Density-functional studies of hydrogen peroxide adsorption and dissociation on MoO_3(100) and $H_{0.33}MoO_3$(100) surfaces.

Supplemental Information

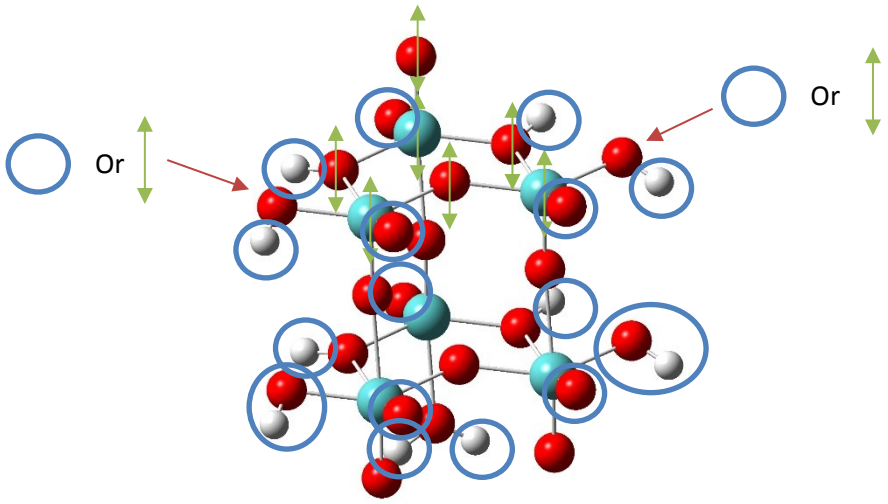
Coordinates and energies for the B3LYP/LanL2DZ + 6-311++G(d,p) optimized geometries and transition states. See Tables 1, 2 and 3 for summaries and Figure 1, 2, 4, 5 and 6 in the text.

Contents

Density-functional studies of hydrogen peroxide adsorption and dissociation on MoO_3(100) and $H_{0.33}MoO_3$(100) surfaces.

SECTION 1

A. Optimization Procedure



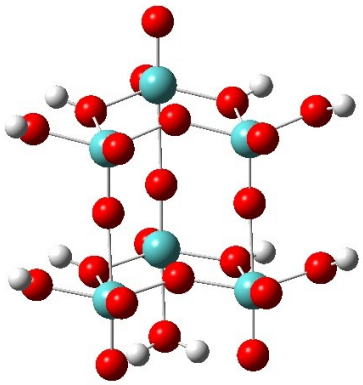
Notations: ◯ atom or group is fully relaxed, ↕ relaxation is allowed only in the vertical direction

Computational procedure details

1. The upper lattice (first layer) Mo and O atoms were allowed to relax in the direction perpendicular to the surface.
2. The lower lattice Mo and O atoms and the lower bridging O atoms, were kept fixed.
3. The lower terminal O and H atoms (including the -OH groups) were allowed to fully relax.
4. Two optimization methods were considered with respect to the terminal –OH groups at the surface: (1) both terminal –H, -O and –OH species were allowed to fully relax, or (2) the O atoms of the terminal –OH groups were allowed to relax only in the vertical direction (perpendicular to the surface), while the remaining atoms had no geometrical constraints. Since the first method resulted in unrealistic positions for the surface O atoms (see text), the structures reported in the paper were optimized using the second method.

SECTION 2

A. $Mo_6O_{23}H_{10}$ Cluster



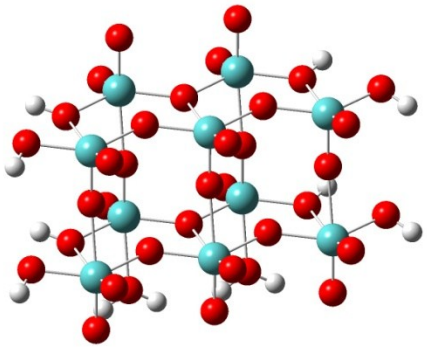
Total B3LYP Energy: -2142.61994446 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	3.47202	0.56329	5.58746
O	1.23364	0.40967	3.71348
O	3.49361	0.59765	1.89105
O	2.83011	2.64679	3.78549
O	1.23364	0.40968	0.01751
Mo	2.87054	0.95327	0.04074
Mo	2.86886	0.95271	3.73669
O	3.50511	0.60147	-1.80713
O	2.82524	2.64712	0.00951
O	-0.47875	-0.21996	-1.86347
Mo	-1.00437	0.16964	-0.00898
O	-0.54415	-0.24006	1.83901
O	-2.64986	-0.37680	-0.03233
O	-1.11651	1.87284	-0.04671
Mo	-1.00437	0.16963	3.68699
O	-0.54073	-0.23268	5.55109
O	-2.64985	-0.37681	3.66364
O	-1.11578	1.87274	3.72372
O	3.87995	-1.16179	0.02877
Mo	4.44443	-1.53381	1.87832
O	-0.21182	-2.02350	-0.02409
O	1.89389	-1.88676	1.84728
O	6.06191	-1.00167	1.90121
O	3.85817	-1.16966	3.72446
O	4.60120	-3.22719	1.87900

Density-functional studies of hydrogen peroxide adsorption and dissociation on MoO_3(100) and $H_{0.33}MoO_3$(100) surfaces.

Atom	Coordinates / Å		
	X	Y	Z
Mo	0.24840	-2.43320	1.82393
O	-1.98961	-2.67323	1.79744
O	-0.21182	-2.02350	3.67191
O	0.42946	-4.12319	1.84283
H	-0.37189	0.52724	6.11836
H	3.54879	1.32388	6.17780
H	-2.41506	-2.29935	1.00443
H	-0.00799	-2.47617	4.49745
H	4.24149	-1.47220	4.55686
H	-2.43244	-2.23428	2.54751
H	3.58537	1.37347	-2.38183
H	-0.31536	0.54765	-2.42192
H	4.31503	-1.40407	-0.79834
H	0.23435	-2.26348	-0.84527

B. $Mo_{10}O_{36}H_{12}$ Cluster

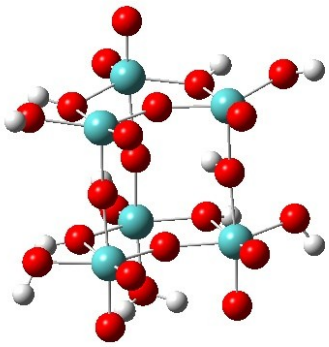


Total B3LYP Energy: -3392.59549584 Hartree

Atom	Coordinates / Å		
	X	Y	Z
Mo	-3.75702	1.53010	-1.45738
O	-5.60935	1.91620	-0.99424
O	-3.70752	-0.12286	-0.93582
O	-1.91441	2.01121	-1.04749
O	-3.77842	1.41553	-3.12431
Mo	-0.06147	1.58435	-1.47072
O	-0.01197	-0.06862	-0.94916
O	1.78115	2.06545	-1.06083
O	-0.08287	1.46977	-3.13765
Mo	3.63411	1.63859	-1.48405
O	3.68361	-0.01437	-0.96250
O	5.47672	2.11969	-1.07416
O	3.61271	1.52402	-3.15099
Mo	3.74373	-2.25510	-0.75622
O	1.89077	-1.82823	-0.33299
O	3.79323	-3.90806	-0.23466
O	5.58635	-1.77399	-0.34633
O	3.72233	-2.36967	-2.42315
Mo	0.04815	-2.30934	-0.74288
O	-1.80478	-1.88247	-0.31965
O	0.09765	-3.96230	-0.22132
O	0.02676	-2.42391	-2.40981
Mo	-3.64740	-2.36358	-0.72955
O	-5.49973	-1.97748	-0.26640
O	-3.59790	-4.01654	-0.20799
O	-3.66879	-2.47815	-2.39648
O	3.64599	2.39850	0.72065
Mo	1.79305	2.82536	1.14388

Atom	Coordinates / Å		
	X	Y	Z
O	3.75562	-1.49534	1.44852
O	1.85318	0.58449	1.35019
O	-0.04956	2.34426	0.73399
O	1.74356	4.47832	0.62232
O	1.81445	2.93993	2.81081
Mo	1.90268	-1.06848	1.87175
Mo	-1.90252	2.77112	1.15722
O	1.96280	-3.30920	2.07802
O	0.06007	-1.54958	1.46185
O	1.92408	-0.95391	3.53868
O	-1.84240	0.53024	1.36352
O	-1.95202	4.42408	0.63566
O	-3.74514	2.29002	0.74732
O	-1.88113	2.88569	2.82415
Mo	-1.79290	-1.12272	1.88508
O	-1.73277	-3.36344	2.09136
O	-3.63551	-1.60382	1.47519
O	-1.77150	-1.00815	3.55201
H	6.07285	1.57029	-1.58835
H	6.18248	-2.32339	-0.86051
H	-6.08299	-2.52658	-0.79545
H	-6.19261	1.36710	-1.52329
H	-0.88887	-3.81931	2.13145
H	1.14454	-3.80895	2.12590
H	-4.42816	-1.21154	1.84859
H	4.54261	-1.08359	1.81281
H	4.43298	2.81025	1.08495
H	-4.53778	2.68230	1.12073
H	-2.55104	-3.86319	2.13924
H	2.80671	-3.76507	2.11811

C. $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze Cluster



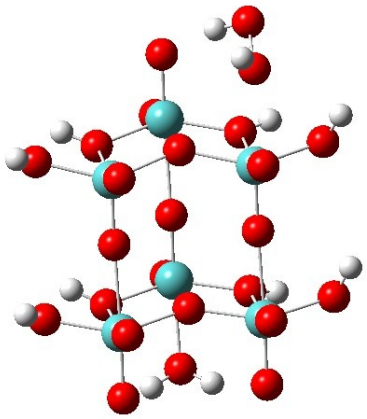
Total B3LYP Energy: -2143.62643222 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.36310	8.26351	5.58070
O	-1.86470	8.01304	3.52094
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.35805	4.08273	5.63378
O	-1.79674	3.99081	3.66175
O	0.08291	5.80887	0.01617
O	0.36332	8.25531	-1.86070
O	-1.86421	8.02318	0.19421
Mo	-0.10311	3.86863	0.00000
Mo	-0.20821	7.81209	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.20832	7.81619	3.72000
O	0.36727	4.09068	-1.90801
O	-1.79789	3.98349	0.03534
O	2.52013	5.86430	1.87546
O	2.41408	9.84349	1.84222
O	4.39611	8.06082	1.86317
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37200	7.92936	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000
O	2.12388	7.76474	-0.00141
Mo	2.69691	8.15127	1.85930
O	2.12348	7.77969	3.72000
O	4.49768	3.81972	1.85407

