

**Combined kinetic and DFT studies on the stabilization of the
pyramidal form of H_3PO_2 at the heterometal site of
 $[\text{Mo}_3\text{M}'\text{S}_4(\text{H}_2\text{O})_{10}]^{4+}$ clusters ($\text{M}' = \text{Pd}, \text{Ni}$)**

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Table S1. Summary of total energies for the different species involved in the proposed mechanism.

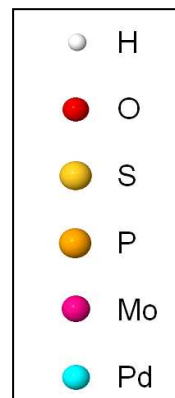
Species	gas phase <i>E</i> (hartrees)	aqueous solution <i>E</i> (hartrees)
H ₂ O	-76.46069560	-76.47397018
H ₃ O ⁺	-76.73277680	-76.87103060
<i>tet</i> -H ₃ PO ₂	-493.7405206	-493.7664040
<i>pyr</i> -H ₃ PO ₂	-493.7313513	-493.7531565
H ₃ PO ₂ -TS ^a	-493.6411556	-493.6623655
H ₄ PO ₂ ⁺	-494.0609353	-494.1823255
1	-1133.3670102	-1134.3192327
<i>osc</i> -1	-1627.1827303	-1628.0883878
TS (1 to I)	-1627.1659552	-1628.0744722
I ··H ₂ O	-1627.1833303	-1628.0863809
I	-1550.6758967	-1551.5989257
TS (I to I ₃) ^b	-1550.5725241	-1551.4982605
I ₂	-1550.5436534	-1551.1473050
I ₃	-1550.6570159	-1551.5927540
TS (I ₃ to 2)	-1550.6449943	-1551.5887665
2	-1550.6828827	-1551.6209159
I -Mo _β ...H ₂ O	-1627.2068235	-1628.10068350
I -Mo _β	-1550.6974064	-1551.60623982
I ₂ -Mo _β	-1550.5820872	-1551.15683811
I ₃ -Mo _β	-1550.6464023	-1551.58177040
2 -Mo _β	-1550.6833204	-1551.60775678
TS (I to I ₃)-Mo _β ^b	-1550.5860916	-1551.50072969
I -Mo _α ...H ₂ O	-1627.2058558	-1628.09729190
<i>osc</i> -2	-1627.2002332	-1628.09029611
I -Mo _α	-1550.6971755	-1551.60639253
I ₂ -Mo _α	-1550.6099981	-1551.17124533
I ₃ -Mo _α	-1550.6561981	-1551.58463340
2 -Mo _α	-1550.6761444	-1551.60189759
TS (I to I ₃)-Mo _α ^b	-1550.5849737	-1551.50078221

^a Transition state for tautomerization in free H₃PO₂. ^b Transition state for direct conversion of **I** to **I**₃ without participation of a second H₃PO₂ molecule.

Table S2. Cartesian Coordinates (in Å) for the different species discussed in the text.

tet-H₃PO₂

O	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.489502
O	1.447730	0.000000	2.243817
H	-0.669194	1.104645	2.064070
H	-0.547825	-1.123526	2.138357
H	2.108980	0.550099	1.797406



pyr-H₃PO₂

O	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.694411
O	1.644057	0.000000	2.103955
H	-0.202743	-0.856595	-0.425289
H	-0.083230	1.425722	1.759438
H	2.008272	-0.856104	2.404218

H₃PO₂-TS

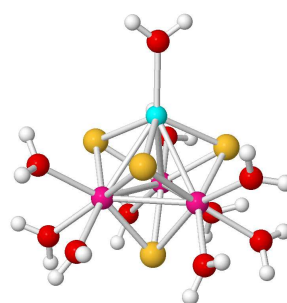
O	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.665568
O	1.491671	0.000000	2.306132
H	0.469689	0.725557	-0.459545
H	-0.634385	-1.283525	1.771161
H	0.419150	0.845668	2.835286

H₄PO₂⁺

O	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.583449
O	1.419008	0.000000	2.286246
H	-0.532605	1.254726	1.914093
H	-0.786852	-1.070662	2.071843
H	0.142601	-0.699094	-0.668677
H	2.081653	-0.699270	2.453930

1

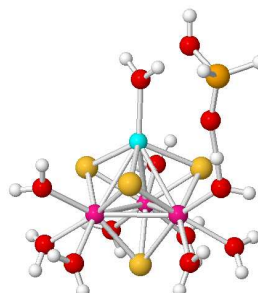
S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.458032
S	2.330806	0.000000	3.116046
Pd	1.413246	2.367672	3.164796
O	2.171296	3.618827	4.796335
Mo	2.159600	0.831344	0.851235
O	4.349010	1.082960	1.078607
Mo	-0.241977	2.294917	0.838090
S	-1.078140	2.081356	3.111361
O	2.979718	-1.086311	0.101423
S	1.988385	3.248872	0.848637
O	-0.836304	4.421887	0.918716
O	-2.432153	2.246064	0.321557



O	-2.136180	-0.732642	2.431465
O	0.086075	-2.207121	2.282799
O	-0.422346	2.830126	-1.308354
O	2.831180	1.193212	-1.270151
O	-0.291910	-0.705999	4.539928
H	-2.384326	-1.599637	2.047336
H	-2.922649	-0.271454	2.788487
H	-1.182703	-0.908557	4.896304
H	0.356080	-0.609913	5.270589
H	0.110886	-2.796428	1.501666
H	0.207925	-2.709709	3.118093
H	-3.194955	2.144975	0.926512
H	-2.720666	2.234688	-0.615731
H	-0.344526	2.260840	-2.101442
H	-0.488812	3.780769	-1.546409
H	-0.264838	5.174217	1.182514
H	-1.783654	4.673547	0.960794
H	2.927021	2.060874	-1.714648
H	3.078364	0.456549	-1.868142
H	4.888433	1.495541	0.370383
H	4.841712	1.070693	1.926363
H	2.533534	-1.846668	-0.324438
H	3.914366	-1.293152	0.322007
H	3.115834	3.786092	4.988599
H	1.601109	4.079732	5.444477

