Supplementary Information

for

Influence of Polyoxometalate Ligand on the Nature of High-Valent Transition Metal-Nitrido Species. A Theoretical Analysis on Experimentally Known and Unprecedented Compounds

by

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XYZ coordinates and energies for several relevant structures

$[PW_{11}O_{39}\{W^{VI}N\}]^{4-}$

P	0.005754	-0.031215	0.000000
W	0.084763	0.053014	-3.603419
W	-2.198414	2.902481	0.000000
W	0.084763	0.053014	3.603419
W	1.999150	-3.003310	0.000000
W	1.065582	2.911132	-1.861074
W	3.080217	0.065275	1.872862
W	-1.004668	-3.004316	1.740021
W	-3.165239	0.063560	-1.731441
W	-3.165239	0.063560	1.731441
W	-1.004668	-3.004316	-1.740021
W	3.080217	0.065275	-1.872862
W	1.065582	2.911132	1.861074
O	0.745581	0.490051	-1.273771
O	-1.472173	0.443603	0.000000
O	0.745581	0.490051	1.273771
O	0.029136	-1.587307	0.000000
O	-2.451222	-1.752363	-1.652333
O	1.559509	3.093543	0.000000
O	-2.451222	-1.752363	1.652333
O	3.417953	0.385221	0.000000
O	-0.711347	3.058294	1.314515
O	2.655519	-1.743014	-1.300483
O	-1.697376	0.377700	2.951345
O	-0.188527	-1.752357	-2.955493
O	-0.188527	-1.752357	2.955493
O	-1.697376	0.377700	-2.951345
O	2.655519	-1.743014	1.300483
O	-0.711347	3.058294	-1.314515
O	2.760899	1.951121	-2.118893

O	-3.991790	-0.249203	0.000000
O	2.760899	1.951121	2.118893
O	-1.529174	-3.689002	0.000000
O	2.004212	-0.246145	-3.455672
O	0.470821	1.936276	3.455252
O	0.767767	-3.688050	-1.334619
O	-3.250042	1.939822	1.371674
O	-3.250042	1.939822	-1.371674
O	0.767767	-3.688050	1.334619
O	0.470821	1.936276	-3.455252
O	2.004212	-0.246145	3.455672
O	-0.160506	-0.130846	-5.303286
N	-2.880253	4.468397	0.000000
O	-0.160506	-0.130846	5.303286
O	3.239098	-4.214566	0.000000
O	1.438287	4.466199	-2.528171
O	4.678346	-0.112705	2.502460
O	-1.614801	-4.229540	2.798494
O	-4.501178	-0.137110	-2.811073
O	-4.501178	-0.137110	2.811073
O	-1.614801	-4.229540	-2.798494
O	4.678346	-0.112705	-2.502460
O	1.438287	4.466199	2.528171

Bond energy LDA + GGA-XC -467.04356 eV

$[PW_{11}O_{39}\{Mo^{VI}N\}]^{4-}$

P	-0.002256	-0.018036	0.000000
W	0.080198	0.047206	-3.611576
Mo	-2.188435	2.929359	0.000000
W	0.080198	0.047206	3.611576
W	2.010365	-3.000177	0.000000
W	1.061788	2.902771	-1.867193
W	3.085208	0.063485	1.875556
W	-1.003594	-3.002253	1.742242
W	-3.169301	0.072271	-1.723052
W	-3.169301	0.072271	1.723052
W	-1.003594	-3.002253	-1.742242
W	3.085208	0.063485	-1.875556
W	1.061788	2.902771	1.867193
O	0.736236	0.504410	-1.271585
O	-1.473394	0.473336	0.000000
O	0.736236	0.504410	1.271585
O	0.020379	-1.579237	0.000000
O	-2.439897	-1.753693	-1.659718
O	1.547038	3.087385	0.000000
O	-2.439897	-1.753693	1.659718
O	3.424523	0.390556	0.000000

O	-0.723919	3.079796	1.350842
O	2.675049	-1.742247	-1.301030
O	-1.700424	0.364769	2.965934
O	-0.182242	-1.760524	-2.966710
O	-0.182242	-1.760524	2.966710
O	-1.700424	0.364769	-2.965934
O	2.675049	-1.742247	1.301030
O	-0.723919	3.079796	-1.350842
O	2.759974	1.945313	-2.117089
O	-3.984995	-0.300235	0.000000
O	2.759974	1.945313	2.117089
O	-1.524065	-3.686054	0.000000
O	1.997722	-0.256644	-3.445602
O	0.494092	1.925256	3.461779
O	0.775651	-3.678577	-1.328029
O	-3.273101	1.925380	1.364162
O	-3.273101	1.925380	-1.364162
O	0.775651	-3.678577	1.328029
O	0.494092	1.925256	-3.461779
O	1.997722	-0.256644	3.445602
O	-0.151305	-0.138039	-5.313043
N	-2.909410	4.456604	0.000000
O	-0.151305	-0.138039	5.313043
O	3.229313	-4.227428	0.000000
O	1.443962	4.455233	-2.532648
O	4.680469	-0.106157	2.519282
O	-1.607190	-4.241505	2.788296
O	-4.513378	-0.131475	-2.793871
O	-4.513378	-0.131475	2.793871
O	-1.607190	-4.241505	-2.788296
O	4.680469	-0.106157	-2.519282
O	1.443962	4.455233	2.532648

Bond energy LDA + GGA-XC -465.98890 eV

$[PW_{11}O_{39}\{Re^{VI}N\}]^{4-}$

P	-0.000610	-0.014536	0.000000
W	0.077837	0.046787	-3.612423
Re	-2.171241	2.909827	0.000000
W	0.077837	0.046787	3.612423
W	2.009675	-2.997578	0.000000
W	1.055872	2.899130	-1.864590
W	3.083360	0.065629	1.876347
W	-1.003149	-3.000887	1.744341
W	-3.165764	0.076199	-1.726038
W	-3.165764	0.076199	1.726038
W	-1.003149	-3.000887	-1.744341
W	3.083360	0.065629	-1.876347

W	1.055872	2.899130	1.864590
O	0.731549	0.509042	-1.270626
O	-1.473928	0.477789	0.000000
O	0.731549	0.509042	1.270626
O	0.017483	-1.570598	0.000000
O	-2.442215	-1.751708	-1.662624
O	1.564566	3.079239	0.000000
O	-2.442215	-1.751708	1.662624
O	3.415478	0.387139	0.000000
O	-0.726273	3.068344	1.331159
O	2.669911	-1.740380	-1.302689
O	-1.698212	0.360006	2.963385
O	-0.176355	-1.763844	-2.965160
O	-0.176355	-1.763844	2.965160
O	-1.698212	0.360006	-2.963385
O	2.669911	-1.740380	1.302689
O	-0.726273	3.068344	-1.331159
O	2.758362	1.949203	-2.114921
O	-3.977515	-0.308679	0.000000
O	2.758362	1.949203	2.114921
O	-1.528212	-3.675045	0.000000
O	1.997503	-0.250930	-3.443316
O	0.482243	1.920973	3.457034
O	0.774609	-3.674098	-1.327749
O	-3.240374	1.928057	1.348943
O	-3.240374	1.928057	-1.348943
O	0.774609	-3.674098	1.327749
O	0.482243	1.920973	-3.457034
O	1.997503	-0.250930	3.443316
O	-0.156013	-0.139980	-5.313401
N	-2.877141	4.431592	0.000000
O	-0.156013	-0.139980	5.313401
O	3.228474	-4.223755	0.000000
O	1.433050	4.450937	-2.533327
O	4.678655	-0.104204	2.518426
O	-1.605406	-4.240618	2.790584
O	-4.512316	-0.119304	-2.793403
O	-4.512316	-0.119304	2.793403
O	-1.605406	-4.240618	-2.790584
O	4.678655	-0.104204	-2.518426
O	1.433050	4.450937	2.533327