Atom	Coordinates / Å		
	X	Y	Z
H	2.55691	8.08262	4.52777
H	-0.31867	8.45085	6.24003
H	2.03537	1.70928	2.63720
H	2.04477	1.70398	1.10856
H	2.63847	3.67967	4.55351
H	0.28073	3.25369	6.11964
H	2.55879	8.05255	-0.81358
H	-0.31824	8.44953	-2.51823
H	0.26178	3.27388	-2.40926
H	2.65907	3.74358	-0.84840
H	1.05390	5.88113	3.56160
H	1.02034	5.87716	0.32848

SECTION 3

A. H_2O_2 + $Mo_6O_{23}H_{10}$ "HOOH1" Structure

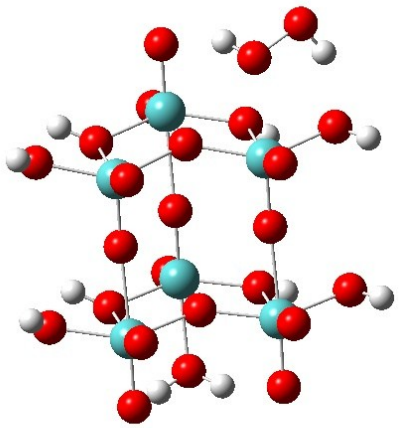


Total B3LYP Energy: -2294.24398027 Hartree BSSE correction: 0.005942359895 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	3.32566	0.51469	5.58534
O	1.23364	0.40967	3.71348
O	3.46476	0.58807	1.89063
O	2.81288	2.65457	3.71873
O	1.23364	0.40968	0.01751
Mo	2.86806	0.95244	0.04070
Mo	2.87722	0.95549	3.73681
O	3.51681	0.60536	-1.80713
O	2.83333	2.64804	0.01315
O	-0.47119	-0.23575	-1.86134
Mo	-1.00437	0.16964	-0.00898
O	-0.54415	-0.24006	1.83901
O	-2.64986	-0.37680	-0.03233
O	-1.11683	1.87205	-0.06325
Mo	-1.00437	0.16963	3.68699
O	-0.60080	-0.17996	5.56271
O	-2.64985	-0.37681	3.66364
O	-1.10572	1.87312	3.63147
O	3.80798	-1.18780	0.02773
Mo	4.32507	-1.57694	1.87658
O	-0.21182	-2.02350	-0.02409
O	1.89389	-1.88676	1.84728
O	5.96041	-1.03686	1.89975
O	3.80305	-1.18958	3.72366
O	4.48914	-3.26706	1.86838

Atom	Coordinates / Å		
	X	Y	Z
Mo	0.24840	-2.43320	1.82393
O	-1.98961	-2.67323	1.79744
O	-0.21182	-2.02350	3.67191
O	0.41669	-4.12409	1.85336
H	0.08721	0.34587	5.98551
H	3.93582	1.12229	6.02450
H	-2.39986	-2.35436	0.97354
H	-0.29192	-2.60069	4.43881
H	4.04575	-1.59681	4.56315
H	-2.43907	-2.17008	2.50392
H	3.60386	1.38007	-2.37677
H	-0.33042	0.52931	-2.42929
H	4.24516	-1.44698	-0.79344
H	0.25814	-2.23035	-0.84166
O	5.31049	1.62570	3.87364
H	5.58604	2.46653	3.47947
O	6.52598	0.85136	3.93130
H	6.43641	0.26172	3.15259

B. H_2O_2 + $Mo_6O_{23}H_{10}$ "HOOH2" Structure

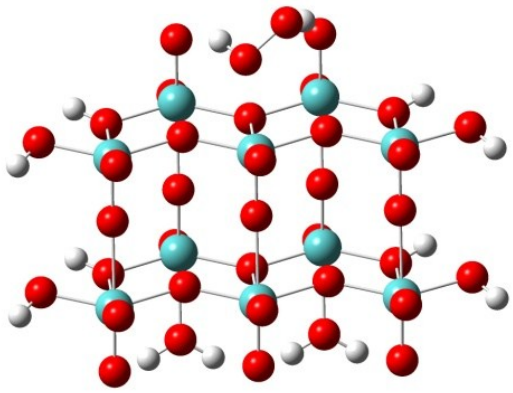


Total B3LYP Energy: -2294.24850922 Hartree BSSE correction: 0.006968162818 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	3.41666	0.54491	5.58666
O	1.23364	0.40967	3.71348
O	3.47547	0.59162	1.89079
O	2.73306	2.64425	3.78113
O	1.23364	0.40968	0.01751
Mo	2.87052	0.95326	0.04074
Mo	2.88393	0.95771	3.73690
O	3.51833	0.60586	-1.80713
O	2.82831	2.64680	0.00375
O	-0.48137	-0.22797	-1.86179
Mo	-1.00437	0.16964	-0.00898
O	-0.54415	-0.24006	1.83901
O	-2.64986	-0.37680	-0.03233
O	-1.11710	1.87211	-0.04461
Mo	-1.00437	0.16963	3.68699
O	-0.54111	-0.23154	5.55661
O	-2.64985	-0.37681	3.66364
O	-1.15172	1.86864	3.72772
O	3.78551	-1.19592	0.02740
Mo	4.30142	-1.58549	1.87624
O	-0.21182	-2.02350	-0.02409
O	1.89389	-1.88676	1.84728
O	5.93161	-1.04684	1.89934
O	3.76630	-1.20286	3.72313
O	4.43596	-3.28040	1.88277
Mo	0.24840	-2.43320	1.82393

Atom	Coordinates / Å		
	X	Y	Z
O	-1.98961	-2.67323	1.79744
O	-0.21182	-2.02350	3.67191
O	0.41113	-4.12422	1.86206
H	-0.82457	0.43946	6.18877
H	3.04601	1.12842	6.26286
H	-2.39244	-2.39400	0.95615
H	-0.41290	-2.62101	4.40071
H	3.38709	-1.85965	4.31864
H	-2.44942	-2.14067	2.47554
H	3.63989	1.38463	-2.36501
H	-0.25733	0.53285	-2.40847
H	4.26688	-1.41454	-0.78115
H	0.27755	-2.21448	-0.83467
O	5.33322	1.23067	3.72919
H	5.81149	0.60624	3.15171
O	5.99478	1.03368	5.00002
H	5.23262	0.69961	5.52345

C. H_2O_2 + $Mo_{10}O_{36}H_{12}$ "HOOH3" Structure

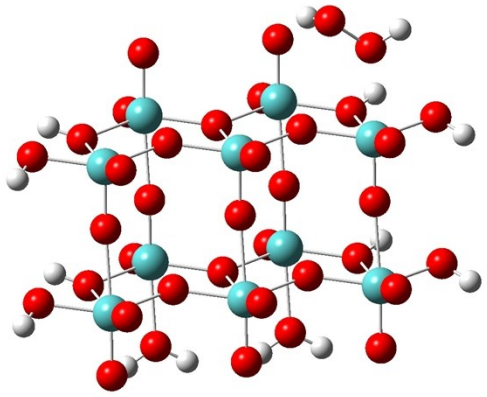


Total B3LYP Energy: -3544.23655985 Hartree BSSE correction: 0.00820678 Hartree

Atom	Coordinates / Å		
	X	Y	Z
Mo	-1.11813	-0.98716	0.37864
O	-1.52042	0.86127	-0.08635
O	0.56723	-0.98714	-0.02916
O	-1.52155	-2.83529	-0.08652
O	-1.11793	-0.98691	2.04964
Mo	-1.07588	-4.68270	0.34143
O	0.60949	-4.68268	-0.06636
O	-1.47930	-6.53083	-0.12373
O	-1.07568	-4.68246	2.01243
Mo	-1.03363	-8.37827	0.30423
O	0.65174	-8.37825	-0.10357
O	-1.43705	-10.22640	-0.16093
O	-1.03342	-8.37803	1.97523
Mo	2.90211	-8.37847	-0.15675
O	2.45644	-6.53103	-0.58470
O	4.58748	-8.37846	-0.56454
O	2.49869	-10.22660	-0.62191
O	2.90232	-8.37823	1.51425
Mo	2.85986	-4.68290	-0.11955
O	2.41419	-2.83549	-0.54750
O	4.54522	-4.68288	-0.52734
O	2.86006	-4.68266	1.55146
Mo	2.81760	-0.98736	-0.08234
O	2.41532	0.86106	-0.54733
O	4.50297	-0.98734	-0.49013
O	2.81781	-0.98712	1.58866
O	-1.64108	-8.37763	-1.94729

Atom	Coordinates / Å		
	X	Y	Z
Mo	-2.08676	-6.53021	-2.37524
O	2.29481	-8.37783	-2.40828
O	0.16377	-6.53044	-2.42845
O	-1.68334	-4.68208	-1.91009
O	-3.77212	-6.53023	-1.96745
O	-2.08696	-6.53046	-4.04624
Mo	1.84914	-6.53042	-2.83624
Mo	-2.12901	-2.83464	-2.33804
O	4.09951	-6.53064	-2.88942
O	2.25256	-4.68229	-2.37108
O	1.84894	-6.53066	-4.50724
O	0.12152	-2.83487	-2.39124
O	-3.81438	-2.83466	-1.93025
O	-1.72559	-0.98651	-1.87288
O	-2.12921	-2.83488	-4.00904
Mo	1.80689	-2.83485	-2.79903
O	4.05726	-2.83507	-2.85222
O	2.21031	-0.98672	-2.33388
O	1.80668	-2.83509	-4.47003
H	-0.90843	-10.81575	0.38206
H	3.02731	-10.81595	-0.07892
H	2.91159	1.45038	0.02540
H	-1.02415	1.45059	0.48638
H	4.53685	-3.66647	-2.87170
H	4.57965	-5.69935	-2.89263
H	1.82364	-0.19898	-2.72318
H	1.92968	-9.16969	-2.80984
H	-2.00622	-9.16948	-2.34885
H	-2.11226	-0.19878	-2.26219
H	4.53740	-2.00378	-2.85542
H	4.57910	-7.36204	-2.90890
O	-3.48856	-4.89764	0.37144
H	-3.90572	-5.50569	-0.27466
O	-4.43576	-3.83438	0.56539
H	-4.36476	-3.34426	-0.28536

