Redox Properties of Polyoxometalates: New Insights on the Anion Charge Effect

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Supplementary Material

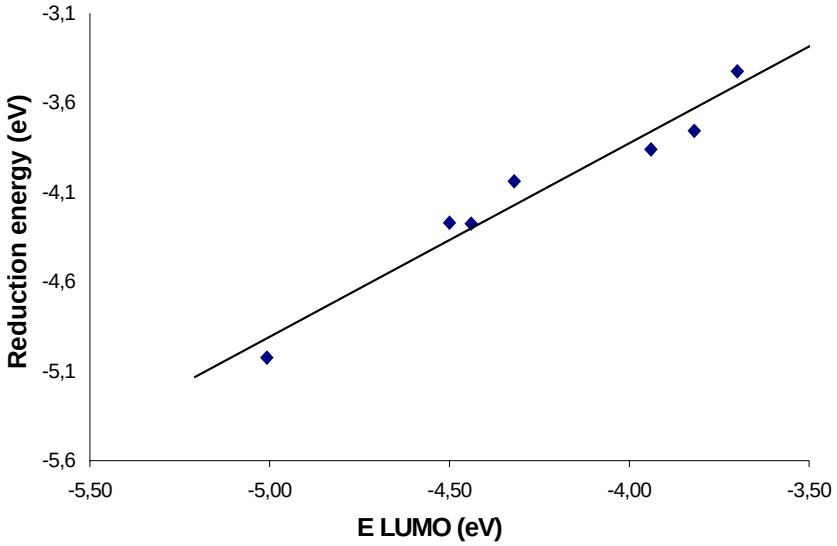

Figure S1. Correlation between the reduction energy and the LUMO's energy for several polyoxotungstates

TABLE S1. XYZ coordinates for several optimized structures
Lindqvist $W_6O_{19}^{2-}$ O(h)

O	0.000000	0.000000	0.000000
W	2.357780	0.000000	0.000000
W	0.000000	2.357780	0.000000
W	-2.357780	0.000000	0.000000
W	0.000000	-2.357780	0.000000
W	0.000000	0.000000	2.357780
W	0.000000	0.000000	-2.357780
O	1.888314	1.888314	0.000000
O	-1.888314	1.888314	0.000000
O	-1.888314	-1.888314	0.000000
O	1.888314	-1.888314	0.000000
O	0.000000	1.888314	1.888314
O	0.000000	-1.888314	1.888314
O	0.000000	-1.888314	-1.888314
O	0.000000	1.888314	-1.888314
O	-1.888314	0.000000	1.888314
O	1.888314	0.000000	1.888314
O	1.888314	0.000000	-1.888314
O	-1.888314	0.000000	-1.888314

O	4.086808	0.000000	0.000000
O	-4.086808	0.000000	0.000000
O	0.000000	0.000000	4.086808
O	0.000000	0.000000	-4.086808
O	0.000000	4.086808	0.000000
O	0.000000	-4.086808	0.000000

Keggin $SiW_{12}O_{40}^{4-}$ T(d)

Si	0.000000	0.000000	0.000000
W	2.529611	2.529611	0.116025
W	-2.529611	2.529611	-0.116025
W	-2.529611	-2.529611	0.116025
W	2.529611	-2.529611	-0.116025
W	0.116025	2.529611	2.529611
W	-0.116025	-2.529611	2.529611
W	0.116025	-2.529611	-2.529611
W	-0.116025	2.529611	-2.529611
W	-2.529611	0.116025	-2.529611
W	2.529611	-0.116025	-2.529611
W	2.529611	0.116025	2.529611
W	-2.529611	-0.116025	2.529611
O	0.950378	0.950378	0.950378
O	-0.950378	0.950378	-0.950378
O	-0.950378	-0.950378	0.950378
O	0.950378	-0.950378	-0.950378
O	1.146732	1.146732	-2.994402
O	-1.146732	1.146732	2.994402
O	-1.146732	-1.146732	-2.994402
O	1.146732	-1.146732	2.994402
O	-2.994402	1.146732	1.146732
O	2.994402	-1.146732	1.146732
O	-2.994402	-1.146732	-1.146732
O	2.994402	1.146732	-1.146732
O	-1.146732	-2.994402	-1.146732
O	1.146732	2.994402	-1.146732
O	1.146732	-2.994402	1.146732
O	-1.146732	2.994402	1.146732
O	1.513802	1.513802	3.415138
O	-1.513802	1.513802	-3.415138
O	-1.513802	-1.513802	3.415138
O	1.513802	-1.513802	-3.415138
O	3.415138	1.513802	1.513802
O	-3.415138	-1.513802	1.513802
O	3.415138	-1.513802	-1.513802