Bond energy LDA + GGA-XC -465.58611 eV

$[PW_{11}O_{39}\{Re^{VII}N\}]^{3-}$

P	0.003886	-0.013854	0.000000
W	0.074295	0.047720	-3.613163

Re	-2.152459	2.893460	0.000000
W	0.074295	0.047720	3.613163
W	2.004590	-2.989297	0.000000
W	1.072433	2.896517	-1.879988
W	3.080271	0.072040	1.870609
W	-1.008870	-3.006051	1.739732
W	-3.159944	0.062428	-1.732492
W	-3.159944	0.062428	1.732492
W	-1.008870	-3.006051	-1.739732
W	3.080271	0.072040	-1.870609
W	1.072433	2.896517	1.879988
O	0.729431	0.518028	-1.271475
O	-1.468780	0.466892	0.000000
O	0.729431	0.518028	1.271475
O	0.021123	-1.566611	0.000000
O	-2.454819	-1.737513	-1.652816
O	1.484776	3.081198	0.000000
O	-2.454819	-1.737513	1.652816
O	3.402850	0.406810	0.000000
O	-0.757785	3.057053	1.320865
O	2.668037	-1.727298	-1.299698
O	-1.715717	0.382744	2.956797
O	-0.191287	-1.746516	-2.964063
O	-0.191287	-1.746516	2.964063
O	-1.715717	0.382744	-2.956797
O	2.668037	-1.727298	1.299698
O	-0.757785	3.057053	-1.320865
O	2.750873	1.971099	-2.127064
O	-3.977721	-0.253406	0.000000
O	2.750873	1.971099	2.127064
O	-1.531925	-3.669734	0.000000
O	1.986117	-0.234153	-3.441565
O	0.462888	1.930416	3.447077
O	0.758230	-3.658014	-1.332448
O	-3.227747	1.962967	1.318035
O	-3.227747	1.962967	-1.318035
O	0.758230	-3.658014	1.332448
O	0.462888	1.930416	-3.447077
O	1.986117	-0.234153	3.441565
O	-0.158976	-0.136624	-5.309727
N	-2.885874	4.406739	0.000000
O	-0.158976	-0.136624	5.309727
O	3.222316	-4.209344	0.000000
O	1.430807	4.448864	-2.533733
O	4.666409	-0.096856	2.513771
O	-1.613020	-4.237620	2.786483
O	-4.514256	-0.118348	-2.787421
O	-4.514256	-0.118348	2.787421
O	-1.613020	-4.237620	-2.786483
O	4.666409	-0.096856	-2.513771

O	1.430807	4.448864	2.533733

Bond energy LDA + GGA-XC -460.86812 eV

$[PW_{11}O_{39}\{Tc^{VI}N\}]^{4-}$

P	-0.002880	-0.014146	0.000000
W	0.079685	0.046194	-3.611782
Tc	-2.174391	2.917606	0.000000
W	0.079685	0.046194	3.611782
W	2.009604	-2.997903	0.000000
W	1.052582	2.897660	-1.863376
W	3.083759	0.064371	1.875524
W	-1.002249	-2.999953	1.742251
W	-3.165117	0.079239	-1.722255
W	-3.165117	0.079239	1.722255
W	-1.002249	-2.999953	-1.742251
W	3.083759	0.064371	-1.875524
W	1.052582	2.897660	1.863376
O	0.733818	0.507366	-1.270655
O	-1.471008	0.480875	0.000000
O	0.733818	0.507366	1.270655
O	0.018292	-1.572567	0.000000
O	-2.437862	-1.751030	-1.660495
O	1.559803	3.077612	0.000000
O	-2.437862	-1.751030	1.660495
O	3.420697	0.386877	0.000000
O	-0.724728	3.069841	1.347824
O	2.671766	-1.741683	-1.301577
O	-1.695205	0.360292	2.967685
O	-0.173986	-1.763978	-2.965600
O	-0.173986	-1.763978	2.965600
O	-1.695205	0.360292	-2.967685
O	2.671766	-1.741683	1.301577
O	-0.724728	3.069841	-1.347824
O	2.759857	1.943815	-2.115309
O	-3.975097	-0.307982	0.000000
O	2.759857	1.943815	2.115309
O	-1.528489	-3.678440	0.000000
O	1.998434	-0.253317	-3.442883
O	0.486078	1.920685	3.464439
O	0.775880	-3.675043	-1.327899
O	-3.258271	1.922392	1.363635
O	-3.258271	1.922392	-1.363635
O	0.775880	-3.675043	1.327899
O	0.486078	1.920685	-3.464439
O	1.998434	-0.253317	3.442883
O	-0.150899	-0.143045	-5.313579

N	-2.877387	4.407734	0.000000
O	-0.150899	-0.143045	5.313579
O	3.231408	-4.222346	0.000000
O	1.431580	4.450671	-2.532485
O	4.678747	-0.106732	2.520075
O	-1.605478	-4.239347	2.789905
O	-4.513671	-0.118986	-2.788930
O	-4.513671	-0.118986	2.788930
O	-1.605478	-4.239347	-2.789905
O	4.678747	-0.106732	-2.520075
O	1.431580	4.450671	2.532485

Bond energy LDA + GGA-XC -464.85698 eV

$[PW_{11}O_{39}\{Os^{VI}N\}]^{4-}$

P	-0.003179	-0.015788	0.000000
W	0.085667	0.041432	-3.619414
Os	-2.172999	2.912007	0.000000
W	0.085667	0.041432	3.619414
W	2.010187	-3.001432	0.000000
W	1.044789	2.890877	-1.861134
W	3.086736	0.069201	1.872709
W	-1.003644	-2.997473	1.742311
W	-3.164021	0.088190	-1.729200
W	-3.164021	0.088190	1.729200
W	-1.003644	-2.997473	-1.742311
W	3.086736	0.069201	-1.872709
W	1.044789	2.890877	1.861134
O	0.731059	0.507613	-1.272238
O	-1.477624	0.485490	0.000000
O	0.731059	0.507613	1.272238
O	0.017674	-1.571980	0.000000
O	-2.440443	-1.749956	-1.664046
O	1.567878	3.076479	0.000000
O	-2.440443	-1.749956	1.664046
O	3.425216	0.384831	0.000000
O	-0.735447	3.050082	1.354173
O	2.675433	-1.744730	-1.303115
O	-1.694503	0.361584	2.976336
O	-0.176760	-1.764403	-2.970349
O	-0.176760	-1.764403	2.970349
O	-1.694503	0.361584	-2.976336
O	2.675433	-1.744730	1.303115
O	-0.735447	3.050082	-1.354173
O	2.759012	1.946047	-2.111903
O	-3.975910	-0.320583	0.000000
O	2.759012	1.946047	2.111903

O	-1.526592	-3.676052	0.000000
O	2.002253	-0.252789	-3.447141
O	0.486349	1.922360	3.473986
O	0.777646	-3.682546	-1.329096
O	-3.255378	1.921594	1.362587
O	-3.255378	1.921594	-1.362587
O	0.777646	-3.682546	1.329096
O	0.486349	1.922360	-3.473986
O	2.002253	-0.252789	3.447141
O	-0.151261	-0.136932	-5.323638
N	-2.872512	4.405846	0.000000
O	-0.151261	-0.136932	5.323638
O	3.232449	-4.226449	0.000000
O	1.417318	4.452706	-2.515061
O	4.680655	-0.108711	2.521348
O	-1.605859	-4.233851	2.795223
O	-4.517736	-0.119550	-2.788406
O	-4.517736	-0.119550	2.788406
O	-1.605859	-4.233851	-2.795223
O	4.680655	-0.108711	-2.521348
O	1.417318	4.452706	2.515061

