	-6.686755	4.376290	0.015293
O	-3.828504	6.358949	0.005419
O	4.239158	3.899668	1.241324
H	3.812704	3.424301	1.977145
O	6.381203	-1.709672	1.260524
H	5.840422	-1.502937	2.045421
O	-1.418477	4.877320	1.175353
H	-1.347557	4.591149	2.102821
O	4.245538	3.896216	-1.206363
H	3.823388	3.418434	-1.943021
O	6.383560	-1.704245	-1.214383
H	5.847440	-1.494011	-2.001506

O	-1.417489	4.867280	-1.154612
H	-1.348669	4.585448	-2.083562
O	-4.239158	-3.899668	1.241324
H	-3.812704	-3.424301	1.977145
O	-6.381203	1.709672	1.260524
H	-5.840422	1.502937	2.045421
O	1.418477	-4.877320	1.175353
H	1.347557	-4.591149	2.102821
O	-4.245538	-3.896216	-1.206363
H	-3.823388	-3.418434	-1.943021
O	-6.383560	1.704245	-1.214383
H	-5.847440	1.494011	-2.001506
O	1.417489	-4.867280	-1.154612
H	1.348669	-4.585448	-2.083562
C	3.271244	0.206127	0.026852
C	1.900925	-0.478229	0.029116
H	1.896331	-1.147624	0.905359
H	1.896780	-1.152571	-0.843395
C	0.653228	0.409076	0.026337
H	0.676544	1.075203	0.903669
H	0.677917	1.073208	-0.852438
C	-0.653228	-0.409076	0.026337
H	-0.676544	-1.075203	0.903669
H	-0.677917	-1.073208	-0.852438
C	-1.900925	0.478229	0.029116
H	-1.896331	1.147624	0.905359
H	-1.896780	1.152571	-0.843395
C	-3.271244	-0.206127	0.026852
O	3.359903	1.471461	0.022880
O	4.276257	-0.596178	0.029031
O	-3.359903	-1.471461	0.022880
O	-4.276257	0.596178	0.029031

(Adipate,H_2O)$^{2-}$@[$Mo_{12}O_{12}S_{12}(OH)_{12}$] ($C_1$ symmetry, Figure 7b)

81 atoms; Bond energy: -533.8943 eV

Mo	4.998865	-3.161528	0.019171
Mo	6.596843	-0.805911	-0.047577
Mo	5.980918	2.509151	-0.042750
Mo	3.864655	4.425296	-0.010769
Mo	0.551167	5.532029	0.022505
Mo	-2.295339	5.370297	0.034689
Mo	-5.105593	3.312840	0.017172
Mo	-6.277898	0.730905	-0.024140
Mo	-5.780414	-2.697616	-0.046366
Mo	-3.896472	-4.833319	-0.038186
Mo	-0.584719	-6.061645	0.030513
Mo	2.157209	-5.220959	0.060439
S	5.637367	-1.930217	-1.882189
S	5.750906	-1.902806	1.859528
S	4.651073	3.232683	-1.858901
S	4.689679	3.211262	1.808257
S	-0.840848	5.071247	-1.797355
S	-0.822771	5.014114	1.841768
S	-5.613972	1.958407	1.875601
S	-5.610612	2.019398	-1.883677
S	-4.466153	-3.465300	-1.849141

S	-4.535521	-3.511079	1.781565
S	0.681816	-5.454463	1.914103
S	0.732557	-5.463532	-1.804294
O	6.101084	-4.461212	-0.001499
O	8.232058	-1.298586	-0.096158
O	7.309276	3.568344	-0.053572
O	4.671192	5.922068	-0.002729
O	0.816729	7.210407	0.050849
O	-2.709668	7.016579	0.063845
O	-6.386657	4.446286	0.048689
O	-7.977053	0.940550	-0.036783
O	-7.216747	-3.601564	-0.066962
O	-4.932539	-6.179993	-0.088512
O	-0.626245	-7.761344	0.029109
O	2.992622	-6.705077	0.099652
O	3.459401	-4.016466	1.245392
H	3.603182	-4.178767	2.194048
O	3.431642	-4.056964	-1.141941
H	3.122352	-3.644176	-1.967395
O	6.766275	0.965669	1.175439
H	6.257483	0.840479	1.999332
O	6.723851	0.964306	-1.288708
H	6.178587	0.840311	-2.088864
O	2.101359	4.710183	-1.158897
H	2.020350	4.490567	-2.104189
O	2.106969	4.654123	1.157582
H	2.047273	4.439082	2.105757
O	-3.742407	4.495734	-1.197566
H	-3.400705	4.004263	-1.967562
O	-3.725368	4.448452	1.252718
H	-3.371279	3.929360	1.998611
O	-6.217185	-1.050651	-1.269238
H	-5.609386	-0.935605	-2.023661
O	-6.241659	-1.073062	1.193179
H	-5.655652	-0.970796	1.966351
O	-2.189259	-5.357718	-1.172623
H	-1.991501	-4.933275	-2.028237
O	-2.259753	-5.422398	1.178125
H	-2.121967	-5.039141	2.063665
O	3.161806	-1.417873	0.058399
O	4.503310	0.377263	-0.032421
O	-3.080795	2.070861	-0.003532
O	-4.054746	0.019660	-0.030678
O	1.079233	-3.011162	0.160258
H	0.789155	-3.047699	1.092673
H	1.825201	-2.326715	0.146656
C	3.342130	-0.155724	0.014611
C	2.145010	0.792168	0.004624
H	2.244624	1.414268	-0.903290
H	2.278533	1.483542	0.855980
C	0.794659	0.089526	0.054968
H	0.740555	-0.506503	0.981995
H	0.739384	-0.639471	-0.769218
C	-0.442221	0.988178	-0.009682
H	-0.468268	1.690832	0.840898
H	-0.430090	1.608912	-0.922464
C	-1.687921	0.101080	0.002641
H	-1.684523	-0.550694	0.894563
H	-1.674463	-0.594026	-0.854689
C	-3.040550	0.798525	-0.014407

(Pimelate)$^{2-}$@[$Mo_{12}O_{12}S_{12}(OH)_{12}$] ($C_2$ symmetry)

