

DFT study of α -Keggin, lacunary Keggin, and iron^{II-VI} substituted Keggin polyoxometalates: The effect of oxidation state and axial ligand in geometry, electronic structures and oxygen transfer

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This Supplementary file contains 6 Tables and 13 Figures:

Table S1: The relative energy differences between spin states of $[\text{PW}_{12}\text{O}_{40}]^{3-}$ and $[\text{PW}_{11}\text{O}_{39}]^{7-}$ obtained by OPTX-PBE/DZVP-GGA calculation.

Table S2: Selected bond lengths (Å) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{n+})]^{(7-n)-}$ and $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{n+}\text{OH}_2)]^{(7-n)-}$ (n=2 and 3) complexes obtained by OPTX-PBE/DZVP-GGA calculation.

Table S3: Optimized geometries of various POM complexes (Å) in the ground state calculated at the DFT/OPTX-PBE/DZVP-GGA level.

Table S4: Calculated vibrational frequencies (cm^{-1}) and assigned bands of POM complexes.

Table S5: XYZ coordinates of optimized the different studied systems at the DFT/OPTX-PBE/DZVP-GGA level.

Table S6: Atomic spin densities (in e) and Mulliken atomic charges (in e) determined for different studied systems.

Figure S1. HOMOs and LUMOs of $[\text{PW}_{12}\text{O}_{40}]^{3-}$ and $[\text{PW}_{11}\text{O}_{39}]^{7-}$ calculated at the UOPBE/6-31G(d) level (LANL2DZ basis set on the metal atom).

Figure S2. The energy level expressions of FMOs for a) $\text{Fe}^{\text{IV}}\text{OH}_2$, b) $\text{Fe}^{\text{IV}}\text{OH}$, c) Fe^{VO} , d) Fe^{VO} and e) Fe^{VO} POMs in the ground state calculated at UOPBE/6-31G(d) level (LANL2DZ basis set on the metal atom).

Figure S3: Simulated IR (cm^{-1}) of $[\text{PW}_{12}\text{O}_{40}]^{3-}$ with spin state=1.

Figure S4: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}]^{7-}$ with spin state=1.

Figure S5: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}\text{Fe}^{+3}]^{-4}$ with spin state=2.

Figure S6: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{+3}\text{OH}_2)]^{-4}$ with spin state=2.

Figure S7: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}\text{Fe}^{+2}]^{-5}$ with spin state=1.

Figure S8: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{+2}\text{OH}_2)]^{-5}$ with spin state=1.

Figure S9: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{IV}}\text{OH}_2)]^{3-}$ with spin state=3.

Figure S10: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{IV}}\text{OH})]^{4-}$ with spin state=3.

Figure S11: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{IV}}\text{O})]^{5-}$ with spin state=3.

Figure S12: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{VO}})]^{4-}$ with spin state=4.

Figure S13: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{VO}})]^{3-}$ with spin state=3.

Table S1: The relative energy differences between spin states of $[\text{PW}_{12}\text{O}_{40}]^{3-}$ and $[\text{PW}_{11}\text{O}_{39}]^{7-}$ obtained by OPTX-PBE/DZVP-GGA calculation.

2S+1	1	3	5
$[\text{PW}_{12}\text{O}_{40}]^{3-}$	0	57.30	125.50
$[\text{PW}_{11}\text{O}_{39}]^{7-}$	0	55.86	-

Table S2: Selected bond lengths (\AA) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{n+}})]^{(7-\text{n})-}$ and $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{n+}}\text{OH}_2)]^{(7-\text{n})-}$ (n=2 and 3) complexes obtained by OPTX-PBE/DZVP-GGA calculation.

	$[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{III}})]^{4-}$	$[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{III}}\text{OH}_2)]^{4-}$	$[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{II}})]^{5-}$	$[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{II}}\text{OH}_2)]^{5-}$
Spin State	2	2	1	1
$\text{Fe}^{\text{I}}-\text{O}_{\text{aqua}}^{53}$	-	2.060	-	2.113
WBI ($\text{Fe}^{\text{I}}-\text{O}_{\text{aqua}}^{53}$)	-	0.3759	-	0.3358
$\text{Fe}^{\text{I}}-\text{O}_{\text{a}}^{48}$	1.907	1.955	1.938	1.982
$\text{Fe}^{\text{I}}-\text{O}_{\text{c}}^{28}$	1.876	1.871	1.932	1.937
$\text{P}^{52}-\text{O}_{\text{a}}^{48}$	1.586	1.578	1.582	1.575
$\text{P}^{52}-\text{O}_{\text{a}}^{50}$	1.554	1.557	1.559	1.562
$\text{W}^{37}-\text{O}_{\text{a}}^{48}$	2.454	2.464	2.461	2.463
$\text{W}^{39}-\text{O}_{\text{a}}^{48}$	2.453	2.451	2.460	2.465
$\text{W}^{37}-\text{O}_{\text{b}}^6$	1.981	1.993	1.945	1.919
$\text{W}^{39}-\text{O}_{\text{b}}^{12}$	1.896	1.880	1.945	1.964
$\text{W}^{37}-\text{O}_{\text{c}}^{26}$	1.900	1.887	1.943	1.967

W ³⁹ -O _c ²⁶	1.971	1.989	1.942	1.919
W ³⁷ -O _d ³⁴	1.712	1.711	1.722	1.722
W ³⁹ -O _d ³¹	1.712	1.712	1.722	1.720

Table S3: Optimized geometries of various POM complexes (Å) in the ground state calculated at the DFT/OPTX-PBE/DZVP-GGA level.

POM	r (Fe-O _{ligand})	WBI(Fe ^I -O _{ligand} ⁵³)	r_{av} (Fe-O _{eq})	r (Fe-O _a)	r (P-O _a)	Angle(O ¹⁹ -Fe ^I -O ²³)	Angle(O ²² -Fe ^I -O ²⁸)
PWFe ^{II} OH ₂	2.113	0.3358	1.927	1.982	1.575	176.452	177.067
PWFe ^{III} OH ₂	2.060	0.3759	1.893	1.955	1.578	176.570	175.421
PWFe ^{IV} OH ₂	2.047	0.3844	1.858	1.920	1.589	177.752	172.304
PWFe ^{IV} OH	1.815	0.9089	1.876	2.043	1.576	173.375	176.671
PWFe ^{IV} O	1.641	1.46	2.026	2.170	1.576	169.40	169.40
PWFe ^V O	1.635	1.3925	1.884	2.140	1.573	170.674	170.581
PWFe ^{VI} O	1.601	1.5416	1.841	2.239	1.570	168.497	157.714

Table S4: Calculated vibrational frequencies (cm⁻¹) and assigned bands of POM complexes.

	PWFe ^{IV} OH ₂	PWFe ^{IV} OH	PWFe ^{IV} O	PWFe ^V O	PWFe ^{VI} O
2S+1	3	3	3	4	3
V _(P-Oa)	1102	1075	1054	1070	1076
V _(P-Oa)	1094	-	-	-	1066
V _(W=Od)	960	943	916	935	954
V _(W-Ob-W)	851	846	842	845	850
V _(W-Oc-W)	781	777	788	781	779
V _(W-Oc-Fe)	748	761	778	754	752
V _(H-O-H)	1670	-	-	-	-

$V_{(H-O-H)}$	3643	-	-	-	-
$V_{(H-O-H)}$	3754	3735	-	-	-

Table S5: The XYZ coordinates of optimized different studied systems at the DFT/OPTX-PBE/DZVP-GGA level.

[PW ₁₂ O ₄₀] ³⁻ 2S+1=1				O	-2.986863	1.059724	1.278300
P	-0.000371	-0.000260	0.000049	O	1.509432	-2.787458	-1.277183
W	-0.156454	0.006770	-3.564432	O	-2.145978	-2.580486	-2.098555
W	2.769945	-2.243392	0.122269	O	3.776013	1.187387	-0.044362
W	0.029693	-0.153208	3.563948	O	-2.217342	-2.520494	2.098583
W	-2.642638	2.389917	-0.121397	O	0.586738	3.916165	0.043679
W	-0.233437	-3.002073	-1.913340	O	-2.008462	-0.279004	-3.401508
W	-2.930362	-0.694927	1.913279	O	0.035969	-2.027393	3.401016
W	0.132304	3.089642	1.773345	O	-1.598204	3.362285	-1.349706
W	3.032047	0.607855	-1.773323	O	3.570002	-1.058569	1.348487
W	3.054170	0.815646	1.653309	O	3.562265	-1.136044	-1.298872
W	0.333974	3.144362	-1.653833	O	-1.673459	3.344199	1.299497
W	-2.949049	-0.906261	-1.786687	O	0.047130	-1.949885	-3.447312
W	-0.439273	-3.054937	1.786860	O	-1.934355	-0.256486	3.448732
O	-0.587016	-0.685223	-1.276940	O	0.006545	0.226616	-5.242128
O	1.556118	-0.144677	0.001086	O	0.222367	0.044009	5.241313
O	-0.587340	-0.685201	1.276811	O	-4.095011	3.272799	-0.141980
O	-0.383096	1.515474	-0.000724	O	-0.205660	-4.570276	-2.568372
O	1.975372	2.253823	-1.644233	O	-4.483923	-0.907276	2.569571
O	-0.698347	-3.346910	-0.037486	O	0.394840	4.407023	2.814775
O	1.920276	2.300635	1.643341	O	4.293636	1.072436	-2.813507
O	-3.198077	-1.208286	0.037949	O	4.316342	1.315342	2.676118
O	1.447642	-2.802030	1.317220	O	0.630721	4.469088	-2.676774
O	-2.990312	0.995453	-1.315468	O	-4.504666	-1.155904	-2.424579

O	1.771644	0.048662	2.922544	O	-0.443814	-4.631747	2.421493
O	-0.226527	1.759070	-2.925028	O	3.867252	-3.541593	0.144878
O	-0.233032	1.693709	2.957349				
O	1.709402	0.032551	-2.958087				

$[PW_{11}O_{39}]^{7-} 2S+1=1$				O	1.475630	-2.813585	-1.296849
P	-0.129367	0.147876	-0.159346	O	-2.151249	-2.646005	-2.140375
W	-0.194683	-0.087396	-3.682572	O	3.682159	1.146919	0.198299
W	2.812979	-2.366469	0.059554	O	-2.151584	-2.526340	2.028487
W	0.045979	0.046839	3.849733	O	0.645233	4.476799	-0.498828
W	-2.731651	2.598441	-0.037049	O	-2.051321	-0.454916	-3.633586
W	-0.321453	-3.077650	-1.895000	O	0.129930	-2.103754	3.245241
W	-2.805317	-0.756912	1.765147	O	-1.739168	3.448919	-1.471707
W	2.854628	0.651399	-1.678923	O	3.407255	-1.296157	1.356045
W	3.291047	0.876952	1.992241	O	3.505982	-1.109463	-1.268183
W	0.195399	3.330965	-1.714282	O	-2.344444	3.720231	1.222490
W	-3.012163	-0.829673	-1.913887	O	0.094750	-2.057270	-3.445668
W	-0.287450	-3.153836	1.849127	O	-1.813754	-0.238045	3.383489
W	-0.702418	-0.634770	-1.427979	O	0.069938	0.020194	-5.404420
O	1.421570	-0.029822	-0.141860	O	0.274522	-0.509577	5.489431
O	-0.671023	-0.550852	1.129704	O	-4.352126	3.123789	-0.422941
O	-0.552611	1.661226	-0.222527	O	-0.270602	-4.696930	-2.532859
O	1.827232	2.287247	-1.637342	O	-4.358464	-0.961543	2.519782
O	-0.707852	-3.368284	-0.033814	O	4.245335	1.190954	-2.575733
O	3.034153	2.533325	2.455082	O	4.787262	0.571955	2.849946
O	-3.229869	-1.255356	-0.055779	O	0.378343	4.315071	-3.145873
O	1.533630	-3.194468	1.255324	O	-4.583950	-1.205685	-2.573403
O	-3.089557	0.904071	-1.531696	O	-0.451797	-4.752692	2.522191
O	1.758044	0.161398	3.002534	O	4.007375	-3.630884	-0.057631
O	-0.307126	1.603153	-3.143434	O	-2.151249	-2.646005	-2.140375

O	-0.164044	1.741723	4.147334	O	3.682159	1.146919	0.198299
O	1.748889	0.026046	-3.006205				
O	-2.973405	1.064724	1.143353				

[PW ₁₁ O ₃₉ Fe] ⁵⁻ 2S+1=1				O	0.862769	-9.278594	-19.373394
Fe	2.128889	-9.180107	-17.917914	O	5.680031	-10.078224	-15.873709
O	4.333534	-14.622408	-15.728143	O	1.236291	-12.842015	-20.392843
O	0.336119	-12.123856	-14.136777	O	5.200566	-9.581994	-21.252524
O	4.506166	-12.240589	-20.224155	O	3.537051	-17.250713	-16.437471
O	3.258594	-14.629979	-20.381530	O	-0.590764	-13.902437	-15.877912
O	-0.408607	-11.600091	-18.856065	O	-0.249779	-10.584951	-21.535078
O	4.635985	-15.419579	-18.272415	W	0.355883	-10.392003	-15.216232
O	5.860208	-13.059074	-18.153382	W	-0.867401	-12.779622	-17.433086
O	2.146306	-10.232993	-14.505691	W	0.799007	-10.883651	-20.202495
O	-1.057351	-11.316455	-16.222428	W	0.918115	-13.811121	-14.681367
O	4.462513	-11.364797	-13.922541	W	4.198278	-10.257914	-20.026322
O	5.440152	-10.524686	-18.552995	W	4.574144	-13.138400	-14.491051
O	6.128663	-12.667208	-15.529422	W	4.843645	-13.929397	-19.520139
O	0.059430	-14.125430	-18.453773	W	3.264969	-15.628288	-16.940897
O	0.638177	-15.552548	-20.836103	W	6.142950	-11.491968	-17.070474
O	2.048151	-15.895306	-18.406279	W	3.938594	-9.733229	-15.031314
O	-0.589056	-9.354962	-14.210856	W	1.449655	-14.553687	-19.694443
O	5.316281	-13.902920	-13.140803	O	6.066724	-14.554365	-20.556046
O	0.780549	-9.349386	-16.612644	O	7.832888	-11.234618	-17.241871
O	2.709533	-13.406190	-14.122146	O	2.492922	-11.015023	-18.422409
O	4.348762	-8.446793	-13.956115	O	2.929039	-13.483921	-18.082549
O	3.312516	-8.884148	-16.481835	O	1.319143	-12.251237	-16.516629
O	3.486490	-8.795558	-19.237525	O	3.831706	-11.789560	-16.386201
O	1.792238	-15.089218	-15.860533	P	2.644735	-12.149287	-17.330490
O	-2.512633	-13.135101	-17.777089				

O	2.551493	-10.609568	-20.994369	
O	0.364312	-14.814281	-13.398636	

[PW ₁₁ O ₃₉ Fe] ⁵⁻ 2S+1=3				O	0.881460	-9.243988	-19.365251
Fe	2.127690	-9.061612	-17.891297	O	5.658487	-10.079485	-15.870001
O	4.324594	-14.631646	-15.726381	O	1.254085	-12.836360	-20.395394
O	0.328288	-12.118860	-14.152797	O	5.203376	-9.595413	-21.236120
O	4.516941	-12.251192	-20.208480	O	3.511742	-17.257276	-16.442939
O	3.269877	-14.639829	-20.389828	O	-0.599622	-13.898279	-15.886229
O	-0.390669	-11.591099	-18.854900	O	-0.222543	-10.583555	-21.509767
O	4.638703	-15.437000	-18.270887	W	0.346470	-10.377027	-15.235643
O	5.870285	-13.070492	-18.139969	W	-0.857959	-12.794560	-17.434688
O	2.138187	-10.239527	-14.533044	W	0.817861	-10.873330	-20.169173
O	-1.046039	-11.302284	-16.245100	W	0.921625	-13.800732	-14.679396
O	4.443082	-11.376030	-13.925831	W	4.190470	-10.262227	-20.012330
O	5.448620	-10.531167	-18.543695	W	4.573989	-13.150939	-14.501541
O	6.129081	-12.666859	-15.517974	W	4.848960	-13.943364	-19.512220
O	0.061055	-14.123088	-18.471423	W	3.245815	-15.634078	-16.950209
O	0.649503	-15.540625	-20.859458	W	6.140511	-11.500734	-17.072719
O	2.039808	-15.911039	-18.422744	W	3.936722	-9.740750	-15.022612
O	-0.604817	-9.375017	-14.201015	W	1.462281	-14.552194	-19.710038
O	5.311069	-13.912581	-13.147167	O	6.076583	-14.565265	-20.544352
O	0.759556	-9.274374	-16.592595	O	7.830646	-11.233195	-17.228273
O	2.701115	-13.413533	-14.120409	O	2.520924	-11.075892	-18.458794
O	4.344879	-8.498529	-13.901952	O	2.936851	-13.541398	-18.064801
O	3.309938	-8.806241	-16.440505	O	1.322197	-12.260787	-16.537808
O	3.510450	-8.780631	-19.219945	O	3.830275	-11.804541	-16.400277
O	1.779870	-15.090363	-15.867467	P	2.650801	-12.177611	-17.356206
O	-2.504995	-13.135586	-17.786296				
O	2.562683	-10.592522	-20.993626				