Bond energy LDA+GGA-XC -463.17811 eV

$[PW_{11}O_{39}\{Ru^{VI}N\}]^{4-}$

P	-0.002138	-0.012921	0.000000
W	0.080649	0.049005	-3.618036
Ru	-2.172696	2.915706	0.000000
W	0.080649	0.049005	3.618036
W	2.010051	-3.000787	0.000000
W	1.046450	2.891638	-1.860060
W	3.084553	0.063338	1.875392
W	-0.999856	-2.996705	1.743129
W	-3.164362	0.083532	-1.722260
W	-3.164362	0.083532	1.722260
W	-0.999856	-2.996705	-1.743129
W	3.084553	0.063338	-1.875392
W	1.046450	2.891638	1.860060
O	0.733971	0.507752	-1.273583
O	-1.475473	0.488731	0.000000
O	0.733971	0.507752	1.273583
O	0.018477	-1.573667	0.000000
O	-2.437290	-1.748433	-1.662756
O	1.564073	3.077121	0.000000
O	-2.437290	-1.748433	1.662756
O	3.424394	0.385565	0.000000
O	-0.730582	3.052695	1.359130

O	2.675187	-1.744797	-1.302630
O	-1.691528	0.363589	2.976114
O	-0.175404	-1.764069	-2.968796
O	-0.175404	-1.764069	2.968796
O	-1.691528	0.363589	-2.976114
O	2.675187	-1.744797	1.302630
O	-0.730582	3.052695	-1.359130
O	2.759948	1.944782	-2.111491
O	-3.974983	-0.314254	0.000000
O	2.759948	1.944782	2.111491
O	-1.526017	-3.675828	0.000000
O	2.002226	-0.253811	-3.445980
O	0.486813	1.920652	3.474937
O	0.777639	-3.680506	-1.328558
O	-3.256565	1.919690	1.367378
O	-3.256565	1.919690	-1.367378
O	0.777639	-3.680506	1.328558
O	0.486813	1.920652	-3.474937
O	2.002226	-0.253811	3.445980
O	-0.150076	-0.140191	-5.320849
N	-2.862196	4.383216	0.000000
O	-0.150076	-0.140191	5.320849
O	3.231901	-4.225075	0.000000
O	1.417069	4.452983	-2.517656
O	4.680049	-0.108235	2.518778
O	-1.604951	-4.233140	2.793085
O	-4.514855	-0.112314	-2.788731
O	-4.514855	-0.112314	2.788731
O	-1.604951	-4.233140	-2.793085
O	4.680049	-0.108235	-2.518778
O	1.417069	4.452983	2.517656

Bond energy LDA+GGA-XC -461.108066 eV

$[PW_{11}O_{39}\{Ru^{V}N\}]^{5-}$

P	-0.006245	-0.012967	0.000000
W	0.085313	0.042319	-3.613178
Ru	-2.159271	2.867806	0.000000
W	0.085313	0.042319	3.613178
W	2.008023	-2.999491	0.000000
W	1.049089	2.906192	-1.864165
W	3.087901	0.067658	1.874824
W	-1.005918	-3.001524	1.743626
W	-3.171992	0.090458	-1.730281
W	-3.171992	0.090458	1.730281
W	-1.005918	-3.001524	-1.743626
W	3.087901	0.067658	-1.874824

W	1.049089	2.906192	1.864165
O	0.731929	0.510545	-1.271777
O	-1.480692	0.484756	0.000000
O	0.731929	0.510545	1.271777
O	0.018242	-1.572581	0.000000
O	-2.440387	-1.759725	-1.661562
O	1.584414	3.083269	0.000000
O	-2.440387	-1.759725	1.661562
O	3.426681	0.393537	0.000000
O	-0.706288	3.082868	1.377624
O	2.673258	-1.738036	-1.306007
O	-1.696441	0.366095	2.973290
O	-0.175316	-1.766153	-2.966473
O	-0.175316	-1.766153	2.966473
O	-1.696441	0.366095	-2.973290
O	2.673258	-1.738036	1.306007
O	-0.706288	3.082868	-1.377624
O	2.772825	1.943874	-2.115024
O	-3.984982	-0.330732	0.000000
O	2.772825	1.943874	2.115024
O	-1.533872	-3.687734	0.000000
O	2.007630	-0.255859	-3.446817
O	0.490771	1.922434	3.470472
O	0.769625	-3.678289	-1.333925
O	-3.281984	1.903662	1.385670
O	-3.281984	1.903662	-1.385670
O	0.769625	-3.678289	1.333925
O	0.490771	1.922434	-3.470472
O	2.007630	-0.255859	3.446817
O	-0.147446	-0.143466	-5.319633
N	-2.894694	4.382487	0.000000
O	-0.147446	-0.143466	5.319633
O	3.230449	-4.228723	0.000000
O	1.439716	4.462467	-2.538295
O	4.684352	-0.116810	2.523504
O	-1.604886	-4.243336	2.796862
O	-4.522574	-0.122115	-2.802092
O	-4.522574	-0.122115	2.802092
O	-1.604886	-4.243336	-2.796862
O	4.684352	-0.116810	-2.523504
O	1.439716	4.462467	2.538295

Bond energy LDA+GGA-XC -464.86467758 eV

$[PW_{11}O_{39}\{Mn^{VI}N\}]^{4-}$

P	-0.007983	-0.019035	0.000000
W	0.081494	0.047257	-3.622433
Mn	-2.100169	2.798459	0.000000

W	0.081494	0.047257	3.622433
W	2.016769	-2.991434	0.000000
W	1.023794	2.883799	-1.846456
W	3.076992	0.068869	1.881423
W	-1.001999	-2.994502	1.742693
W	-3.147942	0.104129	-1.710375
W	-3.147942	0.104129	1.710375
W	-1.001999	-2.994502	-1.742693
W	3.076992	0.068869	-1.881423
W	1.023794	2.883799	1.846456
O	0.732099	0.500842	-1.272203
O	-1.475187	0.471371	0.000000
O	0.732099	0.500842	1.272203
O	0.018928	-1.576489	0.000000
O	-2.437981	-1.734386	-1.663154
O	1.547557	3.065807	0.000000
O	-2.437981	-1.734386	1.663154
O	3.410197	0.384446	0.000000
O	-0.746323	2.997971	1.302850
O	2.667487	-1.744997	-1.306415
O	-1.687039	0.371699	2.969499
O	-0.176078	-1.760595	-2.973086
O	-0.176078	-1.760595	2.973086
O	-1.687039	0.371699	-2.969499
O	2.667487	-1.744997	1.306415
O	-0.746323	2.997971	-1.302850
O	2.746372	1.945672	-2.117908
O	-3.982789	-0.276701	0.000000
O	2.746372	1.945672	2.117908
O	-1.530793	-3.673008	0.000000
O	2.001802	-0.257848	-3.453819
O	0.474152	1.920542	3.467094
O	0.769454	-3.675938	-1.327095
O	-3.182708	1.941393	1.303642
O	-3.182708	1.941393	-1.303642
O	0.769454	-3.675938	1.327095
O	0.474152	1.920542	-3.467094
O	2.001802	-0.257848	3.453819
O	-0.154941	-0.147903	-5.324172
N	-2.736139	4.185565	0.000000
O	-0.154941	-0.147903	5.324172
O	3.223911	-4.231113	0.000000
O	1.388559	4.443686	-2.512818
O	4.673519	-0.097553	2.523844
O	-1.605177	-4.230919	2.794473
O	-4.504611	-0.063099	-2.775020
O	-4.504611	-0.063099	2.775020
O	-1.605177	-4.230919	-2.794473
O	4.673519	-0.097553	-2.523844
O	1.388559	4.443686	2.512818

