Supplementary Material (ESI) for Dalton Transactions

Metastable states associated with a change in the metal-metal bonding network of $(Mo^{V})_6$ polyoxoanions: a DFT study of $[(Mo_2{}^{V}O_4)_3(\mu_6\text{-}CO_3)(\mu\text{-}CO_3)_3(\mu\text{-}OH)_3]^{5-}$.

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SUPPORTING INFORMATION

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$[(Mo_2^{V}O_4)_3(\mu_6\text{-}CO_3)(\mu\text{-}CO_3)_3(\mu\text{-}OH)_3]^{5-}$

Bond energies and Cartesian coordinates of the four energy minima.

1. Global minimum: E = -291.67485eV

Mo	2.5857	0.9253	-1.8540
Mo	-2.8955	0.9269	-1.3143
Mo	0.3123	0.9295	3.1670
Mo	0.3123	0.9295	-3.1670
Mo	-2.8955	0.9269	1.3143
Mo	2.5857	0.9253	1.8540
C	0.0036	0.0926	0.0
O	1.3080	0.0803	0.0
O	-0.6496	0.0918	-1.1305
O	-0.6496	0.0918	1.1305
C	4.4713	-0.8694	0.0
C	-2.2341	-0.8682	-3.8744
C	-2.2341	-0.8682	3.8744
O	3.8732	-0.5722	-1.1450
O	-2.9233	-0.5742	-2.7808
O	-0.9441	-0.5700	3.9290
O	5.5718	-1.5013	0.0
O	-2.7874	-1.4972	-4.8263
O	-2.7874	-1.4972	4.8263
O	3.8732	-0.5722	1.1450
O	-0.9441	-0.5700	-3.9290
O	-2.9233	-0.5742	2.7808
O	1.0690	2.1972	-1.8555
O	-2.1412	2.1979	0.0
O	1.0690	2.1972	1.8555
O	1.6468	-0.4903	-2.8551
O	-3.2847	-0.4910	0.0
O	1.6468	-0.4903	2.8551
O	3.0750	1.9690	0.0
O	-1.5402	1.9867	-2.6667
O	-1.5402	1.9867	2.6667
O	3.7554	1.6626	-2.9265
O	-4.4133	1.6545	-1.7902
O	0.6524	1.6672	4.7170
O	0.6524	1.6672	-4.7170
O	-4.4133	1.6545	1.7902
O	3.7554	1.6626	2.9265
H	2.3215	2.5950	0.0
H	-1.1575	2.6021	-2.0028
H	-1.1575	2.6021	2.0028

2. Local minimum, standard isomer: E = -289.55539eV

Mo	2.7602	1.0157	-1.6470
Mo	-2.8087	1.0163	-1.5667
Mo	0.0473	1.0149	3.2139
Mo	0.0473	1.0149	-3.2139
Mo	-2.8087	1.0163	1.5667
Mo	2.7602	1.0157	1.6470
C	-0.0006	0.1544	0.0
O	1.3027	0.1387	0.0
O	-0.6523	0.1390	-1.1286
O	-0.6523	0.1390	1.1286
C	4.2821	-1.2203	0.0
C	-2.1420	-1.2183	-3.7090
C	-2.1420	-1.2183	3.7090
O	3.8054	-0.7362	-1.1398
O	-2.8900	-0.7349	-2.7251
O	-0.9160	-0.7357	3.8653
O	5.1569	-2.1308	0.0
O	-2.5807	-2.1272	-4.4677
O	-2.5807	-2.1272	4.4677
O	3.8054	-0.7362	1.1398
O	-0.9160	-0.7357	-3.8653
O	-2.8900	-0.7349	2.7251
O	1.1605	2.1606	-2.0099
O	-2.3228	2.1611	0.0
O	1.1605	2.1606	2.0099
O	1.7101	-0.0177	-2.9606
O	-3.4204	-0.0166	0.0
O	1.7101	-0.0177	2.9606
O	2.7876	2.3347	0.0
O	-1.3950	2.3334	-2.4153
O	-1.3950	2.3334	2.4153
O	4.1086	1.7627	-2.4791
O	-4.2028	1.7643	-2.3188
O	0.0935	1.7622	4.7977
O	0.0935	1.7622	-4.7977
O	-4.2028	1.7643	2.3188
O	4.1086	1.7627	2.4791
H	-0.9419	2.7195	-1.6292
H	1.8797	2.7200	0.0
H	-0.9419	2.7195	1.6292