81 atoms; Bond energy: -535.697 eV

Mo	6.873261	0.089844	0.060754
Mo	0.258710	5.174629	-0.018564
Mo	-0.258710	-5.174629	-0.018564
Mo	3.090194	4.882904	0.011205
Mo	-3.090194	-4.882904	0.011205
Mo	5.805099	2.712966	0.047732
Mo	-5.805099	-2.712966	0.047732
Mo	-6.873261	-0.089844	0.060754
Mo	5.554700	-3.003591	0.021010
Mo	-5.554700	3.003591	0.021010
Mo	3.109724	-4.457656	-0.013617
Mo	-3.109724	4.457656	-0.013617
S	1.599188	4.621668	1.814209
S	6.224174	1.368362	1.933731
S	4.099273	-3.427333	1.832239
S	1.637692	4.636657	-1.829034
S	6.281558	1.370989	-1.826769
S	4.142609	-3.416199	-1.832145
S	-1.599188	-4.621668	1.814209
S	-6.224174	-1.368362	1.933731
S	-4.099273	3.427333	1.832239
S	-1.637692	-4.636657	-1.829034
S	-6.281558	-1.370989	-1.826769
S	-4.142609	3.416199	-1.832145
O	0.068356	6.863787	-0.012164
O	3.591090	6.505702	0.021946
O	7.129845	3.794409	0.065517
O	8.579554	0.204201	0.085969
O	6.630269	-4.319229	0.029191
O	3.623441	-6.079150	-0.010772
O	-0.068356	-6.863787	-0.012164
O	-3.591090	-6.505702	0.021946
O	-7.129845	-3.794409	0.065517
O	-8.579554	-0.204201	0.085969
O	-6.630269	4.319229	0.029191
O	-3.623441	6.079150	-0.010772
O	4.457624	3.896345	1.254787
H	4.067244	3.390458	1.991079
O	6.608284	-1.670289	1.280070
H	6.100254	-1.430616	2.077835
O	-1.323074	4.370158	1.126399
H	-1.299121	4.252692	2.092149
O	4.497975	3.911299	-1.197777
H	4.136522	3.417251	-1.956108
O	6.642385	-1.655406	-1.188463
H	6.162867	-1.404785	-2.000151
O	-1.328144	4.390301	-1.178485
H	-1.310234	4.297847	-2.146893
O	-4.457624	-3.896345	1.254787
H	-4.067244	-3.390458	1.991079
O	-6.608284	1.670289	1.280070
H	-6.100254	1.430616	2.077835
O	1.323074	-4.370158	1.126399
H	1.299121	-4.252692	2.092149

O	-4.497975	-3.911299	-1.197777
H	-4.136522	-3.417251	-1.956108
O	-6.642385	1.655406	-1.188463
H	-6.162867	1.404785	-2.000151
O	1.328144	-4.390301	-1.178485
H	1.310234	-4.297847	-2.146893
O	3.708564	1.527860	-0.008458
O	4.560757	-0.558896	0.036821
O	-3.708564	-1.527860	-0.008458
O	-4.560757	0.558896	0.036821
C	3.579886	0.266816	-0.049504
C	2.192262	-0.329074	-0.243936
H	1.909872	-0.818814	0.702257
H	2.313947	-1.146965	-0.972055
C	1.128866	0.664737	-0.733112
H	1.631026	1.408095	-1.367393
H	0.720006	1.235019	0.115367
C	-3.579886	-0.266816	-0.049504
C	-2.192262	0.329074	-0.243936
H	-1.909872	0.818814	0.702257
H	-2.313947	1.146965	-0.972055
C	-1.128866	-0.664737	-0.733112
H	-1.631026	-1.408095	-1.367393
H	-0.720006	-1.235019	0.115367
C	0.000000	0.000000	-1.538131
H	-0.455804	0.752325	-2.203258
H	0.455804	-0.752325	-2.203258

$(Suberate)^{2-}$@$[Mo_{12}O_{12}S_{12}(OH)_{12}]$ (C_1 symmetry)

84 atoms; Bond energy: -551.8864 eV

Mo	4.817177	1.715143	-0.015545
Mo	-4.960615	-1.735746	-0.006467
Mo	-5.003531	1.707672	-0.023409
Mo	4.824981	-1.699507	-0.022133
Mo	4.090661	4.468177	-0.004834
Mo	-4.096937	-4.448386	0.000179
Mo	-4.116220	4.417458	-0.015084
Mo	4.106768	-4.454659	-0.024663
Mo	1.520653	6.657974	0.000947
Mo	-1.355864	-6.539514	0.019382
Mo	-1.310462	6.462780	0.021450
Mo	1.481392	-6.625740	0.008682
O	6.514473	1.794775	-0.075438
O	-6.652268	-1.903788	-0.013451
O	6.523486	-1.772515	-0.002141
O	-6.694862	1.852101	-0.116346
O	5.655776	5.126290	-0.066233
O	-5.599842	-5.238303	0.022756
O	5.661816	-5.135935	0.011665
O	-5.585237	5.265665	-0.104339
O	1.946954	8.314267	-0.043256
O	-1.929756	-8.149351	0.092504
O	1.967191	-8.264884	0.071648
O	-1.935450	8.054570	-0.005173
O	4.310348	0.010234	1.139504

H	4.284900	0.009027	2.112126
O	4.275085	0.000311	-1.162319
H	4.234909	0.000611	-2.134667
O	-4.577783	0.003415	1.157219
H	-4.501942	0.014948	2.127018
O	-4.492811	-0.018375	-1.148845
H	-4.343951	-0.021887	-2.110427
O	3.077580	5.846017	-1.244928
H	2.676880	5.425070	-2.023342
O	3.137348	5.902497	1.230210
H	2.766651	5.513938	2.040354
O	-2.943612	-5.716949	-1.217387
H	-2.564120	-5.271167	-1.997151
O	-2.880316	-5.616729	1.238437
H	-2.493016	-5.139693	1.995686
O	3.084534	-5.853193	-1.236749
H	2.703689	-5.449475	-2.038523
O	3.025429	-5.753151	1.224716
H	2.633946	-5.311169	2.000857
O	-2.809563	5.527765	-1.213125
H	-2.419973	5.046681	-1.966088
O	-2.894190	5.581626	1.232579
H	-2.538873	5.104196	2.004576
S	0.118432	6.524054	1.896915
S	0.093412	6.428731	-1.860399
S	0.072579	-6.415490	1.883169
S	0.052735	-6.589540	-1.872326
S	4.147869	2.982403	1.835359
S	4.005913	2.956461	-1.817104
S	-4.144436	-2.940321	1.816779
S	-4.149821	-2.960830	-1.827657
S	4.056301	-2.948726	1.790922
S	4.115483	-2.966738	-1.858764
S	-4.315332	2.960178	1.826635
S	-4.107685	2.900844	-1.816670
O	1.409245	4.272852	0.089524
O	-0.991746	-4.177011	-0.161000
O	1.263893	-4.250611	-0.181353
O	-0.837616	4.103142	0.180852
C	0.327851	3.610754	0.290287
C	0.150490	-3.653232	-0.375791
C	-0.522586	0.191675	2.020996
H	-1.487808	-0.207680	2.374517
H	0.085313	0.375749	2.923285
C	0.484274	2.161451	0.719786
H	0.846674	1.600519	-0.157823
H	1.315779	2.137863	1.442636
C	-0.557228	-1.204603	-0.137245
H	-0.675662	-0.295170	-0.746739
H	-1.571759	-1.571359	0.086881
C	0.177497	-2.256032	-0.974459
H	1.222675	-1.964635	-1.143622
H	-0.308683	-2.346243	-1.959241
C	0.177353	-0.873428	1.166045
H	1.200916	-0.539189	0.925452
H	0.296447	-1.794078	1.760832
C	-0.777134	1.528744	1.308769
H	-1.232849	2.233331	2.019240
H	-1.525059	1.399739	0.512327