osc-1

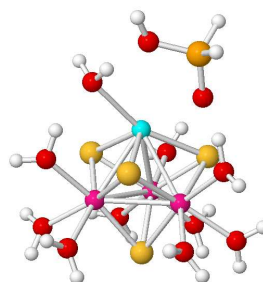
S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.458121
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Mo	-1.572407	-1.704180	0.874664
O	-2.764715	-3.466829	1.032109
Mo	-2.028145	1.077374	0.863537
O	-1.151986	3.104800	0.375362
O	-1.914342	-2.320694	-1.219835
S	-3.737787	-0.629263	0.836024
Pd	-2.739379	-0.454799	3.148656
S	-0.863010	-2.162614	3.138818
O	-2.480746	1.501666	-1.266896
S	-1.526272	1.764440	3.145438
O	1.501722	1.691490	2.428590
O	-4.261558	-0.855148	4.637618
O	-4.806350	-3.557250	2.340836
P	-5.975728	-4.035778	3.212970
O	-6.036915	-3.024689	4.513695
O	2.001230	-0.919955	2.237384
O	-0.019713	-3.284122	0.399910
O	-3.788979	2.423911	0.957515
H	-5.829839	-5.346050	3.731740
H	-1.020513	3.380916	-0.555623
H	-0.796452	3.769498	0.998351
H	-3.668931	3.394926	1.020168
H	-4.688648	2.162827	1.245317
H	-2.006749	1.237786	-2.080722
H	-3.363351	1.882006	-1.466613
H	1.368674	2.614716	2.723313
H	2.395208	1.564926	2.046679
H	2.459449	-1.219118	1.426132
H	2.476208	-1.191049	3.052219



H	0.436376	-0.567104	5.261415
H	1.275236	0.762796	4.896344
H	0.501955	-3.804512	1.044060
H	0.157150	-3.563439	-0.522241
H	-2.304416	-4.330671	1.026701
H	-3.688532	-3.525111	1.587797
H	-1.612778	-1.979109	-2.084921
H	-2.642576	-2.975247	-1.307590
H	-4.879770	-1.630740	4.595996
H	-4.405957	-0.304568	5.430053
H	-6.681174	-3.147702	5.247944
H	-7.233737	-3.943479	2.571620

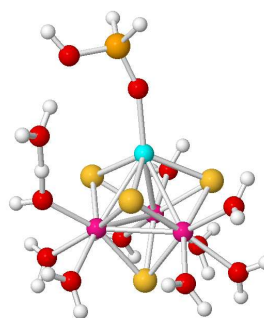
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S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.484247
S	2.331070	0.000000	3.131674
Pd	1.380794	2.379041	3.101536
O	0.711713	4.605329	3.940959
Mo	2.158051	0.804380	0.855779
O	4.349886	1.018527	1.068629
Mo	-0.228734	2.314675	0.846771
S	-1.137122	2.017187	3.060935
O	2.949561	-1.151000	0.151578
S	2.035936	3.206811	0.796802
O	-0.716697	4.399656	1.427519
O	-2.331651	2.201644	0.135086
O	-2.095519	-0.824651	2.416231
O	0.184846	-2.224477	2.411213
O	2.865087	1.071795	-1.277775
O	-0.270307	3.154285	-1.229547
O	-0.244994	-0.448776	4.574365
O	0.494329	1.475771	5.961567
P	0.482497	2.392917	7.201573
O	0.179841	3.930905	6.677729
H	-2.288096	-1.755365	2.180338
H	-2.903032	-0.354061	2.705755
H	-0.970845	-1.001488	4.924569
H	0.078704	0.282796	5.254820
H	0.170609	-2.846737	1.656391
H	0.479204	-2.669383	3.235712
H	-2.973884	2.903735	0.375253
H	-2.778943	1.432404	-0.273417
H	-1.007368	2.960023	-1.845131
H	0.350272	3.808158	-1.609840
H	-0.405177	4.675492	2.336023
H	-0.928824	5.161432	0.851393
H	2.877025	1.897909	-1.801320
H	3.057071	0.292863	-1.840573
H	4.879628	1.380873	0.326961
H	4.847315	1.062209	1.912058
H	2.493957	-1.911574	-0.261822
H	3.873894	-1.371372	0.398707
H	1.357499	5.344986	3.938893
H	0.361331	4.469659	4.862499
H	-0.524443	2.098848	8.155026
H	1.728835	2.443127	7.869430
H	-0.067936	4.646482	7.307755



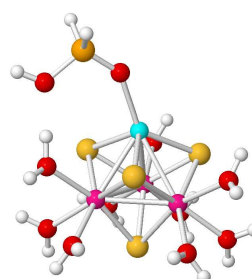
I...H₂O

S	-0.025018	-0.018653	0.013038
Mo	-0.006154	0.077866	2.481903
O	2.189288	0.151193	2.283194
Mo	-0.833418	2.173264	0.791887
O	-0.902145	2.728381	-1.359783
Mo	-2.316695	-0.198537	0.888952
S	-2.086929	-0.965042	3.179722
Pd	-2.327897	1.540251	3.133149
O	-3.292781	2.388429	4.869188
P	-3.643382	2.638832	6.341928
O	-2.431381	2.026797	7.292273
S	-3.251623	2.033047	0.797772
S	0.027815	2.442780	3.026796
O	1.175164	3.068568	0.262957
O	-4.453134	-0.780072	1.037941
O	-2.936009	-0.459738	-1.233481
O	0.630940	-0.084217	4.507673
O	0.094906	1.387876	6.356896
O	-2.280867	-2.403104	0.432533
O	0.703843	-2.074403	2.491191
O	-1.269511	4.352682	0.821422
H	1.436824	3.216113	-0.669621
H	1.885447	3.327677	0.884448
H	-0.545391	5.011863	0.865710
H	-2.121686	4.747331	1.101192
H	-0.712311	2.201871	-2.161818
H	-1.322166	3.588019	-1.580128
H	2.682604	0.249556	3.126434
H	2.769518	0.200453	1.497234
H	1.567385	-2.327980	2.104134
H	0.269517	-2.837927	2.922045
H	0.379813	0.608070	5.350667
H	0.835724	-0.980141	4.845226
H	-2.092381	-3.138032	1.048934
H	-2.335096	-2.717625	-0.494016
H	-4.702274	-1.724466	1.123265
H	-5.184061	-0.195109	1.327721
H	-2.414760	-0.431477	-2.060583
H	-3.901214	-0.445041	-1.412441
H	0.799625	1.733470	6.937838
H	-0.820302	1.600591	6.684116
H	-3.732374	4.015515	6.657379
H	-4.827758	1.996900	6.781054
H	-2.548085	1.912372	8.263776



I

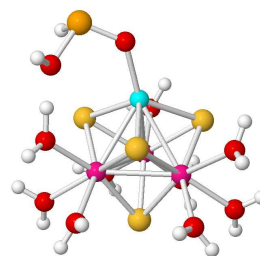
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Mo	0.000000	0.000000	2.464424
O	2.250139	0.000000	2.434379
Mo	-0.612307	-2.237757	0.849281
O	1.405059	-3.048991	0.289685
Mo	-2.307588	0.025589	0.875457
O	-3.073414	0.003139	-1.250584
S	0.300325	-2.307566	3.102839
Pd	-2.145704	-1.726395	3.107860
O	-3.117041	-3.212083	4.353251