Bond energy LDA+GGA-XC -462.80727 eV

$[PW_{11}O_{39}\{Fe^{VI}N\}]^{4-}$

P	-0.011188	-0.013768	0.000000
W	0.084159	0.036393	-3.623307
Fe	-2.091373	2.795956	0.000000
W	0.084159	0.036393	3.623307
W	2.017922	-2.990620	0.000000
W	1.012926	2.878737	-1.842683
W	3.080250	0.072787	1.878441
W	-1.003797	-2.995629	1.741551
W	-3.144809	0.117639	-1.706990
W	-3.144809	0.117639	1.706990
W	-1.003797	-2.995629	-1.741551
W	3.080250	0.072787	-1.878441
W	1.012926	2.878737	1.842683
O	0.729393	0.501273	-1.270648
O	-1.479424	0.482435	0.000000
O	0.729393	0.501273	1.270648
O	0.016446	-1.572149	0.000000
O	-2.431770	-1.734163	-1.660857
O	1.557396	3.068607	0.000000
O	-2.431770	-1.734163	1.660857
O	3.412020	0.380643	0.000000
O	-0.754966	2.995033	1.303450
O	2.675677	-1.743324	-1.305554
O	-1.685440	0.362871	2.974006
O	-0.174501	-1.765101	-2.975326
O	-0.174501	-1.765101	2.975326
O	-1.685440	0.362871	-2.974006
O	2.675677	-1.743324	1.305554
O	-0.754966	2.995033	-1.303450
O	2.744669	1.947913	-2.110868
O	-3.974298	-0.299777	0.000000
O	2.744669	1.947913	2.110868
O	-1.534605	-3.675700	0.000000
O	2.003523	-0.262508	-3.453461
O	0.470353	1.913895	3.462988
O	0.773546	-3.669227	-1.329263
O	-3.182489	1.944437	1.303206
O	-3.182489	1.944437	-1.303206
O	0.773546	-3.669227	1.329263
O	0.470353	1.913895	-3.462988
O	2.003523	-0.262508	3.453461
O	-0.158377	-0.144735	-5.326061
N	-2.715699	4.161927	0.000000

O	-0.158377	-0.144735	5.326061
O	3.232456	-4.222592	0.000000
O	1.378239	4.440593	-2.505205
O	4.678736	-0.097677	2.512741
O	-1.601207	-4.228727	2.800611
O	-4.502188	-0.049951	-2.773102
O	-4.502188	-0.049951	2.773102
O	-1.601207	-4.228727	-2.800611
O	4.678736	-0.097677	-2.512741
O	1.378239	4.440593	2.505205

Bond energy LDA+GGA-XC -460.65576 eV

$[PW_{11}O_{39}\{Mn^{V}N\}]^{5-}$

P	-0.007873	-0.027816	0.000000
W	0.084240	0.044421	-3.618313
Mn	-2.114304	2.837877	0.000000
W	0.084240	0.044421	3.618313
W	2.011169	-3.006924	0.000000
W	1.013152	2.891260	-1.838741
W	3.079144	0.072988	1.887469
W	-1.001170	-2.998968	1.742587
W	-3.152749	0.113174	-1.712242
W	-3.152749	0.113174	1.712242
W	-1.001170	-2.998968	-1.742587
W	3.079144	0.072988	-1.887469
W	1.013152	2.891260	1.838741
O	0.738791	0.492851	-1.270413
O	-1.470182	0.459069	0.000000
O	0.738791	0.492851	1.270413
O	0.030176	-1.589528	0.000000
O	-2.427073	-1.754181	-1.655218
O	1.611480	3.073565	0.000000
O	-2.427073	-1.754181	1.655218
O	3.418142	0.377609	0.000000
O	-0.714205	3.029782	1.292206
O	2.676644	-1.755776	-1.307791
O	-1.677647	0.364891	2.972215
O	-0.162738	-1.776165	-2.971150
O	-0.162738	-1.776165	2.971150
O	-1.677647	0.364891	-2.972215
O	2.676644	-1.755776	1.307791
O	-0.714205	3.029782	-1.292206
O	2.765260	1.930675	-2.117386
O	-3.987657	-0.313264	0.000000
O	2.765260	1.930675	2.117386
O	-1.530194	-3.690632	0.000000

O	2.011480	-0.268594	-3.453786
O	0.477252	1.908145	3.467321
O	0.784814	-3.687727	-1.329851
O	-3.185809	1.913576	1.312538
O	-3.185809	1.913576	-1.312538
O	0.784814	-3.687727	1.329851
O	0.477252	1.908145	-3.467321
O	2.011480	-0.268594	3.453786
O	-0.154980	-0.150032	-5.325037
N	-2.750948	4.216569	0.000000
O	-0.154980	-0.150032	5.325037
O	3.238093	-4.238999	0.000000
O	1.376645	4.456194	-2.512668
O	4.689963	-0.101089	2.519748
O	-1.600537	-4.242560	2.796500
O	-4.513621	-0.045089	-2.779988
O	-4.513621	-0.045089	2.779988
O	-1.600537	-4.242560	-2.796500
O	4.689963	-0.101089	-2.519748
O	1.376645	4.456194	2.512668

Bond energy LDA+GGA-XC -467.58089 eV

$[PW_{11}O_{39}\{Fe^{V}N\}]^{5-}$

P	-0.008555	-0.022358	0.000000
W	0.082468	0.041765	-3.615383
Fe	-2.105216	2.742364	0.000000
W	0.082468	0.041765	3.615383
W	2.011435	-2.994577	0.000000
W	1.017668	2.896292	-1.842774
W	3.085209	0.069365	1.878600
W	-1.002484	-2.994142	1.740372
W	-3.158044	0.114451	-1.707648
W	-3.158044	0.114451	1.707648
W	-1.002484	-2.994142	-1.740372
W	3.085209	0.069365	-1.878600
W	1.017668	2.896292	1.842774
O	0.731665	0.496704	-1.268669
O	-1.479313	0.458496	0.000000
O	0.731665	0.496704	1.268669
O	0.016597	-1.581725	0.000000
O	-2.423642	-1.743872	-1.663212
O	1.599964	3.076553	0.000000
O	-2.423642	-1.743872	1.663212
O	3.412388	0.372774	0.000000
O	-0.711730	3.034994	1.320054
O	2.668351	-1.750809	-1.306984
O	-1.682263	0.363207	2.974414

O	-0.164922	-1.772373	-2.967034
O	-0.164922	-1.772373	2.967034
O	-1.682263	0.363207	-2.974414
O	2.668351	-1.750809	1.306984
O	-0.711730	3.034994	-1.320054
O	2.763748	1.928550	-2.113836
O	-3.987246	-0.321293	0.000000
O	2.763748	1.928550	2.113836
O	-1.534108	-3.681579	0.000000
O	2.009343	-0.264751	-3.448189
O	0.484016	1.907461	3.471582
O	0.770855	-3.677992	-1.326598
O	-3.195074	1.914463	1.318396
O	-3.195074	1.914463	-1.318396
O	0.770855	-3.677992	1.326598
O	0.484016	1.907461	-3.471582
O	2.009343	-0.264751	3.448189
O	-0.152838	-0.155681	-5.321013
N	-2.725779	4.194018	0.000000
O	-0.152838	-0.155681	5.321013
O	3.227867	-4.230238	0.000000
O	1.381668	4.458098	-2.519760
O	4.688773	-0.100841	2.514938
O	-1.600644	-4.235685	2.793327
O	-4.508837	-0.050675	-2.787210
O	-4.508837	-0.050675	2.787210
O	-1.600644	-4.235685	-2.793327
O	4.688773	-0.100841	-2.514938
O	1.381668	4.458098	2.519760