(Muconate)$^{2-}$@[$Mo_{12}O_{12}S_{12}(OH)_{12}$] ($C_s$ symmetry, Figure 7c)

74 atoms; Bond energy: -503.7826 eV

Mo	6.393827	0.259888	0.000000
Mo	5.325616	3.528660	0.000000
Mo	3.039547	5.220673	0.000000
Mo	-0.415321	5.869498	0.000000
Mo	-3.138687	5.023590	0.000000
Mo	-5.468068	2.418905	0.000000
Mo	-6.393827	-0.259888	0.000000
Mo	-5.325616	-3.528660	0.000000
Mo	-3.039547	-5.220673	0.000000
Mo	0.415321	-5.869498	0.000000
Mo	3.138687	-5.023590	0.000000
Mo	5.468068	-2.418905	0.000000
O	8.105573	0.226684	0.000000
O	6.539407	4.715659	0.000000
O	3.752905	6.763707	0.000000
O	-0.536088	7.564884	0.000000
O	-3.969199	6.504802	0.000000
O	-6.866565	3.399363	0.000000
O	-8.105573	-0.226684	0.000000
O	-6.539407	-4.715659	0.000000
O	-3.752905	-6.763707	0.000000
O	0.536088	-7.564884	0.000000
O	3.969199	-6.504802	0.000000
O	6.866565	-3.399363	0.000000
O	6.131722	2.031768	-1.227835
H	5.586783	1.825017	-2.010674
O	1.277907	5.384177	-1.174130
H	1.201359	4.999576	-2.066383
O	-4.266711	3.758050	-1.221034
H	-3.810216	3.340930	-1.974431
O	-6.131722	-2.031768	-1.227835
H	-5.586783	-1.825017	-2.010674
O	-1.277907	-5.384177	-1.174130
H	-1.201359	-4.999576	-2.066383
O	4.266711	-3.758050	-1.221034
H	3.810216	-3.340930	-1.974431
O	6.131722	2.031768	1.227835
H	5.586783	1.825017	2.010674
O	1.277907	5.384177	1.174130
H	1.201359	4.999576	2.066383
O	-4.266711	3.758050	1.221034
H	-3.810216	3.340930	1.974431
O	-6.131722	-2.031768	1.227835
H	-5.586783	-1.825017	2.010674
O	-1.277907	-5.384177	1.174130
H	-1.201359	-4.999576	2.066383
O	4.266711	-3.758050	1.221034
H	3.810216	-3.340930	1.974431
S	5.845144	-1.053578	-1.879107
S	3.916554	4.049634	-1.818308
S	-1.646999	5.078117	-1.819403
S	-5.845144	1.053578	-1.879107
S	-3.916554	-4.049634	-1.818308
S	1.646999	-5.078117	-1.819403

S	5.845144	-1.053578	1.879107
S	3.916554	4.049634	1.818308
S	-1.646999	5.078117	1.819403
S	-5.845144	1.053578	1.879107
S	-3.916554	-4.049634	1.818308
S	1.646999	-5.078117	1.819403
C	3.162777	-0.109397	0.000000
C	-3.162777	0.109397	0.000000
C	-1.790347	-0.457119	0.000000
C	1.790347	0.457119	0.000000
C	0.661637	-0.286288	0.000000
C	-0.661637	0.286288	0.000000
H	-1.737827	-1.549434	0.000000
H	1.737827	1.549434	0.000000
H	-0.758979	1.377188	0.000000
H	0.758979	-1.377188	0.000000
O	4.106154	0.763183	0.000000
O	3.323508	-1.375434	0.000000
O	-3.323508	1.375434	0.000000
O	-4.106154	-0.763183	0.000000

(Muconate,H_2O)$^{2-}$@[$Mo_{12}O_{12}S_{12}(OH)_{12}$] ($C_1$ symmetry, no constraint, Figure 7d)

77 atoms; Bond energy: -517.9760 eV

Mo	4.493207	3.869697	-0.003429
Mo	6.116028	1.551753	-0.035328
Mo	6.460069	-1.930592	-0.028970
Mo	4.629118	-4.123771	-0.016105
Mo	1.401554	-5.526512	0.012296
Mo	-1.441215	-5.337707	0.020830
Mo	-4.530142	-3.708529	0.007250
Mo	-6.457397	-1.626624	-0.039845
Mo	-6.320959	1.742167	-0.027066
Mo	-4.499269	3.930835	0.000779
Mo	-1.358442	5.470122	0.016766
Mo	1.486690	5.624265	0.021704
S	5.111975	2.597225	-1.885001
S	5.246479	2.637224	1.859411
S	5.468917	-2.977263	-1.897163
S	5.366981	-2.870145	1.823488
S	0.011079	-5.045855	-1.815437
S	0.027603	-4.905675	1.807522
S	-5.387782	-2.616319	-1.893451
S	-5.453486	-2.587473	1.862687
S	-5.101254	2.632753	-1.844196
S	-5.114861	2.601056	1.812688
S	0.078360	5.167053	-1.809080
S	0.068564	5.118472	1.832881
O	5.595539	5.175252	-0.039400
O	7.712553	2.142448	-0.098092
O	8.056536	-2.513876	0.010237
O	5.599854	-5.520653	0.040020
O	1.600639	-7.212193	0.078186
O	-1.838862	-6.986852	0.076769
O	-5.425774	-5.163400	0.022578
O	-8.009703	-2.342396	-0.075597
O	-7.777151	2.616497	-0.018446

O	-5.526266	5.286569	-0.005892
O	-1.817785	7.106110	0.019691
O	1.735606	7.303866	0.034633
O	2.980607	4.839252	-1.210177
H	2.676248	4.322288	-1.978605
O	3.016509	4.867831	1.244135
H	2.711338	4.310743	1.984345
O	6.374270	-0.214170	-1.231626
H	5.849896	-0.289733	-2.050816
O	6.441666	-0.190855	1.166574
H	5.885901	-0.248137	1.966695
O	2.981315	-4.810857	-1.196272
H	2.902205	-4.690560	-2.159255
O	2.978697	-4.751770	1.190198
H	2.743127	-4.182707	1.945951
O	-2.891666	-4.468051	-1.204755
H	-2.617651	-3.944463	-1.978975
O	-2.895955	-4.436968	1.237211
H	-2.602537	-3.846494	1.954335
O	-6.837804	0.114502	-1.272994
H	-6.280492	0.067112	-2.073279
O	-6.862695	0.106116	1.191519
H	-6.329722	0.047593	2.007696
O	-2.757872	4.386199	-1.133037
H	-2.660903	4.193808	-2.083609
O	-2.821142	4.490410	1.188873
H	-2.668330	4.165788	2.094477
O	2.997618	-2.164955	-0.143522
H	3.352175	-1.219122	-0.026413
H	2.727516	-2.191332	-1.081101
O	2.657134	2.402167	0.108455
O	3.767599	0.410460	0.109642
O	-4.536068	-0.215502	-0.043312
O	-3.002978	-1.883412	0.045001
C	2.698256	1.132216	0.184599
C	1.422032	0.392561	0.362442
H	1.512347	-0.666557	0.614048
C	0.184250	0.896980	0.150280
H	0.057157	1.951026	-0.118403
C	-0.960800	0.022460	0.211012
H	-0.765913	-1.032224	0.436149
C	-2.245180	0.366170	-0.028696
H	-2.536935	1.394087	-0.258434
C	-3.326621	-0.653505	-0.002630