P	-3.390943	-4.723147	4.413432
O	-2.767314	-5.439737	3.030629
S	-3.040433	-2.263980	0.821851
O	-0.723757	-2.871562	-1.277832
S	-2.167247	0.847149	3.152173
O	-4.436982	0.586372	1.128938
O	0.508789	0.526719	4.555731
O	0.678616	2.118339	2.316954
O	-2.372870	2.137048	0.183313
O	-0.948395	-4.389550	1.168456
H	-0.569290	-2.342001	-2.086891
H	-1.100180	-3.753587	-1.487719
H	-0.223764	-5.033748	1.031481
H	-1.643396	-4.748490	1.799745
H	1.669813	-3.146340	-0.648947
H	2.134086	-3.302822	0.890997
H	-3.467512	-0.755011	-1.728249
H	-3.026542	0.800403	-1.818793
H	-1.699546	2.690568	-0.261200
H	-3.148917	2.669387	0.464508
H	-4.892810	0.702314	1.989621
H	-5.086307	0.450627	0.406766
H	0.824687	2.695476	1.540656
H	0.704442	2.629406	3.155420
H	-0.137460	0.627577	5.286677
H	1.413447	0.385670	4.907381
H	2.738195	0.804914	2.161233
H	2.861100	-0.745018	2.603464
H	-2.750432	-5.371199	5.496801
H	-3.015193	-6.371739	2.823495
H	-4.765210	-5.066460	4.417777

I₂

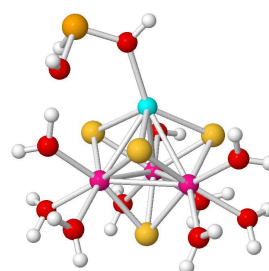
S	-0.008767	0.024103	0.023055
Mo	-0.062359	0.104398	2.505948
S	2.263809	0.115491	3.232713
Pd	1.263216	2.443664	3.204574
S	-1.195178	2.191294	3.069544
Mo	-0.272217	2.337974	0.843544
S	1.934966	3.376399	0.882188
Mo	2.090505	0.936126	0.948768
O	4.251086	1.444415	1.142291
O	3.121369	-1.008745	0.475962
O	-0.884661	4.483167	0.903953
O	-2.465349	2.237376	0.273062
O	-2.100726	-0.787897	2.403238
O	0.229665	-2.132208	2.573214
O	1.668938	3.264955	5.046676
P	0.845402	3.031625	6.408753
O	0.433254	1.288141	6.370246
O	-0.465786	-0.242393	4.604881
O	2.822813	1.048931	-1.180728
O	-0.431792	2.932395	-1.310978
H	-2.645265	-1.043971	1.633739
H	-2.608914	-0.773000	3.241632
H	-0.457962	-1.161643	4.938791
H	-0.141242	0.451012	5.365669
H	-0.426250	-2.763485	2.215732
H	1.001224	-2.584885	2.966746



H	-3.218253	2.103233	0.881401
H	-2.743286	2.269176	-0.664380
H	-0.331025	2.407484	-2.128260
H	-0.379635	3.897033	-1.479746
H	-0.302187	5.185079	1.262163
H	-1.828920	4.727828	0.988604
H	2.357251	0.889790	-2.024160
H	3.650221	1.560155	-1.306559
H	4.567292	2.293540	1.515410
H	4.906569	0.729741	1.278330
H	3.307953	-1.240602	-0.456167
H	3.287914	-1.753658	1.085208
H	-0.493614	3.407616	6.027857
H	0.770192	0.812263	7.159409

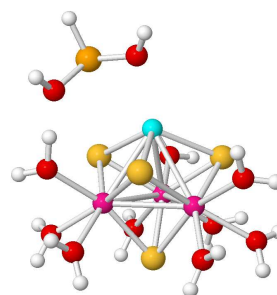
I₃

O	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.211510
O	2.161989	0.000000	1.729793
S	-2.418706	-0.352325	1.950121
Mo	-1.787824	-0.437275	4.322447
O	-1.914622	-2.696927	4.275498
Mo	-1.972903	1.940006	2.783542
O	-2.350175	2.764078	0.722976
S	0.603870	-0.891645	4.398547
Pd	0.188480	1.617886	4.559837
O	1.127376	3.251269	5.783722
P	0.896354	4.961166	5.530167
O	-0.820900	4.966578	5.277242
S	0.322746	2.395612	2.169376
O	-4.145191	2.318842	2.642806
S	-2.257443	1.761020	5.179681
O	-3.903001	-0.991665	4.663523
O	-2.080289	4.049680	3.260753
O	0.354153	-2.131246	1.562006
O	-1.849516	-0.989458	6.468576
H	0.847943	0.160371	-0.468265
H	-0.759424	-0.024593	-0.617336
H	2.664022	-0.835073	1.617845
H	2.773841	0.753138	1.870744
H	0.103204	-2.437675	0.665215
H	0.734838	-2.860684	2.091951
H	-3.254589	2.827211	0.350810
H	-1.684303	3.144807	0.114369
H	-4.890709	1.751775	2.359181
H	-4.461060	3.143284	3.074208
H	-2.775014	-3.149968	4.151310
H	-1.178047	-3.339998	4.312404
H	-4.653311	-1.063392	4.039467
H	-4.200670	-1.059672	5.596980
H	-1.672179	-1.912391	6.749385
H	-1.759895	-0.373552	7.225927
H	1.140274	4.852198	4.127838
H	-1.607523	4.456636	4.098660
H	-2.198285	4.715492	2.552292
H	-1.333756	5.429832	5.977337
H	1.578314	3.026414	6.627855



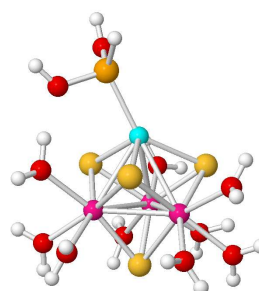
TS (I₃ to 2)