D. H_2O_2 + $Mo_{10}O_{36}H_{12}$ "HOOH1" Structure

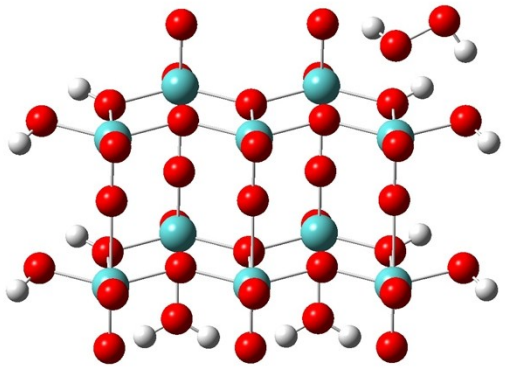


Total B3LYP Energy: -3544.23048866 Hartree BSSE correction: 0.00656181 Hartree

Atom	Coordinates / Å		
	X	Y	Z
Mo	-1.11813	-0.98716	0.37864
O	-1.52042	0.86127	-0.08635
O	0.56723	-0.98714	-0.02916
O	-1.52155	-2.83529	-0.08652
O	-1.11793	-0.98691	2.04964
Mo	-1.07588	-4.68270	0.34143
O	0.60949	-4.68268	-0.06636
O	-1.47930	-6.53083	-0.12373
O	-1.07568	-4.68246	2.01243
Mo	-1.03363	-8.37827	0.30423
O	0.65174	-8.37825	-0.10357
O	-1.43705	-10.22640	-0.16093
O	-1.03342	-8.37803	1.97523
Mo	2.90211	-8.37847	-0.15675
O	2.45644	-6.53103	-0.58470
O	4.58748	-8.37846	-0.56454
O	2.49869	-10.22660	-0.62191
O	2.90232	-8.37823	1.51425
Mo	2.85986	-4.68290	-0.11955
O	2.41419	-2.83549	-0.54750
O	4.54522	-4.68288	-0.52734
O	2.86006	-4.68266	1.55146
Mo	2.81760	-0.98736	-0.08234
O	2.41532	0.86106	-0.54733
O	4.50297	-0.98734	-0.49013

Atom	Coordinates / Å		
	X	Y	Z
O	2.81781	-0.98712	1.58866
O	-1.64108	-8.37763	-1.94729
Mo	-2.08676	-6.53021	-2.37524
O	2.29481	-8.37783	-2.40828
O	0.16377	-6.53044	-2.42845
O	-1.68334	-4.68208	-1.91009
O	-3.77212	-6.53023	-1.96745
O	-2.08696	-6.53046	-4.04624
Mo	1.84914	-6.53042	-2.83624
Mo	-2.12901	-2.83464	-2.33804
O	4.09951	-6.53064	-2.88942
O	2.25256	-4.68229	-2.37108
O	1.84894	-6.53066	-4.50724
O	0.12152	-2.83487	-2.39124
O	-3.81438	-2.83466	-1.93025
O	-1.72559	-0.98651	-1.87288
O	-2.12921	-2.83488	-4.00904
Mo	1.80689	-2.83485	-2.79903
O	4.05726	-2.83507	-2.85222
O	2.21031	-0.98672	-2.33388
O	1.80668	-2.83509	-4.47003
H	-0.90843	-10.81575	0.38206
H	3.02731	-10.81595	-0.07892
H	2.91159	1.45038	0.02540
H	-1.02415	1.45059	0.48638
H	4.53685	-3.66647	-2.87170
H	4.57965	-5.69935	-2.89263
H	1.82364	-0.19898	-2.72318
H	1.92968	-9.16969	-2.80984
H	-2.00622	-9.16948	-2.34885
H	-2.11226	-0.19878	-2.26219
H	4.53740	-2.00378	-2.85542
H	4.57910	-7.36204	-2.90890
O	-4.37841	-2.03350	0.64473
H	-4.45428	-2.40298	-0.26437
O	-3.54198	-0.89076	0.35106
H	-3.99307	-0.16625	0.80721

E. H_2O_2 + $Mo_{10}O_{36}H_{12}$ "HOOH2" Structure

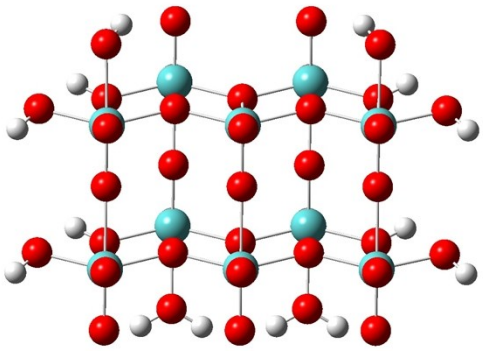


Total B3LYP Energy: -3544.23242632 Hartree BSSE correction: 0.00655391 Hartree

Atom	Coordinates / Å		
	X	Y	Z
Mo	-1.11813	-0.98716	0.37864
O	-1.52042	0.86127	-0.08635
O	0.56723	-0.98714	-0.02916
O	-1.52155	-2.83529	-0.08652
O	-1.11793	-0.98691	2.04964
Mo	-1.07588	-4.68270	0.34143
O	0.60949	-4.68268	-0.06636
O	-1.47930	-6.53083	-0.12373
O	-1.07568	-4.68246	2.01243
Mo	-1.03363	-8.37827	0.30423
O	0.65174	-8.37825	-0.10357
O	-1.43705	-10.22640	-0.16093
O	-1.03342	-8.37803	1.97523
Mo	2.90211	-8.37847	-0.15675
O	2.45644	-6.53103	-0.58470
O	4.58748	-8.37846	-0.56454
O	2.49869	-10.22660	-0.62191
O	2.90232	-8.37823	1.51425
Mo	2.85986	-4.68290	-0.11955
O	2.41419	-2.83549	-0.54750
O	4.54522	-4.68288	-0.52734
O	2.86006	-4.68266	1.55146
Mo	2.81760	-0.98736	-0.08234
O	2.41532	0.86106	-0.54733
O	4.50297	-0.98734	-0.49013
O	2.81781	-0.98712	1.58866

Atom	Coordinates / Å		
	X	Y	Z
O	-1.64108	-8.37763	-1.94729
Mo	-2.08676	-6.53021	-2.37524
O	2.29481	-8.37783	-2.40828
O	0.16377	-6.53044	-2.42845
O	-1.68334	-4.68208	-1.91009
O	-3.77212	-6.53023	-1.96745
O	-2.08696	-6.53046	-4.04624
Mo	1.84914	-6.53042	-2.83624
O	-2.12901	-2.83464	-2.33804
O	4.09951	-6.53064	-2.88942
O	2.25256	-4.68229	-2.37108
O	1.84894	-6.53066	-4.50724
O	0.12152	-2.83487	-2.39124
O	-3.81438	-2.83466	-1.93025
O	-1.72559	-0.98651	-1.87288
O	-2.12921	-2.83488	-4.00904
Mo	1.80689	-2.83485	-2.79903
O	4.05726	-2.83507	-2.85222
O	2.21031	-0.98672	-2.33388
O	1.80668	-2.83509	-4.47003
H	-0.90843	-10.81575	0.38206
H	3.02731	-10.81595	-0.07892
H	2.91159	1.45038	0.02540
H	-1.02415	1.45059	0.48638
H	4.53685	-3.66647	-2.87170
H	4.57965	-5.69935	-2.89263
H	1.82364	-0.19898	-2.72318
H	1.92968	-9.16969	-2.80984
H	-2.00622	-9.16948	-2.34885
H	-2.11226	-0.19878	-2.26219
H	4.53740	-2.00378	-2.85542
H	4.57910	-7.36204	-2.90890
O	-4.16762	0.27300	0.07820
H	-3.36500	0.83430	-0.00076
O	-3.54298	-1.00531	0.35458
H	-3.91457	-1.57709	-0.35007

F. H_2O_2 + $Mo_{10}O_{36}H_{12}$ "HO-OH1" Structure

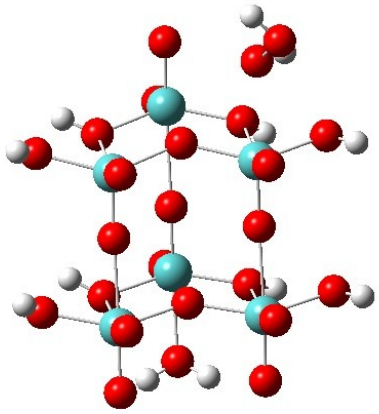


Total B3LYP Energy: -3544.09266029 Hartree

Atom	Coordinates / Å		
	X	Y	Z
Mo	-1.11813	-0.98716	0.37864
O	-1.52042	0.86127	-0.08635
O	0.56723	-0.98714	-0.02916
O	-1.52155	-2.83529	-0.08652
O	-1.11793	-0.98691	2.04964
Mo	-1.07588	-4.68270	0.34143
O	0.60949	-4.68268	-0.06636
O	-1.47930	-6.53083	-0.12373
O	-1.07568	-4.68246	2.01243
Mo	-1.03363	-8.37827	0.30423
O	0.65174	-8.37825	-0.10357
O	-1.43705	-10.22640	-0.16093
O	-1.03342	-8.37803	1.97523
Mo	2.90211	-8.37847	-0.15675
O	2.45644	-6.53103	-0.58470
O	4.58748	-8.37846	-0.56454
O	2.49869	-10.22660	-0.62191
O	2.90232	-8.37823	1.51425
Mo	2.85986	-4.68290	-0.11955
O	2.41419	-2.83549	-0.54750
O	4.54522	-4.68288	-0.52734
O	2.86006	-4.68266	1.55146
Mo	2.81760	-0.98736	-0.08234
O	2.41532	0.86106	-0.54733
O	4.50297	-0.98734	-0.49013
O	2.81781	-0.98712	1.58866
O	-1.64108	-8.37763	-1.94729