O	0.356509	-14.801042	-13.399192				
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[PW ₁₁ O ₃₉ Fe] ⁵⁻ 2S+1=5				O	0.810410	-9.262409	-19.468483
Fe	2.068076	-9.085325	-17.805186	O	5.673919	-10.071459	-15.863695
O	4.336492	-14.620543	-15.714247	O	1.283969	-12.860490	-20.395193
O	0.345975	-12.138209	-14.157482	O	5.281743	-9.639022	-21.252710
O	4.534462	-12.263329	-20.222856	O	3.556633	-17.246793	-16.438829
O	3.263908	-14.673062	-20.392926	O	-0.603442	-13.873393	-15.913906
O	-0.362164	-11.580049	-18.878248	O	-0.158660	-10.677311	-21.622180
O	4.656524	-15.428289	-18.265768	W	0.373406	-10.343889	-15.131047
O	5.872267	-13.079683	-18.153907	W	-0.849851	-12.701160	-17.439723
O	2.145595	-10.151571	-14.539342	W	0.863820	-10.875759	-20.248713
O	-1.026232	-11.267811	-16.218358	W	0.895461	-13.828435	-14.718272
O	4.428409	-11.370990	-13.914706	W	4.235898	-10.215383	-20.008270
O	5.436643	-10.527213	-18.525454	W	4.528999	-13.154736	-14.468771
O	6.110362	-12.653974	-15.498589	W	4.813044	-13.952831	-19.578247
O	0.051449	-14.108439	-18.460179	W	3.289012	-15.628707	-16.959603
O	0.606566	-15.559778	-20.809082	W	6.134643	-11.574743	-17.079320
O	2.054914	-15.911587	-18.403264	W	4.022463	-9.715840	-15.003887
O	-0.566358	-9.451276	-13.995285	W	1.420657	-14.559384	-19.670629
O	5.274714	-13.909226	-13.115425	O	6.049815	-14.580702	-20.596655
O	0.585405	-9.154933	-16.472431	O	7.824223	-11.298853	-17.226237
O	2.689184	-13.423876	-14.104129	O	2.537364	-11.034221	-18.473362
O	4.449864	-8.519367	-13.840564	O	2.940368	-13.517193	-18.085072
O	3.367024	-8.723013	-16.364292	O	1.330997	-12.222652	-16.556516
O	3.585735	-8.715236	-19.308451	O	3.837009	-11.794112	-16.408202
O	1.798101	-15.076614	-15.878974	P	2.660099	-12.151548	-17.374107
O	-2.499725	-13.031362	-17.788891				
O	2.600740	-10.566528	-21.011021				
O	0.319939	-14.843074	-13.454686				

[PW ₁₁ O ₃₉ Fe] ⁴⁻ 2S+1=2				O	0.742854	-9.3606494	-19.330302
Fe	1.983081	-9.238086	-17.928850	O	5.584896	-9.984633	-15.923852
O	4.380736	-14.555103	-15.729148	O	1.207583	-12.877524	-20.368776
O	0.315195	-12.179414	-14.143939	O	5.089216	-9.492147	-21.205449
O	4.438425	-12.161004	-20.241958	O	3.689235	-17.190419	-16.436810
O	3.252673	-14.599875	-20.387822	O	-0.596389	-13.971745	-15.880423
O	-0.472676	-11.676005	-18.850399	O	-0.288436	-10.701711	-21.547162
O	4.690451	-15.345994	-18.296611	W	0.297785	-10.490232	-15.187265
O	5.816982	-12.951860	-18.191002	W	-0.915764	-12.825767	-17.442985
O	2.072389	-10.197218	-14.555566	W	0.768313	-10.983025	-20.230544
O	-1.122334	-11.401530	-16.211170	W	0.902274	-13.880177	-14.724136
O	4.413945	-11.272611	-13.940655	W	4.130601	-10.227636	-19.993095
O	5.344576	-10.430179	-18.550964	W	4.523674	-13.066888	-14.474406
O	6.097034	-12.554413	-15.529590	W	4.805004	-13.869811	-19.566568
O	0.050586	-14.185465	-18.438186	W	3.365269	-15.588535	-16.939217
O	0.654195	-15.621840	-20.777089	W	6.095794	-11.449531	-17.071757
O	2.118765	-15.907706	-18.395543	W	3.873751	-9.706190	-15.069462
O	-0.659083	-9.479096	-14.186902	W	1.439943	-14.613565	-19.641717
O	5.283659	-13.792458	-13.125448	O	6.033170	-14.440447	-20.610167
O	0.664121	-9.423391	-16.627896	O	7.767988	-11.151569	-17.258674
O	2.701557	-13.381989	-14.136036	O	2.425167	-11.026354	-18.421294
O	4.244332	-8.399103	-14.023913	O	2.919445	-13.471465	-18.083994
O	3.170621	-8.874478	-16.529416	O	1.278065	-12.285174	-16.519266
O	3.293460	-8.786358	-19.208251	O	3.778061	-11.760801	-16.385174
O	1.852430	-15.098091	-15.868233	P	2.602260	-12.155762	-17.321724
O	-2.543810	-13.222309	-17.779743				
O	2.461411	-10.566060	-20.985096				
O	0.391780	-14.890082	-13.442480				

[PW ₁₁ O ₃₉ Fe] ⁴⁺ 2S+1=4				O	0.905100	-9.249728	-19.336226
Fe	2.127565	-9.100721	-17.878301	O	5.677037	-10.072587	-15.880126
O	4.325633	-14.619869	-15.723727	O	1.245397	-12.813326	-20.376043
O	0.338395	-12.092725	-14.156309	O	5.210409	-9.589928	-21.187860
O	4.514178	-12.221819	-20.204498	O	3.528791	-17.235012	-16.447409
O	3.253504	-14.613765	-20.385193	O	-0.611370	-13.858167	-15.884702
O	-0.391449	-11.564851	-18.845149	O	-0.194031	-10.574152	-21.504490
O	4.638786	-15.426626	-18.280457	W	0.367504	-10.418389	-15.210076
O	5.862199	-13.062123	-18.150730	W	-0.869668	-12.752095	-17.451393
O	2.156096	-10.200524	-14.571134	W	0.846739	-10.884800	-20.182068
O	-1.041629	-11.272227	-16.239073	W	0.909709	-13.811675	-14.713612
O	4.452094	-11.345729	-13.928618	W	4.207449	-10.272455	-19.980974
O	5.439943	-10.520453	-18.517909	W	4.548707	-13.146094	-14.494364
O	6.122042	-12.653434	-15.508980	W	4.830836	-13.938047	-19.525459
O	0.050053	-14.099557	-18.458926	W	3.266092	-15.622553	-16.954896
O	0.633353	-15.522673	-20.827889	W	6.154393	-11.529609	-17.065842
O	2.038688	-15.894478	-18.415320	W	3.977328	-9.765512	-15.030922
O	-0.539712	-9.381357	-14.193915	W	1.446748	-14.548078	-19.682857
O	5.274012	-13.896373	-13.140077	O	6.047237	-14.547140	-20.560825
O	0.776371	-9.306294	-16.632147	O	7.835015	-11.268300	-17.234204
O	2.693171	-13.382138	-14.137015	O	2.518513	-11.068487	-18.440226
O	4.356193	-8.494669	-13.947984	O	2.937569	-13.527043	-18.059391
O	3.333325	-8.842051	-16.495571	O	1.324890	-12.251592	-16.530749
O	3.475935	-8.778940	-19.190880	O	3.835493	-11.803052	-16.390754
O	1.781870	-15.078085	-15.867417	P	2.655622	-12.176212	-17.337714
O	-2.509461	-13.084398	-17.800385				
O	2.572106	-10.564996	-20.975454				
O	0.351665	-14.795185	-13.431330				

[PW ₁₁ O ₃₉ Fe] ⁴⁺ 2S+1=6				O	0.837855	-9.220462	-19.409950
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Fe	2.175337	-9.100345	-17.883127	O	5.655743	-10.050047	-15.860284
O	4.322330	-14.628624	-15.732871	O	1.235658	-12.828267	-20.402121
O	0.332566	-12.085784	-14.135686	O	5.160622	-9.717297	-21.334981
O	4.487515	-12.257122	-20.193283	O	3.456719	-17.257651	-16.452645
O	3.286375	-14.638923	-20.378184	O	-0.579760	-13.878877	-15.849292
O	-0.388179	-11.582687	-18.823635	O	-0.292353	-10.624157	-21.498132
O	4.627569	-15.427869	-18.245697	W	0.283078	-10.416625	-15.237296
O	5.872232	-13.030074	-18.129030	W	-0.832953	-12.867315	-17.426664
O	2.105373	-10.164072	-14.564726	W	0.750695	-10.867789	-20.161581
O	-1.055832	-11.307143	-16.246497	W	0.974426	-13.776851	-14.639615
O	4.451546	-11.376963	-13.933530	W	4.160056	-10.308734	-20.077802
O	5.413077	-10.504775	-18.561662	W	4.631823	-13.187052	-14.556952
O	6.150223	-12.624472	-15.537937	W	4.881973	-13.937087	-19.452641
O	0.078515	-14.122997	-18.473466	W	3.195893	-15.647694	-16.968178
O	0.689306	-15.516952	-20.900327	W	6.129626	-11.411113	-17.083934
O	2.025643	-15.903669	-18.423452	W	3.919015	-9.798040	-14.940142
O	-0.644776	-9.400388	-14.217887	W	1.502007	-14.532654	-19.762065
O	5.372760	-13.941140	-13.213094	O	6.106341	-14.551967	-20.475645
O	0.727296	-9.299170	-16.619697	O	7.806558	-11.132266	-17.259902
O	2.729925	-13.381278	-14.116934	O	2.490033	-11.037718	-18.414446
O	4.308900	-8.553178	-13.830674	O	2.928121	-13.510929	-18.073549
O	3.379968	-8.851251	-16.451010	O	1.327460	-12.259684	-16.510867
O	3.529771	-8.775139	-19.299500	O	3.835428	-11.799338	-16.393714
O	1.782008	-15.073804	-15.845050	P	2.649136	-12.172367	-17.330981
O	-2.470525	-13.211088	-17.773166				
O	2.509388	-10.585574	-20.981507				
O	0.417800	-14.758739	-13.355023				

[PW ₁₁ O ₃₉ Fe(H ₂ O)] ⁴⁻ 2S+1=2				O	0.720851	-9.360558	-19.359398
Fe	1.958644	-9.171471	-17.968496	O	5.592995	-9.992501	-15.924777

O	4.384457	-14.56186	-15.716219	O	1.211482	-12.885189	-20.361207
O	0.319126	-12.199088	-14.146406	O	5.11199	-9.472158	-21.188872
O	4.437487	-12.15122	-20.256651	O	3.72936	-17.187656	-16.438456
O	3.236167	-14.601716	-20.38762	O	-0.608242	-13.972291	-15.893404
O	-0.465836	-11.663124	-18.846316	O	-0.263391	-10.744517	-21.563399
O	4.692434	-15.347279	-18.307508	W	0.315921	-10.512234	-15.156399
O	5.796885	-12.954953	-18.194572	W	-0.930023	-12.795529	-17.441493
O	2.080249	-10.192338	-14.547605	W	0.794455	-11.01091	-20.245114
O	-1.13202	-11.400584	-16.194589	W	0.897002	-13.910764	-14.753653
O	4.414726	-11.265789	-13.931823	W	4.1455	-10.200453	-19.977832
O	5.342605	-10.426033	-18.545847	W	4.504896	-13.04981	-14.450627
O	6.091264	-12.568485	-15.519948	W	4.780633	-13.854579	-19.592399
O	0.033938	-14.17825	-18.43599	W	3.405818	-15.584137	-16.937217
O	0.636956	-15.644103	-20.742211	W	6.090396	-11.477083	-17.060815
O	2.11871	-15.915708	-18.385673	W	3.883273	-9.686603	-15.092076
O	-0.63749	-9.500224	-14.150114	W	1.4251	-14.637018	-19.607107
O	5.261388	-13.775769	-13.099225	O	6.008104	-14.429554	-20.635145
O	0.642324	-9.453867	-16.619463	O	7.763905	-11.188675	-17.251508
O	2.692642	-13.390359	-14.135828	O	2.442566	-11.012988	-18.413346
O	4.259501	-8.378551	-14.046782	O	2.919374	-13.473371	-18.080346
O	3.172101	-8.878106	-16.53297	O	1.277463	-12.286086	-16.523387
O	3.288338	-8.753805	-19.247978	O	3.777068	-11.766788	-16.376232
O	1.855752	-15.107306	-15.879599	P	2.603702	-12.147285	-17.327839
O	-2.560369	-13.179652	-17.786037	O	1.181195	-7.266735	-17.848837
O	2.470452	-10.563938	-20.986976	H	0.660302	-7.562713	-17.066949
O	0.381373	-14.925708	-13.477955	H	0.594786	-7.489237	-18.604812

[PW ₁₁ O ₃₉ Fe(H ₂ O)] ⁴⁻ 2S+1=4				O	0.897027	-9.274507	-19.343887
Fe	2.099627	-9.104334	-17.873772	O	5.679642	-10.069416	-15.890055
O	4.338153	-14.614936	-15.709079	O	1.259856	-12.826648	-20.366674

O	0.339392	-12.112043	-14.165151	O	5.23047	-9.545627	-21.153984
O	4.522185	-12.206088	-20.216882	O	3.586343	-17.223974	-16.445844
O	3.241287	-14.616455	-20.385704	O	-0.624421	-13.861234	-15.902401
O	-0.393971	-11.567306	-18.857731	O	-0.151306	-10.618251	-21.534341
O	4.65225	-15.418332	-18.291084	W	0.392945	-10.429525	-15.171757
O	5.850655	-13.066474	-18.160423	W	-0.890281	-12.704739	-17.451942
O	2.157937	-10.180448	-14.567724	W	0.880975	-10.920888	-20.20551
O	-1.048397	-11.267101	-16.230429	W	0.890445	-13.842657	-14.751918
O	4.442646	-11.321589	-13.921602	W	4.222099	-10.239783	-19.958965
O	5.435032	-10.515886	-18.506148	W	4.517605	-13.126248	-14.468896
O	6.10659	-12.648595	-15.494792	W	4.80332	-13.925243	-19.571474
O	0.037182	-14.096661	-18.451946	W	3.319483	-15.613304	-16.954579
O	0.608735	-15.549353	-20.781651	W	6.150998	-11.56976	-17.067656
O	2.052372	-15.902302	-18.403072	W	4.006645	-9.750504	-15.050631
O	-0.521746	-9.401997	-14.153699	W	1.419165	-14.573709	-19.636539
O	5.239599	-13.867085	-13.108506	O	6.019729	-14.533404	-20.606616
O	0.739592	-9.313275	-16.626416	O	7.831866	-11.312648	-17.233432
O	2.681213	-13.379993	-14.141035	O	2.5255	-11.068237	-18.442896
O	4.387126	-8.47117	-13.980734	O	2.939995	-13.527113	-18.057267
O	3.307859	-8.847642	-16.501468	O	1.32068	-12.249013	-16.536283
O	3.459225	-8.763158	-19.184774	O	3.830625	-11.801565	-16.386275
O	1.796383	-15.07879	-15.880644	P	2.654002	-12.174521	-17.338898
O	-2.528038	-13.038576	-17.803827	O	-1.383049	-7.436054	-18.202896
O	2.593598	-10.556419	-20.976361	H	-1.095124	-7.907837	-17.397641
O	0.335568	-14.832238	-13.473868	H	-0.870049	-7.940814	-18.86573

$[\text{PW}_{11}\text{O}_{39}\text{Fe}(\text{H}_2\text{O})]^{4-}$ 2S+1=6				O	0.837189	-9.221409	-19.414645
Fe	2.175812	-9.094984	-17.880712	O	5.655898	-10.051481	-15.86013
O	4.320824	-14.627694	-15.730062	O	1.237714	-12.830657	-20.401759
O	0.332022	-12.086459	-14.136821	O	5.164582	-9.709634	-21.33146