Bond energy LDA+GGA-XC -465.26251 eV

$[PW_{11}O_{39}\{Cr^{VI}N\}]^{4-}$

P	-0.000405	-0.032424	0.000000
W	0.085130	0.055147	-3.609007
Cr	-2.126654	2.798798	0.000000
W	0.085130	0.055147	3.609007
W	1.999998	-2.998457	0.000000
W	1.035584	2.894726	-1.849374
W	3.072585	0.065903	1.876997
W	-1.000317	-2.998173	1.740758
W	-3.143979	0.090988	-1.713515
W	-3.143979	0.090988	1.713515
W	-1.000317	-2.998173	-1.740758
W	3.072585	0.065903	-1.876997
W	1.035584	2.894726	1.849374
O	0.739498	0.486838	-1.272038

O	-1.468885	0.438583	0.000000
O	0.739498	0.486838	1.272038
O	0.028863	-1.594126	0.000000
O	-2.446918	-1.741299	-1.651001
O	1.538948	3.088617	0.000000
O	-2.446918	-1.741299	1.651001
O	3.404898	0.389676	0.000000
O	-0.733097	3.002782	1.283729
O	2.657811	-1.742280	-1.306251
O	-1.685530	0.388277	2.949024
O	-0.184682	-1.754037	-2.963101
O	-0.184682	-1.754037	2.963101
O	-1.685530	0.388277	-2.949024
O	2.657811	-1.742280	1.306251
O	-0.733097	3.002782	-1.283729
O	2.744553	1.947087	-2.124391
O	-3.991755	-0.217589	0.000000
O	2.744553	1.947087	2.124391
O	-1.530786	-3.679955	0.000000
O	2.000564	-0.247181	-3.462125
O	0.463834	1.931017	3.460429
O	0.771492	-3.690883	-1.333248
O	-3.171783	1.951086	1.309409
O	-3.171783	1.951086	-1.309409
O	0.771492	-3.690883	1.333248
O	0.463834	1.931017	-3.460429
O	2.000564	-0.247181	3.462125
O	-0.162999	-0.130432	-5.309533
N	-2.750437	4.220164	0.000000
O	-0.162999	-0.130432	5.309533
O	3.231708	-4.212922	0.000000
O	1.397348	4.457663	-2.508179
O	4.672306	-0.113649	2.506619
O	-1.612563	-4.221619	2.800281
O	-4.484709	-0.088314	-2.794730
O	-4.484709	-0.088314	2.794730
O	-1.612563	-4.221619	-2.800281
O	4.672306	-0.113649	-2.506619
O	1.397348	4.457663	2.508179

Bond energy LDA+GGA-XC -464.00319863 eV

$[PW_{11}O_{39}\{Cr^{V}N\}]^{5-}$

P	-0.000581	-0.035692	0.000000
W	0.083613	0.045833	-3.614137
Cr	-2.140013	2.871530	0.000000
W	0.083613	0.045833	3.614137

W	2.012080	-3.006127	0.000000
W	1.030646	2.903466	-1.844325
W	3.085958	0.066955	1.879927
W	-1.002931	-3.002321	1.743775
W	-3.164705	0.102748	-1.709206
W	-3.164705	0.102748	1.709206
W	-1.002931	-3.002321	-1.743775
W	3.085958	0.066955	-1.879927
W	1.030646	2.903466	1.844325
O	0.744210	0.488384	-1.269346
O	-1.467789	0.435659	0.000000
O	0.744210	0.488384	1.269346
O	0.036736	-1.599578	0.000000
O	-2.427449	-1.757496	-1.645290
O	1.614541	3.086033	0.000000
O	-2.427449	-1.757496	1.645290
O	3.417502	0.386028	0.000000
O	-0.706577	3.056181	1.306394
O	2.670099	-1.750125	-1.303618
O	-1.677167	0.363500	2.961830
O	-0.171587	-1.773146	-2.969868
O	-0.171587	-1.773146	2.969868
O	-1.677167	0.363500	-2.961830
O	2.670099	-1.750125	1.303618
O	-0.706577	3.056181	-1.306394
O	2.766674	1.929848	-2.122063
O	-4.007784	-0.300205	0.000000
O	2.766674	1.929848	2.122063
O	-1.525206	-3.697161	0.000000
O	2.006680	-0.267597	-3.455047
O	0.486693	1.916536	3.464169
O	0.782818	-3.689310	-1.333181
O	-3.208413	1.910007	1.334033
O	-3.208413	1.910007	-1.334033
O	0.782818	-3.689310	1.333181
O	0.486693	1.916536	-3.464169
O	2.006680	-0.267597	3.455047
O	-0.161617	-0.141943	-5.319767
N	-2.809517	4.275068	0.000000
O	-0.161617	-0.141943	5.319767
O	3.247525	-4.226698	0.000000
O	1.400681	4.462427	-2.523625
O	4.691307	-0.112832	2.513313
O	-1.605229	-4.243384	2.798968
O	-4.510184	-0.079592	-2.794400
O	-4.510184	-0.079592	2.794400
O	-1.605229	-4.243384	-2.798968
O	4.691307	-0.112832	-2.513313
O	1.400681	4.462427	2.523625

Bond energy LDA+GGA-XC -469.04977209 eV

$[PW_{11}O_{39}\{Os^{V}N\}]^{5-}$

P	-0.005893	-0.013647	0.000000
W	0.084624	0.052637	-3.620710
Os	-2.174086	2.923430	0.000000
W	0.084624	0.052637	3.620710
W	2.005701	-3.007465	0.000000
W	1.050753	2.898345	-1.862004
W	3.093223	0.063494	1.869501
W	-1.006797	-3.000052	1.743013
W	-3.169507	0.073651	-1.725352
W	-3.169507	0.073651	1.725352
W	-1.006797	-3.000052	-1.743013
W	3.093223	0.063494	-1.869501
W	1.050753	2.898345	1.862004
O	0.732777	0.508608	-1.271459
O	-1.479587	0.490544	0.000000
O	0.732777	0.508608	1.271459
O	0.012603	-1.571146	0.000000
O	-2.443768	-1.749157	-1.662284
O	1.570558	3.084280	0.000000
O	-2.443768	-1.749157	1.662284
O	3.427988	0.387705	0.000000
O	-0.749714	3.066907	1.358589
O	2.666622	-1.747514	-1.305445
O	-1.689077	0.367167	2.974891
O	-0.168337	-1.767240	-2.976459
O	-0.168337	-1.767240	2.976459
O	-1.689077	0.367167	-2.974891
O	2.666622	-1.747514	1.305445
O	-0.749714	3.066907	-1.358589
O	2.759964	1.946252	-2.116111
O	-3.975439	-0.328208	0.000000
O	2.759964	1.946252	2.116111
O	-1.523452	-3.681811	0.000000
O	1.994027	-0.258672	-3.453844
O	0.480583	1.918778	3.478153
O	0.792181	-3.682535	-1.329830
O	-3.257187	1.930477	1.359582
O	-3.257187	1.930477	-1.359582
O	0.792181	-3.682535	1.329830
O	0.480583	1.918778	-3.478153
O	1.994027	-0.258672	3.453844
O	-0.155145	-0.146154	-5.328385
N	-2.875480	4.425013	0.000000
O	-0.155145	-0.146154	5.328385

O	3.241907	-4.227831	0.000000
O	1.423599	4.463639	-2.519542
O	4.692343	-0.101876	2.517251
O	-1.609807	-4.247314	2.790900
O	-4.518057	-0.130321	-2.798323
O	-4.518057	-0.130321	2.798323
O	-1.609807	-4.247314	-2.790900
O	4.692343	-0.101876	-2.517251
O	1.423599	4.463639	2.519542