(Muconate,$2H_2O$)$^{2-}$@[$Mo_{12}O_{12}S_{12}(OH)_{12}$] ($C_i$ symmetry, figure 7e)

80 atoms; Bond energy: -532.0904 eV

Mo	6.369038	0.266122	-0.038034
Mo	5.288949	3.552088	0.019679
Mo	3.018186	5.286886	0.017389
Mo	-0.415029	6.140082	-0.016598
Mo	-3.095920	5.105109	-0.044245
Mo	-5.477461	2.455917	0.022010
Mo	-6.369038	-0.266122	0.038034
Mo	-5.288949	-3.552088	-0.019679
Mo	-3.018186	-5.286886	-0.017389
Mo	0.415029	-6.140082	0.016598
Mo	3.095920	-5.105109	0.044245

Mo	5.477461	-2.455917	-0.022010
O	8.077825	0.233057	-0.082648
O	6.507016	4.732401	0.080422
O	3.775961	6.806072	0.089236
O	-0.435173	7.839148	0.039691
O	-4.067549	6.503085	-0.006326
O	-6.911419	3.375164	0.076012
O	-8.077825	-0.233057	0.082648
O	-6.507016	-4.732401	-0.080422
O	-3.775961	-6.806072	-0.089236
O	0.435173	-7.839148	-0.039691
O	4.067549	-6.503085	0.006326
O	6.911419	-3.375164	-0.076012
O	6.100136	2.069615	-1.229316
H	5.576170	1.895220	-2.033804
O	1.282077	5.556424	-1.171955
H	1.214968	5.310597	-2.112455
O	-4.310908	3.809624	-1.211488
H	-4.098113	3.587664	-2.134911
O	-6.124957	-2.028659	-1.215607
H	-5.603460	-1.817595	-2.012584
O	-1.239781	-5.483315	-1.145992
H	-1.108698	-5.106452	-2.035121
O	4.176080	-3.746141	-1.161545
H	3.797078	-3.434419	-2.002878
O	6.124957	2.028659	1.215607
H	5.603460	1.817595	2.012584
O	1.239781	5.483315	1.145992
H	1.108698	5.106452	2.035121
O	-4.176080	3.746141	1.161545
H	-3.797078	3.434419	2.002878
O	-6.100136	-2.069615	1.229316
H	-5.576170	-1.895220	2.033804
O	-1.282077	-5.556424	1.171955
H	-1.214968	-5.310597	2.112455
O	4.310908	-3.809624	1.211488
H	4.098113	-3.587664	2.134911
S	5.761067	-1.051935	-1.899343
S	3.930334	4.158463	-1.812939
S	-1.684972	5.587389	-1.915405
S	-5.860247	1.063112	-1.840460
S	-3.830096	-4.023339	-1.812313
S	1.681657	-5.452328	-1.818047
S	5.860247	-1.063112	1.840460
S	3.830096	4.023339	1.812313
S	-1.681657	5.452328	1.818047
S	-5.761067	1.051935	1.899343
S	-3.930334	-4.158463	1.812939
S	1.684972	-5.587389	1.915405
C	3.141917	-0.016849	0.065561
C	-3.141917	0.016849	-0.065561
C	-1.763369	-0.500978	-0.191234
C	1.763369	0.500978	0.191234
C	0.668627	-0.247097	-0.077472
C	-0.668627	0.247097	0.077472
H	-1.674294	-1.545176	-0.505148
H	1.674294	1.545176	0.505148
H	-0.779002	1.275348	0.425384
H	0.779002	-1.275348	-0.425384
O	4.081197	0.838812	0.025771
O	3.331986	-1.288950	0.021589

O	-3.331986	1.288950	-0.021589
O	-4.081197	-0.838812	-0.025771
O	1.622088	-3.137161	0.272589
H	1.385651	-3.226326	1.217087
H	2.266080	-2.339847	0.214331
O	-1.622088	3.137161	-0.272589
H	-1.385651	3.226326	-1.217087
H	-2.266080	2.339847	-0.214331

(Terephthalate)$^{2-}$@[$Mo_{12}O_{12}S_{12}(OH)_{12}$] (Planar conformation; D_{2h} symmetry, Figure 7f)

76 atoms; Bond energy: -522.2069 eV

Mo	5.860659	1.411031	0.000000
Mo	4.246612	4.486844	0.000000
Mo	1.754005	5.860540	0.000000
Mo	-1.754005	5.860540	0.000000
Mo	-4.246612	4.486844	0.000000
Mo	-5.860659	1.411031	0.000000
Mo	-5.860659	-1.411031	0.000000
Mo	-4.246612	-4.486844	0.000000
Mo	-1.754005	-5.860540	0.000000
Mo	1.754005	-5.860540	0.000000
Mo	4.246612	-4.486844	0.000000
Mo	5.860659	-1.411031	0.000000
O	7.501605	1.897782	0.000000
O	5.345275	5.781906	0.000000
O	2.220474	7.495445	0.000000
O	-2.220474	7.495445	0.000000
O	-5.345275	5.781906	0.000000
O	-7.501605	1.897782	0.000000
O	-7.501605	-1.897782	0.000000
O	-5.345275	-5.781906	0.000000
O	-2.220474	-7.495445	0.000000
O	2.220474	-7.495445	0.000000
O	5.345275	-5.781906	0.000000
O	7.501605	-1.897782	0.000000
O	5.122411	3.040139	-1.227226
H	4.577094	2.736449	-1.975840
O	0.000000	5.734054	-1.179294
H	0.000000	5.298542	-2.050741
O	-5.122411	3.040139	-1.227226
H	-4.577094	2.736449	-1.975840
O	-5.122411	-3.040139	-1.227226
H	-4.577094	-2.736449	-1.975840
O	0.000000	-5.734054	-1.179294
H	0.000000	-5.298542	-2.050741
O	5.122411	-3.040139	-1.227226
H	4.577094	-2.736449	-1.975840
O	5.122411	3.040139	1.227226
H	4.577094	2.736449	1.975840
O	0.000000	5.734054	1.179294
H	0.000000	5.298542	2.050741
O	-5.122411	3.040139	1.227226
H	-4.577094	2.736449	1.975840
O	-5.122411	-3.040139	1.227226
H	-4.577094	-2.736449	1.975840
O	0.000000	-5.734054	1.179294
H	0.000000	-5.298542	2.050741

