Electronic Properties of Polyoxometalates: Electron and Proton Affinity of Mixed-Addenda Keggin and Wells–Dawson Anions

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Supporting Information

Molecule: A- α -[SiW₉Mo₃O₄₀]⁴⁻
Total Binding Energy: -448.8992 eV

Si	0.000000	0.000000	-0.029223
W	0.103925	3.520351	0.075124
Mo	-2.153751	0.000000	2.829006
W	0.103925	-3.520351	0.075124
W	1.939412	0.000000	-2.964560
Mo	1.076876	1.865203	2.829006
W	2.996751	-1.850177	0.075124
W	-0.969706	-1.679580	-2.964560
W	-3.100676	1.670174	0.075124
W	-3.100676	-1.670174	0.075124
W	-0.969706	1.679580	-2.964560
W	2.996751	1.850177	0.075124
Mo	1.076876	-1.865203	2.829006
O	0.786545	1.362337	0.510094
O	-1.573091	0.000000	0.510094
O	0.786545	-1.362337	0.510094
O	0.000000	0.000000	-1.698439
O	-2.430994	1.594683	-1.721810
O	1.484591	0.000000	2.937456
O	-2.430994	-1.594683	-1.721810
O	3.339527	0.000000	0.430101
O	-0.742296	-1.285694	2.937456
O	2.596532	1.307961	-1.721810
O	-1.669764	-2.892115	0.430101
O	-0.165539	2.902644	-1.721810
O	-0.165539	-2.902644	-1.721810
O	-1.669764	2.892115	0.430101
O	2.596532	-1.307961	-1.721810
O	-0.742296	1.285694	2.937456
O	2.788037	2.160955	1.983530
O	-4.035065	0.000000	-0.220697
O	2.788037	-2.160955	1.983530
O	-1.550517	0.000000	-3.738790
O	2.017532	3.494469	-0.220697
O	0.477424	-3.494988	1.983530
O	0.775258	1.342787	-3.738790
O	-3.265461	-1.334033	1.983530
O	-3.265461	1.334033	1.983530
O	0.775258	-1.342787	-3.738790
O	0.477424	3.494988	1.983530
O	2.017532	-3.494469	-0.220697
O	-0.194052	5.225291	-0.123035
O	-2.791642	0.000000	4.445244
O	-0.194052	-5.225291	-0.123035
O	3.217394	0.000000	-4.147696
O	1.395821	2.417633	4.445244
O	4.622261	-2.444592	-0.123035
O	-1.608697	-2.786345	-4.147696
O	-4.428209	2.780700	-0.123035
O	-4.428209	-2.780700	-0.123035
O	-1.608697	2.786345	-4.147696
O	4.622261	2.444592	-0.123035
O	1.395821	-2.417633	4.445244

Molecule: A- α -[SiW₉V₃O₄₀]⁷⁻
Total Binding Energy: -417.2731 eV

Si	0.000000	0.000000	-0.079774
W	0.122328	3.522214	0.107502
V	-2.042957	0.000000	2.863542
W	0.122328	-3.522214	0.107502

W	1.965501	0.000000	-2.987677
V	1.021479	1.769253	2.863542
W	2.989163	-1.867046	0.107502
W	-0.982751	-1.702174	-2.987677
W	-3.111491	1.655168	0.107502
W	-3.111491	-1.655168	0.107502
W	-0.982751	1.702174	-2.987677
W	2.989163	1.867046	0.107502
V	1.021479	-1.769253	2.863542
O	0.784621	1.359003	0.427961
O	-1.569242	0.000000	0.427961
O	0.784621	-1.359003	0.427961
O	0.000000	0.000000	-1.756764
O	-2.441273	1.604837	-1.770015
O	1.460569	0.000000	3.005745
O	-2.441273	-1.604837	-1.770015
O	3.363212	0.000000	0.368846
O	-0.730284	-1.264890	3.005745
O	2.610466	1.311786	-1.770015
O	-1.681606	-2.912627	0.368846
O	-0.169193	2.916623	-1.770015
O	-0.169193	-2.916623	-1.770015
O	-1.681606	2.912627	0.368846
O	2.610466	-1.311786	-1.770015
O	-0.730284	1.264890	3.005745
O	2.746997	2.133885	1.939254
O	-4.061971	0.000000	-0.279764
O	2.746997	-2.133885	1.939254
O	-1.556856	0.000000	-3.784695
O	2.030986	3.517770	-0.279764
O	0.474500	-3.445912	1.939254
O	0.778428	1.348277	-3.784695
O	-3.221497	-1.312027	1.939254
O	-3.221497	1.312027	1.939254
O	0.778428	-1.348277	-3.784695
O	0.474500	3.445912	1.939254
O	2.030986	-3.517770	-0.279764
O	-0.168873	5.262589	-0.099953
O	-2.767216	0.000000	4.347318
O	-0.168873	-5.262589	-0.099953
O	3.236720	0.000000	-4.227768
O	1.383608	2.396479	4.347318
O	4.641972	-2.485047	-0.099953
O	-1.618360	-2.803082	-4.227768
O	-4.473099	2.777542	-0.099953
O	-4.473099	-2.777542	-0.099953
O	-1.618360	2.803082	-4.227768
O	4.641972	2.485047	-0.099953
O	1.383608	-2.396479	4.347318

Molecule: A- α -[SiW₉Nb₃O₄₀]⁷⁻
Total Binding Energy: -427.3954 eV

Si	0.000000	0.000000	-0.043468
W	0.114562	3.545398	0.070926
Nb	-2.176252	0.000000	2.975332
W	0.114562	-3.545398	0.070926
W	1.956562	0.000000	-2.995039
Nb	1.088126	1.884689	2.975332
W	3.013124	-1.871912	0.070926
W	-0.978281	-1.694433	-2.995039
W	-3.127686	1.673486	0.070926
W	-3.127686	-1.673486	0.070926
W	-0.978281	1.694433	-2.995039