Bond energy LDA+GGA-XC -466.91701655 eV

$[PW_{11}O_{39}\{W^{V}N\}]^{5-}$

P	0.005119	-0.027552	0.000000
W	0.081103	0.053367	-3.606450
W	-2.196297	2.911041	0.000000
W	0.081103	0.053367	3.606450
W	2.008363	-3.003248	0.000000
W	1.065751	2.913184	-1.864458
W	3.078700	0.056982	1.878367
W	-1.001376	-3.006791	1.739804
W	-3.167030	0.064457	-1.732772
W	-3.167030	0.064457	1.732772
W	-1.001376	-3.006791	-1.739804
W	3.078700	0.056982	-1.878367
W	1.065751	2.913184	1.864458
O	0.740380	0.497897	-1.271481
O	-1.469250	0.444716	0.000000
O	0.740380	0.497897	1.271481
O	0.028566	-1.591005	0.000000
O	-2.458163	-1.758268	-1.639198
O	1.555160	3.090407	0.000000
O	-2.458163	-1.758268	1.639198
O	3.419049	0.402001	0.000000
O	-0.718187	3.078904	1.326351
O	2.663086	-1.739254	-1.309167
O	-1.706840	0.380788	2.952182
O	-0.192142	-1.753032	-2.950893
O	-0.192142	-1.753032	2.950893
O	-1.706840	0.380788	-2.952182
O	2.663086	-1.739254	1.309167
O	-0.718187	3.078904	-1.326351
O	2.762136	1.953856	-2.114184
O	-3.993099	-0.250725	0.000000
O	2.762136	1.953856	2.114184
O	-1.539382	-3.699100	0.000000
O	2.003245	-0.245450	-3.451782

O	0.474724	1.943717	3.453869
O	0.769322	-3.682280	-1.335809
O	-3.245578	1.935236	1.373525
O	-3.245578	1.935236	-1.373525
O	0.769322	-3.682280	1.335809
O	0.474724	1.943717	-3.453869
O	2.003245	-0.245450	3.451782
O	-0.168607	-0.135214	-5.308448
N	-2.893681	4.479571	0.000000
O	-0.168607	-0.135214	5.308448
O	3.236769	-4.219745	0.000000
O	1.443063	4.470142	-2.531936
O	4.686950	-0.107569	2.506533
O	-1.608961	-4.239067	2.801200
O	-4.508971	-0.142352	-2.810363
O	-4.508971	-0.142352	2.810363
O	-1.608961	-4.239067	-2.801200
O	4.686950	-0.107569	-2.506533
O	1.443063	4.470142	2.531936

Bond energy LDA+GGA-XC -470.95595624 eV

$[PW_{11}O_{39}\{Mo^{V}N\}]^{5-}$

P	0.007116	-0.017933	0.000000
W	0.077145	0.045711	-3.604759
Mo	-2.205764	2.963178	0.000000
W	0.077145	0.045711	3.604759
W	2.011470	-3.004924	0.000000
W	1.058058	2.913362	-1.865408
W	3.087396	0.059201	1.878391
W	-1.001669	-3.005313	1.739854
W	-3.173806	0.074040	-1.727656
W	-3.173806	0.074040	1.727656
W	-1.001669	-3.005313	-1.739854
W	3.087396	0.059201	-1.878391
W	1.058058	2.913362	1.865408
O	0.741364	0.504104	-1.273330
O	-1.461264	0.470781	0.000000
O	0.741364	0.504104	1.273330
O	0.030993	-1.582698	0.000000
O	-2.435742	-1.775486	-1.654255
O	1.593604	3.086562	0.000000
O	-2.435742	-1.775486	1.654255
O	3.424896	0.381742	0.000000
O	-0.690567	3.122664	1.351698
O	2.673265	-1.752117	-1.304834
O	-1.697730	0.352119	2.967482

O	-0.169723	-1.773730	-2.962102
O	-0.169723	-1.773730	2.962102
O	-1.697730	0.352119	-2.967482
O	2.673265	-1.752117	1.304834
O	-0.690567	3.122664	-1.351698
O	2.778562	1.930351	-2.116282
O	-3.982024	-0.321576	0.000000
O	2.778562	1.930351	2.116282
O	-1.523165	-3.700134	0.000000
O	2.005979	-0.262912	-3.443179
O	0.489863	1.916559	3.459245
O	0.782255	-3.685134	-1.332023
O	-3.281666	1.892980	1.381865
O	-3.281666	1.892980	-1.381865
O	0.782255	-3.685134	1.332023
O	0.489863	1.916559	-3.459245
O	2.005979	-0.262912	3.443179
O	-0.156241	-0.143823	-5.309644
N	-2.933175	4.488775	0.000000
O	-0.156241	-0.143823	5.309644
O	3.235613	-4.233577	0.000000
O	1.456043	4.464622	-2.540647
O	4.686227	-0.116167	2.522419
O	-1.601217	-4.244782	2.793720
O	-4.518384	-0.140218	-2.805724
O	-4.518384	-0.140218	2.805724
O	-1.601217	-4.244782	-2.793720
O	4.686227	-0.116167	-2.522419
O	1.456043	4.464622	2.540647

Bond energy LDA+GGA-XC -470.20722672 eV

$[PW_{11}O_{39}\{Re^{V}N\}]^{5-}$

P	-0.003220	-0.016672	0.000000
W	0.078921	0.045639	-3.615413
Re	-2.178604	2.925766	0.000000
W	0.078921	0.045639	3.615413
W	2.019349	-2.998071	0.000000
W	1.049079	2.901281	-1.861116
W	3.085230	0.064392	1.881566
W	-1.008137	-2.996547	1.755799
W	-3.169128	0.079478	-1.730155
W	-3.169128	0.079478	1.730155
W	-1.008137	-2.996547	-1.755799
W	3.085230	0.064392	-1.881566
W	1.049079	2.901281	1.861116
O	0.736855	0.509932	-1.270428

O	-1.469990	0.478413	0.000000
O	0.736855	0.509932	1.270428
O	0.029147	-1.577204	0.000000
O	-2.440348	-1.775940	-1.653416
O	1.630089	3.065825	0.000000
O	-2.440348	-1.775940	1.653416
O	3.421883	0.384798	0.000000
O	-0.708634	3.085918	1.323142
O	2.671933	-1.751428	-1.306771
O	-1.694236	0.340289	2.969029
O	-0.165366	-1.781496	-2.964253
O	-0.165366	-1.781496	2.964253
O	-1.694236	0.340289	-2.969029
O	2.671933	-1.751428	1.306771
O	-0.708634	3.085918	-1.323142
O	2.773973	1.938096	-2.118049
O	-3.972710	-0.366920	0.000000
O	2.773973	1.938096	2.118049
O	-1.519014	-3.693108	0.000000
O	2.011510	-0.267800	-3.444845
O	0.489222	1.915582	3.458664
O	0.782257	-3.690427	-1.328032
O	-3.253238	1.906490	1.347586
O	-3.253238	1.906490	-1.347586
O	0.782257	-3.690427	1.328032
O	0.489222	1.915582	-3.458664
O	2.011510	-0.267800	3.444845
O	-0.151400	-0.142617	-5.320707
N	-2.887380	4.443390	0.000000
O	-0.151400	-0.142617	5.320707
O	3.234335	-4.231576	0.000000
O	1.428022	4.459247	-2.531630
O	4.688698	-0.111015	2.516672
O	-1.602534	-4.251236	2.794070
O	-4.517058	-0.107520	-2.804811
O	-4.517058	-0.107520	2.804811
O	-1.602534	-4.251236	-2.794070
O	4.688698	-0.111015	-2.516672
O	1.428022	4.459247	2.531630