O	5.122411	-3.040139	1.227226
H	4.577094	-2.736449	1.975840
S	5.757326	0.000000	-1.881604
S	2.789636	4.825299	-1.820324
S	-2.789636	4.825299	-1.820324
S	-5.757326	0.000000	-1.881604
S	-2.789636	-4.825299	-1.820324
S	2.789636	-4.825299	-1.820324
S	5.757326	0.000000	1.881604
S	2.789636	4.825299	1.820324
S	-2.789636	4.825299	1.820324
S	-5.757326	0.000000	1.881604
S	-2.789636	-4.825299	1.820324
S	2.789636	-4.825299	1.820324
C	1.407948	0.000000	0.000000
C	-1.407948	0.000000	0.000000
C	0.696157	1.208599	0.000000
C	0.696157	-1.208599	0.000000
C	-0.696157	1.208599	0.000000
C	-0.696157	-1.208599	0.000000
H	1.258786	2.140433	0.000000
H	1.258786	-2.140433	0.000000
H	-1.258786	2.140433	0.000000
H	-1.258786	-2.140433	0.000000
C	2.914487	0.000000	0.000000
C	-2.914487	0.000000	0.000000
O	3.500160	1.135132	0.000000
O	3.500160	-1.135132	0.000000
O	-3.500160	1.135132	0.000000
O	-3.500160	-1.135132	0.000000

(Terephthalate)$^{2-}$@[$Mo_{12}O_{12}S_{12}(OH)_{12}$] (Perpendicular conformation; D_{2h} symmetry, Figure 7g)

76 atoms; Bond energy: -521.7970 eV

Mo	5.863605	1.413948	0.000000
Mo	4.240942	4.487625	0.000000
Mo	1.750326	5.863197	0.000000
Mo	-1.750326	5.863197	0.000000
Mo	-4.240942	4.487625	0.000000
Mo	-5.863605	1.413948	0.000000
Mo	-5.863605	-1.413948	0.000000
Mo	-4.240942	-4.487625	0.000000
Mo	-1.750326	-5.863197	0.000000
Mo	1.750326	-5.863197	0.000000
Mo	4.240942	-4.487625	0.000000
Mo	5.863605	-1.413948	0.000000
O	7.504002	1.899601	0.000000
O	5.347228	5.776978	0.000000
O	2.212700	7.499720	0.000000
O	-2.212700	7.499720	0.000000
O	-5.347228	5.776978	0.000000
O	-7.504002	1.899601	0.000000
O	-7.504002	-1.899601	0.000000
O	-5.347228	-5.776978	0.000000
O	-2.212700	-7.499720	0.000000
O	2.212700	-7.499720	0.000000

O	5.347228	-5.776978	0.000000
O	7.504002	-1.899601	0.000000
O	5.117976	3.035458	-1.226383
H	4.569957	2.733325	-1.973407
O	0.000000	5.748910	-1.185156
H	0.000000	5.270527	-2.033535
O	-5.117976	3.035458	-1.226383
H	-4.569957	2.733325	-1.973407
O	-5.117976	-3.035458	-1.226383
H	-4.569957	-2.733325	-1.973407
O	0.000000	-5.748910	-1.185156
H	0.000000	-5.270527	-2.033535
O	5.117976	-3.035458	-1.226383
H	4.569957	-2.733325	-1.973407
O	5.117976	3.035458	1.226383
H	4.569957	2.733325	1.973407
O	0.000000	5.748910	1.185156
H	0.000000	5.270527	2.033535
O	-5.117976	3.035458	1.226383
H	-4.569957	2.733325	1.973407
O	-5.117976	-3.035458	1.226383
H	-4.569957	-2.733325	1.973407
O	0.000000	-5.748910	1.185156
H	0.000000	-5.270527	2.033535
O	5.117976	-3.035458	1.226383
H	4.569957	-2.733325	1.973407
S	5.754612	0.000000	-1.881229
S	2.793196	4.839166	-1.823164
S	-2.793196	4.839166	-1.823164
S	-5.754612	0.000000	-1.881229
S	-2.793196	-4.839166	-1.823164
S	2.793196	-4.839166	-1.823164
S	5.754612	0.000000	1.881229
S	2.793196	4.839166	1.823164
S	-2.793196	4.839166	1.823164
S	-5.754612	0.000000	1.881229
S	-2.793196	-4.839166	1.823164
S	2.793196	-4.839166	1.823164
C	1.407404	0.000000	0.000000
C	-1.407404	0.000000	0.000000
C	0.697792	0.000000	1.206758
C	0.697792	0.000000	-1.206758
C	-0.697792	0.000000	1.206758
C	-0.697792	0.000000	-1.206758
H	1.242596	0.000000	2.152400
H	1.242596	0.000000	-2.152400
H	-1.242596	0.000000	2.152400
H	-1.242596	0.000000	-2.152400
C	2.917760	0.000000	0.000000
C	-2.917760	0.000000	0.000000
O	3.493709	1.135285	0.000000
O	3.493709	-1.135285	0.000000
O	-3.493709	1.135285	0.000000
O	-3.493709	-1.135285	0.000000

$(TMT)^{2-}$@$[Mo_{12}O_{12}S_{12}(OH)_{12}]$ (Perpendicular conformation; D_{2h} symmetry, Figure 7h) TMT = Tetramethylterephthalate

