

Transition Metal Substitution Effects on Metal-to-Polyoxometalate Charge Transfer

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Table S1. Crystal data, data collection parameters and refinement statistics for $[\text{NH}_4]_7[\text{Co}(\text{H}_2\text{O})_6]_{0.5}[\text{Co}^{\text{II}}\text{Co}^{\text{II}}][\text{Co}_2(\text{H}_2\text{O})\text{W}_{11}\text{O}_{39}]$.

Empirical formula	$\text{Co}_{2.5}\text{H}_{68}\text{N}_7\text{O}_{59}\text{W}_{11}$
$F_w / \text{g mol}^{-1}$	3280.29
T / K	173(2)
$\lambda / \text{\AA}$	0.71073
Crystal system	cubic
Space group	$Fm-3m$
$a / \text{\AA}$	22.376(8)
$b / \text{\AA}$	22.376(8)
$c / \text{\AA}$	22.376(8)
$\alpha / ^\circ$	90
$\beta / ^\circ$	90
$\gamma / ^\circ$	90
$V / \text{\AA}^3$	11203(7)
Z	8
$\rho_{\text{calc}} / \text{g cm}^{-3}$	3.890
μ / mm^{-1}	23.331
Crystal size / mm³	0.16 × 0.14 × 0.10
No. reflections (unique)	57069 (918)
R_{int}	0.0557
θ_{max}	30.46
Completeness to θ_{max}	99.7%
Data / restraints / parameters	918 / 6 / 53
Goodness-of-fit on F^2	1.217
Residuals: R_1; wR_2	0.0231 (0.0616)
Final difference peak and hole / e\AA^{-3}	1.259, -2.524

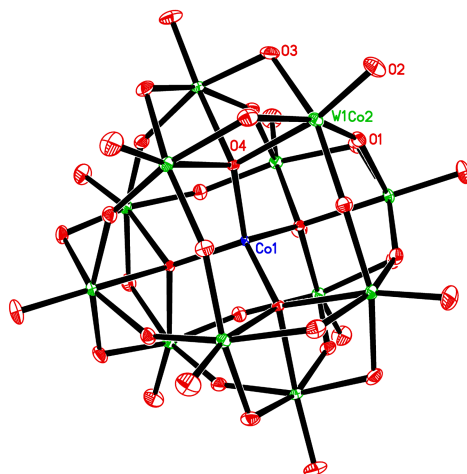


Figure S1. ORTEP representation of the $\text{Co}^{\text{II}}\text{Co}^{\text{II}}$ anion, $[\text{Co}^{\text{II}}\text{Co}^{\text{II}}(\text{H}_2\text{O})\text{W}_{11}\text{O}_{39}]^{8-}$. Thermal ellipsoids are at the 30% probability level. Color scheme: W, green; O, red; Co, blue. H atoms were not located. W1Co2 is modelled as 16.7% Co, 83.3% W.

Table S2. Coordinate bond lengths (Å) and angles (°) in the $\text{Co}^{\text{II}}\text{Co}^{\text{II}}$ anion by x-ray diffraction

<i>Distances / Å</i>		<i>Angles / °</i>	
Co1-O4	1.914(7)	O4-Co1-O4*	109.471(1)
W1/Co2-O1	1.923(2)	O1-W1/Co2-O1*	86.5(3)
W1/Co2-O2	1.753(5)	O1-W1/Co2-O2	100.6(2)
W1/Co2-O3	1.965(3)	O1-W1/Co2-O3	88.8(2)
W1/Co2-O4	2.147(4)	O1-W1/Co2-O3*	162.3(2)
		O1-W1/Co2-O4	88.3(2)
		O2-W1/Co2-O3	97.1(2)
		O2-W1/Co2-O4	167.7(3)
		O3-W1/Co2-O3*	90.6(3)
		O3-W1/Co2-O4	74.5(2)
		Co1-O4-W1/Co2	118.7(2)
		W1/Co2-O1-W1/Co2*	151.2(3)
		W1/Co2-O3-W1/Co2*	112.1(2)
		W1/Co2-O4-W1/Co2*	98.8(2)