W	3.013124	1.871912	0.070926
Nb	1.088126	-1.884689	2.975332
O	0.788711	1.366087	0.487718
O	-1.577421	0.000000	0.487718
O	0.788711	-1.366087	0.487718
O	0.000000	0.000000	-1.724237
O	-2.431834	1.599573	-1.779669
O	1.586318	0.000000	3.179517
O	-2.431834	-1.599573	-1.779669
O	3.350726	0.000000	0.364787
O	-0.793159	-1.373791	3.179517
O	2.601188	1.306244	-1.779669
O	-1.675363	-2.901814	0.364787
O	-0.169354	2.905817	-1.779669
O	-0.169354	-2.905817	-1.779669
O	-1.675363	2.901814	0.364787
O	2.601188	-1.306244	-1.779669
O	-0.793159	1.373791	3.179517
O	2.856015	2.206666	1.901971
O	-4.047940	0.000000	-0.293708
O	2.856015	-2.206666	1.901971
O	-1.539914	0.000000	-3.794005
O	2.023970	3.505619	-0.293708
O	0.483022	-3.576714	1.901971
O	0.769957	1.333605	-3.794005
O	-3.339036	-1.370048	1.901971
O	-3.339036	1.370048	1.901971
O	0.769957	-1.333605	-3.794005
O	0.483022	3.576714	1.901971
O	2.023970	-3.505619	-0.293708
O	-0.200850	5.265033	-0.213049
O	-3.051458	0.000000	4.562909
O	-0.200850	-5.265033	-0.213049
O	3.243271	0.000000	-4.213969
O	1.525729	2.642640	4.562909
O	4.660077	-2.458575	-0.213049
O	-1.621635	-2.808755	-4.213969
O	-4.459227	2.806457	-0.213049
O	-4.459227	-2.806457	-0.213049
O	-1.621635	2.808755	-4.213969
O	4.660077	2.458575	-0.213049
O	1.525729	-2.642640	4.562909

Molecule: A- α -[SiW₉Mo₃O₄₀ 1e]⁵⁻
Total Binding Energy: -442.4571 eV

Si	0.000000	0.000000	-0.030628
W	0.106488	3.527018	0.079672
Mo	-2.148217	0.000000	2.840194
W	0.106488	-3.527018	0.079672
W	1.944913	0.000000	-2.968834
Mo	1.074108	1.860410	2.840194
W	3.001243	-1.855730	0.079672
W	-0.972456	-1.684344	-2.968834
W	-3.107731	1.671287	0.079672
W	-3.107731	-1.671287	0.079672
W	-0.972456	1.684344	-2.968834
W	3.001243	1.855730	0.079672
Mo	1.074108	-1.860410	2.840194
O	0.787995	1.364847	0.499574
O	-1.575989	0.000000	0.499574
O	0.787995	-1.364847	0.499574
O	0.000000	0.000000	-1.699609
O	-2.437316	1.600590	-1.740211
O	1.520667	0.000000	2.924447
O	-2.437316	-1.600590	-1.740211

O	3.341406	0.000000	0.424590
O	-0.760333	-1.316936	2.924447
O	2.604810	1.310482	-1.740211
O	-1.670703	-2.893742	0.424590
O	-0.167494	2.911072	-1.740211
O	-0.167494	-2.911072	-1.740211
O	-1.670703	2.893742	0.424590
O	2.604810	-1.310482	-1.740211
O	-0.760333	1.316936	2.924447
O	2.802499	2.165770	1.964150
O	-4.051047	0.000000	-0.230221
O	2.802499	-2.165770	1.964150
O	-1.559671	0.000000	-3.750885
O	2.025523	3.508310	-0.230221
O	0.474362	-3.509921	1.964150
O	0.779836	1.350715	-3.750885
O	-3.276861	-1.344151	1.964150
O	-3.276861	1.344151	1.964150
O	0.779836	-1.350715	-3.750885
O	0.474362	3.509921	1.964150
O	2.025523	-3.508310	-0.230221
O	-0.193331	5.242488	-0.119219
O	-2.793249	0.000000	4.462123
O	-0.193331	-5.242488	-0.119219
O	3.223554	0.000000	-4.168681
O	1.396624	2.419024	4.462123
O	4.636793	-2.453815	-0.119219
O	-1.611777	-2.791679	-4.168681
O	-4.443462	2.788673	-0.119219
O	-4.443462	-2.788673	-0.119219
O	-1.611777	2.791679	-4.168681
O	4.636793	2.453815	-0.119219
O	1.396624	-2.419024	4.462123

Molecule: A- α -[SiW₉V₃O₄₀ 1e]⁸⁻
Total Binding Energy: -402.5393 eV

Si	0.000000	0.000000	-0.084391
W	0.122183	3.536024	0.113395
V	-2.024849	0.000000	2.885032
W	0.122183	-3.536024	0.113395
W	1.973771	0.000000	-2.994512
V	1.012425	1.753571	2.885032
W	3.001195	-1.873826	0.113395
W	-0.986885	-1.709336	-2.994512
W	-3.123379	1.662198	0.113395
W	-3.123379	-1.662198	0.113395
W	-0.986885	1.709336	-2.994512
W	3.001195	1.873826	0.113395
V	1.012425	-1.753571	2.885032
O	0.788756	1.366166	0.418594
O	-1.577513	0.000000	0.418594
O	0.788756	-1.366166	0.418594
O	0.000000	0.000000	-1.764450
O	-2.445215	1.610029	-1.786971
O	1.496170	0.000000	2.950291
O	-2.445215	-1.610029	-1.786971
O	3.370439	0.000000	0.359349
O	-0.748085	-1.295722	2.950291
O	2.616933	1.312603	-1.786971
O	-1.685220	-2.918886	0.359349
O	-0.171719	2.922632	-1.786971
O	-0.171719	-2.922632	-1.786971
O	-1.685220	2.918886	0.359349
O	2.616933	-1.312603	-1.786971
O	-0.748085	1.295722	2.950291

O	2.766988	2.137112	1.928293
O	-4.071061	0.000000	-0.289360
O	2.766988	-2.137112	1.928293
O	-1.558780	0.000000	-3.795234
O	2.035530	3.525642	-0.289360
O	0.467299	-3.464838	1.928293
O	0.779390	1.349944	-3.795234
O	-3.234287	-1.327726	1.928293
O	-3.234287	1.327726	1.928293
O	0.779390	-1.349944	-3.795234
O	0.467299	3.464838	1.928293
O	2.035530	-3.525642	-0.289360
O	-0.171756	5.288292	-0.092785
O	-2.757183	0.000000	4.382387
O	-0.171756	-5.288292	-0.092785
O	3.250134	0.000000	-4.247013
O	1.378591	2.387790	4.382387
O	4.665673	-2.495401	-0.092785
O	-1.625067	-2.814698	-4.247013
O	-4.493917	2.792891	-0.092785
O	-4.493917	-2.792891	-0.092785
O	-1.625067	2.814698	-4.247013
O	4.665673	2.495401	-0.092785
O	1.378591	-2.387790	4.382387