O	4.48844	-12.254323	-20.196174	O	3.463093	-17.254066	-16.45242
O	3.283109	-14.639765	-20.377329	O	-0.584199	-13.876285	-15.850285
O	-0.385464	-11.581332	-18.825022	O	-0.283705	-10.639183	-21.501087
O	4.62615	-15.426303	-18.247359	W	0.286667	-10.42214	-15.229349
O	5.867731	-13.031768	-18.129161	W	-0.836501	-12.863302	-17.42602
O	2.105385	-10.1609	-14.569388	W	0.757636	-10.880782	-20.165147
O	-1.052103	-11.30397	-16.248233	W	0.973977	-13.781853	-14.645697
O	4.44974	-11.374441	-13.931089	W	4.163203	-10.300228	-20.075649
O	5.410868	-10.505505	-18.560841	W	4.628042	-13.184702	-14.552509
O	6.146716	-12.625278	-15.535081	W	4.877204	-13.932257	-19.460339
O	0.075527	-14.120459	-18.47315	W	3.203804	-15.644964	-16.969026
O	0.685499	-15.521514	-20.892468	W	6.127033	-11.417273	-17.084349
O	2.024082	-15.903286	-18.420771	W	3.924227	-9.797098	-14.942254
O	-0.643128	-9.406042	-14.21369	W	1.498937	-14.538697	-19.754744
O	5.367246	-13.939142	-13.208761	O	6.10157	-14.547883	-20.481846
O	0.718885	-9.288132	-16.616697	O	7.803495	-11.140166	-17.26033
O	2.727124	-13.379786	-14.117197	O	2.487083	-11.033545	-18.413127
O	4.312592	-8.5518	-13.834478	O	2.926763	-13.507658	-18.074735
O	3.381044	-8.854262	-16.45458	O	1.327358	-12.257973	-16.510076
O	3.529007	-8.770364	-19.300191	O	3.834933	-11.797472	-16.394339
O	1.781083	-15.07115	-15.84854	P	2.648115	-12.169489	-17.331337
O	-2.473205	-13.204742	-17.774137	O	-1.065202	-7.083098	-18.127777
O	2.513042	-10.584971	-20.979799	H	-0.835291	-7.591728	-17.326054
O	0.416627	-14.762917	-13.361867	H	-0.668177	-7.668661	-18.804551

[PW ₁₁ O ₃₉ Fe(H ₂ O)] ⁵⁻ 2S+1=1				O	0.848794	-9.286266	-19.379689
Fe	2.120203	-9.178909	-17.918849	O	5.680776	-10.07777	-15.880098
O	4.339562	-14.62125	-15.722289	O	1.238802	-12.848482	-20.383563
O	0.342246	-12.133826	-14.13822	O	5.212928	-9.55974	-21.235439
O	4.503781	-12.229157	-20.233966	O	3.565101	-17.243828	-16.436755

O	3.249729	-14.628248	-20.38241	O	-0.598327	-13.902275	-15.883467
O	-0.405711	-11.599676	-18.856381	O	-0.224368	-10.618758	-21.551489
O	4.639527	-15.415367	-18.280441	W	0.370648	-10.404707	-15.195298
O	5.846535	-13.05769	-18.160916	W	-0.876622	-12.757061	-17.436697
O	2.151761	-10.226193	-14.505539	W	0.822646	-10.90261	-20.21737
O	-1.05726	-11.315971	-16.213553	W	0.907251	-13.82873	-14.70207
O	4.46285	-11.352204	-13.919803	W	4.212511	-10.241884	-20.01266
O	5.438444	-10.519248	-18.549842	W	4.556581	-13.127029	-14.475111
O	6.11926	-12.668541	-15.524973	W	4.826383	-13.921457	-19.543112
O	0.049037	-14.126058	-18.448569	W	3.292377	-15.622129	-16.939521
O	0.62426	-15.565681	-20.812219	W	6.139276	-11.51218	-17.067318
O	2.052706	-15.896866	-18.400832	W	3.952358	-9.722164	-15.043384
O	-0.578307	-9.37082	-14.193102	W	1.43484	-14.568104	-19.670225
O	5.298535	-13.888089	-13.123741	O	6.049594	-14.544456	-20.578799
O	0.768242	-9.352748	-16.604764	O	7.828852	-11.259749	-17.239946
O	2.70596	-13.406267	-14.124926	O	2.490259	-11.012783	-18.422962
O	4.36172	-8.432426	-13.974152	O	2.927646	-13.482208	-18.081883
O	3.305391	-8.882541	-16.488119	O	1.316611	-12.250601	-16.517556
O	3.473299	-8.78852	-19.236679	O	3.827979	-11.786319	-16.385576
O	1.798098	-15.08857	-15.868415	P	2.642208	-12.147064	-17.331048
O	-2.521214	-13.109724	-17.781293	O	-1.127188	-7.262386	-18.087491
O	2.557649	-10.603455	-20.994412	H	-0.878937	-7.742095	-17.272258
O	0.356929	-14.833989	-13.420724	H	-0.657557	-7.831952	-18.734483

[PW ₁₁ O ₃₉ Fe(H ₂ O)] ⁵⁻ 2S+1=3				O	0.87343	-9.254927	-19.371703
Fe	2.120339	-9.062104	-17.889674	O	5.65991	-10.080959	-15.872376
O	4.329197	-14.633246	-15.718254	O	1.262191	-12.841173	-20.386835
O	0.331942	-12.126607	-14.159354	O	5.212865	-9.572052	-21.220032
O	4.520316	-12.240667	-20.217756	O	3.537288	-17.25115	-16.442183
O	3.262978	-14.638421	-20.390765	O	-0.607726	-13.896562	-15.895199

O	-0.390042	-11.591414	-18.8585	O	-0.199762	-10.615637	-21.524092
O	4.641836	-15.434408	-18.277914	W	0.359905	-10.38662	-15.216399
O	5.856952	-13.072293	-18.14441	W	-0.869239	-12.773282	-17.436226
O	2.141156	-10.230298	-14.533344	W	0.836565	-10.897298	-20.181306
O	-1.045852	-11.298472	-16.241446	W	0.914482	-13.816065	-14.701204
O	4.440604	-11.364987	-13.91937	W	4.199284	-10.244524	-20.001439
O	5.444515	-10.527852	-18.538419	W	4.559807	-13.139473	-14.485697
O	6.118487	-12.669439	-15.511511	W	4.8329	-13.93566	-19.536529
O	0.050349	-14.121441	-18.470203	W	3.274712	-15.627953	-16.948565
O	0.636836	-15.552443	-20.836866	W	6.13522	-11.520205	-17.07283
O	2.043686	-15.912149	-18.418709	W	3.951581	-9.731042	-15.031565
O	-0.596299	-9.391044	-14.183711	W	1.448182	-14.567397	-19.685037
O	5.293984	-13.898685	-13.129331	O	6.06205	-14.556751	-20.566179
O	0.743742	-9.270717	-16.587091	O	7.825292	-11.257973	-17.228208
O	2.696565	-13.413046	-14.125048	O	2.522013	-11.073735	-18.458485
O	4.360057	-8.485382	-13.91692	O	2.937271	-13.53975	-18.063915
O	3.304291	-8.807098	-16.4447	O	1.320267	-12.258574	-16.540234
O	3.501671	-8.770114	-19.215234	O	3.827462	-11.802631	-16.397564
O	1.783785	-15.087757	-15.878503	P	2.650093	-12.175775	-17.356167
O	-2.515194	-13.111853	-17.789297	O	-1.19444	-7.267992	-18.144486
O	2.571819	-10.586214	-20.991903	H	-0.895767	-7.725231	-17.332611
O	0.350365	-14.817816	-13.42299	H	-0.736528	-7.835413	-18.800626

$[\text{PW}_{11}\text{O}_{39}\text{Fe}(\text{H}_2\text{O})]^{5-}$ 2S+1=5				O	0.804363	-9.285271	-19.467328
Fe	2.041446	-9.090695	-17.80448	O	5.680668	-10.070709	-15.871974
O	4.344031	-14.619605	-15.70827	O	1.291901	-12.861835	-20.376584
O	0.351381	-12.146002	-14.163154	O	5.300143	-9.612089	-21.231032
O	4.536166	-12.251901	-20.236296	O	3.591101	-17.237694	-16.439096
O	3.25198	-14.669315	-20.395633	O	-0.615754	-13.872989	-15.922172
O	-0.369872	-11.577462	-18.880057	O	-0.122854	-10.711628	-21.639382

O	4.660935	-15.425793	-18.278825	W	0.387928	-10.361237	-15.100859
O	5.861914	-13.081476	-18.165066	W	-0.869087	-12.667713	-17.443529
O	2.15357	-10.137613	-14.535341	W	0.894236	-10.906184	-20.264553
O	-1.038302	-11.266162	-16.207035	W	0.879354	-13.848516	-14.748989
O	4.431029	-11.354664	-13.910462	W	4.251391	-10.193709	-19.992516
O	5.437496	-10.523425	-18.520452	W	4.508025	-13.138348	-14.451218
O	6.100778	-12.6562	-15.495343	W	4.796764	-13.943457	-19.608215
O	0.036996	-14.105207	-18.453727	W	3.324699	-15.619486	-16.957453
O	0.590271	-15.571269	-20.778004	W	6.134146	-11.597702	-17.07765
O	2.058849	-15.911727	-18.39598	W	4.038383	-9.703949	-15.019933
O	-0.54729	-9.471244	-13.962572	W	1.403634	-14.576096	-19.636004
O	5.250788	-13.89	-13.095518	O	6.030782	-14.571882	-20.628813
O	0.560975	-9.174783	-16.468085	O	7.824013	-11.328863	-17.225076
O	2.682895	-13.419966	-14.112586	O	2.541693	-11.032885	-18.471766
O	4.468558	-8.49757	-13.869447	O	2.942477	-13.516405	-18.081034
O	3.359104	-8.731452	-16.379994	O	1.326599	-12.220911	-16.559384
O	3.577464	-8.701738	-19.307033	O	3.83357	-11.792263	-16.403146
O	1.80407	-15.076434	-15.888203	P	2.658607	-12.15001	-17.372209
O	-2.516505	-13.002573	-17.792904	O	-1.560903	-7.633181	-18.276687
O	2.61578	-10.558258	-21.011155	H	-1.218426	-8.065353	-17.467298
O	0.309888	-14.863742	-13.484483	H	-1.007175	-8.107856	-18.932133

[PW ₁₁ O ₃₉ Fe(H ₂ O)] ³⁻ 2S+I=1				O	0.912686	-9.373714	-19.269773
Fe	2.138249	-9.261526	-18.017598	O	5.675475	-10.179093	-15.875449
O	4.346895	-14.750887	-15.775493	O	1.251279	-12.902550	-20.453312
O	0.321786	-12.236043	-14.150701	O	5.192333	-9.753845	-21.229594
O	4.490558	-12.327401	-20.262121	O	3.497737	-17.352545	-16.445335
O	3.269772	-14.681091	-20.412764	O	-0.580868	-14.031770	-15.887397
O	-0.391546	-11.665806	-18.829206	O	-0.269965	-10.725030	-21.468345
O	4.629146	-15.546819	-18.312322	W	0.341921	-10.531298	-15.251345

O	5.850006	-13.123551	-18.196942	W	-0.855079	-12.944728	-17.403530
O	2.131181	-10.339636	-14.548189	W	0.775464	-11.109864	-20.179615
O	-1.055614	-11.434819	-16.248350	W	0.946115	-13.904435	-14.665029
O	4.477156	-11.497667	-13.941593	W	4.216441	-10.491475	-20.044139
O	5.413884	-10.607249	-18.542818	W	4.610024	-13.275199	-14.539483
O	6.145757	-12.774549	-15.569778	W	4.872370	-14.090267	-19.479149
O	0.099599	-14.170662	-18.512736	W	3.233668	-15.743288	-16.928678
O	0.688444	-15.647532	-20.859786	W	6.150314	-11.563720	-17.068594
O	2.052441	-16.008395	-18.460192	W	3.924348	-9.915919	-15.010179
O	-0.579599	-9.489294	-14.262602	W	1.503061	-14.693076	-19.712169
O	5.347565	-14.043003	-13.213540	O	6.083077	-14.678011	-20.519050
O	0.817860	-9.475694	-16.634015	O	7.819130	-11.296145	-17.258580
O	2.732161	-13.535105	-14.163825	O	2.483546	-11.127209	-18.417692
O	4.304577	-8.629300	-13.954637	O	2.934505	-13.585795	-18.097835
O	3.299361	-9.054580	-16.501129	O	1.327344	-12.376285	-16.514303
O	3.486539	-8.922441	-19.136627	O	3.835377	-11.910041	-16.393881
O	1.784282	-15.210163	-15.890942	P	2.646233	-12.266903	-17.328668
O	-2.475702	-13.299805	-17.775662	O	2.003266	-7.235482	-17.838694
O	2.513065	-10.563828	-20.926691	H	2.767576	-7.088286	-18.435562
O	0.407559	-14.902038	-13.396882	H	2.402294	-7.240681	-16.941785

[PW ₁₁ O ₃₉ Fe(H ₂ O)] ³⁻ 2S+1=3				O	0.862885	-9.417128	-19.406132
Fe	2.037088	-9.311267	-17.929877	O	5.710743	-10.169573	-15.907551
O	4.321587	-14.692385	-15.720780	O	1.244737	-12.966332	-20.375746
O	0.322302	-12.244590	-14.106243	O	5.207952	-9.670359	-21.157214
O	4.515253	-12.321289	-20.243987	O	3.667907	-17.333464	-16.450137
O	3.250402	-14.738921	-20.368442	O	-0.613543	-13.969163	-15.876316
O	-0.404476	-11.701440	-18.882555	O	-0.175391	-10.756005	-21.591106
O	4.689164	-15.521710	-18.290149	W	0.405079	-10.669642	-15.095576
O	5.850838	-13.159103	-18.184291	W	-0.880411	-12.820893	-17.465687

O	2.165415	-10.273470	-14.612372	W	0.846215	-11.055812	-20.262181
O	-1.022137	-11.384201	-16.234045	W	0.906093	-14.045090	-14.767954
O	4.444053	-11.405816	-13.933741	W	4.222422	-10.401245	-19.977600
O	5.396428	-10.625083	-18.513122	W	4.500591	-13.210685	-14.466854
O	6.104574	-12.750870	-15.503760	W	4.816602	-14.045274	-19.577177
O	0.057721	-14.217950	-18.418766	W	3.368193	-15.740113	-16.963382
O	0.618258	-15.685232	-20.742664	W	6.162213	-11.685410	-17.064927
O	2.088508	-15.999097	-18.370196	W	4.033971	-9.849828	-15.089307
O	-0.491614	-9.565352	-14.155030	W	1.427833	-14.687841	-19.627958
O	5.216408	-13.947133	-13.111117	O	6.025230	-14.642768	-20.613585
O	0.807661	-9.606610	-16.743579	O	7.832722	-11.427914	-17.253216
O	2.662150	-13.471745	-14.152164	O	2.458778	-11.126032	-18.392693
O	4.400788	-8.539827	-14.058492	O	2.944133	-13.577654	-18.082408
O	3.328624	-9.001870	-16.555306	O	1.329278	-12.394638	-16.495129
O	3.389600	-8.919775	-19.199399	O	3.835746	-11.889476	-16.381799
O	1.807420	-15.254883	-15.847973	P	2.648621	-12.269557	-17.306133
O	-2.512894	-13.157872	-17.801292	O	1.916258	-7.271133	-17.818241
O	2.575027	-10.706095	-20.978435	H	2.499546	-7.155207	-18.599083
O	0.356152	-15.017334	-13.485066	H	2.540721	-7.258696	-17.056392

[PW ₁₁ O ₃₉ Fe(H ₂ O)] ³⁻ 2S+1=5				O	0.707483	-9.435548	-19.303284
Fe	1.956638	-9.242533	-17.901450	O	5.478892	-9.979349	-15.925415
O	4.398098	-14.672684	-15.743581	O	1.183262	-12.989973	-20.401408
O	0.278139	-12.270326	-14.142312	O	4.915436	-9.703046	-21.290311
O	4.416461	-12.282375	-20.215325	O	3.614594	-17.330433	-16.462971
O	3.329435	-14.704216	-20.379265	O	-0.544145	-14.136977	-15.828237
O	-0.490048	-11.850816	-18.804577	O	-0.443236	-10.818131	-21.412787
O	4.720942	-15.460688	-18.256541	W	0.165155	-10.675442	-15.269580
O	5.840171	-12.984940	-18.157288	W	-0.866701	-13.159851	-17.419528
O	1.965453	-10.306227	-14.628575	W	0.631051	-11.102379	-20.124377