*Signifies symmetry generated position

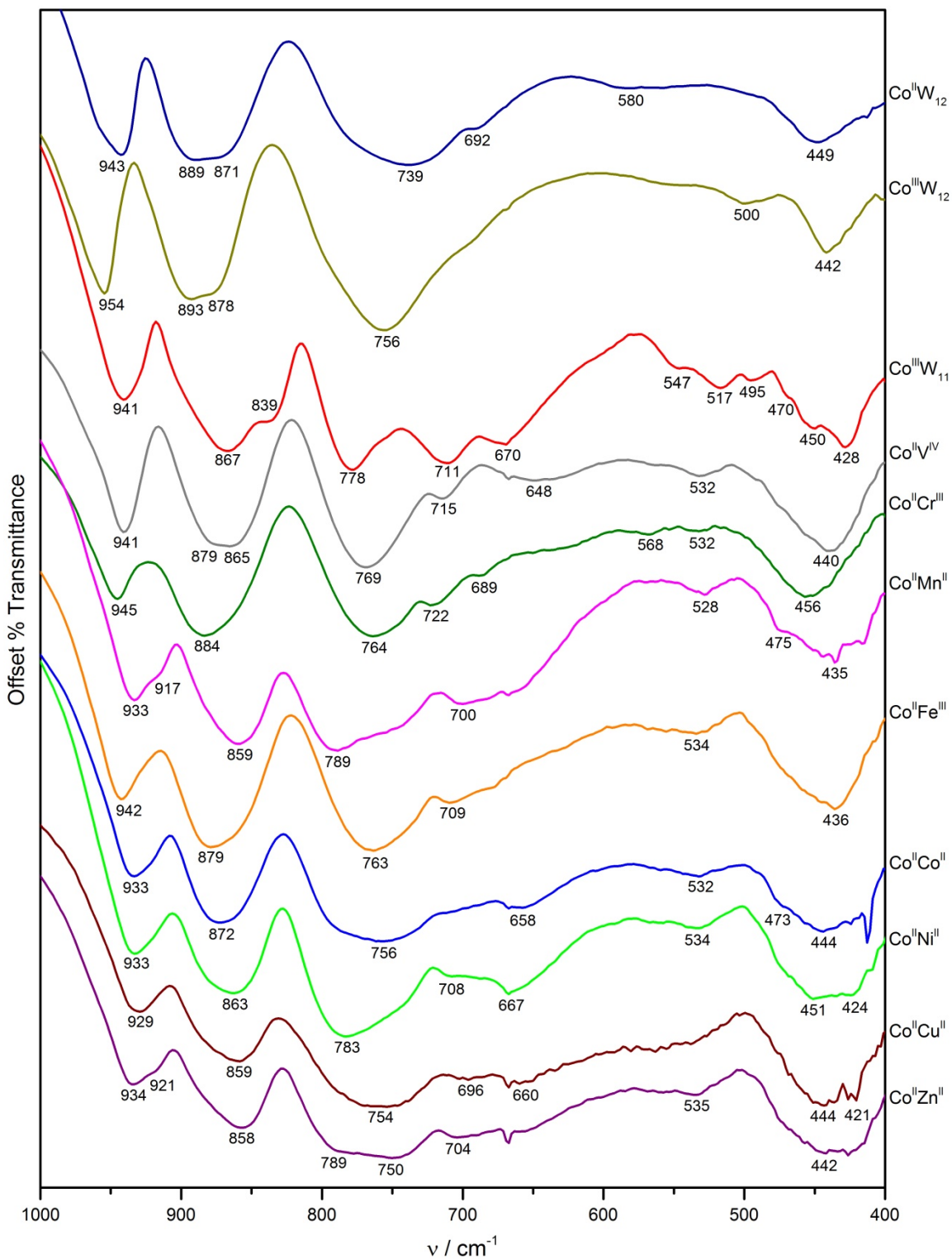


Figure S2. Offset infrared spectra (2% KBr pellet) for the plenary POMs $\text{Co}^{\text{II}}\text{W}_{12}$ and $\text{Co}^{\text{III}}\text{W}_{12}$, the lacunary TMSP-precursor $\text{Co}^{\text{III}}\text{W}_{11}$, and eight TMSP derivatives.

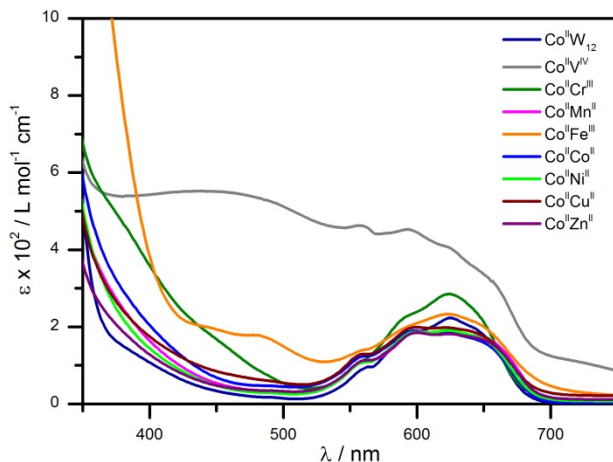


Figure S3. Visible electronic absorption spectra of $\text{Co}^{\text{II}}\text{W}_{12}$ and eight TMSP derivatives in water. The spectra are overlaid for comparison of the extinction coefficients.

Table S3. Measured open circuit potentials (OCP, and OCP_{ox} for the isolated oxidized species where available) and resolved electrochemical potentials for $\text{Co}^{\text{II}}\text{W}_{12}$, $\text{Co}^{\text{III}}\text{W}_{11}$, and eight TMSP derivatives¹

<i>Complex</i>	<i>OCP</i>	<i>OCP_{ox}</i>	<i>Co^{II/III}</i>	<i>M</i>	<i>W₁</i>	<i>W₂</i>	<i>W₃</i>	<i>W₄</i>
	<i>mV</i>			<i>E_{1/2} (ΔE) / mV</i>				
$\text{Co}^{\text{II}}\text{W}_{12}$	610	900	870 (70)		-540 (60)	-660 (60)	-820 (50)	
$\text{Co}^{\text{III}}\text{W}_{11}$	n/a	910	860 (80)		-540 (60)	-660 (60)	-820 (50)	
$\text{Co}^{\text{II}}\text{V}^{\text{IV}}$	200	700 ²	650 (70)	270 (90)	-730 (60)	-880 (50)		
$\text{Co}^{\text{II}}\text{Cr}^{\text{III}}$	180	590	640 (70)	860 (90)	-530 (90)	-720 (80)	-850 (90)	
$\text{Co}^{\text{II}}\text{Mn}^{\text{II}}$	380	570	750 (300)	³	-450 (50)	-550 (40)	-670 (50)	-820 (40)
$\text{Co}^{\text{II}}\text{Fe}^{\text{III}}$	280	n/a	620 (70)	-260 (120)	-570 (40)	-780 (40)	-850 (50)	
$\text{Co}^{\text{II}}\text{Co}^{\text{II}}$	130	620 ⁴	610 (110)	840 (140)	-450 (20)	-560 (10)	-670 (40)	-810 (70)
$\text{Co}^{\text{II}}\text{Ni}^{\text{II}}$	300	760	610 (120)	880 (80)	-460 (40)	-550 (30)	-660 (45)	-800 (80)
$\text{Co}^{\text{II}}\text{Cu}^{\text{II}}$	360	810	610 (100)	850 (120)	-450 (40)	-550 (20)	-670 (50)	-820 (50)
$\text{Co}^{\text{II}}\text{Zn}^{\text{II}}$	600	820	880 (80)		-450 (40)	-550 (40)	-670 (50)	-820 (40)

¹ Peak separations, in mV, are in parentheses after the potential.

² The species measured is the two-electron oxidized species, $\text{Co}^{\text{III}}\text{V}^{\text{V}}$.

³ Protonation and disproportionation reactions obscure the Mn redox couple.

⁴ Static electronic spectroscopy, transient absorption spectroscopy, and electrochemistry indicate that the isolated one-electron oxidized species is incompletely oxidized, retaining some $\text{Co}^{\text{II}}_{\text{Td}}$ in the sample.