Molecule: A- α -[SiW₉Nb₃O₄₀ 1e]⁸⁻
Total Binding Energy: -412.3280 eV

Si	0.000000	0.000000	-0.045411
W	0.114799	3.555950	0.074614
Nb	-2.182411	0.000000	2.976380
W	0.114799	-3.555950	0.074614
W	1.964880	0.000000	-3.004743
Nb	1.091205	1.890023	2.976380
W	3.022143	-1.877394	0.074614
W	-0.982440	-1.701636	-3.004743
W	-3.136943	1.678556	0.074614
W	-3.136943	-1.678556	0.074614
W	-0.982440	1.701636	-3.004743
W	3.022143	1.877394	0.074614
Nb	1.091205	-1.890023	2.976380
O	0.792397	1.372473	0.488315
O	-1.584795	0.000000	0.488315
O	0.792397	-1.372473	0.488315
O	0.000000	0.000000	-1.732756
O	-2.441783	1.601871	-1.781528
O	1.593009	0.000000	3.174292
O	-2.441783	-1.601871	-1.781528
O	3.363670	0.000000	0.372733
O	-0.796504	-1.379586	3.174292
O	2.608153	1.313710	-1.781528
O	-1.681835	-2.913024	0.372733
O	-0.166370	2.915581	-1.781528
O	-0.166370	-2.915581	-1.781528
O	-1.681835	2.913024	0.372733
O	2.608153	-1.313710	-1.781528
O	-0.796504	1.379586	3.174292
O	2.862701	2.207540	1.920576
O	-4.065198	0.000000	-0.294745
O	2.862701	-2.207540	1.920576
O	-1.550397	0.000000	-3.806949
O	2.032599	3.520565	-0.294745
O	0.480435	-3.582942	1.920576
O	0.775199	1.342683	-3.806949
O	-3.343136	-1.375402	1.920576

O	-3.343136	1.375402	1.920576
O	0.775199	-1.342683	-3.806949
O	0.480435	3.582942	1.920576
O	2.032599	-3.520565	-0.294745
O	-0.199371	5.287979	-0.208252
O	-3.065199	0.000000	4.576460
O	-0.199371	-5.287979	-0.208252
O	3.258389	0.000000	-4.235277
O	1.532599	2.654540	4.576460
O	4.679210	-2.471330	-0.208252
O	-1.629194	-2.821847	-4.235277
O	-4.479839	2.816650	-0.208252
O	-4.479839	-2.816650	-0.208252
O	-1.629194	2.821847	-4.235277
O	4.679210	2.471330	-0.208252
O	1.532599	-2.654540	4.576460

Molecule: α -[P₂W₁₈O₆₂]⁶⁻
Total Binding Energy: -685.2213 eV

P	0.000000	0.000000	-2.002709
W	0.098133	3.530337	-1.881654
W	0.098133	-3.530337	-1.881654
W	1.977087	0.000000	-4.945488
W	3.008296	-1.850154	-1.881654
W	-0.988544	-1.712208	-4.945488
W	-3.106428	1.680183	-1.881654
W	-3.106428	-1.680183	-1.881654
W	-0.988544	1.712208	-4.945488
W	3.008296	1.850154	-1.881654
O	0.749612	1.298366	-1.529431
O	-1.499224	0.000000	-1.529431
O	0.749612	-1.298366	-1.529431
O	0.000000	0.000000	-3.628805
O	-2.433034	1.622559	-3.712643
O	-2.433034	-1.622559	-3.712643
O	3.354128	0.000000	-1.584118
O	2.621695	1.295790	-3.712643
O	-1.677064	-2.904760	-1.584118
O	-0.188661	2.918349	-3.712643
O	-0.188661	-2.918349	-3.712643
O	-1.677064	2.904760	-1.584118
O	2.621695	-1.295790	-3.712643
O	2.960368	2.129161	0.000000
O	-3.994553	0.000000	-2.187560
O	2.960368	-2.129161	0.000000
O	-1.531166	0.000000	-5.686225
O	1.997276	3.459384	-2.187560
O	0.363723	-3.628334	0.000000
O	0.765583	1.326029	-5.686225
O	-3.324091	-1.499174	0.000000
O	-3.324091	1.499174	0.000000
O	0.765583	-1.326029	-5.686225
O	0.363723	3.628334	0.000000
O	1.997276	-3.459384	-2.187560
O	-0.203175	5.217955	-2.189664
O	-0.203175	-5.217955	-2.189664
O	3.221633	0.000000	-6.177759
O	4.620469	-2.433023	-2.189664
O	-1.610817	-2.790016	-6.177759
O	-4.417295	2.784932	-2.189664
O	-4.417295	-2.784932	-2.189664
O	-1.610817	2.790016	-6.177759
O	4.620469	2.433023	-2.189664
P	0.000000	0.000000	2.002709
W	0.098133	3.530337	1.881654

W	0.098133	-3.530337	1.881654
W	1.977087	0.000000	4.945488
W	3.008296	-1.850154	1.881654
W	-0.988544	-1.712208	4.945488
W	-3.106428	1.680183	1.881654
W	-3.106428	-1.680183	1.881654
W	-0.988544	1.712208	4.945488
W	3.008296	1.850154	1.881654
O	0.749612	1.298366	1.529431
O	-1.499224	0.000000	1.529431
O	0.749612	-1.298366	1.529431
O	0.000000	0.000000	3.628805
O	-2.433034	1.622559	3.712643
O	-2.433034	-1.622559	3.712643
O	3.354128	0.000000	1.584118
O	2.621695	1.295790	3.712643
O	-1.677064	-2.904760	1.584118
O	-0.188661	2.918349	3.712643
O	-0.188661	-2.918349	3.712643
O	-1.677064	2.904760	1.584118
O	2.621695	-1.295790	3.712643
O	-3.994553	0.000000	2.187560
O	-1.531166	0.000000	5.686225
O	1.997276	3.459384	2.187560
O	0.765583	1.326029	5.686225
O	0.765583	-1.326029	5.686225
O	1.997276	-3.459384	2.187560
O	-0.203175	5.217955	2.189664
O	-0.203175	-5.217955	2.189664
O	3.221633	0.000000	6.177759
O	4.620469	-2.433023	2.189664
O	-1.610817	-2.790016	6.177759
O	-4.417295	2.784932	2.189664
O	-4.417295	-2.784932	2.189664
O	-1.610817	2.790016	6.177759
O	4.620469	2.433023	2.189664