O	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.209403
O	2.161308	0.000000	1.545447
Pd	-1.560065	0.409982	4.586393
S	-2.092904	-1.978596	5.186729
Mo	-2.236402	-1.639786	2.795909
O	-3.077979	-1.881814	0.718038
S	0.994833	0.438200	4.381985
Mo	0.155397	-1.845067	4.333154
O	0.372344	-4.016299	4.679926
S	-0.047156	-2.445734	1.961417
O	0.345601	2.131041	1.719842
S	-2.312099	0.692681	2.175294
O	2.363704	-2.321744	4.268276
O	-2.967559	-3.719880	2.644214
O	-4.336048	-1.433298	3.251836
O	-5.092353	-0.023642	5.201184
P	-4.216883	1.450025	5.476098
O	-3.165294	1.095729	6.723583
O	0.691026	-1.977702	6.480260
H	-0.019059	0.866708	-0.461259
H	-0.108184	-0.748404	-0.621954
H	1.250814	2.494420	1.616691
H	-0.301444	2.855415	1.856960
H	2.411512	-0.291393	0.643497
H	2.950092	0.245428	2.070026
H	-3.293465	-2.767269	0.357154
H	-3.342511	-1.168265	0.101955
H	-2.526727	-4.555739	2.389949
H	-3.844305	-3.881101	3.058394
H	2.678518	-3.242436	4.148961
H	3.112970	-1.693460	4.304624
H	0.314931	-4.771778	4.060597
H	0.398485	-4.315116	5.615224
H	1.628331	-1.949966	6.768637
H	0.093350	-1.768856	7.229048
H	-5.264133	2.140228	6.169497
H	-4.688536	-0.899420	4.091248
H	-4.986208	-1.406340	2.519391
H	-5.878545	-0.262211	5.742756
H	-3.375685	1.145616	7.683685



2

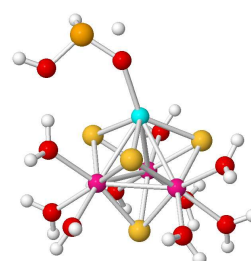
S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.457267
O	2.245082	0.000000	2.386948
Mo	-0.610529	-2.234475	0.862651
O	1.430635	-3.005472	0.360013
Mo	-2.296100	0.033776	0.900111
O	-2.907533	0.291768	-1.196192
S	0.253470	-2.297720	3.149073
Pd	-2.174802	-1.808730	3.177092
P	-3.255295	-3.631549	4.263586
O	-4.861631	-3.587823	4.102424
S	-3.037888	-2.249170	0.885451
O	-0.754275	-2.909153	-1.241890



S	-2.193249	0.772154	3.218101
O	-4.477951	0.436524	1.022607
O	0.563965	0.572755	4.519562
O	-2.654711	-4.901146	3.320575
O	0.633207	2.118241	2.243100
O	-2.393686	2.274271	0.558640
O	-0.973355	-4.374264	1.220940
H	-1.190397	-3.769963	-1.423749
H	-0.542346	-2.437679	-2.072826
H	-0.340767	-5.087257	0.999294
H	-1.629802	-4.657947	1.934368
H	1.774776	-3.038519	-0.556906
H	2.057159	-3.423166	0.985590
H	-3.869726	0.250104	-1.388777
H	-2.374211	0.353044	-2.014248
H	-2.461456	2.680531	-0.330921
H	-2.415458	2.950553	1.267149
H	-5.152399	-0.215918	1.308402
H	-4.816953	1.350516	1.131229
H	0.717669	2.660802	1.432662
H	0.745858	2.653729	3.058398
H	-0.058409	0.711853	5.264336
H	1.477467	0.430995	4.847438
H	2.730905	0.785411	2.058246
H	2.851736	-0.752165	2.538849
H	-3.019428	-4.119757	5.582479
H	-2.885578	-5.835483	3.537369
H	-5.541862	-4.092162	4.601995

TS (I to I₃)

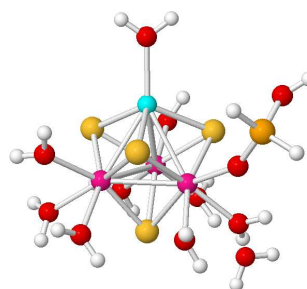
S	-0.000907	0.002694	0.008029
Mo	-0.017313	-0.000522	2.471780
O	2.238736	0.015807	2.462096
Mo	-0.606526	-2.237514	0.855377
O	1.425941	-3.028823	0.324780
Mo	-2.310323	0.011979	0.874489
O	-3.053359	-0.030515	-1.259102
S	0.283278	-2.306192	3.116626
Pd	-2.180280	-1.750849	3.103922
O	-2.996791	-3.277859	4.416130
P	-3.622826	-4.799652	4.294095
O	-2.838362	-5.462401	2.953113
S	-3.042979	-2.282666	0.830412
O	-0.693997	-2.867094	-1.271580
S	-2.192193	0.824613	3.161775
O	-4.443308	0.580523	1.110229
O	0.487476	0.527807	4.562565
O	0.644813	2.123482	2.319100
O	-2.388134	2.122167	0.182079
O	-0.936215	-4.393375	1.161481
H	-0.541168	-2.332546	-2.077425
H	-1.048061	-3.757017	-1.486660
H	-0.204634	-5.034780	1.049611
H	-1.643677	-4.750965	1.776829
H	1.715043	-3.109001	-0.608276
H	2.136772	-3.300450	0.940103
H	-3.453715	-0.789004	-1.730932
H	-2.993261	0.759708	-1.835752
H	-1.717922	2.685659	-0.254457



H	-3.174842	2.642911	0.454932
H	-4.901905	0.704589	1.968069
H	-5.089703	0.441100	0.386140
H	0.802549	2.692530	1.539082
H	0.661164	2.643134	3.152410
H	-0.155965	0.632071	5.295071
H	1.394437	0.390588	4.909379
H	2.724173	0.823107	2.191338
H	2.852808	-0.727689	2.627031
H	-3.011239	-4.112614	5.548181
H	-3.036559	-6.401353	2.720262
H	-4.976180	-4.729613	3.825776