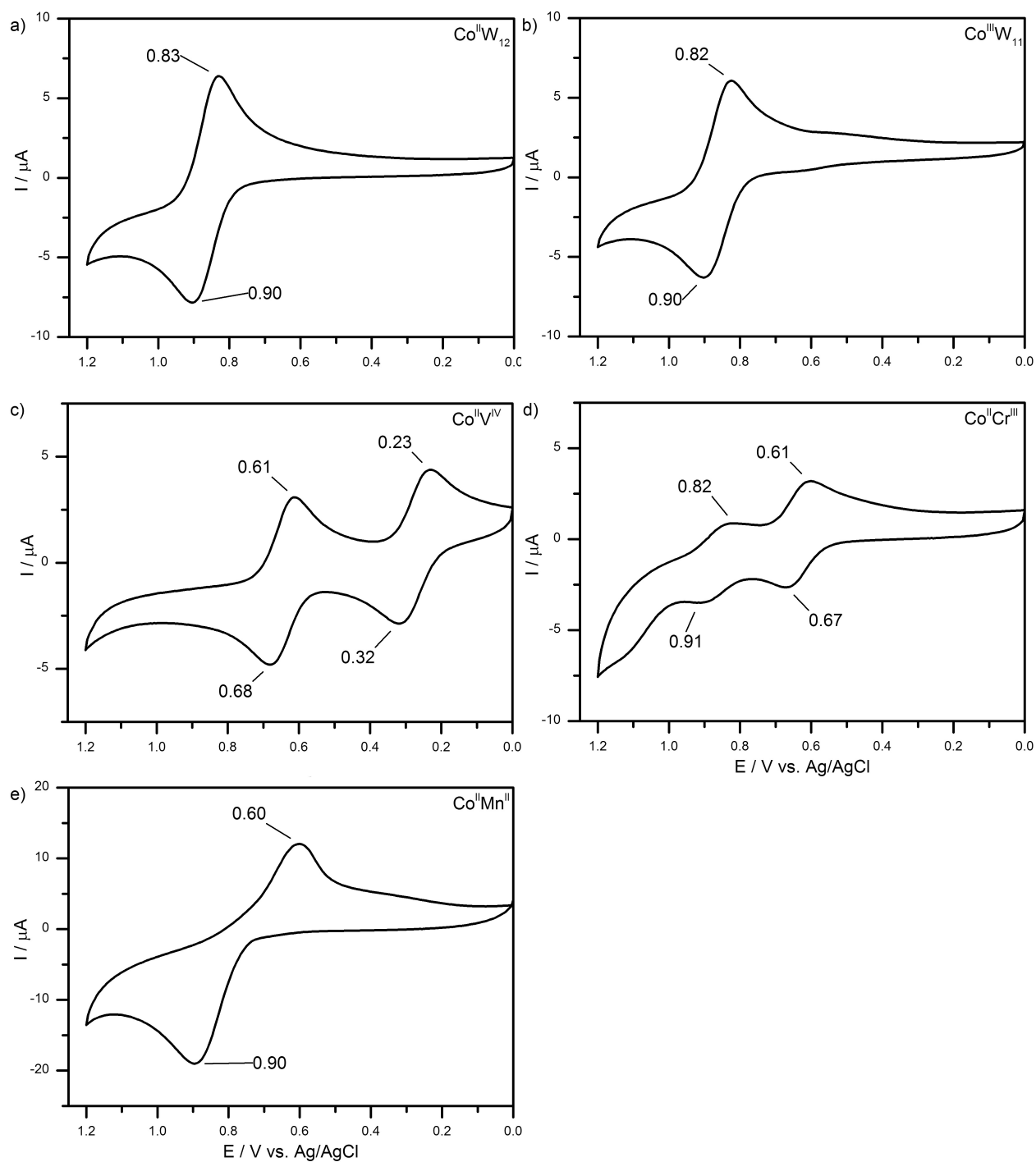


Figure S4. Oxidative cyclic voltammograms of the plenary POM $\text{Co}^{\text{II}}\text{W}_{12}$, the lacunary TMSF-precursor $\text{Co}^{\text{III}}\text{W}_{11}$, and three TMSF derivatives. Each voltammogram, ~ 1 mM POM, was measured in 0.500 M potassium acetate buffer, pH 5, 50 mV/s scan rate. Resolved peaks are annotated.

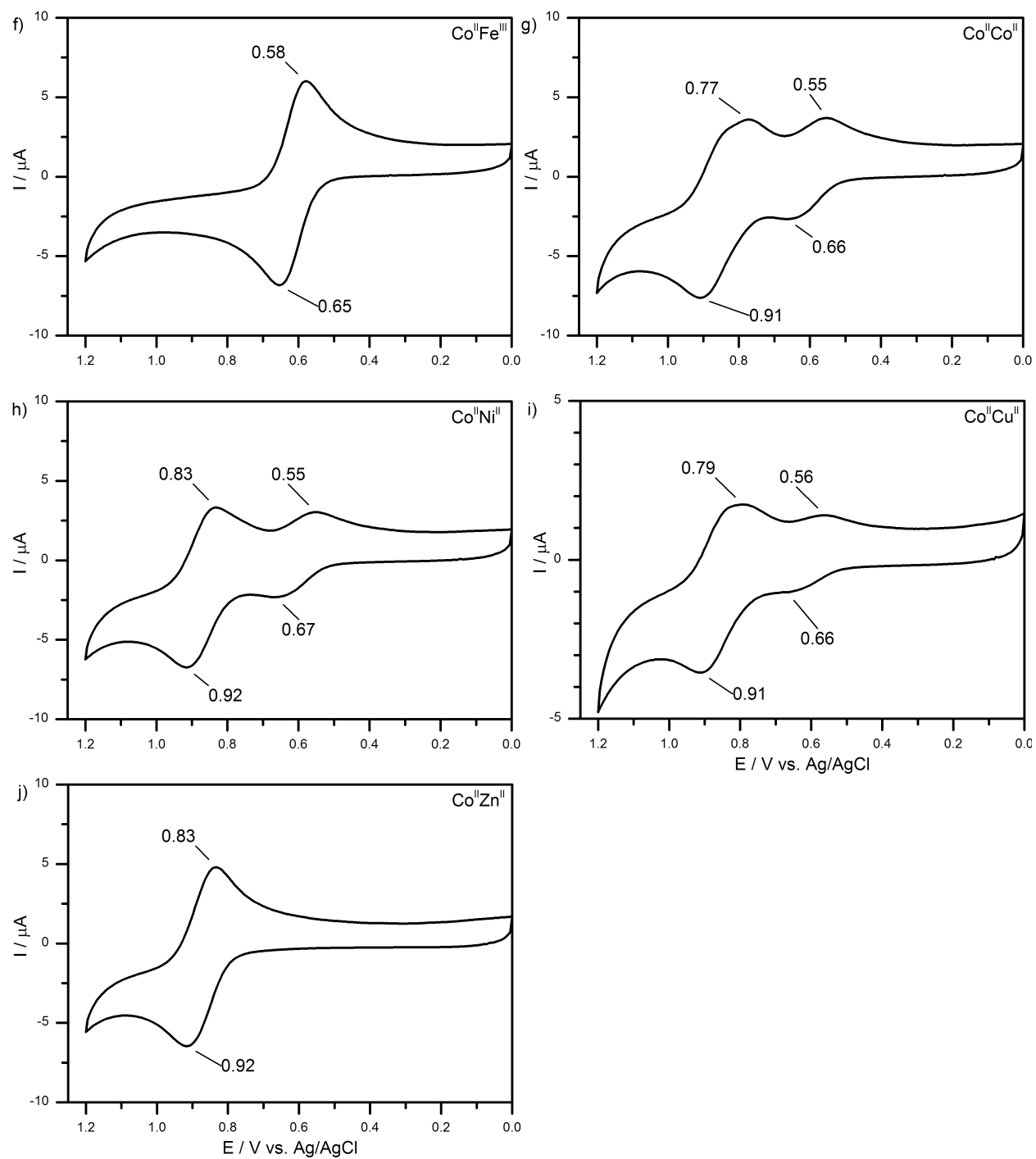


Figure S5. Oxidative cyclic voltammograms of five TMSP derivatives. Each voltammogram, ~ 1 mM POM, was measured in 0.500 M potassium acetate buffer, pH 5, 50 mV/s scan rate. Resolved peaks are annotated.