O	-3.415138	1.513802	-1.513802
O	-1.513802	3.415138	-1.513802
O	1.513802	-3.415138	-1.513802
O	1.513802	3.415138	1.513802
O	-1.513802	-3.415138	1.513802
O	3.738598	3.738598	-0.181099
O	-3.738598	3.738598	0.181099
O	-3.738598	-3.738598	-0.181099
O	3.738598	-3.738598	0.181099
O	-0.181099	3.738598	3.738598
O	0.181099	-3.738598	3.738598
O	-0.181099	-3.738598	-3.738598
O	0.181099	3.738598	-3.738598
O	-3.738598	-0.181099	-3.738598
O	3.738598	0.181099	-3.738598
O	3.738598	-0.181099	3.738598
O	-3.738598	0.181099	3.738598

Dawson $P_2W_{18}O_{62}^{6-}$ D(3)

P	0.000000	0.000000	-2.034766
W	0.097810	3.568708	-1.758075
W	0.077412	-3.561408	-2.073823
W	1.983304	-0.181758	-5.013893
W	3.041687	-1.869061	-1.758075
W	-1.149059	-1.626713	-5.013893
W	-3.122976	1.713663	-2.073823
W	-3.139497	-1.699648	-1.758075
W	-0.834245	1.808471	-5.013893
W	3.045564	1.847745	-2.073823
O	0.755185	1.293286	-1.551594
O	-1.497611	0.007367	-1.551594
O	0.742426	-1.300653	-1.551594
O	0.000000	0.000000	-3.653383
O	-2.425131	1.648709	-3.810878
O	-2.454521	-1.601677	-3.692231
O	3.344592	0.013292	-1.586060
O	2.640389	1.275870	-3.810878
O	-1.660785	-2.903148	-1.586060
O	-0.159833	2.926516	-3.692231
O	-0.215259	-2.924579	-3.810878
O	-1.683807	2.889856	-1.586060
O	2.614354	-1.324839	-3.692231
O	3.055105	2.132923	-0.072170
O	-3.995403	-0.002427	-2.149964
O	3.055105	-2.132923	0.072170
O	-1.548043	0.086983	-5.725089
O	1.995600	3.461334	-2.149964

O	0.319613	-3.712260	-0.072170
O	0.849351	1.297153	-5.725089
O	-3.374718	-1.579337	0.072170
O	-3.374718	1.579337	-0.072170
O	0.698692	-1.384136	-5.725089
O	0.319613	3.712260	0.072170
O	1.999803	-3.458907	-2.149964
O	-0.189514	5.220261	-2.208494
O	-0.188856	-5.260297	-2.292583
O	3.223250	-0.222778	-6.228182
O	4.615636	-2.446007	-2.208494
O	-1.804556	-2.680028	-6.228182
O	-4.461123	2.793702	-2.292583
O	-4.426122	-2.774255	-2.208494
O	-1.418694	2.902805	-6.228182
O	4.649979	2.466595	-2.292583
P	0.000000	0.000000	2.034766
W	0.077412	3.561408	2.073823
W	0.097810	-3.568708	1.758075
W	1.983304	0.181758	5.013893
W	3.045564	-1.847745	2.073823
W	-0.834245	-1.808471	5.013893
W	-3.139497	1.699648	1.758075
W	-3.122976	-1.713663	2.073823
W	-1.149059	1.626713	5.013893
W	3.041687	1.869061	1.758075
O	0.742426	1.300653	1.551594
O	-1.497611	-0.007367	1.551594
O	0.755185	-1.293286	1.551594
O	0.000000	0.000000	3.653383
O	-2.454521	1.601677	3.692231
O	-2.425131	-1.648709	3.810878
O	3.344592	-0.013292	1.586060
O	2.614354	1.324839	3.692231
O	-1.683807	-2.889856	1.586060
O	-0.215259	2.924579	3.810878
O	-0.159833	-2.926516	3.692231
O	-1.660785	2.903148	1.586060
O	2.640389	-1.275870	3.810878
O	-3.995403	0.002427	2.149964
O	-1.548043	-0.086983	5.725089
O	1.999803	3.458907	2.149964
O	0.698692	1.384136	5.725089
O	0.849351	-1.297153	5.725089
O	1.995600	-3.461334	2.149964
O	-0.188856	5.260297	2.292583
O	-0.189514	-5.220261	2.208494
O	3.223250	0.222778	6.228182
O	4.649979	-2.466595	2.292583
O	-1.418694	-2.902805	6.228182