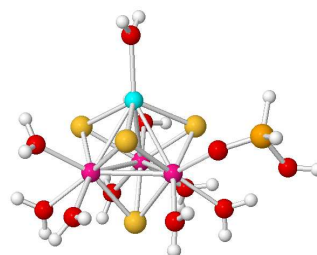
I-Mo_β···H₂O

S	0.082283	-0.246654	0.809019
Mo	-0.145215	-0.672534	3.225416
O	2.088483	-1.060582	3.044634
Mo	-0.795733	-2.497746	1.201931
O	1.243514	-3.148995	0.632286
Mo	-2.266814	-0.109615	1.481909
O	-2.798996	0.373919	-0.648450
S	-0.210304	-3.083996	3.480391
Pd	-2.588207	-2.182606	3.390154
O	-4.044846	-3.181913	4.709147
S	-3.198316	-2.291837	0.933623
O	-0.787966	-2.823087	-1.020252
S	-2.270651	0.271992	3.880581
O	-4.351168	0.638828	1.657230
O	0.756609	1.296075	3.405996
O	0.421471	-0.544953	5.288227
P	0.236130	-0.927193	6.795324
O	-1.127369	-0.308860	7.358146
O	0.273798	3.366514	1.752262
O	-1.998604	2.043216	1.221760
O	-1.028804	-4.694396	1.009155
H	1.334218	-0.435964	7.541024
H	0.071544	-2.849948	-1.491020
H	-1.542858	-2.845886	-1.641475
H	-1.333019	-5.096617	0.168615
H	-1.124055	-5.322612	1.754806
H	2.054347	-2.606564	0.710223
H	1.443348	-4.109799	0.627190
H	-3.251015	-0.177475	-1.317796
H	-2.477368	1.218830	-1.026610
H	-1.152861	2.581853	1.338557
H	-2.808569	2.579114	1.356320
H	-4.856052	0.688904	2.495394
H	-4.954360	0.653712	0.884663
H	0.131586	4.224679	2.215019
H	0.902590	3.513845	1.009488
H	0.676845	2.094883	2.798428
H	0.984621	1.522922	4.332003
H	2.528168	-1.661348	3.682847
H	2.661222	-0.292015	2.835569
H	-4.349862	-2.839434	5.571824
H	-4.516646	-4.005585	4.475542
H	-1.339884	0.040232	8.249922
H	0.158792	-2.330673	6.949700



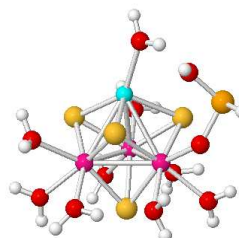
I-Mo_β

S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.459924
O	2.248896	0.000000	2.436098
Mo	-2.305829	-0.109587	0.849932
O	-4.469389	0.318696	1.071412
Mo	-0.490778	-2.251024	0.856714
O	-0.529542	-4.399674	0.913425
P	0.198080	-5.719522	1.292982
O	1.770776	-5.457344	0.919200
O	-3.035486	-0.278928	-1.267490
S	-2.199679	0.777524	3.101366
Pd	-2.127817	-1.777058	3.154139
O	-3.274896	-2.647194	4.813494
S	-2.915261	-2.453595	0.879018
O	1.586557	-2.732606	0.263568
S	0.339960	-2.297314	3.145032
O	0.505852	0.570135	4.543506
O	0.657871	2.116213	2.292594
O	-2.523718	1.956588	0.067242
O	-0.740810	-2.786410	-1.300682
H	2.180962	-2.215427	-0.314272
H	1.904170	-3.663282	0.408587
H	-3.239739	-1.111573	-1.738888
H	-3.083389	0.498679	-1.861697
H	-1.875774	2.549184	-0.364215
H	-3.348360	2.434211	0.304239
H	-4.936117	0.474897	1.919160
H	-5.100144	0.055803	0.367655
H	0.785801	2.684194	1.506358
H	0.685137	2.638497	3.123625
H	-0.136589	0.732672	5.265626
H	1.400720	0.393346	4.903585
H	2.757955	0.808759	2.219635
H	2.829782	-0.779948	2.544455
H	-4.123455	-3.120017	4.702959
H	-3.006424	-2.629668	5.753090
H	-0.301009	-2.386524	-2.078283
H	-1.050821	-3.698157	-1.485768
H	0.125211	-6.028645	2.672275
H	-0.283362	-6.810034	0.530659
H	2.491325	-6.129542	0.938600



I₂-Mo_β

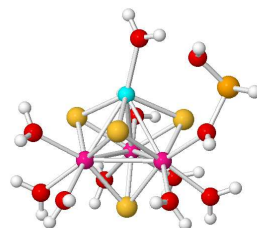
S	1.473064	0.228518	1.923497
Mo	1.378260	-1.223710	-0.058332
O	1.341617	-2.879513	1.451387
Mo	-0.863518	-0.014385	1.087300
O	-1.411186	1.010731	2.956426
Mo	1.174248	1.539881	-0.126059
S	1.985061	0.175429	-1.968480
Pd	-0.568705	0.028468	-1.732689
S	-0.902028	-1.987097	-0.313762
S	-1.210982	1.971413	-0.260134
O	-0.976884	-1.784557	2.693954
O	-2.260233	-0.186499	-3.081347
O	1.414947	3.177592	-1.631775



O	1.084079	3.399732	1.154653
O	1.854785	-2.924370	-1.422299
O	3.511492	-1.658682	0.332816
O	3.255530	2.265176	0.188505
O	-4.011708	-0.800829	-1.134520
P	-4.132826	0.262873	0.196504
O	-2.847223	-0.199939	1.209387
H	-0.850501	-1.526764	3.633533
H	-1.863645	-2.198877	2.579502
H	-0.915576	1.490853	3.647195
H	-2.388388	1.083592	3.033838
H	0.552337	-2.891851	2.044872
H	2.121118	-3.331855	1.828359
H	4.095725	-1.351980	1.052546
H	3.990992	-2.171463	-0.351001
H	1.909156	-2.833184	-2.395899
H	1.572107	-3.827959	-1.168252
H	3.952230	1.922639	0.781354
H	3.623174	2.803763	-0.544080
H	1.435805	3.012358	-2.596936
H	1.080685	4.076984	-1.434939
H	1.899318	3.750246	1.566776
H	0.279293	3.866406	1.454372
H	-3.087190	-0.408285	-2.569425
H	-2.381026	-0.051988	-4.037911
H	-5.136286	-0.469635	0.920260
H	-4.444066	-1.681253	-1.120062

I₃-Mo_β

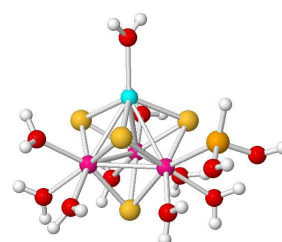
S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.460700
O	2.253653	0.000000	2.431749
Mo	-0.592936	2.243223	0.842490
O	-0.623506	2.828480	-1.296001
Mo	-2.307840	-0.002802	0.869794
S	-2.175178	-0.834567	3.145169
Pd	-2.150296	1.705194	3.139658
S	0.295309	2.313839	3.102652
S	-3.018803	2.297362	0.834244
O	1.475100	2.994563	0.310857
O	-3.120413	3.074324	4.504438
O	-4.447666	-0.539349	1.122926
O	-3.065530	0.066905	-1.258133
O	0.516951	-0.535581	4.549516
O	0.654439	-2.118732	2.302681
O	-2.418494	-2.099569	0.149555
O	-2.037882	5.360003	3.315063
P	-2.236767	5.435166	1.658609
O	-0.818302	4.446659	1.057719
H	1.736093	3.087268	-0.629835
H	2.238045	3.146776	0.904109
H	-0.497702	2.257902	-2.081993
H	-0.937439	3.724556	-1.544709
H	2.862496	0.727232	2.671730
H	2.748235	-0.788987	2.125300
H	0.806118	-2.690401	1.523339
H	0.678532	-2.635215	3.137790
H	-0.123368	-0.630952	5.286161