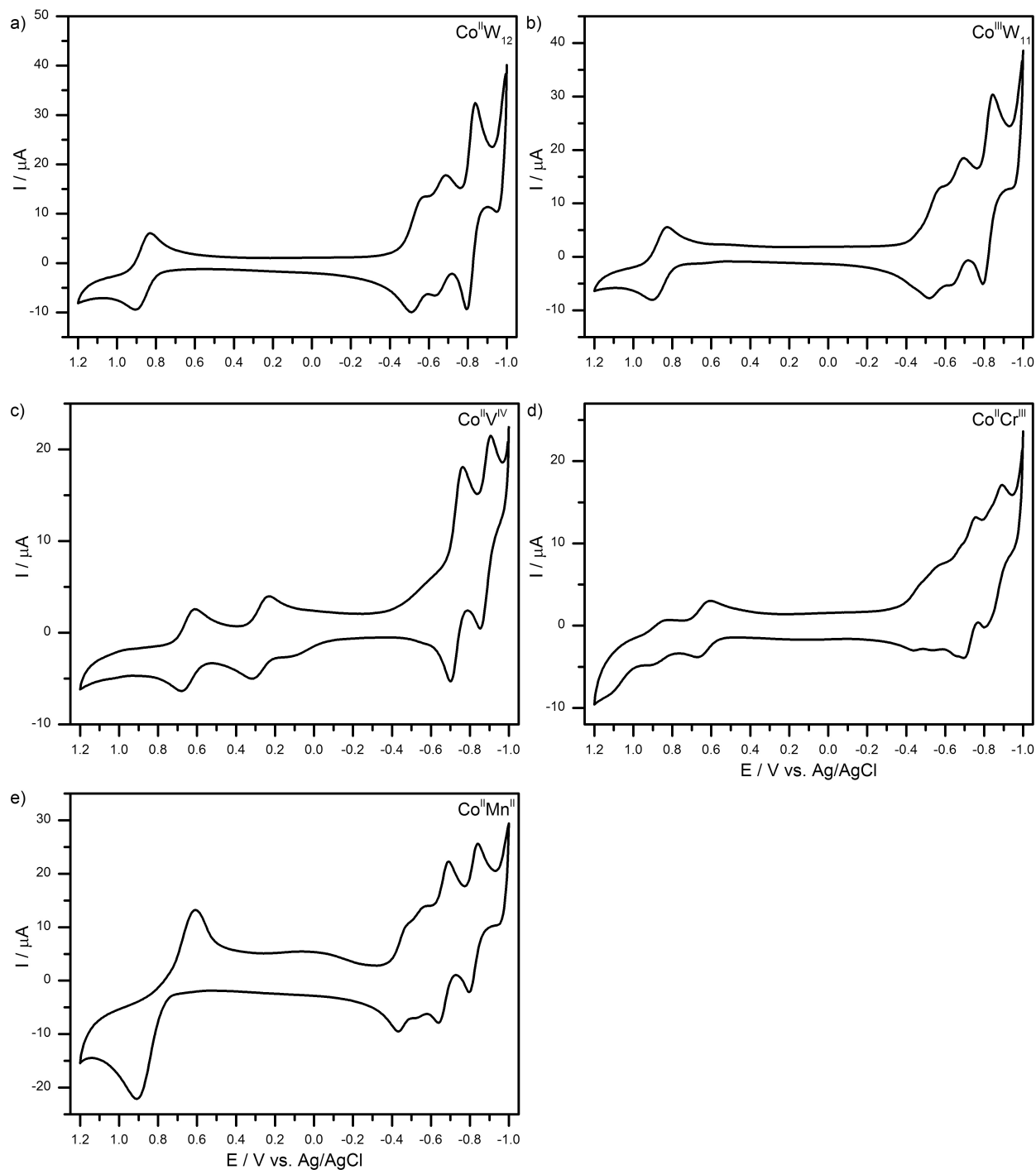


Figure S6. Full cyclic voltammograms of the plenary POM $\text{Co}^{\text{II}}\text{W}_{12}$, the lacunary TMSP-precursor $\text{Co}^{\text{III}}\text{W}_{11}$, and three TMSP derivatives. Each voltammogram, ~ 1 mM POM, was measured in 0.500 M potassium acetate buffer, pH 5, 50 mV/s scan rate.