O	-4.426122	2.774255	2.208494
O	-4.461123	-2.793702	2.292583
O	-1.804556	2.680028	6.228182
O	4.615636	2.446007	2.208494

Preyssler $NaP_5W_{30}O_{110}^{14-}$ C5v

Na	0.000000	0.000000	0.923345
P	-3.613502	0.000000	-0.010804
W	-3.257482	0.000000	3.473292
W	-5.974330	-1.923249	1.712075
W	-5.974330	1.923249	1.712075
O	-2.716224	0.000000	1.268328
O	-4.563388	-1.306522	0.007110
O	-4.563388	1.306522	0.007110
O	-6.477772	0.000000	1.628577
O	-4.590147	1.337550	2.903964
O	-4.590147	-1.337550	2.903964
O	-6.893139	-2.274018	0.007724
O	-6.893139	2.274018	0.007724
O	-1.927234	-1.400218	3.602842
O	-5.052202	-3.670639	1.616002
O	-3.759228	0.000000	5.175759
O	-7.296429	-2.416646	2.813015
O	-7.296429	2.416646	2.813015
P	-1.116634	-3.436645	-0.010804
W	-1.006617	-3.098049	3.473292
W	-0.017051	-6.276242	1.712075
W	-3.675288	-5.087608	1.712075
O	-0.839360	-2.583283	1.268328
O	-0.167588	-4.743777	0.007110
O	-2.652740	-3.936302	0.007110
O	-2.001742	-6.160727	1.628577
O	-2.690519	-3.952163	2.903964
O	-0.146347	-4.778815	2.903964
O	0.032622	-7.258475	0.007724
O	-4.292817	-5.853055	0.007724
O	0.736138	-2.265600	3.602842
O	1.929769	-5.939219	1.616002
O	-1.161665	-3.575238	5.175759
O	0.043646	-7.686101	2.813015
O	-4.553087	-6.192531	2.813015
P	2.923385	-2.123963	-0.010804
W	2.635358	-1.914700	3.473292
W	5.963792	-1.955682	1.712075
W	3.702877	-5.067564	1.712075
O	2.197472	-1.596557	1.268328
O	4.459812	-1.625294	0.007110
O	2.923904	-3.739290	0.007110