88 atoms; Bond energy: -586.9353 eV

Mo	5.860651	1.414890	0.000000
Mo	4.241838	4.494311	0.000000
Mo	1.754260	5.874083	0.000000
Mo	-1.754260	5.874083	0.000000
Mo	-4.241838	4.494311	0.000000
Mo	-5.860651	1.414890	0.000000
Mo	-5.860651	-1.414890	0.000000
Mo	-4.241838	-4.494311	0.000000
Mo	-1.754260	-5.874083	0.000000
Mo	1.754260	-5.874083	0.000000
Mo	4.241838	-4.494311	0.000000
Mo	5.860651	-1.414890	0.000000
O	7.499436	1.906468	0.000000
O	5.347381	5.783881	0.000000
O	2.221760	7.508693	0.000000
O	-2.221760	7.508693	0.000000
O	-5.347381	5.783881	0.000000
O	-7.499436	1.906468	0.000000
O	-7.499436	-1.906468	0.000000
O	-5.347381	-5.783881	0.000000
O	-2.221760	-7.508693	0.000000
O	2.221760	-7.508693	0.000000
O	5.347381	-5.783881	0.000000
O	7.499436	-1.906468	0.000000
O	5.115859	3.040209	-1.224711
H	4.566734	2.735697	-1.970731
O	0.000000	5.756728	-1.180541
H	0.000000	5.281824	-2.032034
O	-5.115859	3.040209	-1.224711
H	-4.566734	2.735697	-1.970731
O	-5.115859	-3.040209	-1.224711
H	-4.566734	-2.735697	-1.970731
O	0.000000	-5.756728	-1.180541
H	0.000000	-5.281824	-2.032034
O	5.115859	-3.040209	-1.224711
H	4.566734	-2.735697	-1.970731
O	5.115859	3.040209	1.224711
H	4.566734	2.735697	1.970731
O	0.000000	5.756728	1.180541
H	0.000000	5.281824	2.032034
O	-5.115859	3.040209	1.224711
H	-4.566734	2.735697	1.970731
O	-5.115859	-3.040209	1.224711
H	-4.566734	-2.735697	1.970731
O	0.000000	-5.756728	1.180541
H	0.000000	-5.281824	2.032034
O	5.115859	-3.040209	1.224711
H	4.566734	-2.735697	1.970731
S	5.762371	0.000000	-1.883369
S	2.796020	4.851535	-1.820628
S	-2.796020	4.851535	-1.820628
S	-5.762371	0.000000	-1.883369
S	-2.796020	-4.851535	-1.820628
S	2.796020	-4.851535	-1.820628
S	5.762371	0.000000	1.883369
S	2.796020	4.851535	1.820628
S	-2.796020	4.851535	1.820628
S	-5.762371	0.000000	1.883369
S	-2.796020	-4.851535	1.820628
S	2.796020	-4.851535	1.820628

C	1.393922	0.000000	0.000000
C	-1.393922	0.000000	0.000000
C	0.706134	0.000000	1.227750
C	0.706134	0.000000	-1.227750
C	-0.706134	0.000000	1.227750
C	-0.706134	0.000000	-1.227750
C	1.460012	0.000000	2.542527
C	1.460012	0.000000	-2.542527
C	-1.460012	0.000000	2.542527
C	-1.460012	0.000000	-2.542527
H	1.203457	0.886239	3.148638
H	1.203457	-0.886239	3.148638
H	2.548363	0.000000	2.391608
H	1.203457	0.886239	-3.148638
H	1.203457	-0.886239	-3.148638
H	2.548363	0.000000	-2.391608
H	-1.203457	0.886239	3.148638
H	-1.203457	-0.886239	3.148638
H	-2.548363	0.000000	2.391608
H	-1.203457	0.886239	-3.148638
H	-1.203457	-0.886239	-3.148638
H	-2.548363	0.000000	-2.391608
C	2.919949	0.000000	0.000000
C	-2.919949	0.000000	0.000000
O	3.503237	1.134475	0.000000
O	3.503237	-1.134475	0.000000
O	-3.503237	1.134475	0.000000
O	-3.503237	-1.134475	0.000000

$(TMT,2H_2O)^{2-}@[Mo_{12}O_{12}S_{12}(OH)_{12}]$ (cis form; C_1 symmetry, Figure 7i)

94 atoms; Bond energy: -615.5205 eV

Mo	5.847821	-2.079211	-0.057237
Mo	3.987269	-4.241328	-0.009316
Mo	0.852752	-5.881917	0.047775
Mo	-1.991154	-6.294984	0.021356
Mo	-5.016061	-4.675849	0.019346
Mo	-6.068469	-2.020995	-0.035165
Mo	-5.737687	1.452224	-0.047896
Mo	-4.587767	4.041343	-0.022329
Mo	-1.584766	5.699566	0.033402
Mo	1.243159	5.404161	0.060151
Mo	4.288767	3.670980	0.024501
Mo	5.918227	1.339450	-0.045470
S	4.881690	-3.081901	1.841876
S	4.769906	-3.066249	-1.901923
S	-0.629224	-5.885383	1.906520
S	-0.595681	-5.803807	-1.808898
S	-5.251159	-3.194088	1.826595
S	-5.142341	-3.231670	-1.836754
S	-5.095527	2.697667	1.846874
S	-5.028378	2.704790	-1.916099
S	-0.217195	5.094335	1.859123
S	-0.172938	5.184347	-1.785370
S	4.853055	2.307128	1.828220
S	4.736726	2.322726	-1.831411
O	7.409683	-2.763780	-0.114564
O	4.951314	-5.648123	-0.046563

O	1.423617	-7.483632	0.032445
O	-2.110181	-7.990498	0.006010
O	-6.434785	-5.609693	0.008958
O	-7.742874	-2.298918	-0.085420
O	-7.423920	1.722254	-0.088785
O	-5.880764	5.161086	-0.034986
O	-1.682700	7.393968	0.065441
O	1.745985	7.026620	0.119614
O	5.454314	4.905507	0.060352
O	7.464546	2.033250	-0.118106
O	6.267719	-0.353400	1.165516
H	5.737615	-0.363660	1.984441
O	6.185362	-0.342905	-1.288695
H	5.605966	-0.348616	-2.073173
O	2.375989	-4.947680	1.225838
H	2.508569	-5.142545	2.170306
O	2.302586	-4.914706	-1.151339
H	2.052590	-4.456503	-1.972420
O	-3.653896	-5.732436	1.246542
H	-3.393421	-5.246045	2.051990
O	-3.706894	-5.847859	-1.178940
H	-3.514170	-5.487568	-2.063929
O	-5.830759	-0.331117	1.180688
H	-5.201233	-0.396267	1.924991
O	-5.761706	-0.341059	-1.252420
H	-5.128448	-0.405606	-1.993879
O	-3.217283	5.146112	1.236444
H	-2.970105	4.620909	2.020073
O	-3.184189	5.177539	-1.225617
H	-2.916945	4.671852	-2.015599
O	2.657057	4.313550	1.207457
H	2.457748	3.936971	2.083439
O	2.695218	4.439026	-1.149370
H	2.463076	4.048676	-2.011276
O	0.175779	-3.399405	0.391561
H	1.037229	-2.859579	0.204653
H	0.152787	-3.508934	1.362580
O	-2.354398	-3.622750	-0.125193
H	-1.400597	-3.340984	0.035116
H	-2.566561	-3.286803	-1.018987
O	3.844052	-0.617126	0.004060
O	2.432008	-2.358704	0.015565
O	-3.438591	0.772231	-0.004542
O	-2.539886	2.855193	-0.005539
C	2.674693	-1.095586	0.009492
C	1.439866	-0.219959	0.004600
C	0.842578	0.117509	1.234423
C	0.830141	0.081151	-1.228938
C	-0.429372	0.729477	1.230632
C	-0.438086	0.700078	-1.230159
C	-1.060855	0.986146	-0.000585
C	-2.457337	1.579679	-0.003174
C	1.530605	-0.196408	2.547932
C	1.501302	-0.272041	-2.540909
H	2.464223	-0.757059	2.401854
H	2.439726	-0.823634	-2.390426
H	1.782113	0.729541	3.093589
H	1.738973	0.637106	-3.119982
H	0.878171	-0.788668	3.211857
H	0.842865	-0.890795	-3.174017
C	-1.105269	1.079912	2.540471