O	-1.150262	-11.598330	-16.262751	W	1.004162	-13.950128	-14.646971
O	4.376936	-11.370351	-13.945751	W	3.980293	-10.428712	-20.069985
O	5.249759	-10.490993	-18.575357	W	4.628103	-13.227024	-14.594078
O	6.106687	-12.537458	-15.555897	W	4.897290	-13.981947	-19.447637
O	0.119682	-14.357738	-18.467274	W	3.281580	-15.744040	-16.977115
O	0.783326	-15.703025	-20.895247	W	6.033695	-11.361654	-17.118005
O	2.139634	-16.050373	-18.434695	W	3.773573	-9.911880	-14.964573
O	-0.788027	-9.643095	-14.309041	W	1.545330	-14.696201	-19.757439
O	5.397500	-13.922877	-13.247209	O	6.138125	-14.525600	-20.473568
O	0.604497	-9.557405	-16.719243	O	7.682550	-10.997149	-17.305173
O	2.745520	-13.443542	-14.153696	O	2.378731	-11.208099	-18.441510
O	4.065840	-8.592100	-13.931348	O	2.936185	-13.633319	-18.060222
O	3.110174	-9.012789	-16.578834	O	1.278275	-12.443817	-16.514674
O	3.225252	-8.900484	-19.199705	O	3.762105	-11.865338	-16.404057
O	1.875518	-15.222031	-15.832117	P	2.593122	-12.301608	-17.335320
O	-2.474224	-13.595158	-17.759581	O	5.656045	-7.074609	-17.701042
O	2.340515	-10.693701	-20.979516	H	4.964722	-7.573264	-18.179065
O	0.519236	-14.928688	-13.344362	H	5.868945	-7.710582	-16.994239

[PW ₁₁ O ₃₉ Fe(OH)] ⁴⁻ 2S+1=1				O	0.898096	-9.332395	-19.374038
Fe	2.157569	-9.139347	-17.977649	O	5.697298	-10.189296	-15.871651
O	4.309460	-14.733886	-15.767245	O	1.257336	-12.913299	-20.398069
O	0.331939	-12.216665	-14.146672	O	5.172498	-9.815144	-21.256825
O	4.501669	-12.378198	-20.218346	O	3.470201	-17.364613	-16.449284
O	3.295750	-14.732333	-20.399548	O	-0.584034	-14.018504	-15.860552
O	-0.401416	-11.694395	-18.825936	O	-0.283752	-10.684722	-21.452394
O	4.638295	-15.563237	-18.275311	W	0.354447	-10.570903	-15.285630
O	5.889500	-13.163945	-18.167186	W	-0.845702	-12.981644	-17.427244
O	2.151298	-10.332472	-14.578994	W	0.764633	-10.994496	-20.136359
O	-1.049665	-11.446706	-16.260786	W	0.956370	-13.912051	-14.649638

O	4.474219	-11.501084	-13.947515	W	4.180188	-10.507027	-20.047670
O	5.432650	-10.645366	-18.544693	W	4.615627	-13.270048	-14.542227
O	6.154812	-12.783898	-15.559063	W	4.893265	-14.106631	-19.455713
O	0.085671	-14.224868	-18.487147	W	3.200803	-15.750246	-16.942231
O	0.700631	-15.608394	-20.900599	W	6.161381	-11.570884	-17.077797
O	2.046463	-15.991425	-18.437893	W	3.937989	-9.886512	-15.029217
O	-0.560709	-9.491255	-14.319221	W	1.512498	-14.636100	-19.752482
O	5.351979	-14.044447	-13.208201	O	6.109429	-14.713786	-20.491921
O	0.857490	-9.561052	-16.708725	O	7.839616	-11.305379	-17.258974
O	2.721276	-13.525710	-14.134084	O	2.475060	-11.114746	-18.402522
O	4.334713	-8.634963	-13.926593	O	2.944781	-13.596550	-18.093620
O	3.356430	-8.978337	-16.487396	O	1.339436	-12.404987	-16.511653
O	3.495951	-8.965153	-19.189484	O	3.846180	-11.906082	-16.401125
O	1.762878	-15.227477	-15.848230	P	2.654425	-12.263478	-17.340250
O	-2.478429	-13.337426	-17.782116	O	1.882384	-7.352519	-17.851888
O	2.524541	-10.672686	-20.968267	H	2.434734	-7.169631	-17.062150
O	0.400923	-14.888704	-13.361458				

[PW ₁₁ O ₃₉ Fe(OH)] ⁴⁻ 2S+1=3				O	0.908467	-9.335700	-19.374967
Fe	2.164296	-9.141036	-17.972279	O	5.695361	-10.189458	-15.872166
O	4.310644	-14.737668	-15.760370	O	1.253591	-12.920033	-20.400903
O	0.329305	-12.212460	-14.148588	O	5.171955	-9.814685	-21.263597
O	4.503752	-12.378898	-20.211168	O	3.465474	-17.365912	-16.448140
O	3.293695	-14.736370	-20.395923	O	-0.583977	-14.013394	-15.861438
O	-0.393638	-11.693660	-18.826423	O	-0.275357	-10.685144	-21.454576
O	4.633644	-15.560613	-18.269973	W	0.349047	-10.565447	-15.284372
O	5.890708	-13.167332	-18.159423	W	-0.844222	-12.980359	-17.428388
O	2.145270	-10.327584	-14.581594	W	0.773143	-11.000601	-20.140197
O	-1.049648	-11.441446	-16.263908	W	0.958778	-13.907110	-14.649087
O	4.470722	-11.500565	-13.946092	W	4.176243	-10.496494	-20.052058

O	5.435821	-10.646676	-18.547342	W	4.620042	-13.276084	-14.545368
O	6.154751	-12.780033	-15.554536	W	4.892177	-14.099361	-19.454611
O	0.084674	-14.225699	-18.487390	W	3.199706	-15.752087	-16.944376
O	0.699348	-15.615897	-20.899069	W	6.161430	-11.567196	-17.082514
O	2.041957	-15.995851	-18.435150	W	3.937739	-9.899434	-15.022656
O	-0.566523	-9.493434	-14.310571	W	1.511150	-14.641903	-19.752489
O	5.353865	-14.047126	-13.208101	O	6.107900	-14.710112	-20.489139
O	0.843140	-9.542369	-16.704979	O	7.840000	-11.302084	-17.260904
O	2.721362	-13.519990	-14.133605	O	2.481376	-11.113469	-18.402173
O	4.333655	-8.644205	-13.924243	O	2.942078	-13.596831	-18.093363
O	3.355419	-8.990239	-16.490318	O	1.339044	-12.399192	-16.512767
O	3.498399	-8.955969	-19.210657	O	3.847616	-11.909973	-16.400278
O	1.764218	-15.220501	-15.849178	P	2.655193	-12.264253	-17.339059
O	-2.477253	-13.333400	-17.784654	O	1.888640	-7.351763	-17.846645
O	2.528793	-10.689275	-20.975309	H	2.339279	-7.188010	-16.991529
O	0.402257	-14.883827	-13.361436				

[PW ₁₁ O ₃₉ Fe(OH)] ⁴⁻ 2S+1=5				O	0.959095	-9.327670	-19.319324
Fe	2.035023	-9.001723	-17.960457	O	5.633336	-10.192111	-15.953742
O	4.394170	-14.770283	-15.705532	O	1.262709	-12.951415	-20.393388
O	0.341904	-12.294794	-14.145160	O	5.279158	-9.741185	-21.270711
O	4.507971	-12.363950	-20.238082	O	3.606459	-17.358047	-16.430375
O	3.226978	-14.756731	-20.400387	O	-0.592742	-14.054501	-15.917576
O	-0.327725	-11.649731	-18.787476	O	-0.136762	-10.771508	-21.464274
O	4.626379	-15.549016	-18.303739	W	0.344044	-10.542159	-15.181286
O	5.861431	-13.215167	-18.173339	W	-0.865296	-12.866239	-17.415557
O	2.136392	-10.328102	-14.579297	W	0.919042	-11.134871	-20.169344
O	-1.096457	-11.466923	-16.175009	W	0.910105	-13.967526	-14.727945
O	4.449495	-11.445817	-13.947057	W	4.265879	-10.342514	-20.026360
O	5.494931	-10.672309	-18.580623	W	4.551296	-13.255059	-14.484944

O	6.111905	-12.760112	-15.520941	W	4.812293	-14.045619	-19.580993
O	0.064309	-14.198786	-18.488544	W	3.345101	-15.742689	-16.925145
O	0.626964	-15.731306	-20.767485	W	6.152887	-11.684589	-17.108806
O	2.045284	-16.064659	-18.405306	W	3.951975	-9.913315	-15.090486
O	-0.565648	-9.546566	-14.122092	W	1.456939	-14.772315	-19.621921
O	5.287859	-13.975208	-13.121694	O	6.020269	-14.668903	-20.618372
O	0.653710	-9.504428	-16.597397	O	7.836568	-11.432039	-17.244797
O	2.719391	-13.535571	-14.149048	O	2.505212	-11.129516	-18.427521
O	4.344879	-8.627594	-14.032281	O	2.927075	-13.628736	-18.086219
O	3.243473	-8.997177	-16.556061	O	1.311720	-12.382353	-16.533427
O	3.630370	-8.855436	-19.280788	O	3.820787	-11.938148	-16.404179
O	1.836755	-15.203332	-15.900006	P	2.632033	-12.275109	-17.361588
O	-2.492489	-13.204658	-17.812460	O	1.767654	-7.144425	-17.875117
O	2.597261	-10.653602	-20.965563	H	2.338379	-6.939117	-17.107539
O	0.374846	-14.990704	-13.467366				

[PW ₁₁ O ₃₉ Fe(O)] ⁵⁻ 2S+1=3				O	0.871246	-9.374401	-19.401254
Fe	2.094906	-9.010466	-17.953738	O	5.700589	-10.224262	-15.880115
O	4.345119	-14.758526	-15.734194	O	1.253812	-12.971943	-20.381643
O	0.351996	-12.260678	-14.145024	O	5.208827	-9.751346	-21.227385
O	4.515656	-12.377457	-20.212378	O	3.541432	-17.378053	-16.445901
O	3.271988	-14.769905	-20.398728	O	-0.582019	-14.037574	-15.878853
O	-0.382166	-11.726084	-18.837102	O	-0.215054	-10.740246	-21.508189
O	4.644267	-15.551913	-18.280170	W	0.380014	-10.534838	-15.252698
O	5.884740	-13.200192	-18.161467	W	-0.849301	-12.933028	-17.434841
O	2.166063	-10.371634	-14.556096	W	0.830828	-11.012512	-20.170099
O	-1.042032	-11.453508	-16.230983	W	0.933790	-13.943499	-14.679412
O	4.478402	-11.508832	-13.930354	W	4.196940	-10.398675	-19.996303
O	5.444045	-10.663879	-18.534756	W	4.584613	-13.278257	-14.490258
O	6.147313	-12.810831	-15.529418	W	4.850399	-14.070249	-19.528254

O	0.062983	-14.261647	-18.464578	W	3.271801	-15.754911	-16.944467
O	0.655855	-15.678519	-20.849120	W	6.162627	-11.653108	-17.070959
O	2.056990	-16.023392	-18.414815	W	3.954932	-9.883152	-15.066175
O	-0.549741	-9.525248	-14.211798	W	1.469817	-14.686754	-19.704419
O	5.328966	-14.044304	-13.143393	O	6.072008	-14.691267	-20.566763
O	0.776693	-9.470019	-16.630405	O	7.851243	-11.391571	-17.244378
O	2.723868	-13.553925	-14.114692	O	2.497959	-11.096158	-18.395422
O	4.360404	-8.630376	-13.955620	O	2.940465	-13.607375	-18.098409
O	3.350508	-9.000879	-16.496362	O	1.335799	-12.391724	-16.525589
O	3.507068	-8.893939	-19.264335	O	3.847959	-11.933654	-16.394992
O	1.800753	-15.221823	-15.866776	P	2.656598	-12.262774	-17.354068
O	-2.495425	-13.279375	-17.781541	O	1.799189	-7.396335	-17.922997
O	2.568196	-10.745727	-20.980457				
O	0.375334	-14.946944	-13.400289				

[PW ₁₁ O ₃₉ Fe(O)] ⁵⁻ 2S+1=5				O	0.767245	-9.396182	-19.496340
Fe	2.036638	-8.950942	-17.982825	O	5.705035	-10.217834	-15.885179
O	4.367168	-14.748314	-15.724952	O	1.269574	-13.000668	-20.373950
O	0.376280	-12.300099	-14.138505	O	5.268708	-9.789199	-21.239148
O	4.504925	-12.375438	-20.236577	O	3.611641	-17.370478	-16.444580
O	3.262332	-14.791028	-20.395415	O	-0.586586	-14.046635	-15.892929
O	-0.377264	-11.731980	-18.854758	O	-0.169870	-10.858748	-21.612848
O	4.667700	-15.537019	-18.282834	W	0.399703	-10.545674	-15.177781
O	5.866998	-13.185811	-18.181456	W	-0.855365	-12.873012	-17.439496
O	2.176131	-10.315908	-14.548321	W	0.855247	-11.036523	-20.241687
O	-1.046830	-11.460057	-16.197138	W	0.906694	-13.992317	-14.715742
O	4.479631	-11.505169	-13.918605	W	4.241027	-10.370946	-19.986763
O	5.426871	-10.647669	-18.531272	W	4.541896	-13.278315	-14.450496
O	6.136301	-12.805667	-15.516560	W	4.815933	-14.064436	-19.579203
O	0.054617	-14.264660	-18.445789	W	3.328850	-15.750876	-16.946355

O	0.625225	-15.711226	-20.793035	W	6.154189	-11.705089	-17.055026
O	2.081265	-16.027602	-18.391466	W	4.000389	-9.858634	-15.058599
O	-0.537505	-9.581940	-14.099582	W	1.436775	-14.705444	-19.658606
O	5.301936	-14.039336	-13.109358	O	6.044780	-14.681353	-20.612152
O	0.694630	-9.471902	-16.573240	O	7.841145	-11.439101	-17.233994
O	2.720102	-13.574558	-14.095765	O	2.490558	-11.057603	-18.396114
O	4.421374	-8.627513	-13.928889	O	2.940042	-13.581944	-18.107803
O	3.380553	-8.953110	-16.460762	O	1.331440	-12.377655	-16.530976
O	3.547006	-8.840008	-19.341160	O	3.839197	-11.917896	-16.391187
O	1.829690	-15.226070	-15.870150	P	2.651353	-12.236170	-17.361546
O	-2.501099	-13.223373	-17.783371	O	1.716042	-7.346244	-17.960564
O	2.577574	-10.716333	-20.983094				
O	0.351108	-15.010923	-13.447529				

[PW ₁₁ O ₃₉ Fe(O)] ⁴⁻ 2S+1=2				O	0.880999	-9.388688	-19.342589
Fe	2.075334	-9.057738	-17.997302	O	5.702793	-10.221139	-15.895375
O	4.369194	-14.754194	-15.737754	O	1.271150	-12.946679	-20.386233
O	0.355322	-12.267641	-14.156708	O	5.230444	-9.720867	-21.162824
O	4.476875	-12.327555	-20.226209	O	3.584182	-17.347595	-16.451874
O	3.246933	-14.729923	-20.419021	O	-0.591422	-14.037812	-15.902002
O	-0.380098	-11.694572	-18.824771	O	-0.192556	-10.782286	-21.498141
O	4.644862	-15.529766	-18.318258	W	0.399138	-10.548668	-15.238248
O	5.855269	-13.165972	-18.192608	W	-0.869950	-12.896557	-17.427012
O	2.176179	-10.352063	-14.578258	W	0.853132	-11.096373	-20.181707
O	-1.049718	-11.444373	-16.221159	W	0.919550	-13.952813	-14.713684
O	4.483513	-11.485530	-13.930480	W	4.238296	-10.410522	-19.952123
O	5.443449	-10.631556	-18.514273	W	4.561478	-13.255790	-14.467426
O	6.145947	-12.811063	-15.520946	W	4.812457	-14.060294	-19.557241
O	0.054118	-14.223878	-18.486286	W	3.312851	-15.729507	-16.931587
O	0.639149	-15.688563	-20.813272	W	6.172180	-11.687697	-17.050521

O	2.066611	-16.024183	-18.434081	W	3.974799	-9.881528	-15.093272
O	-0.517629	-9.532390	-14.207957	W	1.454683	-14.723096	-19.662721
O	5.295951	-14.015345	-13.123862	O	6.026627	-14.647845	-20.606870
O	0.786828	-9.494869	-16.645329	O	7.851501	-11.434785	-17.235081
O	2.721814	-13.557006	-14.136325	O	2.503938	-11.104247	-18.393715
O	4.369028	-8.613732	-14.010774	O	2.937338	-13.605455	-18.095222
O	3.327001	-9.023926	-16.532884	O	1.332640	-12.390657	-16.526437
O	3.469425	-8.882076	-19.212395	O	3.845738	-11.939665	-16.387528
O	1.812854	-15.213531	-15.900001	P	2.656162	-12.265742	-17.345263
O	-2.505137	-13.237242	-17.785410	O	1.768212	-7.441574	-17.936102
O	2.555276	-10.632643	-20.941788				
O	0.370987	-14.961954	-13.448122				