3. Isomer resulting from a concerted transfer of the six protons
Local minimum, E = -289.61178eV

Mo	2.6440	0.9399	-1.7613
Mo	-2.8460	0.9427	-1.4098
Mo	0.2029	0.9394	3.1717
Mo	0.2029	0.9394	-3.1717
Mo	-2.8460	0.9427	1.4098
Mo	2.6440	0.9399	1.7613
C	0.0	0.0776	0.0
O	1.2929	0.1056	0.0
O	-0.6464	0.1118	-1.1194
O	-0.6464	0.1118	1.1194
O	4.4472	-0.9195	0.0
O	-2.2204	-0.9281	-3.8450
O	-2.2204	-0.9281	3.8450
O	3.8276	-0.6687	-1.1505
O	-2.9092	-0.6688	-2.7365
O	-0.9151	-0.6724	3.8879
O	5.5708	-1.4983	0.0
O	-2.7799	-1.5197	-4.8115
O	-2.7799	-1.5197	4.8115
O	3.8276	-0.6687	1.1505
O	-0.9151	-0.6724	-3.8879
O	-2.9092	-0.6688	2.7365
O	1.1075	2.4181	-1.9212
O	-2.2122	2.4177	0.0
O	1.1075	2.4181	1.9212
O	1.6111	-0.4199	-2.7914
O	-3.2247	-0.4159	0.0
O	1.6111	-0.4199	2.7914
O	3.1198	1.7329	0.0
O	-1.5611	1.7327	-2.7070
O	-1.5611	1.7327	2.7070
O	3.7593	1.6809	-2.8857
O	-4.3748	1.6886	-1.8138
O	0.6199	1.6819	4.6988
O	0.6199	1.6819	-4.6988
O	-4.3748	1.6886	1.8138
O	3.7593	1.6809	2.8857
H	0.6281	2.6195	-1.0936
H	-1.2572	2.6264	0.0
H	0.6281	2.6195	1.0936

4. Isomer resulting from a concerted transfer of the six protons
Local minimum, E = -290.24305eV

Mo	2.7921	1.0176	-1.5033
Mo	-2.6980	1.0196	-1.6650
Mo	-0.0956	1.0237	3.1669
Mo	-0.0956	1.0237	-3.1669
Mo	-2.6980	1.0196	1.6650
Mo	2.7921	1.0176	1.5033
C	-0.0015	-0.0229	0.0
O	1.2976	-0.0274	0.0
O	-0.6509	-0.0308	-1.1251
O	-0.6509	-0.0308	1.1251
C	4.3160	-1.2410	0.0
C	-2.1578	-1.2321	-3.7468
C	-2.1578	-1.2321	3.7468
O	3.8414	-0.7567	-1.1419
O	-2.9083	-0.7528	-2.7626
O	-0.9326	-0.7433	3.9092
O	5.1841	-2.1556	0.0
O	-2.5900	-2.1456	-4.5010
O	-2.5900	-2.1456	4.5010
O	3.8414	-0.7567	1.1419
O	-0.9326	-0.7433	-3.9092
O	-2.9083	-0.7528	2.7626
O	1.2770	2.3782	-2.2005
O	-2.5656	2.3837	0.0
O	1.2770	2.3782	2.2005
O	1.6371	0.0956	-2.8417
O	-3.2756	0.0920	0.0
O	1.6371	0.0956	2.8417
O	2.5197	2.2545	0.0
O	-1.2547	2.2565	-2.1663
O	-1.2547	2.2565	2.1663
O	4.1824	1.7410	-2.2862
O	-4.0734	1.7347	-2.4814
O	-0.1134	1.7668	4.7532
O	-0.1134	1.7668	-4.7532
O	-4.0734	1.7347	2.4814
O	4.1824	1.7410	2.2862
H	0.8459	2.8203	-1.4421
H	-1.6959	2.8312	0.0
H	0.8459	2.8203	1.4421