C	-1.115730	1.034114	-2.544136
H	-2.117147	1.478615	2.384899
H	-2.124688	1.442363	-2.393469
H	-1.186675	0.196933	3.197122
H	-1.201994	0.143523	-3.189984
H	-0.526535	1.841760	3.091395
H	-0.532574	1.783716	-3.107327

$(TMT,2H_2O)^{2-}@[Mo_{12}O_{12}S_{12}(OH)_{12}]$ (trans form; C_1 symmetry, Figure 7j)

94 atoms; Bond energy: -615.6294 eV

Mo	-2.194942	-0.050143	-6.067646
Mo	0.626764	-0.073467	-5.672293
Mo	3.683189	-0.097142	-3.914669
Mo	5.576689	-0.079024	-1.766571
Mo	-6.268481	0.010207	-1.734748
Mo	-5.161112	-0.022573	-4.353296
Mo	-2.194942	-0.050143	6.067646
Mo	0.626764	-0.073467	5.672293
Mo	3.683189	-0.097142	3.914669
Mo	5.576689	-0.079024	1.766571
Mo	-6.268481	0.010207	1.734748
Mo	-5.161112	-0.022573	4.353296
S	-0.821988	-1.936534	-5.730696
S	-0.794378	1.815160	-5.745167
S	4.453788	-1.948613	-2.633697
S	4.498678	1.767781	-2.713015
S	-5.370923	-1.829649	-2.854596
S	-5.371469	1.825373	-2.902262
S	-0.821988	-1.936534	5.730696
S	-0.794378	1.815160	5.745167
S	4.453788	-1.948613	2.633697
S	4.498678	1.767781	2.713015
S	-5.370923	-1.829649	2.854596
S	-5.371469	1.825373	2.902262
O	-2.449803	-0.058531	-7.756083
O	1.263133	-0.077281	-7.253632
O	4.738955	-0.149061	-5.249373
O	7.133917	-0.099331	-2.450675
O	-7.943698	0.000376	-2.020414
O	-6.587390	-0.041868	-5.273402
O	-2.449803	-0.058531	7.756083
O	1.263133	-0.077281	7.253632
O	4.738955	-0.149061	5.249373
O	7.133917	-0.099331	2.450675
O	-7.943698	0.000376	2.020414
O	-6.587390	-0.041868	5.273402
O	-3.884075	-1.263191	-5.478760
H	-3.593801	-2.061674	-4.999594
O	-3.875502	1.189548	-5.504312
H	-3.581984	1.996261	-5.040871
O	2.110347	-1.283332	-4.717148
H	1.929029	-2.199595	-4.446995
O	2.134148	1.116919	-4.698874
H	1.869443	1.931168	-4.235747
O	-3.884075	-1.263191	5.478760
H	-3.593801	-2.061674	4.999594

O	-3.875502	1.189548	5.504312
H	-3.581984	1.996261	5.040871
O	2.110347	-1.283332	4.717148
H	1.929029	-2.199595	4.446995
O	2.134148	1.116919	4.698874
H	1.869443	1.931168	4.235747
O	5.721004	-1.249739	0.000000
H	5.281666	-2.120577	0.000000
O	5.627286	1.104254	0.000000
H	5.089409	1.920059	0.000000
O	-6.005700	-1.159133	0.000000
H	-5.603417	-2.045558	0.000000
O	-6.014275	1.193856	0.000000
H	-5.602118	2.075787	0.000000
O	2.090423	-0.109260	-2.003706
H	1.158999	-0.098199	-2.406920
H	2.207778	-1.008804	-1.645220
O	2.090423	-0.109260	2.003706
H	1.158999	-0.098199	2.406920
H	2.207778	-1.008804	1.645220
O	-2.346428	-0.031429	-3.639193
O	-0.119914	-0.041160	-3.328355
O	-2.346428	-0.031429	3.639193
O	-0.119914	-0.041160	3.328355
C	-1.324595	-0.034277	-2.891684
C	-1.478066	-0.031949	-1.385887
C	-1.522578	-1.263832	-0.705670
C	-1.461254	1.199552	-0.705342
C	-1.540116	-2.574724	-1.465941
C	-1.396502	2.510341	-1.461374
H	-1.432302	-2.424744	-2.549292
H	-1.369321	2.359081	-2.549325
H	-2.486791	-3.117126	-1.298721
H	-2.270559	3.144012	-1.233147
H	-0.726533	-3.242179	-1.133675
H	-0.498171	3.084684	-1.176993
C	-1.324595	-0.034277	2.891684
C	-1.478066	-0.031949	1.385887
C	-1.522578	-1.263832	0.705670
C	-1.461254	1.199552	0.705342
C	-1.540116	-2.574724	1.465941
C	-1.396502	2.510341	1.461374
H	-1.432302	-2.424744	2.549292
H	-1.369321	2.359081	2.549325
H	-2.486791	-3.117126	1.298721
H	-2.270559	3.144012	1.233147
H	-0.726533	-3.242179	1.133675
H	-0.498171	3.084684	1.176993

$(TMT,3H_2O)^{2-}$@$[Mo_{12}O_{12}S_{12}(OH)_{12}]$ (C_s symmetry, Figure 7k)

97 atoms; Bond energy: -630.2830 eV

Mo	-2.190713	-0.036329	-6.078034
Mo	0.634425	-0.092388	-5.690648
Mo	3.726993	-0.128578	-3.979270
Mo	5.528267	-0.045058	-1.743125
Mo	-6.267608	0.008110	-1.736598