Bond energy LDA+GGA-XC -469.74301641 eV

$[PW_{11}O_{39}\{Tc^{V}N\}]^{5-}$

P	-0.010400	-0.016552	0.000000
W	0.079676	0.044939	-3.605068
Tc	-2.196602	2.952944	0.000000
W	0.079676	0.044939	3.605068

W	2.015188	-3.005719	0.000000
W	1.046501	2.909886	-1.853094
W	3.087881	0.060714	1.879354
W	-0.999916	-3.002861	1.744721
W	-3.178161	0.086833	-1.721606
W	-3.178161	0.086833	1.721606
W	-0.999916	-3.002861	-1.744721
W	3.087881	0.060714	-1.879354
W	1.046501	2.909886	1.853094
O	0.736298	0.502480	-1.267264
O	-1.482713	0.476682	0.000000
O	0.736298	0.502480	1.267264
O	0.022188	-1.579148	0.000000
O	-2.431340	-1.771678	-1.664050
O	1.633840	3.069177	0.000000
O	-2.431340	-1.771678	1.664050
O	3.425895	0.377000	0.000000
O	-0.693989	3.096043	1.343417
O	2.673679	-1.755153	-1.305414
O	-1.686577	0.351197	2.966732
O	-0.155550	-1.782199	-2.963524
O	-0.155550	-1.782199	2.963524
O	-1.686577	0.351197	-2.966732
O	2.673679	-1.755153	1.305414
O	-0.693989	3.096043	-1.343417
O	2.778830	1.927472	-2.115823
O	-3.986861	-0.354681	0.000000
O	2.778830	1.927472	2.115823
O	-1.514391	-3.698567	0.000000
O	2.009281	-0.270984	-3.444512
O	0.501432	1.906194	3.462841
O	0.787954	-3.687946	-1.329959
O	-3.272332	1.894266	1.375694
O	-3.272332	1.894266	-1.375694
O	0.787954	-3.687946	1.329959
O	0.501432	1.906194	-3.462841
O	2.009281	-0.270984	3.444512
O	-0.149112	-0.144829	-5.313320
N	-2.898682	4.442046	0.000000
O	-0.149112	-0.144829	5.313320
O	3.239482	-4.236983	0.000000
O	1.452091	4.457121	-2.541771
O	4.691646	-0.114711	2.520447
O	-1.592484	-4.254266	2.793910
O	-4.516332	-0.129839	-2.807879
O	-4.516332	-0.129839	2.807879
O	-1.592484	-4.254266	-2.793910
O	4.691646	-0.114711	-2.520447
O	1.452091	4.457121	2.541771

Bond energy LDA+GGA-XC -469.37460087 eV

$[PW_{11}O_{39}\{Mn^{VI}O\}]^{3-}$

P	-0.005737	-0.021677	0.000000
W	0.081021	0.039853	-3.635820
Mn	-2.109256	2.852322	0.000000
W	0.081021	0.039853	3.635820
W	2.016103	-2.988696	0.000000
W	1.021138	2.864883	-1.849820
W	3.078283	0.075442	1.877447
W	-1.005307	-2.996975	1.743981
W	-3.133212	0.100301	-1.715206
W	-3.133212	0.100301	1.715206
W	-1.005307	-2.996975	-1.743981
W	3.078283	0.075442	-1.877447
W	1.021138	2.864883	1.849820
O	0.725781	0.505594	-1.273976
O	-1.472144	0.473365	0.000000
O	0.725781	0.505594	1.273976
O	0.012175	-1.574492	0.000000
O	-2.442768	-1.713896	-1.660325
O	1.529866	3.046805	0.000000
O	-2.442768	-1.713896	1.660325
O	3.402491	0.396728	0.000000
O	-0.797884	2.970587	1.252964
O	2.666151	-1.729696	-1.305725
O	-1.693877	0.373829	2.977226
O	-0.179261	-1.753216	-2.969364
O	-0.179261	-1.753216	2.969364
O	-1.693877	0.373829	-2.977226
O	2.666151	-1.729696	1.305725
O	-0.797884	2.970587	-1.252964
O	2.722942	1.964912	-2.121686
O	-3.976350	-0.248285	0.000000
O	2.722942	1.964912	2.121686
O	-1.537860	-3.657371	0.000000
O	1.996662	-0.241044	-3.454591
O	0.460550	1.929274	3.461729
O	0.763797	-3.661239	-1.324592
O	-3.119803	1.974603	1.260858
O	-3.119803	1.974603	-1.260858
O	0.763797	-3.661239	1.324592
O	0.460550	1.929274	-3.461729
O	1.996662	-0.241044	3.454591
O	-0.152429	-0.156174	-5.332379
O	-2.752238	4.279401	0.000000
O	-0.152429	-0.156174	5.332379

O	3.221698	-4.223267	0.000000
O	1.365699	4.426268	-2.496619
O	4.671382	-0.083531	2.517126
O	-1.602826	-4.232803	2.791063
O	-4.494466	-0.042526	-2.767263
O	-4.494466	-0.042526	2.767263
O	-1.602826	-4.232803	-2.791063
O	4.671382	-0.083531	-2.517126
O	1.365699	4.426268	2.496619

Bond energy LDA+GGA-XC -455.99855679 eV

$[PW_{11}O_{39}\{Mn^{V}O\}]^{4-}$

P	-0.004039	-0.015728	0.000000
W	0.081735	0.046080	-3.624035
Mn	-2.077685	2.732879	0.000000
W	0.081735	0.046080	3.624035
W	2.011385	-2.989351	0.000000
W	1.023964	2.877023	-1.845881
W	3.079518	0.073141	1.876652
W	-1.005311	-2.989649	1.742470
W	-3.147650	0.103778	-1.716456
W	-3.147650	0.103778	1.716456
W	-1.005311	-2.989649	-1.742470
W	3.079518	0.073141	-1.876652
W	1.023964	2.877023	1.845881
O	0.730670	0.500271	-1.270525
O	-1.474300	0.487282	0.000000
O	0.730670	0.500271	1.270525
O	0.009836	-1.567800	0.000000
O	-2.435840	-1.725572	-1.656483
O	1.555407	3.057760	0.000000
O	-2.435840	-1.725572	1.656483
O	3.403372	0.390621	0.000000
O	-0.749791	2.985034	1.293649
O	2.667391	-1.737848	-1.304226
O	-1.688703	0.378576	2.971577
O	-0.174131	-1.755201	-2.966900
O	-0.174131	-1.755201	2.966900
O	-1.688703	0.378576	-2.971577
O	2.667391	-1.737848	1.304226
O	-0.749791	2.985034	-1.293649
O	2.742823	1.947516	-2.117597
O	-3.976840	-0.270119	0.000000
O	2.742823	1.947516	2.117597
O	-1.534969	-3.663393	0.000000
O	2.000208	-0.250648	-3.450035

O	0.474304	1.920678	3.465718
O	0.767158	-3.663464	-1.324916
O	-3.175521	1.943437	1.297145
O	-3.175521	1.943437	-1.297145
O	0.767158	-3.663464	1.324916
O	0.474304	1.920678	-3.465718
O	2.000208	-0.250648	3.450035
O	-0.146189	-0.141939	-5.325507
O	-2.742453	4.201663	0.000000
O	-0.146189	-0.141939	5.325507
O	3.222634	-4.222561	0.000000
O	1.377085	4.441739	-2.496566
O	4.676149	-0.090588	2.514912
O	-1.603811	-4.227618	2.791191
O	-4.507237	-0.059582	-2.773895
O	-4.507237	-0.059582	2.773895
O	-1.603811	-4.227618	-2.791191
O	4.676149	-0.090588	-2.514912
O	1.377085	4.441739	2.496566