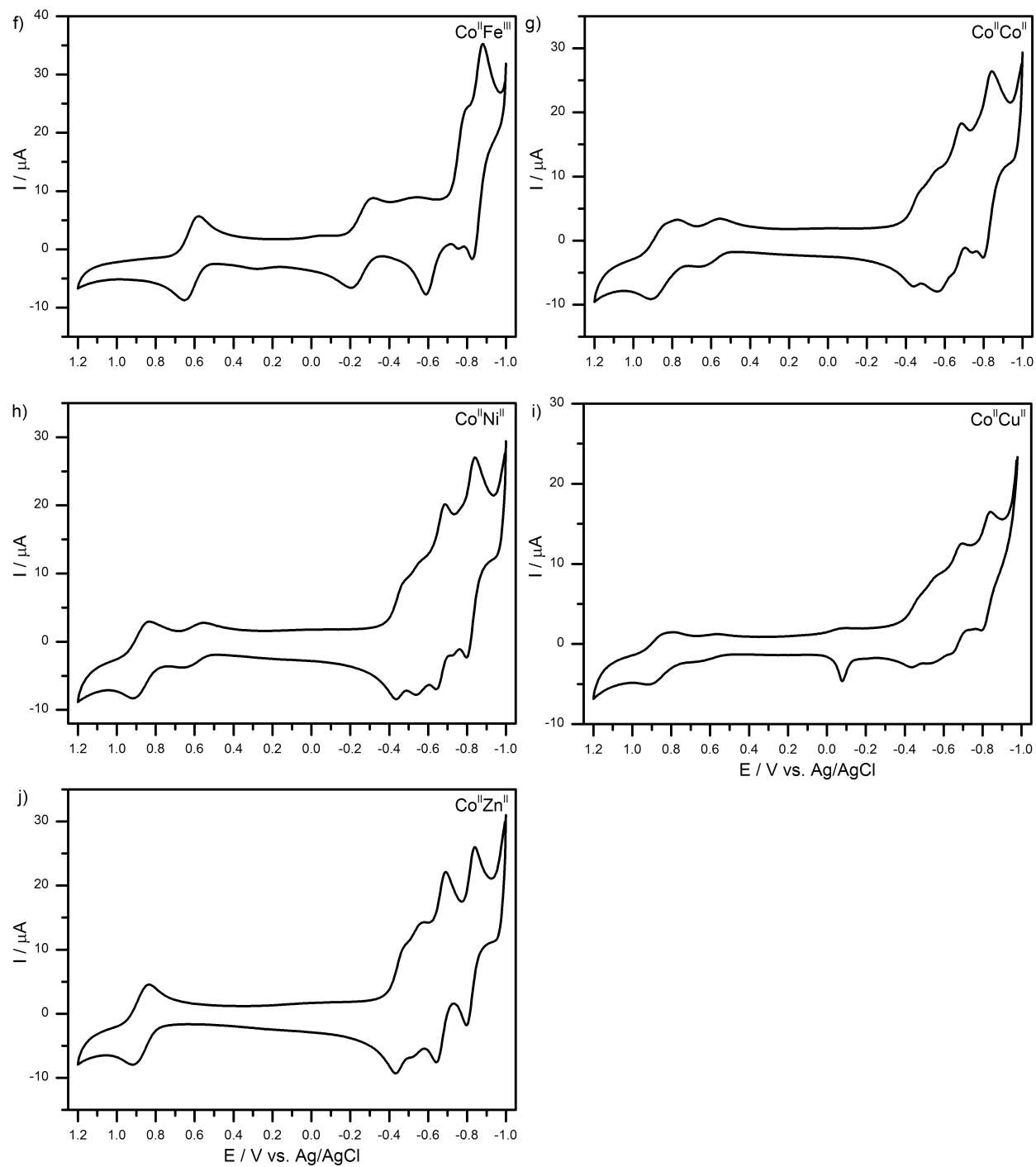


Figure S7. Full cyclic voltammograms of five TMSP derivatives. Each voltammogram, ~ 1 mM POM, was measured in 0.500 M potassium acetate buffer, pH 5, 50 mV/s scan rate.

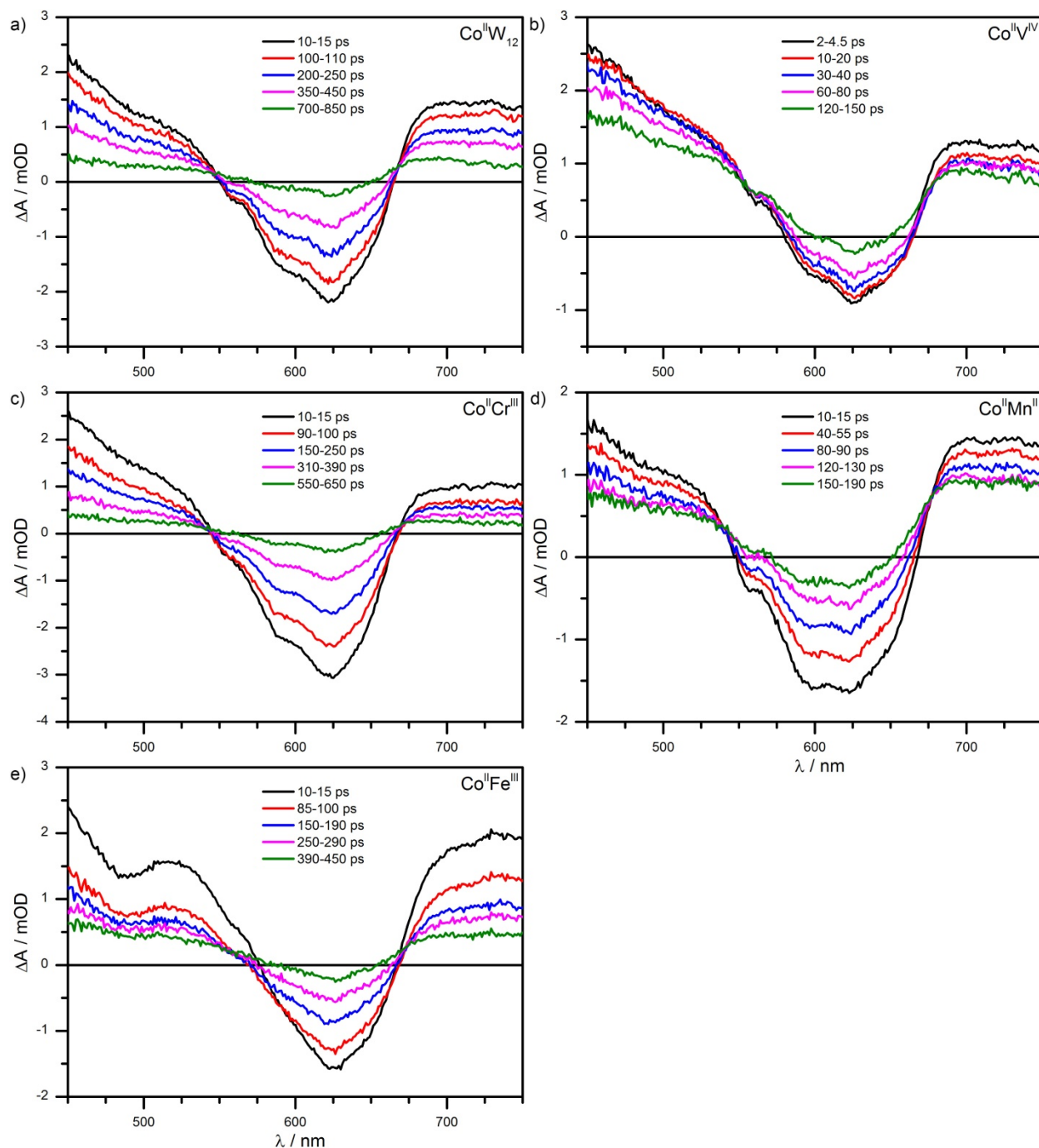


Figure S8. Transient absorption spectra of the plenary POM complex $\text{Co}^{\text{II}}\text{W}_{12}$ and four TMSP derivatives upon excitation by an ultrafast pump pulse at 400 nm. Spectral traces are the average of multiple measurements within the noted time windows. Solvent conditions (0.250 M LiAc buffer, pH 5) and pump power were kept consistent between measurements of all compounds.