Mo	-5.154892	-0.011369	-4.354165
Mo	-2.190713	-0.036329	6.078034
Mo	0.634425	-0.092388	5.690648
Mo	3.726993	-0.128578	3.979270
Mo	5.528267	-0.045058	1.743125
Mo	-6.267608	0.008110	1.736598
Mo	-5.154892	-0.011369	4.354165
S	-0.837644	-1.936803	-5.754731
S	-0.766859	1.809298	-5.749792
S	4.447944	-1.938341	-2.612326
S	4.497968	1.765283	-2.832409
S	-5.361228	-1.824621	-2.862134
S	-5.369077	1.828548	-2.894067
S	-0.837644	-1.936803	5.754731
S	-0.766859	1.809298	5.749792
S	4.447944	-1.938341	2.612326
S	4.497968	1.765283	2.832409
S	-5.361228	-1.824621	2.862134
S	-5.369077	1.828548	2.894067
O	-2.449850	-0.029214	-7.765456
O	1.269793	-0.107709	-7.272349
O	4.787310	-0.236221	-5.305091
O	7.126661	-0.002807	-2.328138
O	-7.941144	-0.001479	-2.030110
O	-6.580821	-0.025168	-5.274705
O	-2.449850	-0.029214	7.765456
O	1.269793	-0.107709	7.272349
O	4.787310	-0.236221	5.305091
O	7.126661	-0.002807	2.328138
O	-7.941144	-0.001479	2.030110
O	-6.580821	-0.025168	5.274705
O	-3.882505	-1.245188	-5.491959
H	-3.594734	-2.051802	-5.024979
O	-3.863801	1.206753	-5.495097
H	-3.567904	2.007639	-5.023268
O	2.093043	-1.293368	-4.687672
H	2.036977	-2.262635	-4.629329
O	2.159807	1.075860	-4.731785
H	1.960992	1.939261	-4.327956
O	-3.882505	-1.245188	5.491959
H	-3.594734	-2.051802	5.024979
O	-3.863801	1.206753	5.495097
H	-3.567904	2.007639	5.023268
O	2.093043	-1.293368	4.687672
H	2.036977	-2.262635	4.629329
O	2.159807	1.075860	4.731785
H	1.960992	1.939261	4.327956
O	5.807844	-1.247762	0.000000
H	5.396032	-2.130986	0.000000
O	5.184458	1.071653	0.000000
H	4.264834	1.553891	0.000000
O	-6.012180	-1.164756	0.000000
H	-5.599305	-2.046172	0.000000
O	-6.023728	1.189408	0.000000
H	-5.627267	2.078379	0.000000
O	2.044867	-0.052969	-1.983279
H	1.122264	-0.085593	-2.430008
H	2.211461	-0.957330	-1.652282
O	2.044867	-0.052969	1.983279
H	1.122264	-0.085593	2.430008
H	2.211461	-0.957330	1.652282

O	2.691390	1.846707	0.000000
H	2.397678	1.292199	-0.770534
H	2.397678	1.292199	0.770534
O	-2.337868	-0.023049	-3.642112
O	-0.113365	-0.070434	-3.336013
O	-2.337868	-0.023049	3.642112
O	-0.113365	-0.070434	3.336013
C	-1.317273	-0.046970	-2.894340
C	-1.470408	-0.047167	-1.387031
C	-1.516672	-1.279226	-0.705924
C	-1.455105	1.184351	-0.705818
C	-1.536724	-2.590302	-1.466241
C	-1.392355	2.496021	-1.460238
H	-1.424701	-2.440734	-2.549406
H	-1.349244	2.345346	-2.547824
H	-2.486140	-3.129197	-1.301626
H	-2.276866	3.119392	-1.244009
H	-0.726202	-3.260396	-1.131684
H	-0.504289	3.078776	-1.162238
C	-1.317273	-0.046970	2.894340
C	-1.470408	-0.047167	1.387031
C	-1.516672	-1.279226	0.705924
C	-1.455105	1.184351	0.705818
C	-1.536724	-2.590302	1.466241
C	-1.392355	2.496021	1.460238
H	-1.424701	-2.440734	2.549406
H	-1.349244	2.345346	2.547824
H	-2.486140	-3.129197	1.301626
H	-2.276866	3.119392	1.244009
H	-0.726202	-3.260396	1.131684
H	-0.504289	3.078776	1.162238

(Trimesate)$^{3-}$@[$Mo_{12}O_{12}S_{12}(OH)_{12}$] ($C_{2v}$ symmetry, Figure 7l)

78 atoms; Bond energy: -541.5208 eV

Mo	0.000000	-4.526386	4.255202
Mo	0.000000	4.352134	-4.151422
Mo	0.000000	-1.416379	5.827200
Mo	0.000000	1.427297	-6.042641
Mo	0.000000	1.416379	5.827200
Mo	0.000000	-1.427297	-6.042641
Mo	0.000000	4.526386	4.255202
Mo	0.000000	-4.352134	-4.151422
Mo	0.000000	5.957021	1.782809
Mo	0.000000	-5.766605	-1.696637
Mo	0.000000	-5.957021	1.782809
Mo	0.000000	5.766605	-1.696637
S	-1.820594	-4.885304	2.812645
S	1.882108	4.977406	-2.876639
S	1.820594	-4.885304	2.812645
S	-1.882108	4.977406	-2.876639
S	-1.882166	0.000000	5.733246
S	1.819904	0.000000	-5.623146
S	1.882166	0.000000	5.733246
S	-1.819904	0.000000	-5.623146
S	1.820594	4.885304	2.812645
S	-1.882108	-4.977406	-2.876639
S	-1.820594	4.885304	2.812645
S	1.882108	-4.977406	-2.876639

O	0.000000	-5.789809	5.397324
O	0.000000	5.528197	-5.399488
O	0.000000	-1.909752	7.469629
O	0.000000	1.774310	-7.709894
O	0.000000	1.909752	7.469629
O	0.000000	-1.774310	-7.709894
O	0.000000	5.789809	5.397324
O	0.000000	-5.528197	-5.399488
O	0.000000	7.576869	2.309041
O	0.000000	-7.435617	-2.091214
O	0.000000	-7.576869	2.309041
O	0.000000	7.435617	-2.091214
O	1.229036	-3.040727	5.089375
H	1.951020	-2.736596	4.509076
O	-1.230299	2.900298	-5.186982
H	-1.951849	2.553562	-4.630509
O	-1.229036	-3.040727	5.089375
H	-1.951020	-2.736596	4.509076
O	1.230299	2.900298	-5.186982
H	1.951849	2.553562	-4.630509
O	1.229036	3.040727	5.089375
H	1.951020	2.736596	4.509076
O	-1.230299	-2.900298	-5.186982
H	-1.951849	-2.553562	-4.630509
O	-1.229036	3.040727	5.089375
H	-1.951020	2.736596	4.509076
O	1.230299	-2.900298	-5.186982
H	1.951849	-2.553562	-4.630509
O	1.229256	-5.939583	0.079244
H	1.952034	-5.285873	0.105673
O	-1.229256	5.939583	0.079244
H	-1.952034	5.285873	0.105673
O	-1.229256	-5.939583	0.079244
H	-1.952034	-5.285873	0.105673
O	1.229256	5.939583	0.079244
H	1.952034	5.285873	0.105673
O	0.000000	2.460979	-2.737538
O	0.000000	-1.134522	3.484449
O	0.000000	1.134522	3.484449
O	0.000000	-2.460979	-2.737538
O	0.000000	-3.593389	-0.771313
O	0.000000	3.593389	-0.771313
C	0.000000	-1.208199	0.688307
H	0.000000	-2.149597	1.231601
C	0.000000	1.215635	-0.711047
C	0.000000	0.000000	1.394325
C	0.000000	0.000000	-1.404627
H	0.000000	0.000000	-2.491538
C	0.000000	-1.215635	-0.711047
C	0.000000	1.208199	0.688307
H	0.000000	2.149597	1.231601
C	0.000000	2.519648	-1.462086
C	0.000000	0.000000	2.898778
C	0.000000	-2.519648	-1.462086