[PW ₁₁ O ₃₉ Fe(O)] ⁴⁻ 2S+1=4				O	0.876581	-9.3887209	-19.350318
Fe	2.072135	-9.052310	-17.980619	O	5.703396	-10.212697	-15.900877
O	4.368264	-14.745061	-15.736499	O	1.264643	-12.952359	-20.374167
O	0.359578	-12.263261	-14.154350	O	5.219017	-9.720525	-21.161639
O	4.490372	-12.333524	-20.225066	O	3.591181	-17.346429	-16.448653
O	3.251839	-14.735364	-20.411417	O	-0.591886	-14.032460	-15.896657
O	-0.382243	-11.704547	-18.828450	O	-0.183982	-10.769420	-21.500782
O	4.655180	-15.530360	-18.309401	W	0.400213	-10.561747	-15.230163
O	5.861807	-13.166533	-18.191655	W	-0.871100	-12.889613	-17.437842
O	2.176346	-10.337526	-14.589121	W	0.863935	-11.076626	-20.184718
O	-1.049562	-11.444662	-16.220109	W	0.913570	-13.959338	-14.719525
O	4.481015	-11.475294	-13.934536	W	4.228699	-10.418024	-19.954248
O	5.431723	-10.631362	-18.512733	W	4.553533	-13.255325	-14.470620
O	6.144576	-12.798921	-15.519390	W	4.816208	-14.066870	-19.557861
O	0.053169	-14.236897	-18.472280	W	3.314429	-15.731519	-16.935209
O	0.638788	-15.685520	-20.807185	W	6.172975	-11.689130	-17.055217
O	2.074071	-16.021704	-18.424526	W	3.985049	-9.884777	-15.091856

O	-0.516017	-9.544725	-14.201101	W	1.450167	-14.713595	-19.659216
O	5.289665	-14.009223	-13.124899	O	6.031125	-14.657954	-20.604501
O	0.779098	-9.503707	-16.652925	O	7.851229	-11.430266	-17.241921
O	2.718933	-13.546341	-14.136237	O	2.502934	-11.106819	-18.395785
O	4.376389	-8.616336	-14.010010	O	2.940850	-13.606387	-18.093315
O	3.333885	-9.018261	-16.538992	O	1.333088	-12.392844	-16.527497
O	3.453658	-8.883395	-19.216916	O	3.845742	-11.936389	-16.388782
O	1.816940	-15.216380	-15.888426	P	2.656724	-12.267149	-17.344947
O	-2.506864	-13.232535	-17.791831	O	1.759205	-7.440692	-17.915677
O	2.561996	-10.663532	-20.952628				
O	0.368216	-14.962992	-13.448316				

$[\text{PW}_{11}\text{O}_{39}\text{Fe}(\text{O})]^{4-}$ $2S+1=6$				O	0.768094	-9.352496	-19.513494
Fe	2.197260	-8.988500	-17.981504	O	5.609367	-10.146816	-15.866316
O	4.368585	-14.780185	-15.728897	O	1.257667	-12.983900	-20.421724
O	0.381142	-12.169554	-14.153910	O	5.160031	-9.886621	-21.353068
O	4.497550	-12.400170	-20.184676	O	3.448430	-17.393344	-16.446170
O	3.305696	-14.794435	-20.379500	O	-0.539887	-13.988927	-15.849660
O	-0.384361	-11.745316	-18.854962	O	-0.299757	-10.810909	-21.548861
O	4.639966	-15.549230	-18.225781	W	0.296617	-10.519644	-15.312383
O	5.887600	-13.165944	-18.120838	W	-0.810645	-12.994707	-17.447586
O	2.132631	-10.233936	-14.527836	W	0.738855	-10.988500	-20.198900
O	-1.053915	-11.428128	-16.277935	W	0.997772	-13.861175	-14.642337
O	4.495783	-11.546280	-13.864835	W	4.145706	-10.460258	-20.100331
O	5.415478	-10.641673	-18.574778	W	4.661559	-13.368733	-14.558448
O	6.159297	-12.718685	-15.521800	W	4.865013	-14.091609	-19.459374
O	0.095277	-14.279873	-18.474806	W	3.191081	-15.786781	-16.969316
O	0.697068	-15.660862	-20.898227	W	6.107006	-11.566316	-17.120918
O	2.048160	-16.042316	-18.419418	W	3.944795	-9.981905	-14.780929
O	-0.647705	-9.492389	-14.320041	W	1.500076	-14.660306	-19.767728

O	5.412652	-14.134406	-13.227747	O	6.101645	-14.703516	-20.467470
O	0.828215	-9.461412	-16.654542	O	7.781796	-11.256417	-17.259244
O	2.771602	-13.504384	-14.116191	O	2.505653	-11.071716	-18.407278
O	4.349263	-8.765549	-13.642843	O	2.930108	-13.590628	-18.102758
O	3.579782	-8.988711	-16.365059	O	1.342817	-12.360474	-16.530586
O	3.577369	-8.896597	-19.331771	O	3.850393	-11.932068	-16.391025
O	1.818752	-15.182353	-15.837270	P	2.663821	-12.237972	-17.360405
O	-2.445277	-13.362770	-17.774414	O	1.978159	-7.367733	-17.867913
O	2.512426	-10.726524	-21.011918				
O	0.436289	-14.829858	-13.351440				

[PW ₁₁ O ₃₉ Fe(O)] ³⁻ 2S+1=3				O	0.973531	-9.385216	-19.280367
Fe	2.165707	-8.962379	-17.918812	O	5.618389	-10.144790	-15.898360
O	4.392031	-14.825708	-15.696640	O	1.243010	-12.948718	-20.408998
O	0.360039	-12.145716	-14.166192	O	5.152732	-9.781787	-21.258241
O	4.500704	-12.364433	-20.176783	O	3.418822	-17.383529	-16.464381
O	3.284417	-14.756412	-20.376298	O	-0.554566	-13.999292	-15.840975
O	-0.369073	-11.722236	-18.804323	O	-0.233446	-10.678853	-21.387768
O	4.615828	-15.534085	-18.235952	W	0.297311	-10.512126	-15.351084
O	5.883895	-13.153547	-18.116792	W	-0.836537	-13.007409	-17.423618
O	2.131893	-10.289817	-14.687772	W	0.823129	-11.070719	-20.110016
O	-1.067724	-11.431437	-16.279011	W	0.988111	-13.828257	-14.648227
O	4.494220	-11.480738	-13.853415	W	4.158909	-10.426791	-20.035718
O	5.421485	-10.619894	-18.549402	W	4.653815	-13.400110	-14.571787
O	6.145105	-12.710051	-15.504502	W	4.866536	-14.055739	-19.458862
O	0.085688	-14.252664	-18.485153	W	3.185627	-15.779405	-16.977019
O	0.699009	-15.649831	-20.889181	W	6.139392	-11.559396	-17.104603
O	2.019516	-16.045978	-18.435800	W	3.978402	-10.075891	-14.901663
O	-0.607110	-9.483375	-14.338348	W	1.504331	-14.685870	-19.744102
O	5.384184	-14.116779	-13.213458	O	6.085845	-14.667320	-20.473822

O	0.756153	-9.392053	-16.715776	O	7.806059	-11.265134	-17.266058
O	2.778946	-13.454489	-14.146050	O	2.518105	-11.118876	-18.407884
O	4.288666	-8.717607	-13.920230	O	2.926731	-13.615015	-18.077988
O	3.331418	-9.227633	-16.708614	O	1.329191	-12.357291	-16.532477
O	3.494374	-8.869328	-19.282564	O	3.849606	-11.962817	-16.376711
O	1.831666	-15.142525	-15.852169	P	2.658767	-12.265559	-17.344027
O	-2.461196	-13.365980	-17.773327	O	1.911517	-7.381232	-17.907078
O	2.534474	-10.712870	-20.973884				
O	0.454872	-14.789662	-13.351130				

$[\text{PW}_{11}\text{O}_{39}\text{Fe}(\text{O})]^{3-} 2\text{S}+1=5$				O	0.924633	-9.326622	-19.331122
Fe	2.200245	-9.077235	-17.953722	O	5.613379	-10.128361	-15.914802
O	4.359513	-14.780883	-15.752813	O	1.280415	-12.885640	-20.392790
O	0.356020	-12.159296	-14.155447	O	5.153714	-9.866298	-21.310286
O	4.518322	-12.393902	-20.233661	O	3.396876	-17.384924	-16.463729
O	3.320530	-14.733006	-20.383488	O	-0.551209	-14.016217	-15.835192
O	-0.403050	-11.708440	-18.806138	O	-0.295803	-10.662923	-21.389143
O	4.640052	-15.569758	-18.243089	W	0.285288	-10.531641	-15.341052
O	5.881654	-13.137785	-18.146479	W	-0.834361	-13.022198	-17.414186
O	2.119116	-10.266736	-14.614283	W	0.751292	-10.992063	-20.088850
O	-1.080231	-11.458259	-16.271932	W	0.987634	-13.844276	-14.628558
O	4.492497	-11.500178	-13.911558	W	4.175727	-10.555537	-20.100167
O	5.419306	-10.629974	-18.582592	W	4.654037	-13.362283	-14.595899
O	6.158867	-12.714356	-15.552477	W	4.908681	-14.128534	-19.420664
O	0.113266	-14.229474	-18.491059	W	3.153724	-15.779211	-16.966200
O	0.729108	-15.565801	-20.927794	W	6.133151	-11.525196	-17.102736
O	2.041270	-16.011161	-18.454929	W	3.933577	-10.011580	-14.894326
O	-0.636474	-9.477154	-14.371322	W	1.532563	-14.614577	-19.770258
O	5.400097	-14.106227	-13.261681	O	6.135701	-14.735200	-20.428154
O	0.806196	-9.494605	-16.719515	O	7.797682	-11.222117	-17.267237

O	2.770542	-13.480570	-14.146690	O	2.506121	-11.114637	-18.400464
O	4.301375	-8.726082	-13.838819	O	2.946270	-13.605740	-18.082872
O	3.402788	-9.028465	-16.541920	O	1.333797	-12.382538	-16.522802
O	3.556038	-8.938125	-19.176831	O	3.843020	-11.929605	-16.385494
O	1.803501	-15.184284	-15.836246	P	2.656074	-12.265883	-17.340399
O	-2.451219	-13.407708	-17.767882	O	1.955538	-7.440753	-17.864445
O	2.518546	-10.641660	-20.960601				
O	0.453892	-14.801553	-13.328817				

Table S6: Atomic spin densities (in e) and Mulliken atomic charges (in e) determined for different studied systems.

[PW ₁₂ O ₄₀] ³⁻		Charge=-3 Multiplicity=1	
		Spin	Charge
1	P	0.0000	1.984646
2	W	0.0000	1.978430
3	W	-0.0000	1.979209
4	W	0.0000	1.978700
5	W	0.0000	1.979674
6	W	0.0000	1.978848
7	W	-0.0000	1.978185
8	W	-0.0000	1.978064
9	W	-0.0000	1.977634
10	W	-0.0000	1.979632
11	W	0.0000	1.979324
12	W	0.0000	1.978113
13	W	-0.0000	1.978438
14	O	-0.0000	-0.739922
15	O	0.0000	-0.739514
16	O	0.0000	-0.739691

17	O	-0.0000	-0.739804
18	O	-0.0000	-0.820696
19	O	-0.0000	-0.819869
20	O	0.0000	-0.821154
21	O	-0.0000	-0.819593
22	O	0.0000	-0.820050
23	O	-0.0000	-0.820654
24	O	0.0000	-0.820322
25	O	0.0000	-0.819794
26	O	0.0000	-0.819767
27	O	-0.0000	-0.819545
28	O	-0.0000	-0.820401
29	O	-0.0000	-0.820737
30	O	0.0000	-0.766580
31	O	0.0000	-0.766176
32	O	-0.0000	-0.766439
33	O	0.0000	-0.766095
34	O	0.0000	-0.765743
35	O	-0.0000	-0.765751
36	O	-0.0000	-0.765977
37	O	0.0000	-0.766355
38	O	-0.0000	-0.766345
39	O	-0.0000	-0.766268
40	O	0.0000	-0.765906
41	O	-0.0000	-0.765743
42	O	0.0000	-0.561262
43	O	-0.0000	-0.561301
44	O	0.0000	-0.561063
45	O	0.0000	-0.561048
46	O	-0.0000	-0.561301

47	O	-0.0000	-0.561085
48	O	-0.0000	-0.561120
49	O	-0.0000	-0.561168
50	O	0.0000	-0.561159
51	O	0.0000	-0.561221
52	O	-0.0000	-0.561078
53	O	-0.0000	-0.561200

[PW ₁₁ O ₃₉] ⁷⁻		Charge=-7 Multiplicity=1	
		Spin	Charge
1	P	0.0000	1.873288
2	W	-0.0000	1.802748
3	W	0.0000	1.906146
4	W	-0.0000	1.730760
5	W	0.0000	1.671733
6	W	0.0000	1.923806
7	W	0.0000	1.825270
8	W	-0.0000	1.805034
9	W	0.0000	1.723688
10	W	0.0000	1.665137
11	W	0.0000	1.805309
12	W	-0.0000	1.912639
13	O	-0.0000	-0.738438
14	O	0.0000	-0.727288
15	O	-0.0000	-0.728109
16	O	0.0000	-0.727854
17	O	0.0000	-0.824791
18	O	0.0000	-0.823510
19	O	-0.0000	-0.635602
20	O	-0.0000	-0.810012

21	O	-0.0000	-0.837832
22	O	-0.0000	-0.693660
23	O	0.0000	-0.870762
24	O	-0.0000	-0.694365
25	O	0.0000	-0.617470
26	O	0.0000	-0.776194
27	O	0.0000	-0.823026
28	O	-0.0000	-0.822522
29	O	0.0000	-0.779498
30	O	-0.0000	-0.783669
31	O	0.0000	-0.785965
32	O	-0.0000	-0.616427
33	O	0.0000	-0.784514
34	O	-0.0000	-0.723258
35	O	-0.0000	-0.819970
36	O	-0.0000	-0.708783
37	O	0.0000	-0.794659
38	O	-0.0000	-0.616314
39	O	0.0000	-0.783093
40	O	-0.0000	-0.804727
41	O	0.0000	-0.690975
42	O	-0.0000	-0.679593
43	O	-0.0000	-0.673286
44	O	0.0000	-0.686809
45	O	0.0000	-0.664242
46	O	-0.0000	-0.666141
47	O	0.0000	-0.687140
48	O	0.0000	-0.672833
49	O	0.0000	-0.691710
50	O	0.0000	-0.689904

		51		O	-0.0000	-0.690610	
[PW ₁₁ O ₃₉ {Fe ⁿ⁺ }] ⁽⁷⁻ⁿ⁾⁻		Charge=-4 Multiplicity=2		Charge=-4 Multiplicity=4		Charge=-4 Multiplicity=6	
		Spin	Charge	Spin	Charge	Spin	Charge
1	Fe	0.906992	0.847686	2.780808	0.873961	3.979211	0.955738
2	O	-0.000288	-0.820433	-0.000209	-0.822472	0.000233	-0.820996
3	O	0.000351	-0.770848	-0.001796	-0.769048	0.007685	-0.769424
4	O	0.000655	-0.818934	-0.001201	-0.812421	0.003963	-0.818833
5	O	-0.000047	-0.775485	-0.000103	-0.777107	0.000161	-0.774516
6	O	-0.000325	-0.815449	-0.000122	-0.823689	0.000090	-0.826895
7	O	-0.000242	-0.775123	0.000231	-0.772995	0.000982	-0.775686
8	O	0.001428	-0.824049	0.001117	-0.822316	0.000710	-0.819158
9	O	0.020784	-0.816653	0.028582	-0.816531	0.032376	-0.815214
10	O	0.000241	-0.775511	0.000642	-0.778617	0.005113	-0.776549
11	O	-0.000181	-0.766258	-0.002887	-0.767965	0.008251	-0.778388
12	O	0.001852	-0.824025	-0.000426	-0.825477	0.001439	-0.818508
13	O	0.001260	-0.773274	0.001288	-0.775195	0.001698	-0.772065
14	O	0.001038	-0.821451	0.001053	-0.822784	0.000404	-0.817456
15	O	0.000077	-0.598325	-0.000103	-0.597793	-0.000165	-0.599232
16	O	-0.000219	-0.776006	0.000269	-0.773795	0.000768	-0.769600
17	O	0.007943	-0.608258	0.016522	-0.603001	0.027126	-0.603314
18	O	0.000114	-0.597412	-0.000206	-0.597167	0.000500	-0.597204
19	O	0.035416	-0.715898	0.066826	-0.742277	0.187850	-0.742966
20	O	-0.000050	-0.820711	0.000010	-0.824641	0.000055	-0.818604
21	O	0.006302	-0.608357	0.002114	-0.606217	0.029077	-0.603414
22	O	0.028470	-0.710797	0.016962	-0.732368	0.254646	-0.757646
23	O	0.009110	-0.678623	0.028455	-0.691946	0.167084	-0.707688
24	O	-0.000298	-0.825569	-0.000058	-0.823018	0.000292	-0.822291
25	O	-0.000288	-0.596134	-0.000201	-0.595857	-0.000034	-0.593909
26	O	0.029867	-0.778251	0.022476	-0.778825	0.020093	-0.780643
27	O	0.000165	-0.596669	-0.000006	-0.596802	0.000703	-0.597635