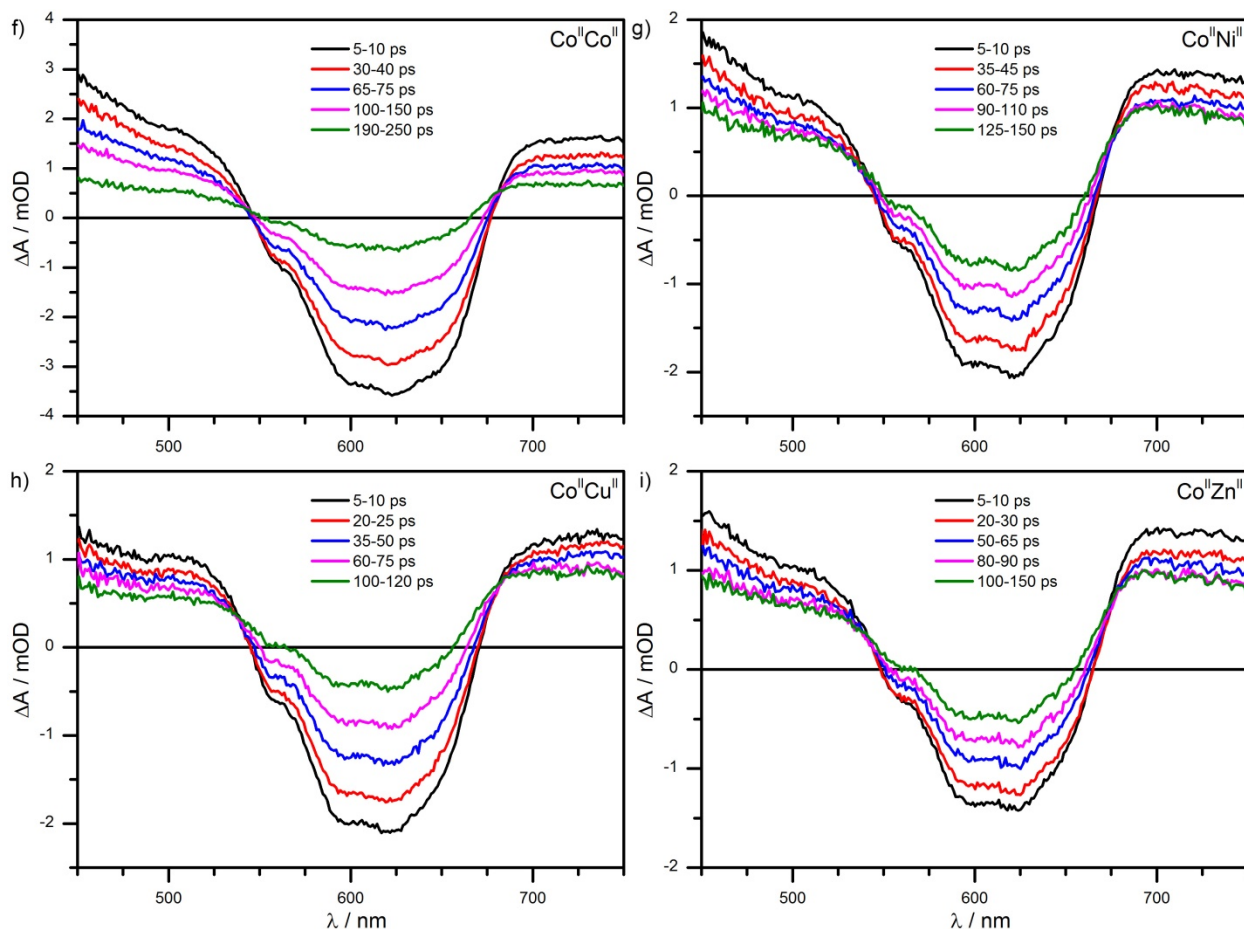


Figure S9. Transient absorption spectra of four TMSP derivatives upon excitation by an ultrafast pump pulse at 400 nm. Spectral traces are the average of multiple measurements within the noted time windows. Solvent conditions (0.250 M LiAc buffer, pH 5) and pump power were kept consistent between measurements of all compounds.