Molecule: α -[P₂W₁₅Mo₃O₆₂]⁶⁻
Total Binding Energy: -680.1069 eV

P	0.000000	0.000000	-2.021136
W	0.093992	3.534351	-1.881797
W	0.093992	-3.534351	-1.881797
Mo	1.994193	0.000000	-4.958960
W	3.013841	-1.848575	-1.881797
Mo	-0.997096	-1.727022	-4.958960
W	-3.107833	1.685776	-1.881797
W	-3.107833	-1.685776	-1.881797
Mo	-0.997096	1.727022	-4.958960
W	3.013841	1.848575	-1.881797
O	0.750828	1.300472	-1.532461
O	-1.501655	0.000000	-1.532461
O	0.750828	-1.300472	-1.532461
O	0.000000	0.000000	-3.636783
O	-2.455425	1.635964	-3.715785
O	-2.455425	-1.635964	-3.715785
O	3.335912	0.000000	-1.575317
O	2.644499	1.308478	-3.715785
O	-1.667956	-2.888985	-1.575317
O	-0.189074	2.944443	-3.715785
O	-0.189074	-2.944443	-3.715785
O	-1.667956	2.888985	-1.575317
O	2.644499	-1.308478	-3.715785
O	2.938972	2.113428	0.002118
O	-3.989583	0.000000	-2.167694
O	2.938972	-2.113428	0.002118

O	-1.536940	0.000000	-5.708749
O	1.994792	3.455081	-2.167694
O	0.360796	-3.601938	0.002118
O	0.768470	1.331029	-5.708749
O	-3.299768	-1.488511	0.002118
O	-3.299768	1.488511	0.002118
O	0.768470	-1.331029	-5.708749
O	0.360796	3.601938	0.002118
O	1.994792	-3.455081	-2.167694
O	-0.187520	5.229688	-2.139127
O	-0.187520	-5.229688	-2.139127
O	3.238700	0.000000	-6.183226
O	4.622803	-2.452447	-2.139127
O	-1.619350	-2.804797	-6.183226
O	-4.435283	2.777242	-2.139127
O	-4.435283	-2.777242	-2.139127
O	-1.619350	2.804797	-6.183226
O	4.622803	2.452447	-2.139127
P	0.000000	0.000000	1.995856
W	0.095102	3.530077	1.884663
W	0.095102	-3.530077	1.884663
W	1.975541	0.000000	4.945473
W	3.009585	-1.847399	1.884663
W	-0.987770	-1.710869	4.945473
W	-3.104687	1.682678	1.884663
W	-3.104687	-1.682678	1.884663
W	-0.987770	1.710869	4.945473
W	3.009585	1.847399	1.884663
O	0.752931	1.304115	1.520279
O	-1.505862	0.000000	1.520279
O	0.752931	-1.304115	1.520279
O	0.000000	0.000000	3.619520
O	-2.434124	1.620276	3.711405
O	-2.434124	-1.620276	3.711405
O	3.351899	0.000000	1.577437
O	2.620262	1.297875	3.711405
O	-1.675950	-2.902830	1.577437
O	-0.186138	2.918151	3.711405
O	-0.186138	-2.918151	3.711405
O	-1.675950	2.902830	1.577437
O	2.620262	-1.297875	3.711405
O	-3.989377	0.000000	2.180543
O	-1.542018	0.000000	5.677149
O	1.994688	3.454902	2.180543
O	0.771009	1.335427	5.677149
O	0.771009	-1.335427	5.677149
O	1.994688	-3.454902	2.180543
O	-0.177525	5.223739	2.166066
O	-0.177525	-5.223739	2.166066
O	3.213502	0.000000	6.176801
O	4.612653	-2.458128	2.166066
O	-1.606751	-2.782975	6.176801
O	-4.435128	2.765610	2.166066
O	-4.435128	-2.765610	2.166066
O	-1.606751	2.782975	6.176801
O	4.612653	2.458128	2.166066

Molecule: α -[P₂W₁₅V₃O₆₂]⁹⁻
Total Binding Energy: -641.4867 eV

P	0.000000	0.000000	-2.023040
W	0.068079	3.505911	-1.949680
W	0.068079	-3.505911	-1.949680
V	1.871448	0.000000	-4.985851
W	3.002168	-1.811914	-1.949680
V	-0.935724	-1.620721	-4.985851

W	-3.070248	1.693997	-1.949680
W	-3.070248	-1.693997	-1.949680
V	-0.935724	1.620721	-4.985851
W	3.002168	1.811914	-1.949680
O	0.752373	1.303148	-1.508176
O	-1.504746	0.000000	-1.508176
O	0.752373	-1.303148	-1.508176
O	0.000000	0.000000	-3.605881
O	-2.419467	1.618655	-3.670803
O	-2.419467	-1.618655	-3.670803
O	3.373029	0.000000	-1.483151
O	2.611530	1.285993	-3.670803
O	-1.686514	-2.921129	-1.483151
O	-0.192063	2.904648	-3.670803
O	-0.192063	-2.904648	-3.670803
O	-1.686514	2.921129	-1.483151
O	2.611530	-1.285993	-3.670803
O	2.987258	2.103699	0.062708
O	-3.995952	0.000000	-2.063545
O	2.987258	-2.103699	0.062708
O	-1.521297	0.000000	-5.653704
O	1.997976	3.460596	-2.063545
O	0.328228	-3.638891	0.062708
O	0.760649	1.317482	-5.653704
O	-3.315486	-1.535191	0.062708
O	-3.315486	1.535191	0.062708
O	0.760649	-1.317482	-5.653704
O	0.328228	3.638891	0.062708
O	1.997976	-3.460596	-2.063545
O	-0.168906	5.232868	-2.202625
O	-0.168906	-5.232868	-2.202625
O	3.077070	0.000000	-6.114246
O	4.616250	-2.470157	-2.202625
O	-1.538535	-2.664821	-6.114246
O	-4.447343	2.762711	-2.202625
O	-4.447343	-2.762711	-2.202625
O	-1.538535	2.664821	-6.114246
O	4.616250	2.470157	-2.202625
P	0.000000	0.000000	2.053190
W	0.096323	3.561099	1.892650
W	0.096323	-3.561099	1.892650
W	1.999703	0.000000	4.987246
W	3.035841	-1.863968	1.892650
W	-0.999851	-1.731793	4.987246
W	-3.132164	1.697131	1.892650
W	-3.132164	-1.697131	1.892650
W	-0.999851	1.731793	4.987246
W	3.035841	1.863968	1.892650
O	0.753065	1.304346	1.574546
O	-1.506129	0.000000	1.574546
O	0.753065	-1.304346	1.574546
O	0.000000	0.000000	3.680418
O	-2.447393	1.625173	3.779396
O	-2.447393	-1.625173	3.779396
O	3.404815	0.000000	1.670314
O	2.631138	1.306918	3.779396
O	-1.702408	-2.948656	1.670314
O	-0.183745	2.932091	3.779396
O	-0.183745	-2.932091	3.779396
O	-1.702408	2.948656	1.670314
O	2.631138	-1.306918	3.779396
O	-3.996015	0.000000	2.234307
O	-1.531682	0.000000	5.738985
O	1.998008	3.460651	2.234307
O	0.765841	1.326475	5.738985
O	0.765841	-1.326475	5.738985
O	1.998008	-3.460651	2.234307