28	O	0.012017	-0.680531	-0.014290	-0.681089	0.131191	-0.692066
29	O	0.000902	-0.779306	0.000618	-0.779073	0.007896	-0.771252
30	O	0.001199	-0.826425	-0.000951	-0.814756	0.003669	-0.798833
31	O	-0.011066	-0.602073	0.001242	-0.598645	0.021226	-0.599884
32	O	-0.000208	-0.597977	0.000629	-0.598473	0.000936	-0.598230
33	O	0.000969	-0.773444	0.000984	-0.775459	0.000917	-0.771111
34	O	-0.011159	-0.601401	-0.007793	-0.600341	0.018959	-0.601494
35	W	-0.001496	1.916754	-0.001045	1.939753	-0.009670	1.930637
36	W	0.003207	1.951565	0.001864	1.957514	0.000275	1.945509
37	W	-0.006025	1.954936	-0.009981	1.944350	-0.014175	1.928827
38	W	-0.000016	1.964741	0.000173	1.966052	0.000446	1.957088
39	W	-0.005455	1.949796	-0.005125	1.946305	-0.013937	1.946789
40	W	0.000085	1.960159	0.000008	1.964644	0.000171	1.963197
41	W	0.000187	1.962349	-0.000195	1.958965	0.000676	1.955620
42	W	0.001373	1.961781	0.001663	1.957303	0.002184	1.960427
43	W	0.001801	1.957324	0.001980	1.957929	0.000576	1.946264
44	W	-0.000636	1.913681	-0.004148	1.935832	-0.007904	1.940963
45	W	-0.000002	1.962833	-0.000827	1.958604	0.000654	1.953141
46	O	0.000086	-0.598099	-0.000067	-0.597653	-0.000232	-0.598653
47	O	-0.000249	-0.594771	-0.000198	-0.595946	0.000053	-0.594887
48	O	-0.042331	-0.767619	0.071981	-0.763527	0.118246	-0.772293
49	O	-0.001596	-0.727267	0.005561	-0.736684	0.010036	-0.730154
50	O	0.000371	-0.727219	-0.000037	-0.731786	0.001626	-0.728137
51	O	0.000449	-0.728083	-0.000248	-0.731719	0.001462	-0.726711
52	P	0.007467	1.989112	-0.001837	1.994260	-0.005591	1.977336

[PW ₁₁ O ₃₉ {Fe ⁿ⁺ }] ⁽⁷⁻ⁿ⁾⁻		Charge=-5 Multiplicity=1		Charge=-5 Multiplicity=3		Charge=-5 Multiplicity=5	
		Spin	Charge	Spin	Charge	Spin	Charge
1	Fe	0.0000	0.666359	2.197634	0.689805	3.705000	0.732828
2	O	0.0000	-0.821017	0.000513	-0.820621	0.000014	-0.822180

3	O	0.0000	-0.762783	-0.006981	-0.758828	0.005338	-0.767729
4	O	0.0000	-0.806839	-0.004673	-0.801446	0.001718	-0.783225
5	O	0.0000	-0.782317	0.000383	-0.781554	-0.000178	-0.778309
6	O	0.0000	-0.823727	0.003707	-0.825379	-0.000126	-0.821873
7	O	0.0000	-0.779252	0.000448	-0.776872	0.000142	-0.775621
8	O	0.0000	-0.820772	-0.001853	-0.819750	0.000349	-0.810150
9	O	0.0000	-0.816459	-0.004992	-0.817677	0.010806	-0.817457
10	O	0.0000	-0.781395	0.004471	-0.783607	0.001524	-0.777882
11	O	0.0000	-0.762969	-0.007399	-0.763879	0.006778	-0.771552
12	O	0.0000	-0.824001	0.003012	-0.822477	-0.000776	-0.828337
13	O	0.0000	-0.780045	-0.003060	-0.779753	0.001414	-0.778897
14	O	0.0000	-0.820889	-0.001718	-0.820354	0.000442	-0.814743
15	O	0.0000	-0.631832	0.000030	-0.631036	-0.000113	-0.631774
16	O	0.0000	-0.779511	0.000623	-0.777035	0.000123	-0.779310
17	O	0.0000	-0.646306	0.009386	-0.642179	0.008755	-0.638327
18	O	0.0000	-0.629487	-0.000215	-0.629058	0.000492	-0.628888
19	O	0.0000	-0.696708	-0.000333	-0.710654	0.054379	-0.744060
20	O	0.0000	-0.824433	0.000719	-0.824857	-0.000085	-0.826177
21	O	0.0000	-0.646400	0.011172	-0.639957	0.004043	-0.639477
22	O	0.0000	-0.696300	0.002932	-0.717961	0.047781	-0.742126
23	O	0.0000	-0.668555	-0.010305	-0.682565	0.033196	-0.676879
24	O	0.0000	-0.820935	0.000554	-0.818562	-0.000024	-0.823526
25	O	0.0000	-0.625671	0.002288	-0.625586	0.000105	-0.623211
26	O	0.0000	-0.792789	-0.006283	-0.788133	0.005931	-0.792267
27	O	0.0000	-0.629559	-0.000265	-0.629447	0.000279	-0.629019
28	O	0.0000	-0.668600	-0.008196	-0.685467	0.036437	-0.688752
29	O	0.0000	-0.781265	0.004632	-0.783834	0.003911	-0.782365
30	O	0.0000	-0.807133	-0.004970	-0.799767	0.001788	-0.800401
31	O	0.0000	-0.637261	-0.000519	-0.635699	0.008713	-0.636041
32	O	0.0000	-0.631670	0.000975	-0.631818	0.000338	-0.630839

33	O	0.0000	-0.780109	-0.003446	-0.779562	0.000550	-0.779868
34	O	0.0000	-0.637184	-0.000381	-0.633828	0.009074	-0.635791
35	W	0.0000	1.842833	-0.044976	1.860533	0.007326	1.867195
36	W	0.0000	1.913043	-0.029490	1.916101	-0.001361	1.913187
37	W	0.0000	1.881705	-0.033065	1.875973	-0.003447	1.874004
38	W	0.0000	1.940090	-0.000420	1.938604	0.000011	1.948552
39	W	0.0000	1.882050	-0.033861	1.879143	-0.002097	1.855116
40	W	0.0000	1.940565	-0.000060	1.941399	-0.000024	1.947070
41	W	0.0000	1.932714	-0.001069	1.929559	0.000638	1.923539
42	W	0.0000	1.941336	-0.005386	1.933156	0.001613	1.945162
43	W	0.0000	1.913589	-0.029405	1.915085	0.000679	1.912701
44	W	0.0000	1.842064	-0.045773	1.864516	0.008836	1.880984
45	W	0.0000	1.933603	-0.001473	1.928981	0.000774	1.924413
46	O	0.0000	-0.631889	-0.000033	-0.631099	-0.000100	-0.631923
47	O	0.0000	-0.625659	0.002270	-0.626092	-0.000052	-0.623433
48	O	0.0000	-0.756771	0.042382	-0.756998	0.040216	-0.766703
49	O	0.0000	-0.728409	0.003208	-0.737521	0.003042	-0.734487
50	O	0.0000	-0.729330	0.000120	-0.732753	0.000161	-0.726462
51	O	0.0000	-0.729486	0.000142	-0.733613	-0.000309	-0.729546
52	P	0.0000	1.985769	-0.000999	1.984424	-0.004024	1.964856

[PW ₁₁ O ₃₉ Fe ⁺ⁿ (H ₂ O)] ⁻⁽⁷⁻ⁿ⁾		Charge=-4 Multiplicity=2		Charge=-4 Multiplicity=4		Charge=-4 Multiplicity=6	
		Spin	Charge	Spin	Charge	Spin	Charge
1	Fe	0.924499	0.661910	2.788609	0.855082	4.396534	0.928167
2	O	-0.000161	-0.815451	-0.000116	-0.820984	0.000063	-0.822076
3	O	0.000261	-0.774359	-0.001877	-0.772919	0.000851	-0.771280
4	O	-0.000059	-0.812757	-0.001232	-0.807004	0.000766	-0.817414
5	O	-0.000217	-0.773525	-0.000095	-0.773546	0.000016	-0.774517
6	O	-0.000635	-0.812974	-0.001159	-0.820979	0.000492	-0.826700
7	O	-0.000266	-0.772843	0.000222	-0.770440	0.000028	-0.775290

8	O	0.001317	-0.823021	0.001166	-0.818069	-0.000062	-0.819692
9	O	0.022416	-0.816673	0.026903	-0.814194	0.000470	-0.817131
10	O	-0.000097	-0.772463	-0.001523	-0.775438	0.000580	-0.776608
11	O	-0.000502	-0.759550	-0.002699	-0.768181	0.000634	-0.778111
12	O	0.002271	-0.821675	0.000709	-0.827407	0.000139	-0.819915
13	O	0.001162	-0.771143	0.001290	-0.774200	-0.000028	-0.771656
14	O	0.000758	-0.819090	0.000802	-0.819823	0.000031	-0.818472
15	O	-0.000059	-0.598304	-0.000036	-0.594903	-0.000009	-0.596359
16	O	-0.000428	-0.774039	0.000308	-0.773627	0.000024	-0.770579
17	O	-0.000532	-0.615358	0.001975	-0.603351	-0.000366	-0.599599
18	O	-0.000274	-0.598029	-0.000127	-0.594346	0.000002	-0.594917
19	O	0.017863	-0.744727	0.019572	-0.760419	-0.058598	-0.770072
20	O	-0.000078	-0.818837	0.000001	-0.821471	0.000031	-0.818871
21	O	-0.001656	-0.612861	0.017496	-0.598383	-0.000464	-0.599520
22	O	0.011224	-0.691848	0.065328	-0.742796	-0.073838	-0.757251
23	O	0.012191	-0.671873	-0.018477	-0.676844	-0.047640	-0.705426
24	O	-0.000243	-0.825451	-0.000098	-0.822984	0.000095	-0.823392
25	O	-0.000272	-0.598808	-0.000136	-0.592144	-0.000014	-0.590530
26	O	0.029329	-0.774738	0.020944	-0.778182	0.000628	-0.780955
27	O	0.000033	-0.596816	-0.000050	-0.594537	0.000000	-0.595035
28	O	0.033623	-0.721473	0.029613	-0.726764	-0.039882	-0.723964
29	O	0.001037	-0.780204	0.002672	-0.776013	0.000386	-0.771430
30	O	-0.000243	-0.827670	-0.001017	-0.821073	0.000773	-0.802957
31	O	-0.006322	-0.603816	-0.008490	-0.597766	-0.000043	-0.597097
32	O	-0.000345	-0.598551	0.000625	-0.595853	-0.000004	-0.595835
33	O	0.001064	-0.772351	0.000351	-0.774023	0.000061	-0.770709
34	O	-0.002715	-0.602174	0.001622	-0.593327	-0.000021	-0.596314
35	W	-0.002868	1.911721	-0.006677	1.923010	-0.020936	1.914269
36	W	0.003929	1.949555	0.002948	1.952955	0.001053	1.953801
37	W	-0.004908	1.955959	-0.005573	1.937331	-0.034168	1.919795

38	W	0.000071	1.963504	0.000148	1.965474	-0.000425	1.959231
39	W	-0.002068	1.949955	-0.009360	1.943359	-0.029450	1.952672
40	W	0.000316	1.954354	0.000192	1.963945	-0.000439	1.966404
41	W	-0.000170	1.955597	-0.000698	1.956558	-0.000217	1.957861
42	W	0.000975	1.959725	0.001562	1.956824	-0.000499	1.964335
43	W	0.001689	1.950690	0.000897	1.956070	0.000521	1.949225
44	W	-0.003279	1.907935	-0.000391	1.947657	-0.017188	1.951991
45	W	-0.000395	1.960766	-0.000111	1.958264	-0.000379	1.957267
46	O	0.000022	-0.598398	-0.000078	-0.595725	-0.000010	-0.596522
47	O	-0.000197	-0.594218	-0.000180	-0.593149	0.000004	-0.592180
48	O	-0.023059	-0.742804	0.070904	-0.763075	-0.071873	-0.772325
49	O	-0.002618	-0.731037	0.005457	-0.737063	-0.000296	-0.730148
50	O	0.000174	-0.730691	-0.000319	-0.730804	0.001477	-0.728258
51	O	-0.000005	-0.732519	-0.000015	-0.733373	0.001617	-0.726875
52	P	-0.001881	1.998839	-0.002445	1.993396	-0.023337	1.976817
53	O	-0.008116	-0.752187	0.000428	-0.885871	0.000673	-0.885613
54	H	-0.000837	0.488688	-0.000019	0.463256	-0.001121	0.463559
55	H	-0.000721	0.486105	0.000257	0.467867	-0.001376	0.466203

[PW ₁₁ O ₃₉ Fe ⁺ⁿ (H ₂ O)] ⁻⁽⁷⁻ⁿ⁾		Charge=-5 Multiplicity=1		Charge=-5 Multiplicity=3		Charge=-5 Multiplicity=5	
		Spin	Charge	Spin	Charge	Spin	Charge
1	Fe	0.0000	0.641991	2.204576	0.667702	3.684524	0.698439
2	O	0.0000	-0.819221	0.000511	-0.819428	0.000079	-0.820438
3	O	0.0000	-0.766887	-0.006819	-0.763180	0.005570	-0.774767
4	O	0.0000	-0.804943	-0.004756	-0.798376	0.001863	-0.778141
5	O	0.0000	-0.781363	0.000387	-0.780684	-0.000197	-0.774305
6	O	0.0000	-0.821237	0.003044	-0.825110	-0.001068	-0.817594
7	O	0.0000	-0.778055	0.000400	-0.775640	0.000130	-0.772754
8	O	0.0000	-0.821236	-0.002477	-0.819259	0.000316	-0.807127
9	O	0.0000	-0.817283	-0.005437	-0.818436	0.006855	-0.815000

10	O	0.0000	-0.779659	0.003711	-0.782008	0.000129	-0.773977
11	O	0.0000	-0.761537	-0.007591	-0.762689	0.006700	-0.770313
12	O	0.0000	-0.826227	0.003648	-0.824535	-0.000897	-0.830864
13	O	0.0000	-0.779610	-0.003513	-0.779555	0.001304	-0.777373
14	O	0.0000	-0.820260	-0.001066	-0.820350	0.000418	-0.810112
15	O	0.0000	-0.628950	0.000056	-0.628050	-0.000148	-0.628288
16	O	0.0000	-0.780023	0.000699	-0.777665	0.000202	-0.780099
17	O	0.0000	-0.642086	0.008951	-0.636971	0.009803	-0.633357
18	O	0.0000	-0.627227	-0.000222	-0.626721	0.000598	-0.626180
19	O	0.0000	-0.727869	-0.002520	-0.742424	0.048871	-0.777448
20	O	0.0000	-0.823965	0.000733	-0.825508	-0.000047	-0.822439
21	O	0.0000	-0.642519	0.010869	-0.636428	0.010924	-0.633803
22	O	0.0000	-0.695702	0.003478	-0.717336	0.053884	-0.751265
23	O	0.0000	-0.667115	-0.009420	-0.681044	0.028355	-0.662262
24	O	0.0000	-0.822748	0.000594	-0.820266	-0.000105	-0.823566
25	O	0.0000	-0.622135	0.002138	-0.621754	-0.000065	-0.618835
26	O	0.0000	-0.792008	-0.006743	-0.788472	0.005729	-0.790992
27	O	0.0000	-0.626775	-0.000274	-0.626608	0.000330	-0.625877
28	O	0.0000	-0.705815	-0.010778	-0.719886	0.042480	-0.732617
29	O	0.0000	-0.782227	0.005345	-0.784048	0.004212	-0.779363
30	O	0.0000	-0.813622	-0.004918	-0.807442	0.002319	-0.812642
31	O	0.0000	-0.634450	-0.000683	-0.632745	0.007513	-0.634724
32	O	0.0000	-0.629241	0.000992	-0.629431	0.000318	-0.628009
33	O	0.0000	-0.779252	-0.002897	-0.779582	0.000745	-0.777798
34	O	0.0000	-0.630135	-0.000266	-0.627674	0.007894	-0.628283
35	W	0.0000	1.830893	-0.041712	1.848607	0.011033	1.872550
36	W	0.0000	1.917333	-0.027561	1.923929	0.001221	1.901948
37	W	0.0000	1.875412	-0.029659	1.870823	-0.000316	1.875822
38	W	0.0000	1.943269	-0.000426	1.941939	-0.000340	1.949439
39	W	0.0000	1.888363	-0.036622	1.884515	-0.003645	1.853632