Atom	Coordinates / Å		
	X	Y	Z
Mo	-2.08676	-6.53021	-2.37524
O	2.29481	-8.37783	-2.40828
O	0.16377	-6.53044	-2.42845
O	-1.68334	-4.68208	-1.91009
O	-3.77212	-6.53023	-1.96745
O	-2.08696	-6.53046	-4.04624
Mo	1.84914	-6.53042	-2.83624
Mo	-2.12901	-2.83464	-2.33804
O	4.09951	-6.53064	-2.88942
O	2.25256	-4.68229	-2.37108
O	1.84894	-6.53066	-4.50724
O	0.12152	-2.83487	-2.39124
O	-3.81438	-2.83466	-1.93025
O	-1.72559	-0.98651	-1.87288
O	-2.12921	-2.83488	-4.00904
Mo	1.80689	-2.83485	-2.79903
O	4.05726	-2.83507	-2.85222
O	2.21031	-0.98672	-2.33388
O	1.80668	-2.83509	-4.47003
H	-0.90843	-10.81575	0.38206
H	3.02731	-10.81595	-0.07892
H	2.91159	1.45038	0.02540
H	-1.02415	1.45059	0.48638
H	4.53685	-3.66647	-2.87170
H	4.57965	-5.69935	-2.89263
H	1.82364	-0.19898	-2.72318
H	1.92968	-9.16969	-2.80984
H	-2.00622	-9.16948	-2.34885
H	-2.11226	-0.19878	-2.26219
H	4.53740	-2.00378	-2.85542
H	4.57910	-7.36204	-2.90890
H	-3.73640	-8.00997	-0.36622
O	-3.24277	-8.42887	0.36224
O	-3.32145	-0.97224	0.42248
H	-3.79736	-1.41511	-0.30397

G. H_2O_2 + $Mo_6O_{23}H_{10}$ "TS1-Oxide" Transition State Structure.

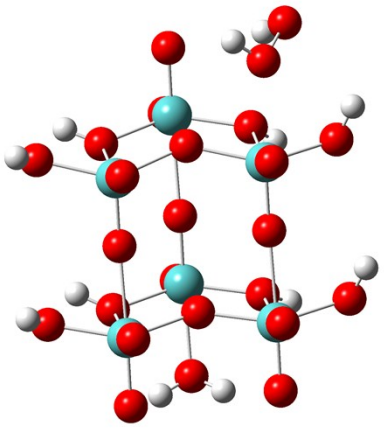


Total B3LYP Energy: -2294.23829964 Hartree BSSE correction: 0.005884851424 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	3.37031	0.52952	5.58599
O	1.23364	0.40967	3.71348
O	3.47944	0.59294	1.89084
O	2.75292	2.64592	3.76375
O	1.23364	0.40968	0.01751
Mo	2.87190	0.95372	0.04076
Mo	2.87951	0.95625	3.73684
O	3.51813	0.60579	-1.80713
O	2.83158	2.64845	0.00144
O	-0.48051	-0.22457	-1.86391
Mo	-1.00437	0.16964	-0.00898
O	-0.54415	-0.24006	1.83901
O	-2.64986	-0.37680	-0.03233
O	-1.11643	1.87287	-0.04611
Mo	-1.00437	0.16963	3.68699
O	-0.54765	-0.23264	5.55638
O	-2.64985	-0.37681	3.66364
O	-1.14528	1.86977	3.73188
O	3.86431	-1.16744	0.02855
Mo	4.42507	-1.54081	1.87804
O	-0.21182	-2.02350	-0.02409
O	1.89389	-1.88676	1.84728
O	6.04315	-1.00817	1.90094
O	3.88263	-1.16082	3.72481
O	4.55082	-3.23837	1.90712
Mo	0.24840	-2.43320	1.82393
O	-1.98961	-2.67323	1.79744

Atom	Coordinates / Å		
	X	Y	Z
O	-0.21182	-2.02350	3.67191
O	0.40977	-4.12610	1.86080
H	-0.73151	0.48301	6.17554
H	3.13678	1.19953	6.24171
H	-2.39414	-2.39119	0.95816
H	-0.38536	-2.61714	4.41035
H	3.53769	-1.81703	4.34135
H	-2.44705	-2.14249	2.47829
H	3.60138	1.38186	-2.37539
H	-0.25556	0.54003	-2.40474
H	4.32576	-1.37882	-0.79292
H	0.29673	-2.19621	-0.82663
O	5.38130	1.18979	3.89037
H	5.54613	0.64420	4.67794
O	5.84744	2.48836	4.32589
H	6.52614	2.66242	3.65662

H. H_2O_2 + $Mo_6O_{23}H_{10}$ "TS2-Oxide" Transition State Structure.



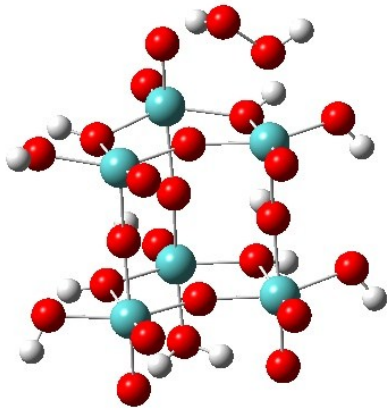
Total B3LYP Energy: -2294.2406737 Hartree BSSE correction: 0.006542648089 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	3.26855	0.49573	5.58451
O	1.23364	0.40967	3.71348
O	3.48786	0.59574	1.89096
O	2.81344	2.65212	3.69012
O	1.23364	0.40968	0.01751
Mo	2.86955	0.95294	0.04073
Mo	2.87917	0.95613	3.73683
O	3.51867	0.60597	-1.80713
O	2.83152	2.64772	0.00514
O	-0.47127	-0.23779	-1.86086
Mo	-1.00437	0.16964	-0.00898
O	-0.54415	-0.24006	1.83901
O	-2.64986	-0.37680	-0.03233
O	-1.11716	1.87182	-0.06298
Mo	-1.00437	0.16963	3.68699
O	-0.60213	-0.17684	5.56229
O	-2.64985	-0.37681	3.66364
O	-1.10812	1.87229	3.62830
O	3.81348	-1.18581	0.02781
Mo	4.33945	-1.57174	1.87679
O	-0.21182	-2.02350	-0.02409
O	1.89389	-1.88676	1.84728
O	5.96812	-1.03418	1.89986
O	3.84727	-1.17360	3.72430

Atom	Coordinates / Å		
	X	Y	Z
O	4.47159	-3.26764	1.90359
Mo	0.24840	-2.43320	1.82393
O	-1.98961	-2.67323	1.79744
O	-0.21182	-2.02350	3.67191
O	0.40849	-4.12543	1.86019
H	0.08684	0.34739	5.98597
H	4.01185	0.93901	6.01532
H	-2.38972	-2.39276	0.95529
H	-0.43662	-2.62674	4.38906
H	3.46940	-1.80130	4.35200
H	-2.44820	-2.13595	2.47317
H	3.60015	1.38071	-2.37757
H	-0.32055	0.52666	-2.42709
H	4.26426	-1.42338	-0.79266
H	0.26990	-2.21967	-0.83778
O	5.32640	1.38058	3.90680
H	5.85825	1.72699	3.17394
O	6.23184	0.52666	4.62551
H	6.08933	-0.33139	4.18761

SECTION 4

A. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "HOOH1" Structure

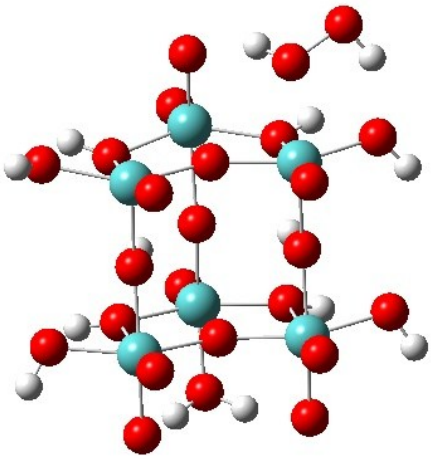


Total B3LYP Energy: -2295.27491653 Hartree BSSE correction: 0.006000678683 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37065	7.98047	5.58070
O	-1.88637	7.92301	3.60865
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.37207	4.09597	5.64423
O	-1.79569	3.97313	3.66515
O	0.08291	5.80887	0.01617
O	0.36306	8.26535	-1.86070
O	-1.85970	8.05409	0.19113
Mo	-0.10311	3.86863	0.00000
Mo	-0.20822	7.81274	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.20988	7.87483	3.72000
O	0.38154	4.08937	-1.90706
O	-1.79771	3.97996	0.02448
O	2.52013	5.86430	1.87546
O	2.41578	9.77979	1.84275
O	4.39704	7.98792	1.84622
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37223	7.92081	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000

Atom	Coordinates / Å		
	X	Y	Z
O	2.12527	7.71240	-0.00141
Mo	2.69934	8.05998	1.85930
O	2.12576	7.69407	3.72000
O	4.49773	3.82052	1.86018
H	2.54031	8.02952	4.52420
H	0.34936	7.16780	6.10652
H	2.02354	1.71492	2.63348
H	2.04568	1.70626	1.10582
H	2.62626	3.62641	4.54173
H	0.28097	3.27070	6.13433
H	2.58209	7.97944	-0.80876
H	-0.32004	8.47588	-2.51129
H	0.26133	3.27592	-2.41046
H	2.64921	3.74263	-0.85350
H	1.06142	5.90003	3.70545
H	1.02054	5.87730	0.32229
O	0.27225	9.98835	3.95922
O	0.21432	10.96124	2.89628
H	1.06826	10.74502	2.44168
H	0.10100	10.48234	4.77595

B. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "HOOH2" Structure

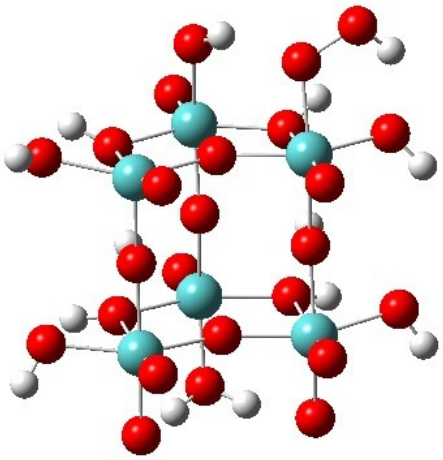


Total B3LYP Energy: -2295.28055853 Hartree BSSE correction: 0.006410875207 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.36793	8.08228	5.58070
O	-1.88470	7.93744	3.62444
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.37398	4.08938	5.64392
O	-1.79572	3.97347	3.66824
O	0.08291	5.80887	0.01617
O	0.36329	8.25675	-1.86070
O	-1.85998	8.04501	0.19101
Mo	-0.10311	3.86863	0.00000
Mo	-0.20810	7.80796	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.21014	7.88461	3.72000
O	0.37948	4.09323	-1.90615
O	-1.79748	3.98207	0.02674
O	2.52013	5.86430	1.87546
O	2.41595	9.77350	1.84280
O	4.39720	7.98253	1.85184
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37248	7.91144	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000

Atom	Coordinates / Å		
	X	Y	Z
O	2.12541	7.70733	-0.00141
Mo	2.69943	8.05692	1.85930
O	2.12537	7.70866	3.72000
O	4.49759	3.82074	1.85990
H	2.62591	7.91461	4.51766
H	0.32873	7.34050	6.19885
H	2.02242	1.71380	2.63219
H	2.04832	1.70507	1.10460
H	2.61698	3.60989	4.53993
H	0.27660	3.26281	6.13074
H	2.57115	7.99928	-0.80665
H	-0.31680	8.47092	-2.51351
H	0.26346	3.28095	-2.41246
H	2.65280	3.74853	-0.85289
H	1.05982	5.89877	3.67715
H	1.02383	5.87684	0.31302
O	0.31101	10.00955	3.74414
H	1.07215	10.21603	3.14979
O	0.68082	10.61523	5.01123
H	0.63383	9.81363	5.59267

C. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "HOO-H1" Structure

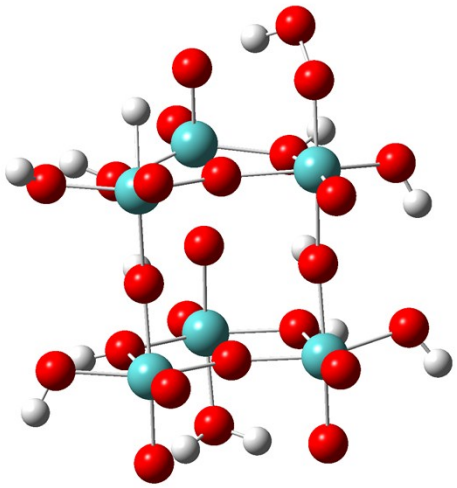


Total B3LYP Energy: -2295.27758605 Hartree BSSE correction: 0.007085973133 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.36958	8.02031	5.58070
O	-1.89767	7.90133	3.70447
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.37360	4.09492	5.64207
O	-1.79423	3.96021	3.65019
O	0.08291	5.80887	0.01617
O	0.36307	8.26486	-1.86070
O	-1.83435	8.17447	0.23986
Mo	-0.10311	3.86863	0.00000
Mo	-0.20855	7.82482	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.21180	7.94698	3.72000
O	0.39525	4.10319	-1.90258
O	-1.79576	3.98294	0.03213
O	2.52013	5.86430	1.87546
O	2.41813	9.69170	1.84348
O	4.39052	7.88808	1.77774
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37249	7.91117	1.85930
O	2.22673	3.90565	-0.00141

Atom	Coordinates / Å		
	X	Y	Z
O	2.22590	3.93672	3.72000
O	2.12578	7.69351	-0.00141
Mo	2.70640	7.79521	1.85930
O	2.12591	7.68850	3.72000
O	4.49679	3.87779	1.84029
H	2.49344	8.18438	4.46360
H	0.08941	7.32527	6.19203
H	2.03073	1.71536	2.63978
H	2.04648	1.70374	1.10676
H	2.64632	3.70033	4.55666
H	0.31319	3.26484	6.12866
H	2.56407	8.08222	-0.76992
H	-0.30710	8.54932	-2.49668
H	0.29623	3.29374	-2.41687
H	2.65504	3.77054	-0.85618
H	1.04025	5.90354	3.91405
H	1.06281	5.88690	0.05180
O	0.24810	9.84832	3.71347
H	1.65160	10.09543	2.29385
O	-0.01778	10.62551	4.88727
H	0.09397	9.95697	5.59669

D. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "HOO-H2" Structure

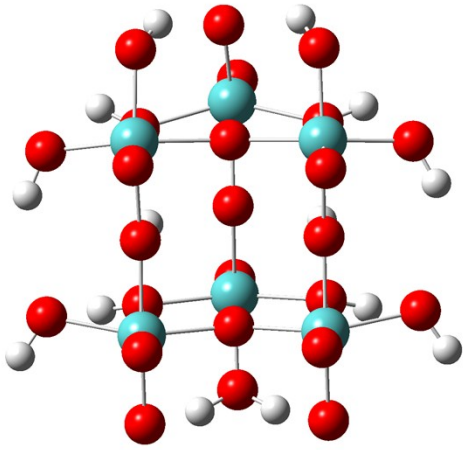


Total B3LYP Energy: -2295.24634195 Hartree BSSE correction: 0.008059861099 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37846	7.68713	5.58071
O	-1.91871	7.69760	3.77261
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.36589	4.15941	5.64216
O	-1.79452	3.96952	3.66581
O	0.08291	5.80887	0.01617
O	0.36774	8.08980	-1.86070
O	-1.81308	8.38969	-0.06846
Mo	-0.10311	3.86863	0.00000
Mo	-0.21697	7.86551	-0.04647
O	0.18602	1.94025	0.01617
Mo	-0.24702	7.89043	3.76723
O	0.38183	4.09681	-1.90635
O	-1.79697	3.97945	0.03530
O	2.52013	5.86430	1.87546
O	2.40623	9.69193	1.83184
O	4.48250	8.00200	1.88453
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546

Atom	Coordinates / Å		
	X	Y	Z
O	0.32928	7.83325	1.85278
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000
O	2.14928	7.53300	0.01438
Mo	2.78844	7.97940	1.86402
O	2.17629	7.67126	3.73174
O	4.49693	3.82356	1.85379
H	2.60701	8.00225	4.53021
H	0.27670	6.79989	5.96590
H	2.03548	1.71051	2.63920
H	2.03829	1.70687	1.11050
H	2.64666	3.66440	4.54506
H	0.23981	3.37047	6.18198
H	2.57251	7.90546	-0.77094
H	-0.16547	8.54222	-2.52815
H	0.25157	3.29060	-2.41891
H	2.65337	3.71293	-0.84556
H	1.06138	5.90370	3.70673
H	1.06128	5.90309	0.10807
O	-0.12761	9.76887	3.84793
H	1.44566	10.40706	2.99585
O	0.86456	10.72723	3.74172
H	0.44874	9.39327	0.15496

E. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "HO-OH2" Structure

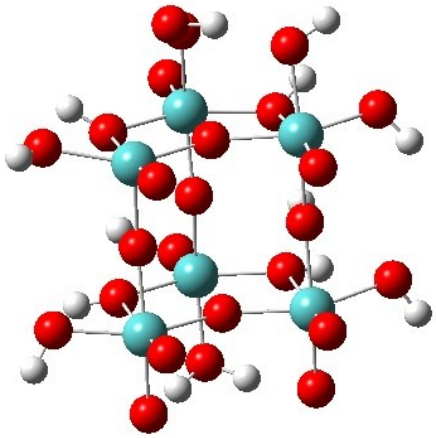


Total B3LYP Energy: -2295.40272383 Hartree BSSE correction: 0.010196094226 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37858	7.68274	5.58071
O	-1.89302	7.72811	3.83127
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.36271	4.14537	5.64505
O	-1.79452	3.96618	3.66868
O	0.08291	5.80887	0.01617
O	0.37997	7.63066	-1.86070
O	-1.83150	7.85475	-0.07001
Mo	-0.10311	3.86863	0.00000
Mo	-0.15159	7.93224	-0.05430
O	0.18602	1.94025	0.01617
Mo	-0.22543	7.89990	3.76323
O	0.37652	4.17179	-1.91993
O	-1.79517	3.95570	0.02347
O	2.52013	5.86430	1.87546
O	2.43829	9.66597	1.77593
O	4.52566	7.98546	1.99712
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.33309	7.79831	1.87487
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000

Atom	Coordinates / Å		
	X	Y	Z
O	2.21476	7.59696	0.02117
Mo	2.83477	7.96048	1.90046
O	2.16223	7.65580	3.74221
O	4.49693	3.82368	1.85202
H	2.62174	7.86102	4.56574
H	0.15013	6.85337	6.03276
H	2.03108	1.71229	2.63769
H	2.03808	1.70747	1.10942
H	2.63926	3.65134	4.54458
H	0.24045	3.34690	6.17167
H	2.66625	7.91971	-0.76869
H	0.25760	6.74669	-2.24962
H	0.21563	3.39955	-2.47475
H	2.66302	3.70995	-0.83991
H	1.05987	5.89970	3.68859
H	1.04941	5.89306	0.17665
O	0.03268	9.75840	3.72810
O	0.23019	9.75792	0.01097
H	1.04186	10.07247	0.46346
H	0.83596	10.16352	3.35916

F. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "HO-OH3" Structure

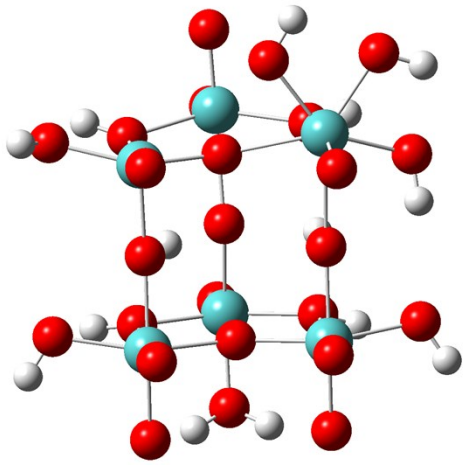


Total B3LYP Energy: -2295.27824496 Hartree BSSE correction: 0.008040614696 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.36960	8.01987	5.58070
O	-1.88559	7.75749	3.66890
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.36965	4.09121	5.64341
O	-1.79384	3.95984	3.64276
O	0.08291	5.80887	0.01617
O	0.36229	8.29414	-1.86070
O	-1.87338	7.99354	0.10170
Mo	-0.10311	3.86863	0.00000
Mo	-0.20899	7.84146	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.21127	7.92723	3.72000
O	0.37956	4.10325	-1.90755
O	-1.79494	3.98272	0.06153
O	2.52013	5.86430	1.87546
O	2.41765	9.70963	1.84333
O	4.39098	7.92068	1.89144
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37295	7.89386	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000