O	-0.163009	5.271776	2.228415
O	-0.163009	-5.271776	2.228415
O	3.246332	0.000000	6.250561
O	4.646997	-2.494718	2.228415
O	-1.623166	-2.811406	6.250561
O	-4.483988	2.777058	2.228415
O	-4.483988	-2.777058	2.228415
O	-1.623166	2.811406	6.250561
O	4.646997	2.494718	2.228415

Molecule: $\alpha\text{-[P}_2\text{Mo}_{18}\text{O}_{62}]^{6-}$

Total Binding Energy: -653.2920 eV

P	0.000000	0.000000	-2.106719
Mo	0.112054	3.563354	-1.760132
Mo	0.074619	-3.554045	-2.128069
Mo	1.987223	-0.201262	-5.077579
Mo	3.029928	-1.878719	-1.760132
Mo	-1.167909	-1.620354	-5.077579
Mo	-3.115203	1.712401	-2.128069
Mo	-3.141982	-1.684635	-1.760132
Mo	-0.819313	1.821616	-5.077579
Mo	3.040584	1.841644	-2.128069
O	0.759951	1.296522	-1.624616
O	-1.502797	0.009876	-1.624616
O	0.742845	-1.306398	-1.624616
O	0.000000	0.000000	-3.726381
O	-2.456591	1.666656	-3.860993
O	-2.451633	-1.609036	-3.764619
O	3.328973	0.013085	-1.610882
O	2.671662	1.294142	-3.860993
O	-1.653155	-2.889518	-1.610882
O	-0.167650	2.927695	-3.764619
O	-0.215072	-2.960798	-3.860993
O	-1.675818	2.876433	-1.610882
O	2.619283	-1.318658	-3.764619
O	3.054758	2.144097	-0.039515
O	-4.011341	0.015089	-2.194180
O	3.054758	-2.144097	0.039515
O	-1.557049	0.068175	-5.818804
O	2.018738	3.466379	-2.194180
O	0.329464	-3.717546	-0.039515
O	0.837566	1.314356	-5.818804
O	-3.384221	-1.573449	0.039515
O	-3.384221	1.573449	-0.039515
O	0.719483	-1.382532	-5.818804
O	0.329464	3.717546	0.039515
O	1.992604	-3.481468	-2.194180
O	-0.163610	5.222686	-2.207464
O	-0.201068	-5.255194	-2.341545
O	3.241056	-0.235083	-6.289766
O	4.604783	-2.469652	-2.207464
O	-1.824116	-2.689296	-6.289766
O	-4.450597	2.801727	-2.341545
O	-4.441173	-2.753033	-2.207464
O	-1.416941	2.924378	-6.289766
O	4.651665	2.453466	-2.341545
P	0.000000	0.000000	2.106719
Mo	0.074619	3.554045	2.128069
Mo	0.112054	-3.563354	1.760132
Mo	1.987223	0.201262	5.077579
Mo	3.040584	-1.841644	2.128069
Mo	-0.819313	-1.821616	5.077579
Mo	-3.141982	1.684635	1.760132
Mo	-3.115203	-1.712401	2.128069
Mo	-1.167909	1.620354	5.077579

Mo	3.029928	1.878719	1.760132
O	0.742845	1.306398	1.624616
O	-1.502797	-0.009876	1.624616
O	0.759951	-1.296522	1.624616
O	0.000000	0.000000	3.726381
O	-2.451633	1.609036	3.764619
O	-2.456591	-1.666656	3.860993
O	3.328973	-0.013085	1.610882
O	2.619283	1.318658	3.764619
O	-1.675818	-2.876433	1.610882
O	-0.215072	2.960798	3.860993
O	-0.167650	-2.927695	3.764619
O	-1.653155	2.889518	1.610882
O	2.671662	-1.294142	3.860993
O	-4.011341	-0.015089	2.194180
O	-1.557049	-0.068175	5.818804
O	1.992604	3.481468	2.194180
O	0.719483	1.382532	5.818804
O	0.837566	-1.314356	5.818804
O	2.018738	-3.466379	2.194180
O	-0.201068	5.255194	2.341545
O	-0.163610	-5.222686	2.207464
O	3.241056	0.235083	6.289766
O	4.651665	-2.453466	2.341545
O	-1.416941	-2.924378	6.289766
O	-4.441173	2.753033	2.207464
O	-4.450597	-2.801727	2.341545
O	-1.824116	2.689296	6.289766
O	4.604783	2.469652	2.207464