Bond energy LDA+GGA-XC -461.81850497 eV

$[PW_{11}O_{39}\{Re^{VI}O\}]^{3-}$

P	0.003913	0.001812	0.000000
W	0.078705	0.046807	-3.621754
Re	-2.174910	2.915743	0.000000
W	0.078705	0.046807	3.621754
W	2.008137	-2.987867	0.000000
W	1.055220	2.881880	-1.862199
W	3.085172	0.066524	1.876783
W	-1.005415	-3.000384	1.747309
W	-3.158040	0.066058	-1.729464
W	-3.158040	0.066058	1.729464
W	-1.005415	-3.000384	-1.747309
W	3.085172	0.066524	-1.876783
W	1.055220	2.881880	1.862199
O	0.731964	0.520995	-1.275318
O	-1.465214	0.524341	0.000000
O	0.731964	0.520995	1.275318
O	0.008226	-1.549193	0.000000
O	-2.450314	-1.731940	-1.664852
O	1.551936	3.049997	0.000000
O	-2.450314	-1.731940	1.664852
O	3.408258	0.395487	0.000000
O	-0.765544	3.050693	1.296915
O	2.660508	-1.727469	-1.302512
O	-1.695029	0.375509	2.960757

O	-0.187817	-1.753914	-2.964789
O	-0.187817	-1.753914	2.964789
O	-1.695029	0.375509	-2.960757
O	2.660508	-1.727469	1.302512
O	-0.765544	3.050693	-1.296915
O	2.748036	1.955349	-2.123749
O	-3.963182	-0.277164	0.000000
O	2.748036	1.955349	2.123749
O	-1.541198	-3.655738	0.000000
O	1.994716	-0.237949	-3.447222
O	0.462195	1.931377	3.452827
O	0.766015	-3.658669	-1.326875
O	-3.198578	1.949657	1.319090
O	-3.198578	1.949657	-1.319090
O	0.766015	-3.658669	1.326875
O	0.462195	1.931377	-3.452827
O	1.994716	-0.237949	3.447222
O	-0.156185	-0.129861	-5.320426
O	-2.886686	4.454364	0.000000
O	-0.156185	-0.129861	5.320426
O	3.225930	-4.211093	0.000000
O	1.433921	4.434794	-2.506913
O	4.679650	-0.101962	2.510817
O	-1.601455	-4.242765	2.787393
O	-4.498275	-0.106441	-2.797513
O	-4.498275	-0.106441	2.797513
O	-1.601455	-4.242765	-2.787393
O	4.679650	-0.101962	-2.510817
O	1.433921	4.434794	2.506913

Bond energy LDA+GGA-XC -460.05041617 eV

$[PW_{11}O_{39}\{Re^{VII}O\}]^{2-}$

P	-0.015496	0.014985	0.000000
W	0.065471	0.059771	-3.605103
Re	-2.134142	2.847583	0.000000
W	0.065471	0.059771	3.605103
W	2.003742	-2.984832	0.000000
W	1.097130	2.897532	-1.886199
W	3.086503	0.069828	1.868799
W	-1.010301	-3.000281	1.740365
W	-3.175018	0.042269	-1.749075
W	-3.175018	0.042269	1.749075
W	-1.010301	-3.000281	-1.740365
W	3.086503	0.069828	-1.868799
W	1.097130	2.897532	1.886199
O	0.709450	0.541647	-1.268258

O	-1.493315	0.525068	0.000000
O	0.709450	0.541647	1.268258
O	-0.038516	-1.534618	0.000000
O	-2.475554	-1.726628	-1.653865
O	1.459121	3.100727	0.000000
O	-2.475554	-1.726628	1.653865
O	3.399091	0.419721	0.000000
O	-0.782988	3.004944	1.278736
O	2.650550	-1.709871	-1.300067
O	-1.724500	0.404137	2.949984
O	-0.216267	-1.721045	-2.944389
O	-0.216267	-1.721045	2.944389
O	-1.724500	0.404137	-2.949984
O	2.650550	-1.709871	1.300067
O	-0.782988	3.004944	-1.278736
O	2.749998	1.989690	-2.112776
O	-3.985996	-0.167203	0.000000
O	2.749998	1.989690	2.112776
O	-1.536777	-3.662496	0.000000
O	1.975395	-0.201534	-3.428191
O	0.430004	1.962539	3.431342
O	0.762708	-3.632459	-1.329626
O	-3.188359	1.975441	1.302453
O	-3.188359	1.975441	-1.302453
O	0.762708	-3.632459	1.329626
O	0.430004	1.962539	-3.431342
O	1.975395	-0.201534	3.428191
O	-0.165098	-0.116304	-5.299948
O	-2.839262	4.401811	0.000000
O	-0.165098	-0.116304	5.299948
O	3.213463	-4.206609	0.000000
O	1.442165	4.443309	-2.548871
O	4.668056	-0.105356	2.515107
O	-1.587915	-4.242100	2.782171
O	-4.531557	-0.138259	-2.786714
O	-4.531557	-0.138259	2.786714
O	-1.587915	-4.242100	-2.782171
O	4.668056	-0.105356	-2.515107
O	1.442165	4.443309	2.548871

Bond energy LDA+GGA-XC -455.08541681 eV

$[PW_{11}O_{39}\{Re^{V}O\}]^{4-}$

P	0.002443	-0.000423	0.000000
W	0.081648	0.043795	-3.621006
Re	-2.176435	2.923461	0.000000
W	0.081648	0.043795	3.621006

W	2.012062	-2.996590	0.000000
W	1.044218	2.891392	-1.852212
W	3.088350	0.064698	1.880266
W	-1.005298	-3.000915	1.748014
W	-3.164509	0.081396	-1.728947
W	-3.164509	0.081396	1.728947
W	-1.005298	-3.000915	-1.748014
W	3.088350	0.064698	-1.880266
W	1.044218	2.891392	1.852212
O	0.730958	0.518219	-1.271442
O	-1.471375	0.518152	0.000000
O	0.730958	0.518219	1.271442
O	0.012230	-1.550908	0.000000
O	-2.443255	-1.755562	-1.662984
O	1.616881	3.049952	0.000000
O	-2.443255	-1.755562	1.662984
O	3.415511	0.381215	0.000000
O	-0.737346	3.062654	1.293409
O	2.673586	-1.740833	-1.300135
O	-1.692753	0.340554	2.966675
O	-0.173513	-1.771160	-2.970558
O	-0.173513	-1.771160	2.970558
O	-1.692753	0.340554	-2.966675
O	2.673586	-1.740833	1.300135
O	-0.737346	3.062654	-1.293409
O	2.758224	1.941419	-2.118717
O	-3.957994	-0.353416	0.000000
O	2.758224	1.941419	2.118717
O	-1.523432	-3.675553	0.000000
O	2.008456	-0.257808	-3.449359
O	0.485224	1.918147	3.460422
O	0.772811	-3.675383	-1.324559
O	-3.225389	1.925145	1.325355
O	-3.225389	1.925145	-1.325355
O	0.772811	-3.675383	1.324559
O	0.485224	1.918147	-3.460422
O	2.008456	-0.257808	3.449359
O	-0.158485	-0.128345	-5.325204
O	-2.897053	4.455013	0.000000
O	-0.158485	-0.128345	5.325204
O	3.233545	-4.223184	0.000000
O	1.416188	4.447186	-2.509425
O	4.689923	-0.101136	2.513087
O	-1.600117	-4.244865	2.795392
O	-4.508885	-0.102774	-2.800558
O	-4.508885	-0.102774	2.800558
O	-1.600117	-4.244865	-2.795392
O	4.689923	-0.101136	-2.513087
O	1.416188	4.447186	2.509425

Bond energy LDA+GGA-XC -464.54446086 eV