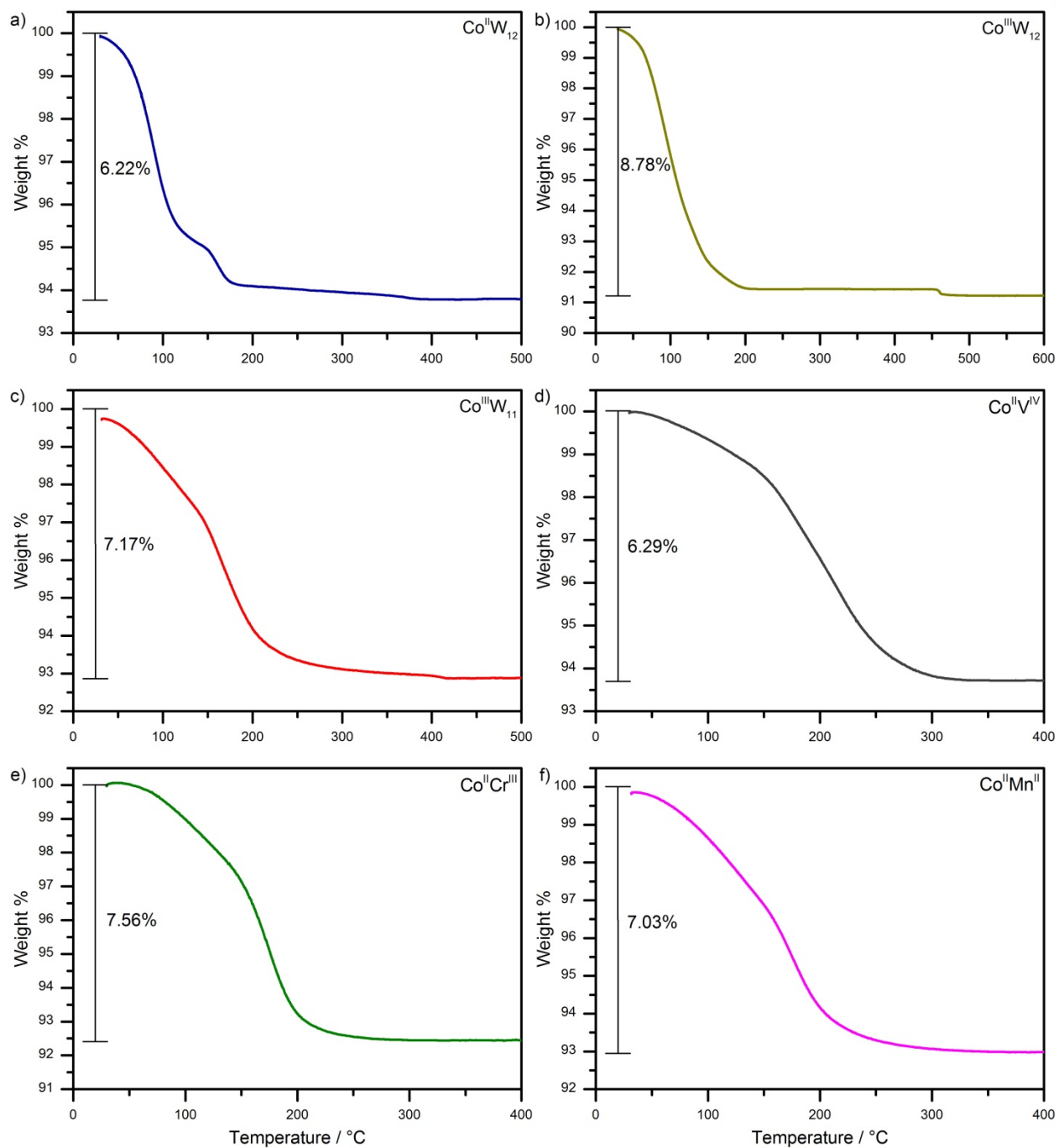


Figure S10. Thermogravimetric analyses of the plenary POMs $\text{Co}^{\text{II}}\text{W}_{12}$ and $\text{Co}^{\text{III}}\text{W}_{12}$, the lacunary TMSP-precursor $\text{Co}^{\text{III}}\text{W}_{11}$, and three TMSP derivatives. The total weight loss, attributed to water in all cases, is annotated.

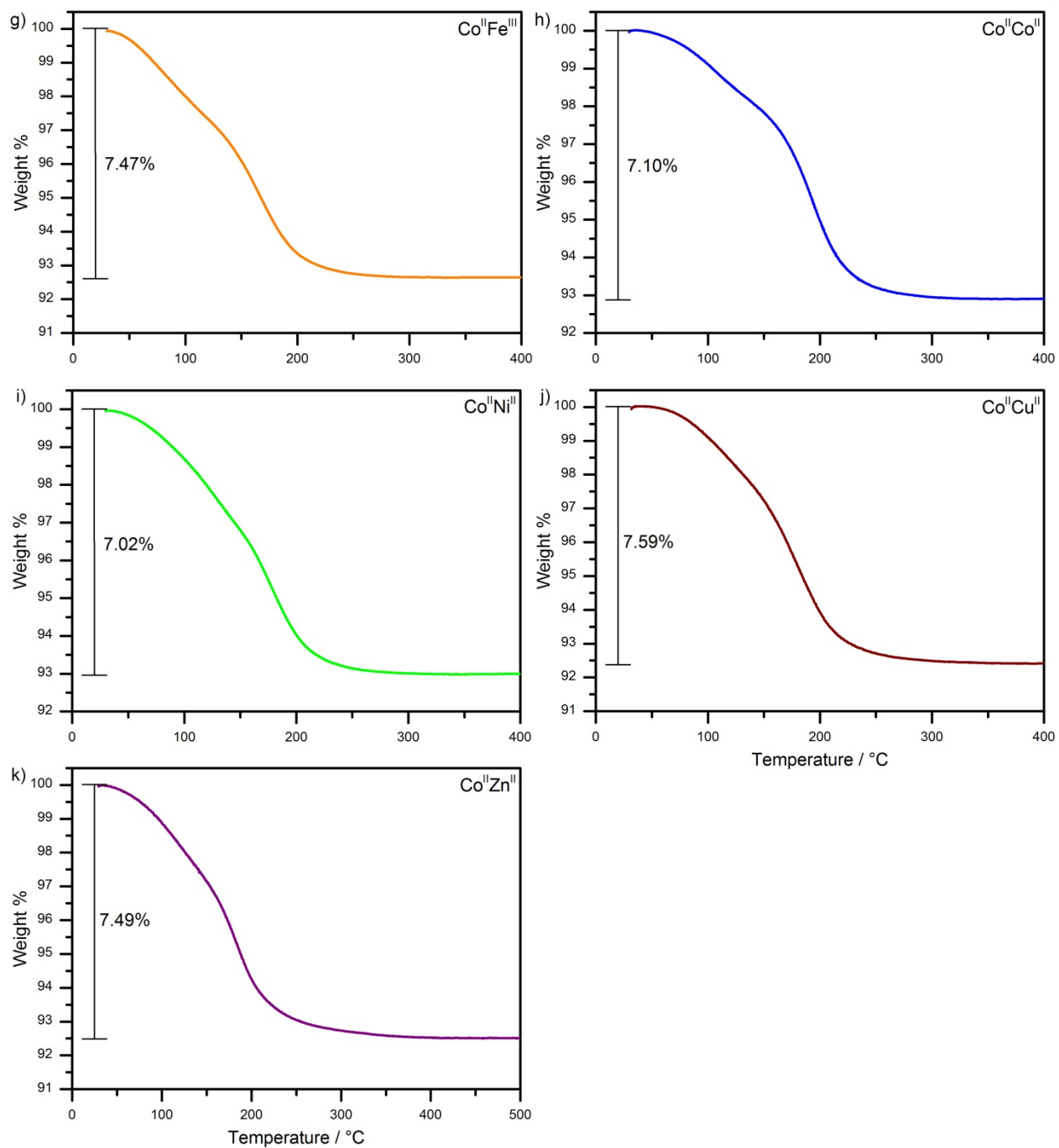


Figure S11. Thermogravimetric analyses of five TMSP derivatives. The total weight loss, attributed to water in all cases, is annotated.

Table S4. Full calculated geometries (Cartesian coordinates, in Å) for all reported TMSPs at their lower-lying electronic states