O	5.240628	-3.807539	1.628577
O	2.927315	-3.780122	2.903964
O	4.499699	-1.615920	2.903964
O	6.913301	-2.211967	0.007724
O	4.240033	-5.891405	0.007724
O	2.382193	0.000000	3.602842
O	6.244865	0.000000	1.616002
O	3.041280	-2.209619	5.175759
O	7.323404	-2.333626	2.813015
O	4.482466	-6.243841	2.813015
P	2.923385	2.123963	-0.010804
W	2.635358	1.914700	3.473292
W	3.702877	5.067564	1.712075
W	5.963792	1.955682	1.712075
O	2.197472	1.596557	1.268328
O	2.923904	3.739290	0.007110
O	4.459812	1.625294	0.007110
O	5.240628	3.807539	1.628577
O	4.499699	1.615920	2.903964
O	2.927315	3.780122	2.903964
O	4.240033	5.891405	0.007724
O	6.913301	2.211967	0.007724
O	0.736138	2.265600	3.602842
O	1.929769	5.939219	1.616002
O	3.041280	2.209619	5.175759
O	4.482466	6.243841	2.813015
O	7.323404	2.333626	2.813015
P	-1.116634	3.436645	-0.010804
W	-1.006617	3.098049	3.473292
W	-3.675288	5.087608	1.712075
W	-0.017051	6.276242	1.712075
O	-0.839360	2.583283	1.268328
O	-2.652740	3.936302	0.007110
O	-0.167588	4.743777	0.007110
O	-2.001742	6.160727	1.628577
O	-0.146347	4.778815	2.903964
O	-2.690519	3.952163	2.903964
O	-4.292817	5.853055	0.007724
O	0.032622	7.258475	0.007724
O	-1.927234	1.400218	3.602842
O	-5.052202	3.670639	1.616002
O	-1.161665	3.575238	5.175759
O	-4.553087	6.192531	2.813015
O	0.043646	7.686101	2.813015
W	-3.252722	0.000000	-3.470072
W	-5.976163	1.924181	-1.712702
W	-5.976163	-1.924181	-1.712702
O	-2.773610	0.000000	-1.313622
O	-6.479350	0.000000	-1.618577
O	-4.608265	-1.346885	-2.909740

O	-4.608265	1.346885	-2.909740
O	-1.936609	1.407029	-3.614413
O	-5.057319	3.674358	-1.610119
O	-3.782524	0.000000	-5.167041
O	-7.311310	2.420907	-2.795763
O	-7.311310	-2.420907	-2.795763
W	-1.005146	3.093522	-3.470072
W	-0.016731	6.278274	-1.712702
W	-3.676741	5.089065	-1.712702
O	-0.857093	2.637860	-1.313622
O	-2.002229	6.162228	-1.618577
O	-2.704996	3.966510	-2.909740
O	-0.143068	4.798930	-2.909740
O	0.739719	2.276621	-3.614413
O	1.931724	5.945236	-1.610119
O	-1.168864	3.597395	-5.167041
O	0.043101	7.701570	-2.795763
O	-4.561738	6.205367	-2.795763
W	2.631507	1.911902	-3.470072
W	5.965823	1.956006	-1.712702
W	3.703813	5.069396	-1.712702
O	2.243897	1.630287	-1.313622
O	5.241905	3.808467	-1.618577
O	2.936485	3.798323	-2.909740
O	4.519844	1.619017	-2.909740
O	2.393781	0.000000	-3.614413
O	6.251191	0.000000	-1.610119
O	3.060127	2.223312	-5.167041
O	7.337947	2.338925	-2.795763
O	4.492000	6.256035	-2.795763
W	2.631507	-1.911902	-3.470072
W	3.703813	-5.069396	-1.712702
W	5.965823	-1.956006	-1.712702
O	2.243897	-1.630287	-1.313622
O	5.241905	-3.808467	-1.618577
O	4.519844	-1.619017	-2.909740
O	2.936485	-3.798323	-2.909740
O	0.739719	-2.276621	-3.614413
O	1.931724	-5.945236	-1.610119
O	3.060127	-2.223312	-5.167041
O	4.492000	-6.256035	-2.795763
O	7.337947	-2.338925	-2.795763
W	-1.005146	-3.093522	-3.470072
W	-3.676741	-5.089065	-1.712702
W	-0.016731	-6.278274	-1.712702
O	-0.857093	-2.637860	-1.313622
O	-2.002229	-6.162228	-1.618577
O	-0.143068	-4.798930	-2.909740
O	-2.704996	-3.966510	-2.909740
O	-1.936609	-1.407029	-3.614413

O	-5.057319	-3.674358	-1.610119
O	-1.168864	-3.597395	-5.167041
O	-4.561738	-6.205367	-2.795763
O	0.043101	-7.701570	-2.795763