H	1.427121	-0.416154	4.894510
H	-1.748764	-2.670701	-0.277629
H	-3.220595	-2.608938	0.398940
H	-4.896352	-0.674939	1.984445
H	-5.104982	-0.363860	0.416322
H	-3.025236	-0.723894	-1.835857
H	-3.476137	0.827475	-1.718235
H	-2.916738	4.026205	4.336932
H	-3.730953	2.919132	5.250033
H	-1.552953	6.673937	1.414902
H	-1.546510	6.033080	3.838042
H	0.057793	4.895371	1.051361

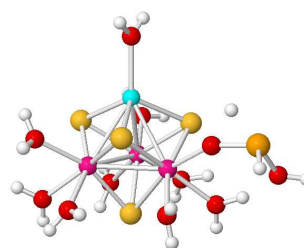
2-Mo_β

S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.456315
O	2.247260	0.000000	2.424661
Mo	-2.306273	-0.185558	0.824836
O	-4.483303	0.196002	1.015363
Mo	-0.433385	-2.269949	0.871946
P	-0.360628	-4.856051	1.065811
O	1.247290	-5.194058	1.156269
O	-3.014508	-0.419513	-1.295308
S	-2.224299	0.751849	3.059260
Pd	-2.104173	-1.784870	3.173897
O	-3.223425	-2.655530	4.856037
S	-2.859095	-2.544255	0.896668
O	1.679335	-2.699994	0.376257
S	0.363734	-2.284082	3.179255
O	0.495116	0.597006	4.534510
O	-0.926230	-5.370039	-0.391724
O	-0.602849	-2.885845	-1.243740
O	-2.580969	1.858124	0.005945
O	0.643384	2.116033	2.283456
H	2.246761	-2.255528	-0.284522
H	1.998928	-3.611201	0.619828
H	-3.204111	-1.264530	-1.751400
H	-3.067389	0.344431	-1.907021
H	-1.939468	2.466933	-0.412902
H	-3.426800	2.311790	0.214172
H	-4.965728	0.375065	1.849871
H	-5.099973	-0.096336	0.310627
H	0.764315	2.681133	1.493745
H	0.677562	2.641399	3.112550
H	-0.148425	0.766808	5.254349
H	1.389407	0.423060	4.898401
H	2.759760	0.808389	2.213873
H	2.824663	-0.786142	2.505522
H	-4.154759	-2.949478	4.810254
H	-2.857758	-2.799317	5.751287
H	-0.227261	-2.449453	-2.033975
H	-0.834807	-3.842656	-1.394324
H	-0.967904	-5.722360	2.016762
H	1.662659	-6.068707	1.336892
H	-1.135094	-6.295420	-0.656696



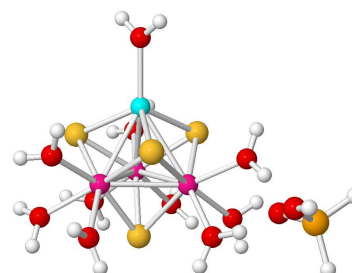
TS (I to I₃)-Mo_β

S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.461546
O	2.255093	0.000000	2.443677
Mo	-0.485533	-2.257694	0.843261
O	1.539979	-2.742836	0.164910
Mo	-2.302885	-0.111414	0.850611
O	-3.025552	-0.218189	-1.269452
S	0.356870	-2.301150	3.125593
Pd	-2.115001	-1.797515	3.141416
O	-3.229145	-2.716958	4.795652
S	-2.911998	-2.455872	0.855541
O	-0.522363	-4.420021	1.020848
P	0.252336	-5.903446	0.848724
O	1.815959	-5.416101	0.578017
S	-2.203489	0.756707	3.109890
O	-4.465971	0.316299	1.059750
O	0.490098	0.565505	4.552575
O	-2.508159	1.980590	0.122457
O	0.655384	2.115243	2.293408
O	-0.795984	-2.797641	-1.333745
H	2.183713	-2.162772	-0.285394
H	1.866222	-3.679711	0.285818
H	-3.164546	-1.034624	-1.789304
H	-3.081147	0.583317	-1.830498
H	-1.860732	2.575309	-0.306676
H	-3.322615	2.462086	0.385017
H	-4.949142	0.453522	1.901532
H	-5.082247	0.073303	0.336210
H	0.783234	2.683882	1.507744
H	0.690232	2.635610	3.125476
H	-0.163790	0.718683	5.266472
H	1.380451	0.393928	4.926002
H	2.763877	0.805389	2.214209
H	2.841396	-0.764045	2.617932
H	-4.129260	-3.089755	4.713637
H	-2.893204	-2.819413	5.707916
H	-0.194851	-2.537498	-2.062161
H	-1.336594	-3.577432	-1.577410
H	-0.672314	-5.398382	1.995598
H	-0.135989	-6.452222	-0.417282
H	2.591253	-6.025766	0.571908



osc-2

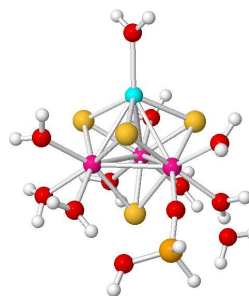
S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.447027
S	2.345067	0.000000	3.093098
Pd	1.379051	2.345500	3.196375
S	-1.118489	2.061350	3.085553
Mo	-0.216090	2.297650	0.836274
S	2.000315	3.265187	0.908596
Mo	2.160666	0.839759	0.840804
O	4.285304	1.226645	0.906457
O	2.992285	-0.957893	0.017407
O	-0.815416	4.427321	0.910667
O	-2.342820	2.245589	0.135555
O	-2.113653	-0.792618	2.438083