40	W	0.0000	1.941121	-0.000080	1.943103	0.000012	1.944980
41	W	0.0000	1.934056	-0.000917	1.930622	0.000636	1.921545
42	W	0.0000	1.943236	-0.005726	1.935231	0.001722	1.943925
43	W	0.0000	1.915484	-0.032430	1.915545	0.000551	1.913109
44	W	0.0000	1.852326	-0.049695	1.872239	0.019829	1.897035
45	W	0.0000	1.937256	-0.001525	1.933379	0.000636	1.926939
46	O	0.0000	-0.629456	-0.000035	-0.628887	-0.000055	-0.630161
47	O	0.0000	-0.622558	0.002531	-0.623223	-0.000090	-0.620499
48	O	0.0000	-0.757042	0.042272	-0.757433	0.043155	-0.765811
49	O	0.0000	-0.728537	0.003165	-0.737602	0.002991	-0.734858
50	O	0.0000	-0.729441	0.000121	-0.732781	0.000570	-0.725728
51	O	0.0000	-0.729917	0.000156	-0.734078	0.000617	-0.730946
52	P	0.0000	1.985109	-0.001278	1.984404	-0.007441	1.967348
53	O	0.0000	-0.901897	0.000274	-0.900231	-0.000220	-0.906691
54	H	0.0000	0.468710	-0.000428	0.468781	-0.000380	0.468737
55	H	0.0000	0.475670	-0.000177	0.472722	-0.000022	0.469855

		[PW ₁₁ O ₃₉ Fe ⁺⁴ (H ₂ O)] ⁻³		[PW ₁₁ O ₃₉ Fe ⁺⁴ (OH)] ⁻⁴		[PW ₁₁ O ₃₉ Fe ⁺⁴ (O)] ⁻⁵	
		Charge=-3 Multiplicity=3		Charge=-4 Multiplicity=3		Charge=-5 Multiplicity=3	
		Spin	Charge	Spin	Charge	Spin	Charge
1	Fe	1.594526	0.824400	1.712700	0.866888	3.072304	0.864579
2	O	-0.000242	-0.825998	-0.000233	-0.827017	0.000003	-0.822341
3	O	-0.003249	-0.757088	-0.001427	-0.763799	0.005836	-0.765162
4	O	-0.000505	-0.820081	-0.001423	-0.825011	0.002901	-0.794625
5	O	-0.000009	-0.770321	-0.000383	-0.774428	-0.000730	-0.779264
6	O	0.000175	-0.816851	0.001736	-0.823539	0.000016	-0.818709
7	O	-0.000253	-0.769156	-0.000360	-0.773828	-0.000114	-0.779316
8	O	0.001183	-0.823013	0.001142	-0.821474	0.001159	-0.818523
9	O	0.036849	-0.810635	0.029470	-0.815030	0.018262	-0.821640
10	O	0.009536	-0.765318	0.001609	-0.775975	0.001748	-0.776146

11	O	-0.002145	-0.763684	-0.002372	-0.764781	0.005856	-0.758673
12	O	0.002408	-0.823805	0.001557	-0.817999	0.001163	-0.825683
13	O	-0.000475	-0.767538	0.001017	-0.774924	0.001231	-0.775539
14	O	0.001069	-0.822888	0.000990	-0.822096	0.000571	-0.818819
15	O	0.000026	-0.566297	-0.000068	-0.596126	-0.000167	-0.629075
16	O	-0.000827	-0.773949	-0.000374	-0.774351	-0.000142	-0.782004
17	O	0.034270	-0.571370	0.013117	-0.603428	0.002069	-0.636053
18	O	-0.000192	-0.564999	-0.000201	-0.594548	0.000495	-0.627033
19	O	0.390904	-0.667352	0.062899	-0.691548	0.076055	-0.695852
20	O	-0.000007	-0.820729	-0.000143	-0.821120	-0.000253	-0.823383
21	O	-0.001923	-0.583148	-0.002225	-0.608851	0.002146	-0.635423
22	O	-0.000390	-0.732202	0.006498	-0.709238	0.071281	-0.689892
23	O	0.032096	-0.695804	0.097714	-0.666052	0.084550	-0.678881
24	O	0.000289	-0.813477	-0.000254	-0.820238	-0.000106	-0.827407
25	O	0.000286	-0.564793	-0.000182	-0.593073	-0.000060	-0.621340
26	O	0.021834	-0.776994	0.043242	-0.771796	0.020056	-0.784422
27	O	0.000319	-0.565547	0.000099	-0.595249	0.000369	-0.626228
28	O	-0.021702	-0.656911	0.006243	-0.653165	0.089756	-0.680461
29	O	-0.002191	-0.772492	-0.000994	-0.775394	0.002303	-0.783595
30	O	-0.001072	-0.826055	-0.002184	-0.810026	0.003331	-0.806585
31	O	-0.000505	-0.568975	0.003713	-0.594140	0.010108	-0.627343
32	O	-0.000852	-0.564833	-0.000415	-0.595806	-0.000416	-0.627777
33	O	0.001048	-0.767387	0.001787	-0.773130	0.000902	-0.778342
34	O	-0.010850	-0.570806	-0.007630	-0.596184	0.009679	-0.627009
35	W	-0.020640	1.959814	-0.012659	1.937771	-0.001635	1.881166
36	W	0.002686	1.978119	0.001425	1.958131	0.000826	1.922440
37	W	-0.002464	1.996914	-0.010434	1.945708	-0.010141	1.898952
38	W	0.000944	1.967686	-0.000073	1.963165	0.000524	1.952672
39	W	-0.004324	1.989505	-0.015879	1.974463	-0.009378	1.889303
40	W	0.000567	1.976689	0.000345	1.966913	0.000580	1.944398

41	W	0.000215	1.982521	-0.000051	1.964746	0.000754	1.938371
42	W	0.001215	1.985363	0.001194	1.963668	0.001648	1.957710
43	W	0.001059	1.977084	0.003176	1.958853	0.000253	1.925730
44	W	-0.009520	1.942731	-0.009115	1.907354	-0.002733	1.879113
45	W	0.000351	1.979699	0.000120	1.959983	0.000700	1.940288
46	O	0.000058	-0.565474	-0.000042	-0.595887	-0.000143	-0.628965
47	O	-0.000163	-0.565843	-0.000221	-0.594292	-0.000072	-0.620421
48	O	-0.032818	-0.740547	-0.012093	-0.735207	-0.014603	-0.732885
49	O	-0.006680	-0.722770	-0.002177	-0.730835	-0.002454	-0.728936
50	O	0.005015	-0.726178	0.000841	-0.733520	0.000347	-0.733474
51	O	0.000205	-0.727193	-0.000038	-0.731757	0.000339	-0.734165
52	P	-0.001025	1.987708	-0.003022	1.990663	-0.001934	1.966850
53	O	-0.014931	-0.731814	0.098916	-0.641052	0.554961	-0.440183
54	H	0.000957	0.495642	-0.004876	0.427608	-	-
55	H	-0.000135	0.496441	-	-	-	-

		[PW ₁₁ O ₃₉ Fe ⁺⁵ (O)] ⁻⁴		[PW ₁₁ O ₃₉ Fe ⁺⁶ (O)] ⁻³	
		Charge=-4 Multiplicity=4		Charge=-3 Multiplicity=3	
		Spin	Charge	Spin	Charge
1	Fe	1.985691	0.960527	1.332332	1.108209
2	O	-0.000189	-0.818415	-0.000753	-0.802579
3	O	-0.001929	-0.760071	0.000416	-0.748490
4	O	-0.003827	-0.817999	-0.003269	-0.814634
5	O	-0.000448	-0.774153	0.000282	-0.768965
6	O	0.001091	-0.821785	0.003681	-0.819883
7	O	-0.000426	-0.775879	-0.000201	-0.772433
8	O	0.001174	-0.824021	0.001204	-0.822075
9	O	0.032430	-0.817284	0.058968	-0.812384
10	O	-0.001272	-0.774491	-0.004877	-0.771326
11	O	-0.002505	-0.755607	-0.003298	-0.736558

12	O	0.003176	-0.821607	0.001350	-0.817079
13	O	0.001578	-0.773576	-0.004457	-0.771949
14	O	0.000663	-0.824043	0.001318	-0.823731
15	O	-0.000143	-0.595289	-0.000110	-0.562080
16	O	-0.000488	-0.774088	-0.001051	-0.768470
17	O	0.002920	-0.602384	0.008499	-0.567384
18	O	-0.000123	-0.594535	-0.000136	-0.563657
19	O	0.041682	-0.683624	0.053888	-0.679966
20	O	-0.000147	-0.826034	-0.001404	-0.826964
21	O	0.002970	-0.601977	-0.007192	-0.565003
22	O	0.038836	-0.679033	0.171397	-0.598323
23	O	0.054076	-0.660905	0.037020	-0.640413
24	O	-0.000182	-0.824860	-0.002302	-0.822869
25	O	-0.000188	-0.593386	-0.000080	-0.562771
26	O	0.060524	-0.768620	0.035483	-0.767084
27	O	-0.000092	-0.593943	0.000129	-0.561789
28	O	0.071136	-0.661263	-0.046421	-0.617844
29	O	-0.000011	-0.777711	-0.012975	-0.765139
30	O	-0.003446	-0.822267	-0.002305	-0.816406
31	O	-0.004467	-0.593330	0.001560	-0.561677
32	O	-0.000402	-0.595629	-0.000330	-0.561693
33	O	0.001579	-0.776016	-0.001735	-0.767782
34	O	-0.004549	-0.592782	-0.025821	-0.557126
35	W	-0.015714	1.925810	-0.019302	1.950805
36	W	0.002640	1.963095	0.001178	1.982700
37	W	-0.023749	1.961875	0.004735	1.983677
38	W	0.000040	1.968232	0.001116	1.974443
39	W	-0.021696	1.954407	-0.014667	1.960691
40	W	0.000112	1.962396	0.002173	1.962920
41	W	0.000240	1.967469	0.000906	1.979370

42	W	0.001044	1.961982	0.001253	1.980273
43	W	0.001260	1.961633	0.004910	1.983102
44	W	-0.015085	1.922782	-0.006391	1.950743
45	W	0.000189	1.968334	0.000612	1.984112
46	O	-0.000129	-0.594962	-0.000191	-0.563354
47	O	-0.000185	-0.592871	0.000233	-0.562725
48	O	-0.014173	-0.734089	-0.016483	-0.719959
49	O	-0.001879	-0.733058	-0.001586	-0.733972
50	O	0.000136	-0.733989	-0.000266	-0.735549
51	O	0.000146	-0.734532	-0.001353	-0.734080
52	P	-0.002627	1.987260	-0.001341	1.976980
53	O	0.814739	-0.365696	0.455651	-0.311861

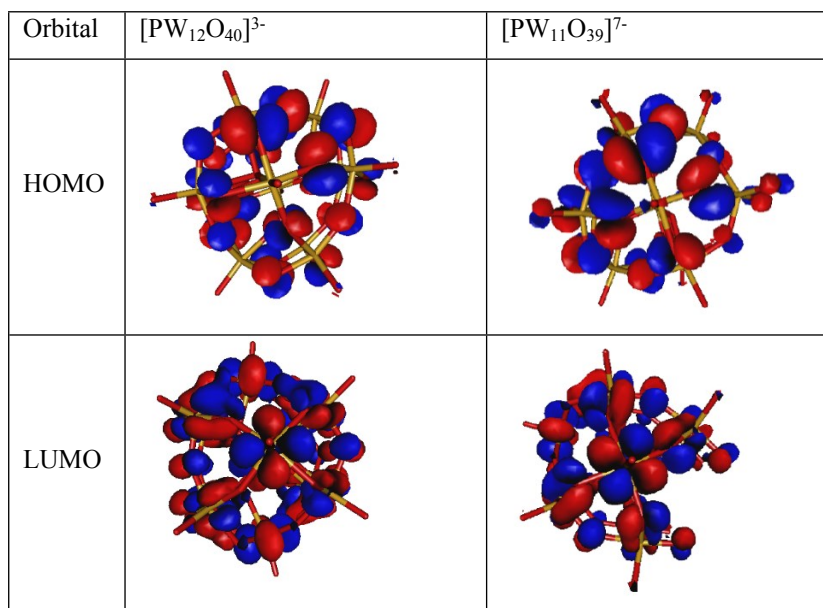


Figure S1. HOMOs and LUMOs of [PW₁₂O₄₀]³⁻ and [PW₁₁O₃₉]⁷⁻ calculated at the UOPBE/6-31G(d) level (LANL2DZ basis set on the metal atom).

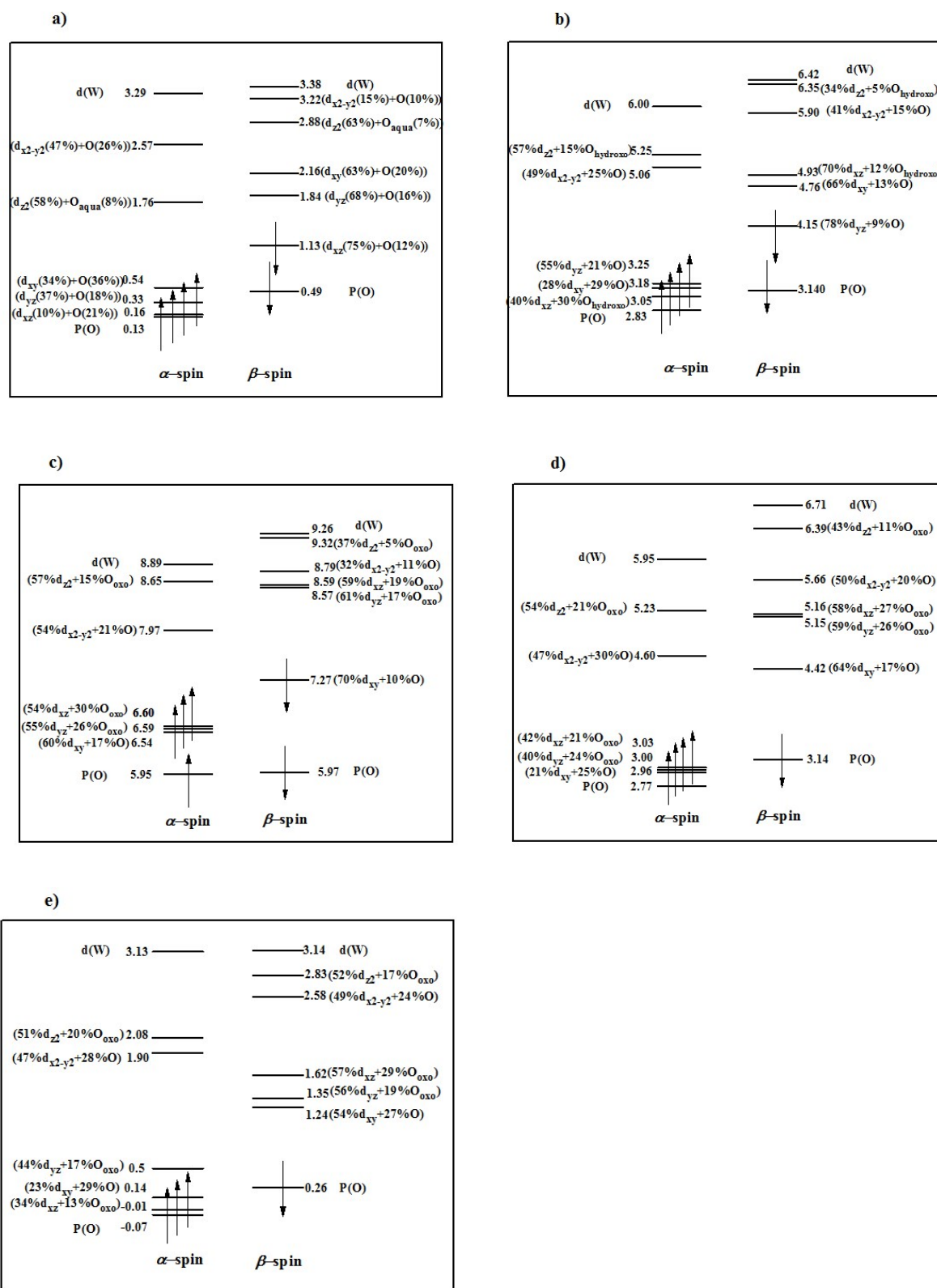


Figure S2. The energy level expressions of FMOs for a) $\text{Fe}^{\text{IV}}\text{OH}_2$, b) $\text{Fe}^{\text{IV}}\text{OH}$, c) $\text{Fe}^{\text{IV}}\text{O}$, d) Fe^{VO} , and e) $\text{Fe}^{\text{VI}}\text{O}$ POMs in the ground state calculated at UOPBE/6-31G(d) level (LANL2DZ basis set on the metal atom).