Atom	Coordinates / Å		
	X	Y	Z
O	2.12430	7.74876	-0.00141
Mo	2.70733	7.76054	1.85930
O	2.12700	7.64747	3.72000
O	4.49710	3.87830	1.85178
H	2.47351	8.17757	4.45068
H	0.08142	7.30319	6.16397
H	2.03210	1.71835	2.64323
H	2.03821	1.70490	1.11075
H	2.65652	3.73341	4.55989
H	0.30816	3.25969	6.12739
H	2.50470	8.27222	-0.72042
H	-0.31227	8.40892	-2.54226
H	0.30911	3.28804	-2.41713
H	2.66241	3.71194	-0.84062
H	1.04355	5.89887	3.90307
H	1.04884	5.89629	-0.13985
O	0.08609	9.87548	3.68325
O	1.24672	10.33066	1.35756
H	0.70760	10.37376	2.19510
H	0.11588	10.32124	4.53889

G. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "HO-OH4" Structure

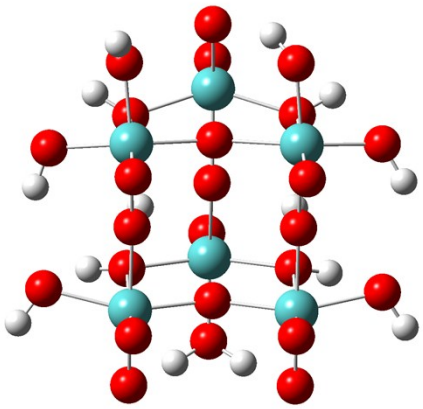


Total B3LYP Energy: -2295.31661206 Hartree BSSE correction: 0.007248789717 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.38106	7.58974	5.58071
O	-1.72676	7.81523	3.84417
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.34746	4.09223	5.64854
O	-1.79535	3.94485	3.64899
O	0.08291	5.80887	0.01617
O	0.36459	8.20766	-1.86070
O	-1.75266	8.03690	-0.08142
Mo	-0.10311	3.86863	0.00000
Mo	-0.09390	7.75880	-0.04078
O	0.18602	1.94025	0.01617
Mo	-0.10636	8.22033	3.76544
O	0.36579	4.15612	-1.90217
O	-1.79758	3.98974	0.01910
O	2.52013	5.86430	1.87546
O	2.75345	9.88903	1.70980
O	4.54392	7.90316	1.82860
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.49085	7.76130	1.69166

Atom	Coordinates / Å		
	X	Y	Z
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000
O	2.14297	7.85935	-0.09027
Mo	2.86950	8.17786	1.80139
O	2.21479	7.95413	3.64754
O	4.49767	3.81712	1.85865
H	2.69319	8.00181	4.48380
H	0.11460	6.65740	5.67023
H	2.01176	1.71665	2.62681
H	2.07236	1.69070	1.09905
H	2.61735	3.59808	4.53536
H	0.21893	3.28161	6.15431
H	2.59748	8.09500	-0.90865
H	-0.34909	8.36358	-2.49702
H	0.20868	3.37754	-2.44898
H	2.67096	3.77961	-0.84792
H	1.05058	5.92126	3.65722
H	0.92920	5.83710	0.55814
O	0.06817	9.80462	4.94093
O	-0.21048	9.82265	2.65196
H	-0.11169	10.62775	3.18132
H	0.16100	9.47994	5.84878

H. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "HO-OH5" Structure

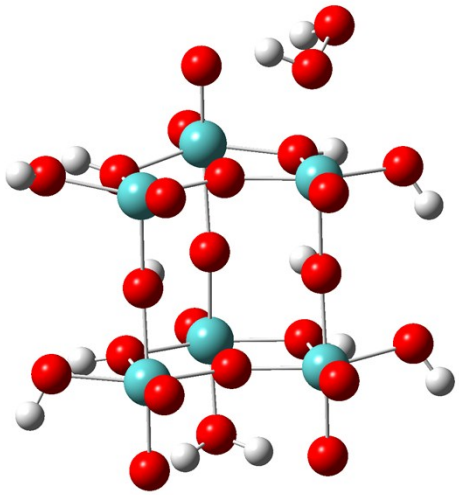


Total B3LYP Energy: -2295.39602049 Hartree BSSE correction: 0.0095389515 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37744	7.72543	5.58071
O	-1.84254	7.79997	3.83704
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.35298	4.14826	5.64676
O	-1.79509	3.96908	3.66492
O	0.08291	5.80887	0.01617
O	0.38137	7.57833	-1.86070
O	-1.84171	7.82562	-0.05365
Mo	-0.10311	3.86863	0.00000
Mo	-0.16468	7.91938	-0.04567
O	0.18602	1.94025	0.01617
Mo	-0.16720	7.91984	3.76200
O	0.37690	4.18119	-1.92010
O	-1.79618	3.95718	0.01969
O	2.52013	5.86430	1.87546
O	2.48150	9.71619	1.82372
O	4.52841	8.00012	1.91034
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37017	7.80019	1.83011
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000

Atom	Coordinates / Å		
	X	Y	Z
O	2.20015	7.60770	0.01728
Mo	2.83374	8.01059	1.87031
O	2.21162	7.64571	3.73689
O	4.49737	3.81895	1.85530
H	2.66616	7.93823	4.53619
H	0.12663	6.92381	6.06922
H	2.03371	1.71063	2.63733
H	2.03920	1.70731	1.10948
H	2.64423	3.64586	4.53963
H	0.24019	3.34619	6.16986
H	2.62072	7.96908	-0.77372
H	0.35482	6.64760	-2.14972
H	0.20918	3.41655	-2.48312
H	2.66223	3.70175	-0.83793
H	1.06268	5.88540	3.67818
H	1.03951	5.89310	0.23070
O	0.14777	9.75720	3.61113
O	0.13723	9.76495	-0.22474
H	-0.49404	10.47465	-0.39589
H	0.91621	10.10659	3.11388

I. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS1" Transition State Structure

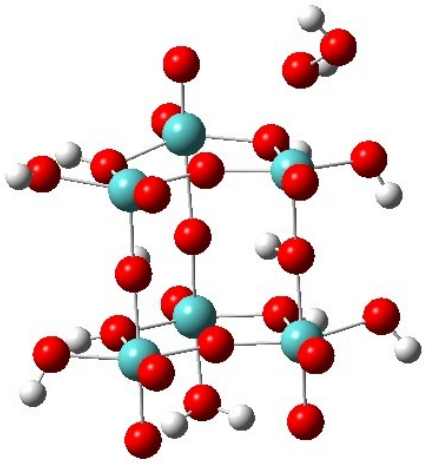


Total B3LYP Energy: -2295.2607711 Hartree BSSE correction: 0.006482805682 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37431	7.84281	5.58071
O	-1.88365	7.95997	3.60300
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.37385	4.10428	5.64246
O	-1.79598	3.97239	3.67683
O	0.08291	5.80887	0.01617
O	0.36315	8.26190	-1.86070
O	-1.84764	8.12643	0.21462
Mo	-0.10311	3.86863	0.00000
Mo	-0.20832	7.81627	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.20962	7.86519	3.72000
O	0.37913	4.09016	-1.90636
O	-1.79774	3.97924	0.02644
O	2.52013	5.86430	1.87546
O	2.41490	9.81288	1.84247
O	4.39541	8.00766	1.86504
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546

Atom	Coordinates / Å		
	X	Y	Z
O	0.37247	7.91204	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000
O	2.12462	7.73702	-0.00141
Mo	2.69827	8.10019	1.85930
O	2.12176	7.84415	3.72000
O	4.49765	3.81902	1.85655
H	2.60525	7.72612	4.54504
H	0.26851	7.00953	6.06465
H	2.02481	1.71117	2.63229
H	2.04776	1.70567	1.10461
H	2.60808	3.60356	4.54162
H	0.25345	3.29087	6.14616
H	2.56639	8.00412	-0.81718
H	-0.31484	8.47857	-2.51453
H	0.25988	3.27708	-2.41065
H	2.65317	3.75522	-0.85392
H	1.04695	5.88618	3.56084
H	1.01385	5.87642	0.34324
O	0.10988	10.10795	3.72424
H	0.13029	10.52716	2.84732
O	1.20721	10.72004	4.42298
H	1.97423	10.38170	3.92064

J. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS2" Transition State Structure

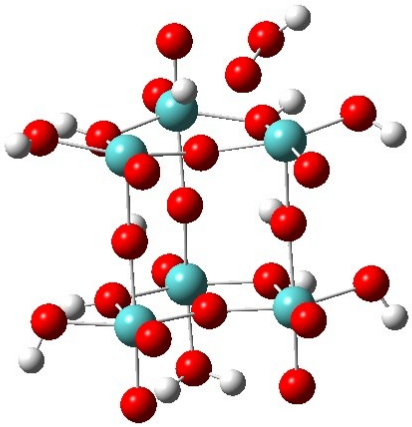


Total B3LYP Energy: -2295.2623555 Hartree BSSE correction: 0.005478846939 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37638	7.76532	5.58071
O	-1.87675	8.01586	3.56203
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.37129	4.12188	5.64307
O	-1.79742	3.95890	3.69251
O	0.08291	5.80887	0.01617
O	0.36319	8.26038	-1.86070
O	-1.85532	8.10013	0.19090
Mo	-0.10311	3.86863	0.00000
Mo	-0.20849	7.82277	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.20922	7.85019	3.72000
O	0.36763	4.08778	-1.90886
O	-1.79766	3.98206	0.03754
O	2.52013	5.86430	1.87546
O	2.41301	9.88378	1.84188
O	4.39402	8.06965	1.86639
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37208	7.92663	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000