O	0.119148	-2.209294	2.281483
O	2.113200	3.521241	4.901628
O	5.454358	-0.892365	0.217770
P	6.812225	-1.683432	0.204583
O	6.945642	-2.467645	1.589850
O	-0.200376	2.803564	-1.315722
O	-0.276556	-0.697221	4.532018
O	2.483870	1.353081	-1.412363
H	-2.300283	-1.710220	2.149599
H	-2.939079	-0.300104	2.619958
H	-1.176096	-0.853904	4.889467
H	0.372552	-0.576988	5.256651
H	0.216450	-2.787875	1.499453
H	0.262912	-2.700779	3.118923
H	-3.168977	2.231365	0.658965
H	-2.516175	2.112676	-0.820641
H	0.388596	2.322269	-1.935332
H	-0.377480	3.722210	-1.611789
H	-0.234403	5.168313	1.180996
H	-1.756368	4.701098	0.909353
H	3.149699	2.053537	-1.593023
H	2.625389	0.593504	-2.018851
H	4.701255	2.016086	1.301348
H	4.948936	0.465268	0.699608
H	2.501370	-1.715975	-0.349735
H	4.039630	-1.113257	0.065706
H	3.031995	3.518678	5.234438
H	1.553453	4.124779	5.429175
H	7.680091	-3.014432	1.940891
H	7.893524	-0.784099	0.053168
H	6.834638	-2.608240	-0.865561

I-Mo_α···H₂O

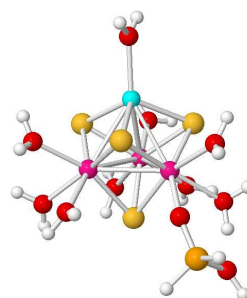
S	0.988826	-0.297379	0.321256
Mo	0.723254	-0.078523	2.752090
S	2.895966	0.487041	3.650641
Pd	1.516970	2.577266	3.336947
S	-0.849404	1.756380	3.041632
Mo	0.238551	1.971007	0.876502
S	2.226719	3.340700	1.019834
Mo	2.841077	1.003394	1.276687
O	4.884044	1.805176	1.534381
O	3.541494	1.130995	-0.792061
O	-0.760578	3.947191	0.693436
O	-1.788798	1.423138	0.084852
O	-1.119184	-1.349897	2.592796
O	1.364328	-2.178014	2.815574
O	1.807232	4.058356	4.935075
O	4.089550	-0.790756	1.113263
P	4.524566	-2.227737	0.750762
O	3.338767	-3.250946	1.265387
O	0.255922	2.313251	-1.287787
O	0.319536	-0.622805	4.865669
O	2.020630	1.331725	-3.018295
H	-1.003094	-2.284639	2.321916
H	-2.062112	-1.100277	2.659915
H	-0.567400	-0.927160	5.151218
H	0.845511	-0.310458	5.631421



H	2.024212	-2.611789	2.204785
H	1.367304	-2.583372	3.708636
H	-2.619870	1.236093	0.564799
H	-1.870297	1.250715	-0.876306
H	0.862243	1.907525	-1.987338
H	-0.080923	3.195357	-1.552803
H	-0.348205	4.803451	0.932797
H	-1.737815	4.022605	0.676946
H	2.364159	2.003743	-3.651443
H	1.781199	0.520789	-3.520852
H	5.124400	2.745148	1.669563
H	5.592013	1.206875	1.851914
H	3.025938	1.121040	-1.652047
H	4.468784	1.423209	-0.902396
H	2.673216	4.383763	5.250073
H	1.076390	4.479142	5.429513
H	3.372106	-4.225001	1.112695
H	5.717846	-2.598516	1.414965
H	4.674290	-2.457478	-0.638702

I-Mo₆

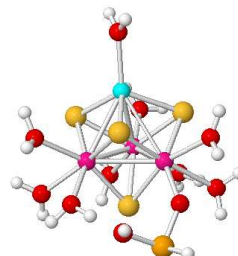
S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.456167
O	2.246423	0.000000	2.445620
Mo	-0.528010	2.247123	0.844452
O	-0.962036	2.750226	-1.338286
Mo	-2.304163	0.094864	0.852389
S	-2.198190	-0.792339	3.102761
Pd	-2.097486	1.758757	3.188300
S	0.353690	2.307776	3.108328
S	-2.955097	2.422329	0.912523
O	1.403380	2.884144	0.112021
P	2.428614	3.119403	-1.035378
O	1.584387	3.017999	-2.429767
O	-3.165210	2.666326	4.877684
O	-4.468952	-0.338408	1.015496
O	-2.945824	0.267447	-1.275641
O	0.499345	-0.564685	4.544435
O	0.653244	-2.117484	2.299191
O	-2.499126	-1.982256	0.084096
O	-0.657959	4.440375	1.030672
H	-0.207022	2.708376	-1.982732
H	-1.492423	3.562791	-1.488400
H	2.828485	0.776184	2.571580
H	2.753139	-0.811523	2.235268
H	0.767090	-2.696464	1.519042
H	0.674396	-2.630376	3.136408
H	-0.150740	-0.706345	5.264676
H	1.391552	-0.386108	4.910358
H	-1.854979	-2.548924	-0.385939
H	-3.306964	-2.481431	0.333197
H	-4.960900	-0.525280	1.842439
H	-5.077076	-0.035823	0.307034
H	-3.120074	-0.511772	-1.842972
H	-2.817437	1.083307	-1.802076
H	-2.729526	3.106822	5.634088
H	-4.138017	2.702311	4.968718
H	-1.429862	4.957445	1.341586
H	0.166777	4.965705	1.088857



H	3.021779	4.402062	-0.952303
H	3.447328	2.137078	-1.073290
H	1.948077	3.151436	-3.336416

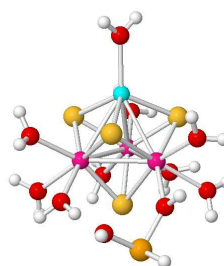
I₂-Mo_α

S	-0.809635	-0.025947	-1.951150
Mo	-0.854879	-1.102509	0.273090
S	1.391332	-2.007889	0.675000
Pd	1.339887	0.332585	1.680224
O	2.351920	0.553759	3.633044
Mo	1.464610	-0.352580	-1.079538
O	3.642838	-0.804416	-1.146182
Mo	-0.336245	1.605913	-0.194216
S	-1.170599	0.673325	1.877317
O	1.406760	-2.204078	-2.321960
S	2.101386	1.824558	-0.184724
O	-0.313257	3.544940	0.876645
O	-2.388364	2.304215	-0.417507
O	-2.778293	-1.483488	0.014584
P	-4.037716	-0.809696	-0.879615
O	-4.252903	0.679973	-0.018325
O	-0.816778	-3.165886	-1.044369
O	2.123957	0.299119	-3.100798
O	-0.302548	3.142502	-1.829524
O	-1.382311	-2.527586	1.867007
H	-1.653823	-3.273671	-1.549644
H	-0.684055	-3.942246	-0.454708
H	-3.216999	1.708287	-0.207330
H	-2.568091	2.965775	-1.114135
H	-0.380905	3.022096	-2.795520
H	0.041512	4.028636	-1.591658
H	0.421452	3.883885	1.426965
H	-1.184756	3.874771	1.181895
H	1.598462	0.584572	-3.872784
H	3.085486	0.436109	-3.229040
H	4.324192	-0.310644	-0.646275
H	3.910544	-1.737200	-1.285805
H	1.655410	-2.263307	-3.264593
H	0.692416	-2.838512	-2.051655
H	1.926395	0.397243	4.497558
H	3.292066	0.793541	3.740108
H	-2.352336	-2.648219	1.951446
H	-0.878495	-2.827680	2.648613
H	-5.098169	-1.508587	-0.209152
H	-4.918806	0.760690	0.696622