Molecule: α -[P₂Mo₁₅V₃O₆₂]⁹⁻
Total Binding Energy: -614.6037 eV

P	0.000000	0.000000	-2.031064
Mo	0.070069	3.542156	-1.978564
Mo	0.070069	-3.542156	-1.978564
V	1.872756	0.000000	-5.026514
Mo	3.032563	-1.831760	-1.978564
V	-0.936378	-1.621854	-5.026514
Mo	-3.102632	1.710396	-1.978564
Mo	-3.102632	-1.710396	-1.978564
V	-0.936378	1.621854	-5.026514
Mo	3.032563	1.831760	-1.978564
O	0.751673	1.301935	-1.533804
O	-1.503345	0.000000	-1.533804
O	0.751673	-1.301935	-1.533804
O	0.000000	0.000000	-3.625645
O	-2.426048	1.632735	-3.706115
O	-2.426048	-1.632735	-3.706115
O	3.403322	0.000000	-1.512978
O	2.627013	1.284652	-3.706115
O	-1.701661	-2.947363	-1.512978
O	-0.200966	2.917386	-3.706115
O	-0.200966	-2.917386	-3.706115
O	-1.701661	2.947363	-1.512978
O	2.627013	-1.284652	-3.706115
O	3.018519	2.125790	0.060841
O	-4.031323	0.000000	-2.099741
O	3.018519	-2.125790	0.060841
O	-1.521942	0.000000	-5.693299
O	2.015662	3.491228	-2.099741
O	0.331729	-3.677009	0.060841
O	0.760971	1.318040	-5.693299
O	-3.350248	-1.551219	0.060841
O	-3.350248	1.551219	0.060841
O	0.760971	-1.318040	-5.693299
O	0.331729	3.677009	0.060841

O	2.015662	-3.491228	-2.099741
O	-0.161640	5.271618	-2.229716
O	-0.161640	-5.271618	-2.229716
O	3.078709	0.000000	-6.153504
O	4.646175	-2.495824	-2.229716
O	-1.539355	-2.666240	-6.153504
O	-4.484535	2.775794	-2.229716
O	-4.484535	-2.775794	-2.229716
O	-1.539355	2.666240	-6.153504
O	4.646175	2.495824	-2.229716
P	0.000000	0.000000	2.093015
Mo	0.098258	3.600675	1.908531
Mo	0.098258	-3.600675	1.908531
Mo	2.018294	0.000000	5.036645
Mo	3.069147	-1.885431	1.908531
Mo	-1.009147	-1.747894	5.036645
Mo	-3.167405	1.715243	1.908531
Mo	-3.167405	-1.715243	1.908531
Mo	-1.009147	1.747894	5.036645
Mo	3.069147	1.885431	1.908531
O	0.750925	1.300641	1.599689
O	-1.501851	0.000000	1.599689
O	0.750925	-1.300641	1.599689
O	0.000000	0.000000	3.719705
O	-2.464467	1.641490	3.811597
O	-2.464467	-1.641490	3.811597
O	3.433474	0.000000	1.683514
O	2.653806	1.313546	3.811597
O	-1.716737	-2.973476	1.683514
O	-0.189339	2.955036	3.811597
O	-0.189339	-2.955036	3.811597
O	-1.716737	2.973476	1.683514
O	2.653806	-1.313546	3.811597
O	-4.030369	0.000000	2.250807
O	-1.545268	0.000000	5.789110
O	2.015185	3.490402	2.250807
O	0.772634	1.338242	5.789110
O	0.772634	-1.338242	5.789110
O	2.015185	-3.490402	2.250807
O	-0.144724	5.314500	2.248249
O	-0.144724	-5.314500	2.248249
O	3.260578	0.000000	6.299850
O	4.674854	-2.531915	2.248249
O	-1.630289	-2.823743	6.299850
O	-4.530130	2.782585	2.248249
O	-4.530130	-2.782585	2.248249
O	-1.630289	2.823743	6.299850
O	4.674854	2.531915	2.248249

Molecule: α -[P₂W₁₅Mo₃O₆₂]⁷⁻
Total Binding Energy: -670.9731 eV

P	0.000000	0.000000	-2.031983
W	0.095090	3.534276	-1.883651
W	0.095090	-3.534276	-1.883651
Mo	1.999533	0.000000	-4.978472
W	3.013228	-1.849489	-1.883651
Mo	-0.999766	-1.731646	-4.978472
W	-3.108318	1.684788	-1.883651
W	-3.108318	-1.684788	-1.883651
Mo	-0.999766	1.731646	-4.978472
W	3.013228	1.849489	-1.883651
O	0.752807	1.303900	-1.542200
O	-1.505614	0.000000	-1.542200
O	0.752807	-1.303900	-1.542200
O	0.000000	0.000000	-3.650192

O	-2.458183	1.626286	-3.741504
O	-2.458183	-1.626286	-3.741504
O	3.338140	0.000000	-1.596895
O	2.637497	1.315706	-3.741504
O	-1.669070	-2.890914	-1.596895
O	-0.179314	2.941992	-3.741504
O	-0.179314	-2.941992	-3.741504
O	-1.669070	2.890914	-1.596895
O	2.637497	-1.315706	-3.741504
O	2.954243	2.106704	0.002911
O	-3.991502	0.000000	-2.168574
O	2.954243	-2.106704	0.002911
O	-1.541200	0.000000	-5.726977
O	1.995751	3.456742	-2.168574
O	0.347337	-3.611801	0.002911
O	0.770600	1.334719	-5.726977
O	-3.301580	-1.505098	0.002911
O	-3.301580	1.505098	0.002911
O	0.770600	-1.334719	-5.726977
O	0.347337	3.611801	0.002911
O	1.995751	-3.456742	-2.168574
O	-0.181040	5.236087	-2.154469
O	-0.181040	-5.236087	-2.154469
O	3.241234	0.000000	-6.215022
O	4.625105	-2.461258	-2.154469
O	-1.620617	-2.806991	-6.215022
O	-4.444064	2.774829	-2.154469
O	-4.444064	-2.774829	-2.154469
O	-1.620617	2.806991	-6.215022
O	4.625105	2.461258	-2.154469
P	0.000000	0.000000	2.014058
W	0.092598	3.538724	1.886918
W	0.092598	-3.538724	1.886918
W	1.983896	0.000000	4.955908
W	3.018326	-1.849554	1.886918
W	-0.991948	-1.718105	4.955908
W	-3.110924	1.689170	1.886918
W	-3.110924	-1.689170	1.886918
W	-0.991948	1.718105	4.955908
W	3.018326	1.849554	1.886918
O	0.752312	1.303043	1.542674
O	-1.504625	0.000000	1.542674
O	0.752312	-1.303043	1.542674
O	0.000000	0.000000	3.642189
O	-2.446014	1.622165	3.739892
O	-2.446014	-1.622165	3.739892
O	3.354851	0.000000	1.599744
O	2.627843	1.307228	3.739892
O	-1.677426	-2.905386	1.599744
O	-0.181829	2.929393	3.739892
O	-0.181829	-2.929393	3.739892
O	-1.677426	2.905386	1.599744
O	2.627843	-1.307228	3.739892
O	-3.986274	0.000000	2.174420
O	-1.540769	0.000000	5.700271
O	1.993137	3.452214	2.174420
O	0.770384	1.334345	5.700271
O	0.770384	-1.334345	5.700271
O	1.993137	-3.452214	2.174420
O	-0.176785	5.239628	2.170685
O	-0.176785	-5.239628	2.170685
O	3.229635	0.000000	6.194024
O	4.626043	-2.466713	2.170685
O	-1.614817	-2.796946	6.194024
O	-4.449258	2.772914	2.170685
O	-4.449258	-2.772914	2.170685
O	-1.614817	2.796946	6.194024