Atom	Coordinates / Å		
	X	Y	Z
O	2.12362	7.77443	-0.00141
Mo	2.69582	8.19233	1.85930
O	2.11941	7.93227	3.72000
O	4.49791	3.81456	1.84542
H	2.61349	7.48365	4.41490
H	0.36875	6.88624	5.98938
H	2.02727	1.70888	2.63202
H	2.04868	1.70515	1.10491
H	2.59259	3.58465	4.54050
H	0.20779	3.32699	6.16401
H	2.55853	8.04651	-0.81888
H	-0.31719	8.44494	-2.52181
H	0.26549	3.26841	-2.40655
H	2.66122	3.73767	-0.84618
H	0.95578	5.86865	3.27618
H	1.02925	5.88436	0.29475
O	0.30160	10.00651	4.14616
H	0.97956	9.92373	4.84333
O	-0.75732	10.71883	4.83604
H	-0.86344	11.47758	4.23966

K. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS3" Transition State Structure

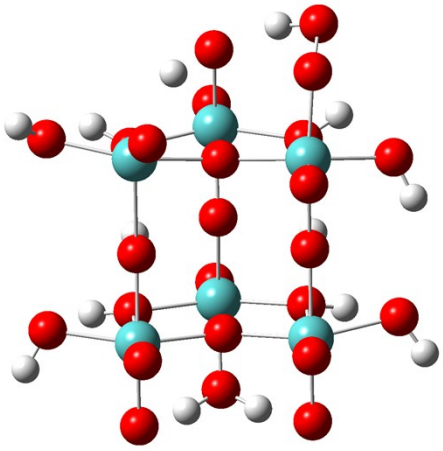


Total B3LYP Energy: -2295.18082852 Hartree BSSE correction: 0.007526024726 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.36688	8.12185	5.58070
O	-1.85091	7.51253	3.93641
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.35839	4.10108	5.64096
O	-1.79667	3.98413	3.67092
O	0.08291	5.80887	0.01617
O	0.35935	8.40436	-1.86070
O	-1.88888	7.93407	-0.01445
Mo	-0.10311	3.86863	0.00000
Mo	-0.21077	7.90837	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.20877	7.83329	3.72000
O	0.37400	4.07087	-1.91121
O	-1.79834	3.97032	0.02869
O	2.52013	5.86430	1.87546
O	2.41627	9.76135	1.84290
O	4.40017	7.98407	1.87174
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.38029	7.61837	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000
O	2.12435	7.74690	-0.00141

Atom	Coordinates / Å		
	X	Y	Z
Mo	2.69918	8.06633	1.85930
O	2.12585	7.69058	3.72000
O	4.49815	3.81809	1.85572
H	2.55957	7.98759	4.52891
H	-0.17141	7.67390	6.24967
H	2.03595	1.71005	2.63773
H	2.03879	1.70870	1.10953
H	2.64297	3.67778	4.55049
H	0.27484	3.27366	6.12862
H	2.57415	8.03878	-0.80386
H	-0.32728	8.46584	-2.53821
H	0.26161	3.24728	-2.39961
H	2.65220	3.74602	-0.85246
H	1.05540	5.88118	3.57965
H	1.01279	5.89828	0.32875
O	0.30903	10.11864	3.52942
O	-0.80033	9.64247	2.70544
H	-0.38087	9.30722	1.40186
H	-0.14598	10.65774	4.20121

L. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS4" Transition State Structure

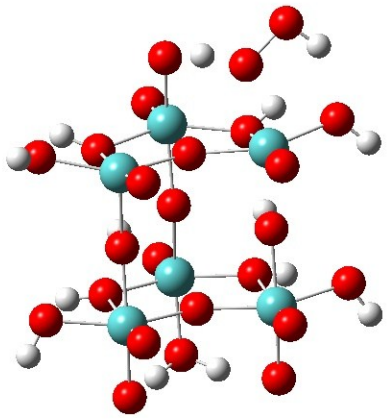


Total B3LYP Energy: -2295.19272773 Hartree BSSE correction: 0.008183934595 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37780	7.71220	5.58071
O	-1.89385	7.82413	3.66375
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.38004	4.15154	5.63842
O	-1.79370	3.96663	3.66234
O	0.08291	5.80887	0.01617
O	0.36096	8.34396	-1.86070
O	-1.69871	8.77655	0.21908
Mo	-0.10311	3.86863	0.00000
Mo	-0.21360	8.01440	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.21053	7.89927	3.72000
O	0.40210	4.06822	-1.90618
O	-1.79671	3.96673	0.03295
O	2.52013	5.86430	1.87546
O	2.41968	9.63345	1.84397
O	4.40149	7.84080	1.84829
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37607	7.77687	1.85930
O	2.22673	3.90565	-0.00141

Atom	Coordinates / Å		
	X	Y	Z
O	2.22590	3.93672	3.72000
O	2.12820	7.60241	-0.00141
Mo	2.70553	7.82794	1.85930
O	2.12655	7.66451	3.72000
O	4.49678	3.84788	1.85171
H	2.51068	8.07014	4.50923
H	0.22414	6.84382	5.98722
H	2.03670	1.71157	2.64228
H	2.02910	1.71233	1.11156
H	2.66174	3.72751	4.55627
H	0.28582	3.35336	6.17098
H	2.59051	7.94033	-0.78044
H	-0.21461	8.81481	-2.47889
H	0.29267	3.24772	-2.40067
H	2.64340	3.75500	-0.86013
H	1.05191	5.89704	3.85653
H	1.05214	5.94732	0.02703
O	0.00974	9.78265	3.86418
O	1.20035	10.49572	4.05649
H	1.69483	10.33300	3.20815
H	1.18269	9.48678	0.92051

M. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS5" Transition State Structure

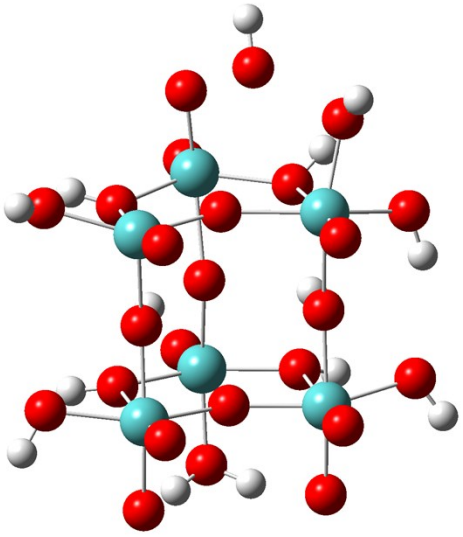


Total B3LYP Energy: -2295.26640455 Hartree BSSE correction: 0.007457737366 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.36260	8.28228	5.58070
O	-1.88912	8.06290	3.67209
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.39063	4.06623	5.63958
O	-1.79510	3.96158	3.66682
O	0.08291	5.80887	0.01617
O	0.36271	8.27844	-1.86070
O	-1.85454	8.06852	0.21923
Mo	-0.10311	3.86863	0.00000
Mo	-0.20844	7.82105	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.21239	7.96912	3.72000
O	0.40414	4.08551	-1.90230
O	-1.79615	3.97719	0.02096
O	2.52013	5.86430	1.87546
O	2.41843	9.68022	1.84358
O	4.39597	7.88700	1.78830
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37330	7.88085	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000
O	2.12724	7.63855	-0.00141
Mo	2.70406	7.88314	1.85930

Atom	Coordinates / Å		
	X	Y	Z
O	2.12745	7.63051	3.72000
O	4.49670	3.84414	1.86119
H	2.55306	8.02551	4.49316
H	0.16361	7.65336	6.28546
H	2.02222	1.71951	2.63801
H	2.03911	1.70714	1.10781
H	2.63655	3.70515	4.56347
H	0.31179	3.22968	6.11264
H	2.58094	7.97604	-0.78518
H	-0.30933	8.53661	-2.50521
H	0.28387	3.27555	-2.41148
H	2.64252	3.76929	-0.86280
H	1.05243	5.92448	3.80605
H	1.05181	5.88927	0.16908
O	0.55653	9.89260	3.43752
H	1.50974	9.93805	2.57505
O	0.94275	10.69677	4.57544
H	0.78009	10.06718	5.31253

N. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS6" Transition State Structure

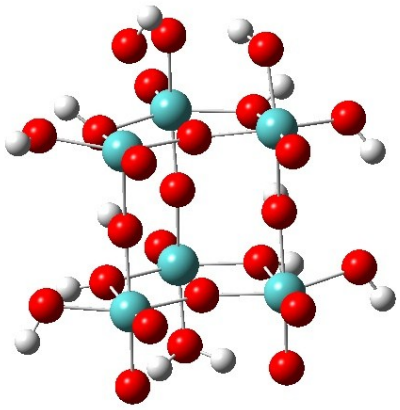


Total B3LYP Energy: -2295.22928909 Hartree BSSE correction: 0.007614363472 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.38036	7.61594	5.58070
O	-1.88961	7.89998	3.65310
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.36320	4.13600	5.64160
O	-1.79482	3.96579	3.65510
O	0.08291	5.80887	0.01617
O	0.36129	8.33181	-1.86070
O	-1.84452	8.05519	0.03404
Mo	-0.10311	3.86863	0.00000
Mo	-0.19074	7.79106	-0.08081
O	0.18602	1.94025	0.01617
Mo	-0.20296	7.91738	3.73028
O	0.37194	4.12324	-1.90538
O	-1.79757	3.98424	0.02170
O	2.52013	5.86430	1.87546
O	2.86141	9.72057	1.65138
O	4.65036	7.72965	1.99383
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.35397	7.94780	1.73778