I₃-Mo_α

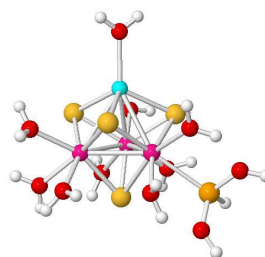
S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.455216
S	2.342177	0.000000	3.113131
Pd	1.435797	2.347055	3.164649
O	2.178167	3.596898	4.807351
Mo	2.152460	0.842675	0.841466
O	4.322544	1.298878	0.913255
Mo	-0.264486	2.299997	0.852399
S	-1.074232	2.072036	3.118721
O	3.088492	-1.152421	0.342002



S	1.967160	3.251273	0.837529
O	-0.894191	4.409165	0.992777
O	-2.382425	2.230591	0.308804
O	-2.042326	-0.934836	2.368065
P	-3.295073	-1.008015	1.096336
O	-3.983788	0.526467	1.329424
O	0.284704	-2.228623	2.408546
O	2.757833	0.915512	-1.284767
O	-0.384202	2.919580	-1.297508
O	-0.460238	-0.570564	4.566297
H	-0.409425	-2.805194	2.026628
H	1.073215	-2.745113	2.670517
H	-3.112893	1.659042	0.743976
H	-2.643740	2.543229	-0.580892
H	-0.451673	2.370807	-2.104976
H	-0.291012	3.871851	-1.516543
H	-0.345596	5.181085	1.244151
H	-1.851355	4.604091	1.086184
H	2.251270	0.743874	-2.103828
H	3.631751	1.320135	-1.477624
H	4.714209	2.158856	1.175287
H	4.990590	0.582800	0.966655
H	3.192051	-1.436098	-0.590482
H	3.407127	-1.840822	0.959823
H	1.729188	4.392322	5.156434
H	3.005775	3.423668	5.298820
H	-0.161825	-1.428634	4.937674
H	-0.621397	0.075570	5.287094
H	-4.226863	-1.748418	1.895909
H	-4.827718	0.682661	1.810348
H	-2.325704	-1.058483	3.305516

2-Mo_α

S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.423094
O	2.222451	0.000000	2.402923
Mo	-0.646648	2.193728	0.779288
O	-0.893485	2.556711	-1.400504
Pd	-2.416906	-0.024904	0.834388
S	-3.066676	2.408336	0.995753
Mo	-2.151085	1.646551	3.104388
P	-2.717158	4.053207	4.131474
O	-1.962858	4.110755	5.588309
O	1.343466	2.959623	0.164892
S	0.202931	2.360048	3.083642
O	-3.760864	-1.250754	-0.384091
S	-2.127059	-0.791579	3.239710
O	0.545619	-2.129212	2.194323
O	-4.230827	1.412942	3.745290
O	-4.344121	3.969205	4.349966
O	-0.789533	4.450388	0.670974
O	-1.862595	1.467414	5.323401
O	0.667597	-0.543567	4.491072
H	-1.231073	3.406938	-1.753038
H	-0.959151	1.852816	-2.080219
H	2.151362	3.140383	0.686290
H	1.528938	2.969399	-0.799647
H	0.025171	4.993855	0.629847
H	-1.595179	4.999534	0.584807



H	2.867301	0.704190	2.616559
H	2.664946	-0.796412	2.036248
H	0.461593	-2.672727	1.382691
H	0.593234	-2.697427	2.993408
H	-4.505269	-0.899566	-0.912253
H	-3.721291	-2.225726	-0.448432
H	1.612464	-0.553323	4.750559
H	0.079838	-0.572198	5.273233
H	-2.509728	5.354037	3.589395
H	-4.950192	4.683705	4.654199
H	-1.901251	4.880913	6.199132
H	-4.729537	2.232815	4.006119
H	-4.806979	0.634152	3.610367
H	-1.577323	2.267993	5.836475
H	-2.510879	0.930803	5.828878

TS (I to I₃)-Mo_α

S	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.460343
S	2.337880	0.000000	3.136420
Pd	1.443747	2.365550	3.155106
S	-1.061259	2.091134	3.101623
Mo	-0.208396	2.299461	0.844072
S	2.036687	3.212391	0.823379
Mo	2.163998	0.797839	0.859964
O	4.347412	1.160585	0.965450
O	3.020064	-1.216153	0.381030
O	-0.756646	4.451018	0.922370
O	-2.408681	2.266856	0.355169
O	-1.987200	-0.898521	2.347040
P	-2.925474	-2.309756	2.376262
O	-1.962385	-3.399882	1.599982
O	0.404235	-2.205907	2.283528
O	2.184134	3.621593	4.795901
O	2.797498	0.845192	-1.270920
O	-0.406632	2.881316	-1.288188
O	-0.320181	-0.549714	4.585495
H	-0.237815	-2.797743	1.809433
H	0.844951	-2.678533	3.020144
H	-3.148256	2.196988	0.991879
H	-2.726940	2.299114	-0.570954
H	-0.358679	2.346476	-2.105747
H	-0.397146	3.843611	-1.483315
H	-0.155113	5.176900	1.191711
H	-1.693479	4.733086	0.988617
H	2.305452	0.620262	-2.085995
H	3.660064	1.268455	-1.473402
H	4.787031	2.003636	1.203072
H	4.956599	0.400297	1.081915
H	3.294719	-1.453561	-0.528957
H	2.962709	-2.004248	0.957587
H	1.619246	4.194341	5.351721
H	3.118064	3.675723	5.080037
H	0.380361	-0.581024	5.270113
H	-1.204507	-0.478942	5.000638
H	-2.930125	-2.786253	3.726119
H	-3.264157	-0.887918	1.846503
H	-2.287231	-4.199114	1.123436