O	4.626043	2.466713	2.170685
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Molecule: α -[P₂W₁₅V₃O₆₂1e]¹⁰⁻

Total Binding Energy: -625.3212 eV

P	0.000000	0.000000	-2.055588
W	0.067458	3.510565	-1.974309
W	0.067458	-3.510565	-1.974309
V	1.875202	0.000000	-5.058237
W	3.006509	-1.813703	-1.974309
V	-0.937601	-1.623972	-5.058237
W	-3.073967	1.696862	-1.974309
W	-3.073967	-1.696862	-1.974309
V	-0.937601	1.623972	-5.058237
W	3.006509	1.813703	-1.974309
O	0.751483	1.301606	-1.532725
O	-1.502965	0.000000	-1.532725
O	0.751483	-1.301606	-1.532725
O	0.000000	0.000000	-3.633255
O	-2.433764	1.624254	-3.675092
O	-2.433764	-1.624254	-3.675092
O	3.374731	0.000000	-1.495327
O	2.623527	1.295575	-3.675092
O	-1.687366	-2.922603	-1.495327
O	-0.189763	2.919829	-3.675092
O	-0.189763	-2.919829	-3.675092
O	-1.687366	2.922603	-1.495327
O	2.623527	-1.295575	-3.675092
O	2.997428	2.101624	0.088636
O	-4.003179	0.000000	-2.084368
O	2.997428	-2.101624	0.088636
O	-1.540894	0.000000	-5.699882
O	2.001589	3.466855	-2.084368
O	0.321346	-3.646661	0.088636
O	0.770447	1.334453	-5.699882
O	-3.318774	-1.545037	0.088636
O	-3.318774	1.545037	0.088636
O	0.770447	-1.334453	-5.699882
O	0.321346	3.646661	0.088636
O	2.001589	-3.466855	-2.084368
O	-0.163395	5.253519	-2.217586
O	-0.163395	-5.253519	-2.217586
O	3.113472	0.000000	-6.160829
O	4.631379	-2.485255	-2.217586
O	-1.556736	-2.696345	-6.160829
O	-4.467983	2.768264	-2.217586
O	-4.467983	-2.768264	-2.217586
O	-1.556736	2.696345	-6.160829
O	4.631379	2.485255	-2.217586
P	0.000000	0.000000	2.073120
W	0.094998	3.570925	1.906333
W	0.094998	-3.570925	1.906333
W	2.006242	0.000000	5.018431
W	3.045013	-1.867733	1.906333
W	-1.003121	-1.737457	5.018431
W	-3.140011	1.703192	1.906333
W	-3.140011	-1.703192	1.906333
W	-1.003121	1.737457	5.018431
W	3.045013	1.867733	1.906333
O	0.752359	1.303123	1.599935
O	-1.504717	0.000000	1.599935
O	0.752359	-1.303123	1.599935
O	0.000000	0.000000	3.703058
O	-2.447775	1.627311	3.813742
O	-2.447775	-1.627311	3.813742
O	3.399525	0.000000	1.691416

O	2.633180	1.306180	3.813742
O	-1.699763	-2.944075	1.691416
O	-0.185405	2.933491	3.813742
O	-0.185405	-2.933491	3.813742
O	-1.699763	2.944075	1.691416
O	2.633180	-1.306180	3.813742
O	-3.996868	0.000000	2.253174
O	-1.541260	0.000000	5.774345
O	1.998434	3.461390	2.253174
O	0.770630	1.334771	5.774345
O	0.770630	-1.334771	5.774345
O	1.998434	-3.461390	2.253174
O	-0.154067	5.289315	2.255582
O	-0.154067	-5.289315	2.255582
O	3.253712	0.000000	6.297173
O	4.657715	-2.511231	2.255582
O	-1.626856	-2.817797	6.297173
O	-4.503648	2.778083	2.255582
O	-4.503648	-2.778083	2.255582
O	-1.626856	2.817797	6.297173
O	4.657715	2.511231	2.255582

Molecule: α -[P₂Mo₁₈O₆₂ 1e]⁶⁻
Total Binding Energy: -633.4207 eV

P	0.000000	0.000000	-2.123795
Mo	0.098622	3.582055	-1.757603
Mo	0.084316	-3.561357	-2.102934
Mo	2.008022	-0.174676	-5.083294
Mo	3.052840	-1.876437	-1.757603
Mo	-1.155285	-1.651660	-5.083294
Mo	-3.126384	1.707659	-2.102934
Mo	-3.151462	-1.705618	-1.757603
Mo	-0.852737	1.826336	-5.083294
Mo	3.042068	1.853698	-2.102934
O	0.751060	1.302798	-1.637247
O	-1.503786	-0.000962	-1.637247
O	0.752726	-1.301835	-1.637247
O	0.000000	0.000000	-3.737279
O	-2.467965	1.642600	-3.874563
O	-2.470112	-1.638863	-3.820654
O	3.328216	0.012219	-1.634467
O	2.656516	1.316020	-3.874563
O	-1.653526	-2.888429	-1.634467
O	-0.184241	2.958611	-3.820654
O	-0.188551	-2.958620	-3.874563
O	-1.674690	2.876210	-1.634467
O	2.654353	-1.319748	-3.820654
O	3.065564	2.143365	-0.057873
O	-4.009679	-0.004532	-2.182247
O	3.065564	-2.143365	0.057873
O	-1.559241	0.041741	-5.831037
O	2.000914	3.474750	-2.182247
O	0.323427	-3.726539	-0.057873
O	0.815769	1.329472	-5.831037
O	-3.388991	-1.583174	0.057873
O	-3.388991	1.583174	-0.057873
O	0.743472	-1.371213	-5.831037
O	0.323427	3.726539	0.057873
O	2.008765	-3.470217	-2.182247
O	-0.179152	5.249379	-2.203712
O	-0.191260	-5.274484	-2.329651
O	3.260087	-0.160481	-6.327836
O	4.635671	-2.469539	-2.203712
O	-1.769024	-2.743077	-6.327836
O	-4.472207	2.802878	-2.329651