Atom	Coordinates / Å		
	X	Y	Z
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000
O	2.11940	7.69502	0.02478
Mo	2.97816	7.96869	1.82328
O	2.18543	7.80287	3.63168
O	4.49648	3.83110	1.83467
H	2.49496	8.36724	4.35515
H	0.35027	6.67868	5.83737
H	2.02558	1.71514	2.63459
H	2.05627	1.69728	1.10487
H	2.64631	3.67393	4.54838
H	0.25835	3.33660	6.17013
H	2.57089	7.90615	-0.80315
H	-0.29538	8.59104	-2.52178
H	0.23797	3.32542	-2.43001
H	2.66540	3.75806	-0.84765
H	1.06080	5.89885	3.72479
H	0.99640	5.88904	0.40035
O	0.02067	9.76471	4.18368
O	1.44438	10.53308	2.70488
H	1.81057	11.43487	2.69948
H	-0.72586	10.35892	4.33667

O. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS7" Transition State Structure

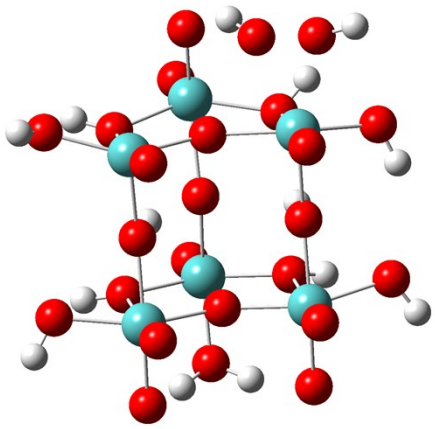


Total B3LYP Energy: -2295.25241536 Hartree BSSE correction: 0.009744753109 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37561	7.79403	5.58071
O	-1.89466	7.86912	3.69684
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.34637	4.12696	5.64614
O	-1.79404	3.96820	3.63683
O	0.08291	5.80887	0.01617
O	0.36239	8.29048	-1.86070
O	-1.87216	8.04794	-0.00432
Mo	-0.10311	3.86863	0.00000
Mo	-0.20920	7.84933	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.21148	7.93482	3.72000
O	0.36308	4.11690	-1.90898
O	-1.79533	3.99207	0.06594
O	2.52013	5.86430	1.87546
O	2.41801	9.69621	1.84345
O	4.39834	7.86587	1.82621
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37580	7.78714	1.85930
O	2.22673	3.90565	-0.00141
O	2.22590	3.93672	3.72000
O	2.12775	7.61939	-0.00141
Mo	2.70694	7.77510	1.85930

Atom	Coordinates / Å		
	X	Y	Z
O	2.12642	7.66916	3.72000
O	4.49706	3.86759	1.87324
H	2.51927	8.07665	4.50115
H	0.09709	6.99769	6.06001
H	2.03253	1.71314	2.63847
H	2.04594	1.70482	1.10729
H	2.65705	3.65969	4.53753
H	0.27880	3.30999	6.15335
H	2.46769	8.21008	-0.68847
H	-0.32335	8.38093	-2.53661
H	0.30683	3.30173	-2.42025
H	2.67192	3.70867	-0.83428
H	1.04655	5.90412	3.89029
H	1.05504	5.91142	-0.11186
O	0.17034	9.78723	3.64618
H	1.03817	10.02729	3.25922
O	1.19577	9.94747	0.61046
H	0.77532	10.70818	1.04000

P. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS8" Transition State Structure

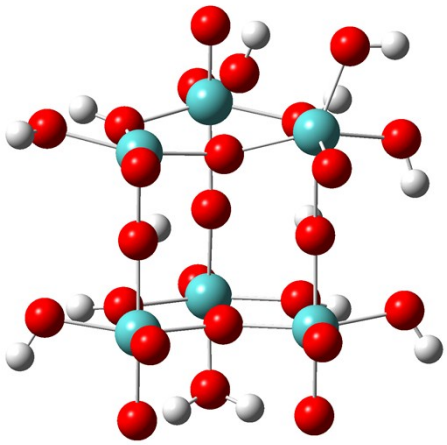


Total B3LYP Energy: -2295.23260243 Hartree BSSE correction: 0.006561538891 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37848	7.68645	5.58071
O	-1.82243	8.01737	3.60987
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.35594	4.14087	5.64225
O	-1.79419	3.97064	3.64879
O	0.08291	5.80887	0.01617
O	0.36045	8.36310	-1.86070
O	-1.80561	8.04145	0.06518
Mo	-0.10311	3.86863	0.00000
Mo	-0.15558	7.78936	-0.07449
O	0.18602	1.94025	0.01617
Mo	-0.14538	7.90003	3.70339
O	0.37875	4.11294	-1.90428
O	-1.79751	3.97756	0.01937
O	2.52013	5.86430	1.87546
O	2.56296	9.70143	1.80417
O	4.57703	7.96308	1.83269
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.41503	7.87518	1.78281
O	2.22673	3.90565	-0.00141

Atom	Coordinates / Å		
	X	Y	Z
O	2.22590	3.93672	3.72000
O	2.14215	7.68770	-0.00571
Mo	2.88097	7.99720	1.84549
O	2.31619	7.63637	3.71492
O	4.49650	3.82924	1.85989
H	2.58358	8.24115	4.42055
H	0.28133	6.79005	5.94141
H	2.03261	1.71230	2.63821
H	2.04718	1.70180	1.10803
H	2.67091	3.71535	4.54744
H	0.28206	3.33291	6.16300
H	2.62811	7.89947	-0.81259
H	-0.30137	8.61366	-2.51917
H	0.23036	3.31723	-2.42839
H	2.65342	3.75625	-0.85387
H	1.06326	5.89143	3.77784
H	0.98596	5.87089	0.42648
O	-0.30421	10.19306	2.89483
H	0.53474	10.41474	2.44524
O	0.68417	9.76684	4.39941
H	0.16924	10.04267	5.17788

Q. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS9" Transition State Structure

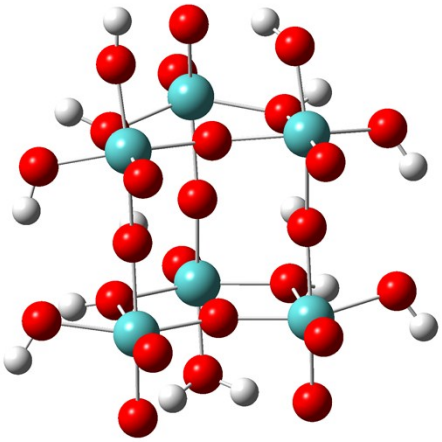


Total B3LYP Energy: -2295.2935978 Hartree BSSE correction: 0.007443492324 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37688	7.74646	5.58071
O	-1.84673	7.67210	3.82416
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.34355	4.09200	5.64834
O	-1.79462	3.95339	3.64116
O	0.08291	5.80887	0.01617
O	0.36535	8.17933	-1.86070
O	-1.86630	7.81520	-0.19010
Mo	-0.10311	3.86863	0.00000
Mo	-0.20627	7.73957	0.00000
O	0.18602	1.94025	0.01617
Mo	-0.21526	8.07676	3.72000
O	0.35838	4.15122	-1.90385
O	-1.79776	3.99704	0.02549
O	2.52013	5.86430	1.87546
O	2.41501	9.80852	1.84251
O	4.39788	8.02905	1.83426
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.38274	7.52674	1.85930
O	2.22673	3.90565	-0.00141

Atom	Coordinates / Å		
	X	Y	Z
O	2.22590	3.93672	3.72000
O	2.12342	7.78202	-0.00141
Mo	2.69771	8.12126	1.85930
O	2.12390	7.76369	3.72000
O	4.49759	3.81786	1.86461
H	2.50622	8.13605	4.52449
H	0.19892	6.82850	5.84492
H	2.01858	1.71432	2.62921
H	2.07015	1.69165	1.10028
H	2.64328	3.63518	4.53657
H	0.24888	3.27031	6.14366
H	2.57805	8.05468	-0.80725
H	-0.34052	8.22552	-2.52347
H	0.22906	3.36157	-2.44192
H	2.67763	3.79431	-0.84640
H	1.05451	5.93154	3.72746
H	0.94865	5.86029	0.52165
O	-0.03800	9.84762	4.44504
O	-0.62682	9.47595	2.04430
H	-0.91435	10.34840	2.34871
H	0.08111	9.81306	5.40626

R. HOOH + $Mo_6O_{23}H_{10}$ + 2H Hydrogen Bronze "TS10" Transition State Structure



Total B3LYP Energy: -2295.39473788 Hartree BSSE correction: 0.011032539061 Hartree

Atom	Coordinates / Å		
	X	Y	Z
O	0.08291	5.80887	3.73617
O	0.37774	7.71430	5.58071
O	-1.84499	7.80048	3.83335
Mo	-0.10311	3.86863	3.72000
O	0.18602	1.94025	3.73617
O	0.48023	3.86863	1.85930
O	0.35413	4.14534	5.64706
O	-1.79512	3.96735	3.66678
O	0.08291	5.80887	0.01617
O	0.38176	7.56352	-1.86070
O	-1.84253	7.79717	-0.05950
Mo	-0.10311	3.86863	0.00000
Mo	-0.16650	7.90315	-0.05026
O	0.18602	1.94025	0.01617
Mo	-0.16998	7.92111	3.75984
O	0.37343	4.18968	-1.92000
O	-1.79582	3.95734	0.02229
O	2.52013	5.86430	1.87546
O	2.46393	9.72289	1.81665
O	4.52294	8.01643	1.91331
Mo	2.80924	3.93672	1.85930
O	2.62324	1.99568	1.87546
O	0.37132	7.79141	1.83966
O	2.22673	3.90565	-0.00141

Atom	Coordinates / Å		
	X	Y	Z
O	2.22590	3.93672	3.72000
O	2.21909	7.60654	0.01603
Mo	2.82794	8.01725	1.87028
O	2.20544	7.65627	3.73457
O	4.49741	3.81833	1.85462
H	2.67203	7.91057	4.53978
H	0.13685	6.90056	6.05405
H	2.03152	1.71109	2.63620
H	2.04159	1.70657	1.10844
H	2.63743	3.63331	4.53860
H	0.23580	3.34398	6.17005
H	2.63186	7.98429	-0.77100
H	0.33663	6.63918	-2.16774
H	0.20293	3.42921	-2.48785
H	2.66533	3.70812	-0.83779
H	1.06151	5.88676	3.66844
H	1.04074	5.89038	0.22994
O	0.14422	9.76332	3.63278
O	0.13266	9.72599	-0.18923
H	0.08552	10.68299	-0.13315
H	0.93325	10.10370	3.16480