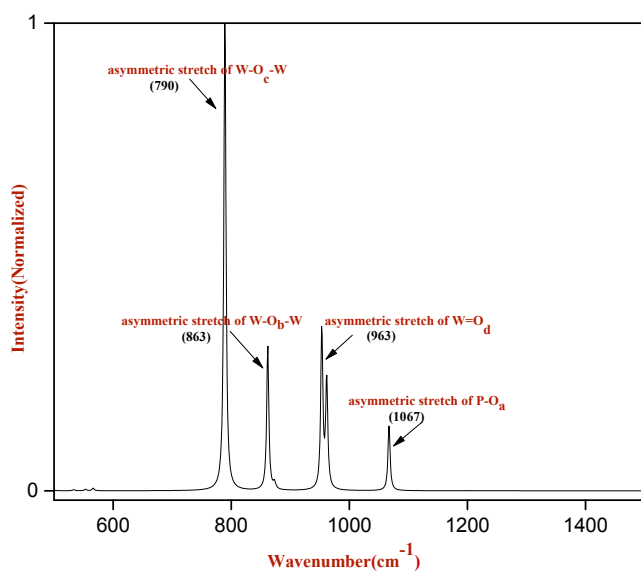


Figure S3: Simulated IR (cm⁻¹) of [PW₁₂O₄₀]⁻³ with spin state=1.

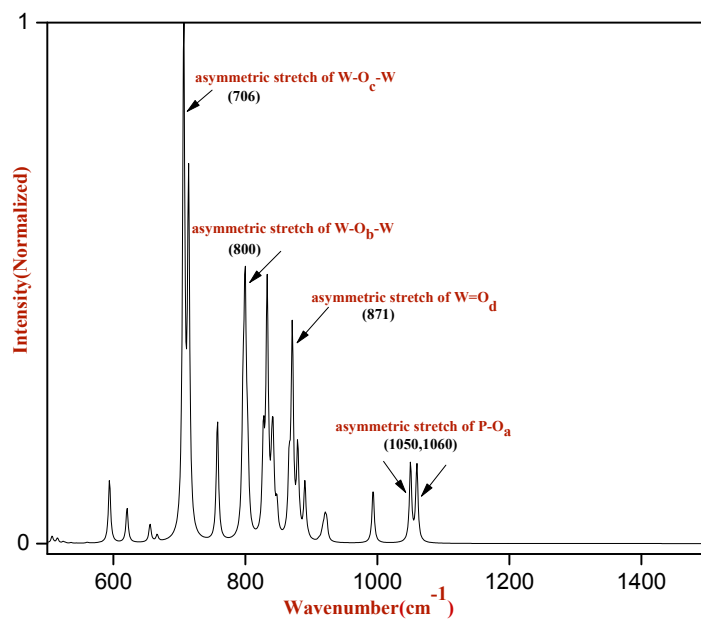


Figure S4: Simulated IR (cm⁻¹) of [PW₁₁O₃₉]⁻⁷ with spin state=1.

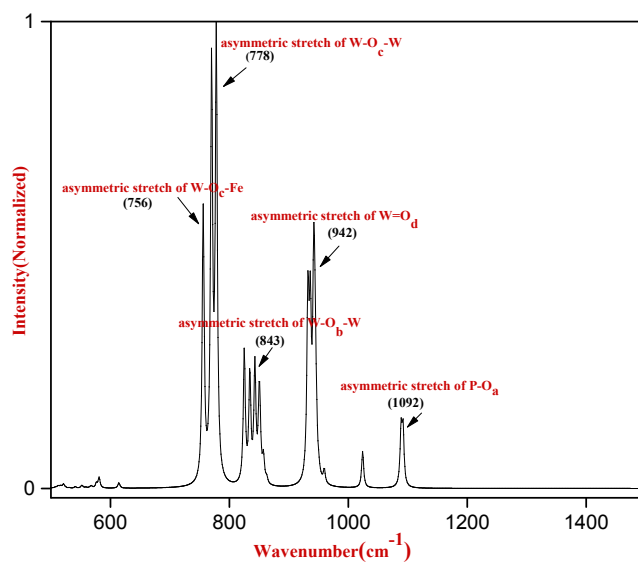


Figure S5: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}\text{Fe}^{+3}]^{-4}$ with spin state=2.

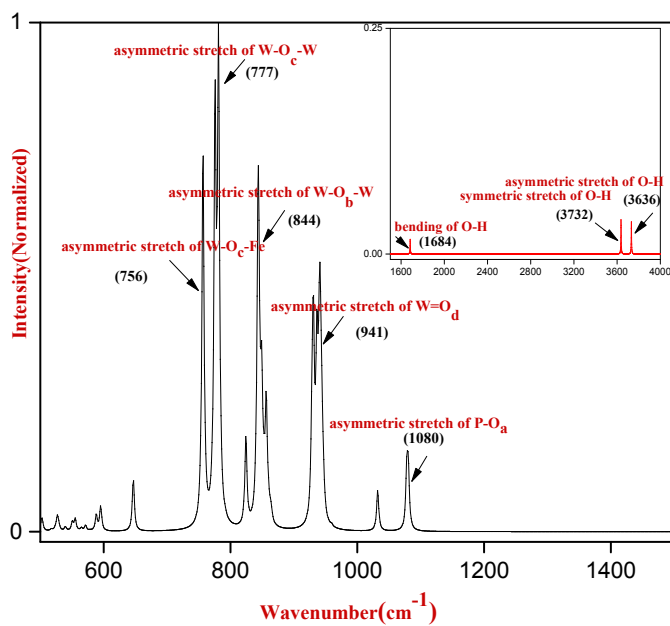


Figure S6: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{+3}\text{OH}_2)]^{-4}$ with spin state=2.

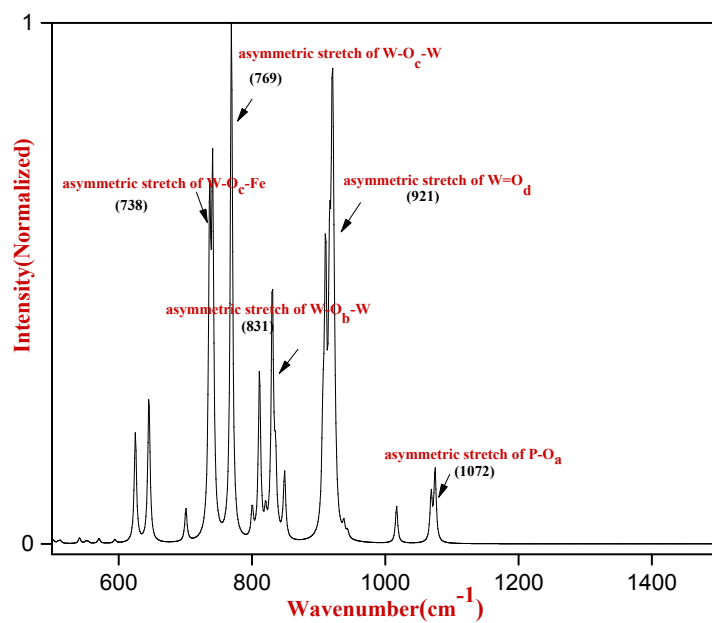


Figure S7: Simulated IR (cm^{-1}) of $[PW_{11}O_{39}Fe^{+2}]^{-5}$ with spin state=1.

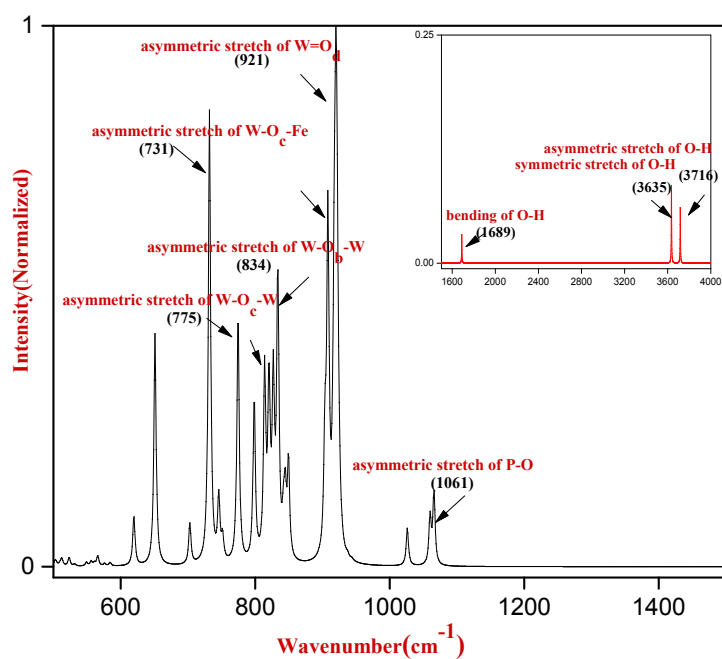


Figure S8: Simulated IR (cm^{-1}) of $[PW_{11}O_{39}(Fe^{+2}OH_2)]^{-5}$ with spin state=1.

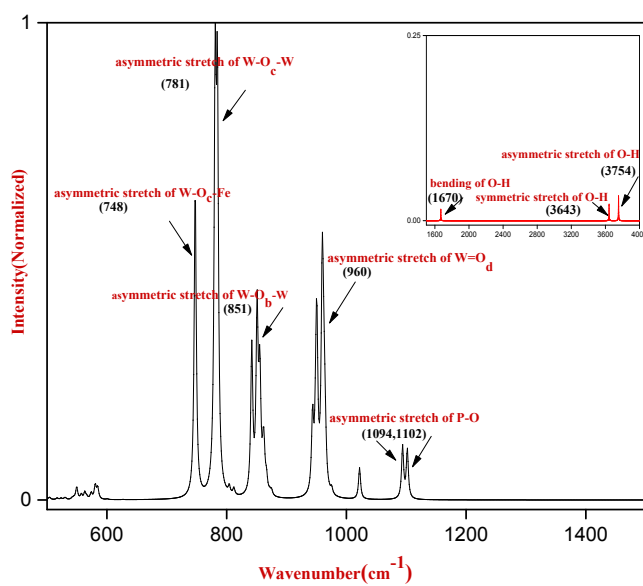


Figure S9: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{IV}}\text{OH}_2)]^{3-}$ with spin state=3.

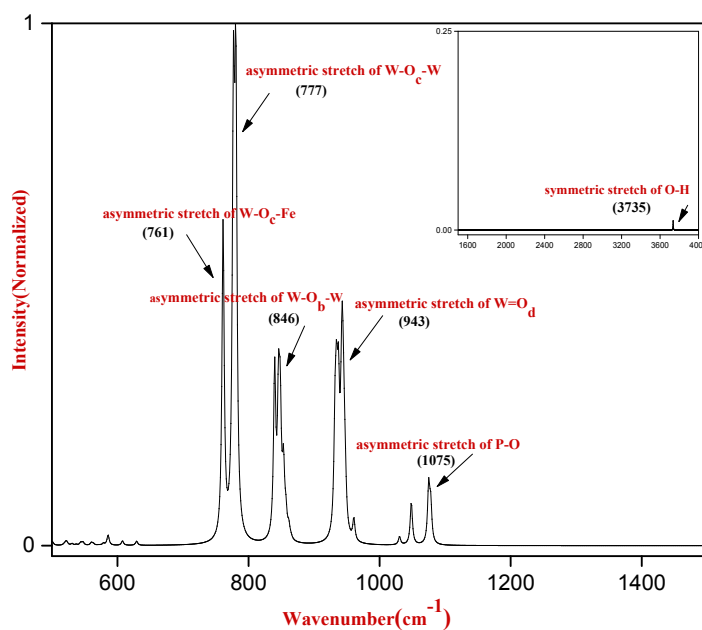


Figure S10: Simulated IR (cm^{-1}) of $[\text{PW}_{11}\text{O}_{39}(\text{Fe}^{\text{IV}}\text{OH})]^{4-}$ with spin state=3.

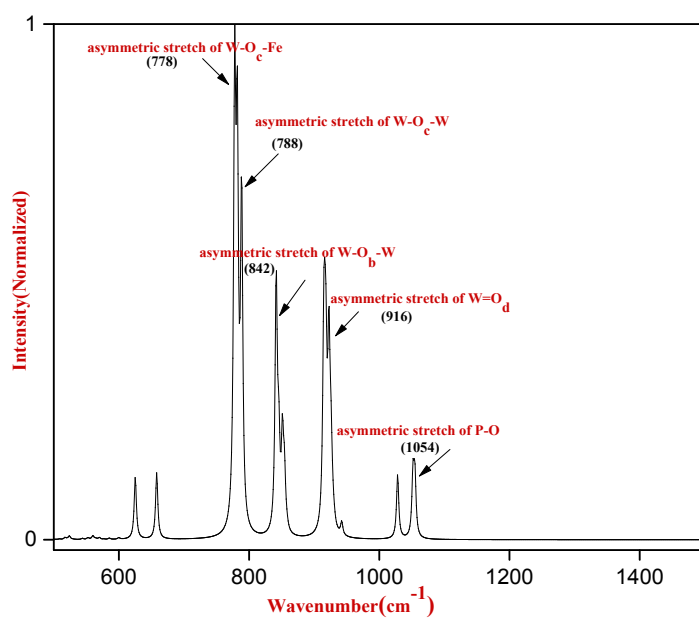


Figure S11: Simulated IR (cm^{-1}) of $[PW_{11}O_{39}(Fe^{IV}O)]^{5-}$ with spin state=3.

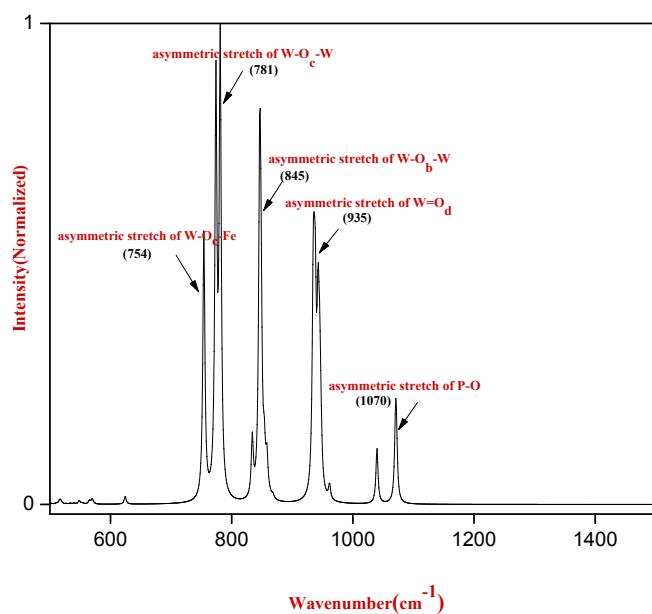


Figure S12: Simulated IR (cm^{-1}) of $[PW_{11}O_{39}(Fe^{VO})]^{4+}$ with spin state=4.

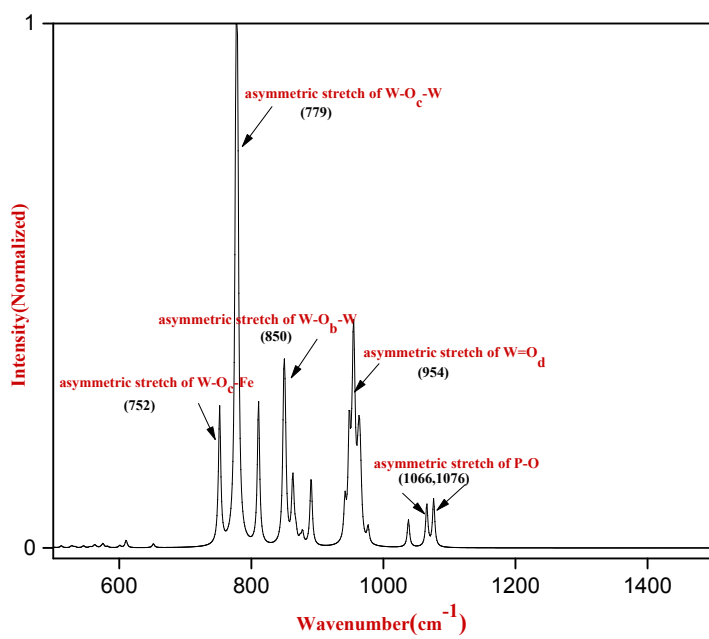


Figure S13: Simulated IR (cm⁻¹) of [PW₁₁O₃₉(Fe^{VI}O)]³⁻ with spin state=3.