O	-4.456520	-2.779840	-2.203712
O	-1.491062	2.903559	-6.327836
O	4.663467	2.471606	-2.329651
P	0.000000	0.000000	2.123795
Mo	0.084316	3.561357	2.102934
Mo	0.098622	-3.582055	1.757603
Mo	2.008022	0.174676	5.083294
Mo	3.042068	-1.853698	2.102934
Mo	-0.852737	-1.826336	5.083294
Mo	-3.151462	1.705618	1.757603
Mo	-3.126384	-1.707659	2.102934
Mo	-1.155285	1.651660	5.083294
Mo	3.052840	1.876437	1.757603
O	0.752726	1.301835	1.637247
O	-1.503786	0.000962	1.637247
O	0.751060	-1.302798	1.637247
O	0.000000	0.000000	3.737279
O	-2.470112	1.638863	3.820654
O	-2.467965	-1.642600	3.874563
O	3.328216	-0.012219	1.634467
O	2.654353	1.319748	3.820654
O	-1.674690	-2.876210	1.634467
O	-0.188551	2.958620	3.874563
O	-0.184241	-2.958611	3.820654
O	-1.653526	2.888429	1.634467
O	2.656516	-1.316020	3.874563
O	-4.009679	0.004532	2.182247
O	-1.559241	-0.041741	5.831037
O	2.008765	3.470217	2.182247
O	0.743472	1.371213	5.831037
O	0.815769	-1.329472	5.831037
O	2.000914	-3.474750	2.182247
O	-0.191260	5.274484	2.329651
O	-0.179152	-5.249379	2.203712
O	3.260087	0.160481	6.327836
O	4.663467	-2.471606	2.329651
O	-1.491062	-2.903559	6.327836
O	-4.456520	2.779840	2.203712
O	-4.472207	-2.802878	2.329651
O	-1.769024	2.743077	6.327836
O	4.635671	2.469539	2.203712

Molecule: α -[P₂Mo₁₅V₃O₆₂ 1e]¹⁰⁻
Total Binding Energy: -598.8649 eV

P	0.000000	0.000000	-2.059187
Mo	0.066450	3.543262	-1.999316
Mo	0.066450	-3.543262	-1.999316
V	1.875017	0.000000	-5.060495
Mo	3.035330	-1.829178	-1.999316
V	-0.937508	-1.623812	-5.060495
Mo	-3.101779	1.714084	-1.999316
Mo	-3.101779	-1.714084	-1.999316
V	-0.937508	1.623812	-5.060495
Mo	3.035330	1.829178	-1.999316
O	0.751595	1.301800	-1.561187
O	-1.503189	0.000000	-1.561187
O	0.751595	-1.301800	-1.561187
O	0.000000	0.000000	-3.653460
O	-2.432092	1.643459	-3.715620
O	-2.432092	-1.643459	-3.715620
O	3.400547	0.000000	-1.516033
O	2.639323	1.284524	-3.715620
O	-1.700273	-2.944960	-1.516033
O	-0.207231	2.927983	-3.715620
O	-0.207231	-2.927983	-3.715620

O	-1.700273	2.944960	-1.516033
O	2.639323	-1.284524	-3.715620
O	3.024037	2.112115	0.082618
O	-4.013803	0.000000	-2.121038
O	3.024037	-2.112115	0.082618
O	-1.534570	0.000000	-5.719047
O	2.006902	3.476056	-2.121038
O	0.317127	-3.674951	0.082618
O	0.767285	1.328977	-5.719047
O	-3.341164	-1.562835	0.082618
O	-3.341164	1.562835	0.082618
O	0.767285	-1.328977	-5.719047
O	0.317127	3.674951	0.082618
O	2.006902	-3.476056	-2.121038
O	-0.155922	5.282105	-2.241605
O	-0.155922	-5.282105	-2.241605
O	3.094972	0.000000	-6.187397
O	4.652398	-2.506020	-2.241605
O	-1.547486	-2.680324	-6.187397
O	-4.496476	2.776084	-2.241605
O	-4.496476	-2.776084	-2.241605
O	-1.547486	2.680324	-6.187397
O	4.652398	2.506020	-2.241605
P	0.000000	0.000000	2.119332
Mo	0.093050	3.605271	1.915522
Mo	0.093050	-3.605271	1.915522
Mo	2.026715	0.000000	5.060152
Mo	3.075731	-1.883220	1.915522
Mo	-1.013357	-1.755186	5.060152
Mo	-3.168782	1.722052	1.915522
Mo	-3.168782	-1.722052	1.915522

Mo	-1.013357	1.755186	5.060152
Mo	3.075731	1.883220	1.915522
O	0.750938	1.300663	1.631272
O	-1.501876	0.000000	1.631272
O	0.750938	-1.300663	1.631272
O	0.000000	0.000000	3.737818
O	-2.463256	1.648851	3.842260
O	-2.463256	-1.648851	3.842260
O	3.434158	0.000000	1.700387
O	2.659575	1.308816	3.842260
O	-1.717079	-2.974068	1.700387
O	-0.196319	2.957668	3.842260
O	-0.196319	-2.957668	3.842260
O	-1.717079	2.974068	1.700387
O	2.659575	-1.308816	3.842260
O	-4.013853	0.000000	2.255416
O	-1.547898	0.000000	5.808682
O	2.006926	3.476099	2.255416
O	0.773949	1.340519	5.808682
O	0.773949	-1.340519	5.808682
O	2.006926	-3.476099	2.255416
O	-0.133890	5.324741	2.283083
O	-0.133890	-5.324741	2.283083
O	3.270076	0.000000	6.344041
O	4.678306	-2.546418	2.283083
O	-1.635038	-2.831969	6.344041
O	-4.544416	2.778323	2.283083
O	-4.544416	-2.778323	2.283083
O	-1.635038	2.831969	6.344041
O	4.678306	2.546418	2.283083