$[\text{Co}^{\text{II}}(\text{V}^{\text{IV}}\text{O})\text{W}_{11}\text{O}_{39}]^{8-}$, $^5\text{A-state}$ $E_{\text{tot}} = -3975.61782189$ a.u.				$[\text{Co}^{\text{II}}(\text{V}^{\text{IV}}\text{O})\text{W}_{11}\text{O}_{39}]^{8-}$, $^3\text{A-state}$ $E_{\text{tot}} = -3975.61780865$ a.u.			
	X	Y	Z		X	Y	Z
Co	-0.000063	0.023694	-0.160221	Co	-0.000063	0.023694	-0.160221
W	-3.541614	-0.142859	-0.116891	W	-3.541614	-0.142859	-0.116891
O	-2.883171	1.138932	-1.386962	O	-2.883171	1.138932	-1.386962
O	-5.265402	0.233157	-0.098266	O	-5.265402	0.233157	-0.098266
O	-3.592506	-1.510766	-1.511392	O	-3.592506	-1.510766	-1.511392
O	-1.566725	-1.098723	-0.166476	O	-1.566725	-1.098723	-0.166476
W	-1.883552	-2.560554	1.457764	W	-1.883552	-2.560554	1.457764
O	-1.297571	-1.15523	2.687435	O	-1.297571	-1.15523	2.687435
O	-2.476043	-3.759992	2.60883	O	-2.476043	-3.759992	2.60883
O	-3.568645	-1.56748	1.233245	O	-3.568645	-1.56748	1.233245
W	-1.855141	-2.389063	-1.890111	W	-1.855141	-2.389063	-1.890111
O	-0.002311	-2.929554	-1.710858	O	-0.002311	-2.929554	-1.710858
O	-2.486581	-3.653959	-2.954203	O	-2.486581	-3.653959	-2.954203
O	-2.192471	-3.491666	-0.168441	O	-2.192471	-3.491666	-0.168441
V	-0.001047	0.244753	-3.719292	V	-0.001047	0.244753	-3.719292
O	-1.318558	-1.081869	-3.053024	O	-1.318558	-1.081869	-3.053024
O	-1.420048	1.69318	-3.686816	O	-1.420048	1.69318	-3.686816
O	0.000044	1.185563	-1.675408	O	0.000044	1.185563	-1.675408
W	1.638832	2.508303	-2.043204	W	1.638832	2.508303	-2.043204
O	2.883844	1.137749	-1.3893	O	2.883844	1.137749	-1.3893
O	2.776568	3.795747	-2.474388	O	2.776568	3.795747	-2.474388
O	1.419393	1.692949	-3.687247	O	1.419393	1.692949	-3.687247
W	-1.640169	2.507181	-2.041988	W	-1.640169	2.507181	-2.041988
O	-1.572249	2.929189	-0.054377	O	-1.572249	2.929189	-0.054377
O	-2.775614	3.796419	-2.473685	O	-2.775614	3.796419	-2.473685
O	0.000347	3.592182	-2.213911	O	0.000347	3.592182	-2.213911
W	-0.000812	0.085201	3.38402	W	-0.000812	0.085201	3.38402
O	1.296371	-1.154879	2.684787	O	1.296371	-1.154879	2.684787
O	0.000336	-0.338382	5.099235	O	0.000336	-0.338382	5.099235
O	1.375737	1.473757	3.456216	O	1.375737	1.473757	3.456216
O	0.00038	1.088799	1.442506	O	0.00038	1.088799	1.442506
W	-1.654612	2.482832	1.765114	W	-1.654612	2.482832	1.765114
O	-2.883856	1.081124	1.219067	O	-2.883856	1.081124	1.219067
O	-2.779688	3.681576	2.412488	O	-2.779688	3.681576	2.412488
O	-1.373561	1.476027	3.456801	O	-1.373561	1.476027	3.456801
W	1.65978	2.477736	1.76418	W	1.65978	2.477736	1.76418
O	1.574204	2.926728	-0.05477	O	1.574204	2.926728	-0.05477
O	2.784723	3.676941	2.411057	O	2.784723	3.676941	2.411057
O	0.002328	3.467027	2.145278	O	0.002328	3.467027	2.145278
W	3.542554	-0.145531	-0.124091	W	3.542554	-0.145531	-0.124091
O	2.886051	1.077181	1.21704	O	2.886051	1.077181	1.21704
O	5.266273	0.230891	-0.103824	O	5.266273	0.230891	-0.103824
O	3.56987	-1.569555	1.23116	O	3.56987	-1.569555	1.23116
O	1.566058	-1.0992	-0.167711	O	1.566058	-1.0992	-0.167711
W	1.848146	-2.391896	-1.889878	W	1.848146	-2.391896	-1.889878
O	1.318024	-1.083403	-3.053831	O	1.318024	-1.083403	-3.053831
O	2.480502	-3.657734	-2.952504	O	2.480502	-3.657734	-2.952504
O	3.590622	-1.51462	-1.512963	O	3.590622	-1.51462	-1.512963
W	1.886809	-2.559034	1.458457	W	1.886809	-2.559034	1.458457
O	-0.000388	-2.991417	1.408684	O	-0.000388	-2.991417	1.408684
O	2.47522	-3.759088	2.610975	O	2.47522	-3.759088	2.610975
O	2.189379	-3.492996	-0.167034	O	2.189379	-3.492996	-0.167034

[Co^{II}(V^VO)W₁₁O₃₉]⁷⁻, ⁴A-stateE_{tot} = -3975.46054334 a.u.

	X	Y	Z
Co	-0.000489	-0.003003	-0.142712
W	-3.558586	-0.13828	-0.110918
O	-2.870912	1.069122	-1.466811
O	-5.269772	0.266511	-0.119327
O	-3.597081	-1.554239	-1.442309
O	-1.577301	-1.096413	-0.104614
W	-1.899351	-2.468646	1.579143
O	-1.307448	-0.992595	2.740316
O	-2.504504	-3.595321	2.787151
O	-3.581815	-1.465106	1.31082
W	-1.861349	-2.461028	-1.766939
O	-0.01986	-3.006265	-1.566784
O	-2.498209	-3.750942	-2.787337
O	-2.218971	-3.470854	0.000535
V	-0.00102	0.107605	-3.727131
O	-1.282826	-1.191086	-2.969457
O	-1.332043	1.374148	-3.754046
O	0.005494	1.114127	-1.678816
W	1.652898	2.372578	-2.11336
O	2.882644	1.032913	-1.469556
O	2.771354	3.557474	-2.790853
O	1.345325	1.356768	-3.754897
W	-1.625809	2.392876	-2.112462
O	-1.566885	2.961509	-0.249682
O	-2.729009	3.592868	-2.788561
O	0.020315	3.415248	-2.478306
W	0.002393	0.255888	3.351737
O	1.297296	-1.008137	2.738834
O	0.001873	-0.033629	5.088325
O	1.386678	1.675467	3.348098
O	0.007871	1.170536	1.371712
W	-1.644671	2.587322	1.638845
O	-2.87165	1.185012	1.122216
O	-2.753598	3.833639	2.196557
O	-1.362033	1.693292	3.349689
W	1.679403	2.565744	1.638148
O	1.603161	2.9406	-0.250833
O	2.804373	3.798644	2.193447
O	0.023764	3.584342	1.903625
W	3.557159	-0.18236	-0.115179
O	2.88891	1.149274	1.119634
O	5.273195	0.201335	-0.125564
O	3.564978	-1.509483	1.306877
O	1.563062	-1.115053	-0.105827
W	1.827959	-2.483717	-1.768088
O	1.264505	-1.206515	-2.970538
O	2.448428	-3.780695	-2.789552
O	3.575892	-1.599228	-1.445466
W	1.870419	-2.490764	1.577707
O	-0.017182	-2.902104	1.561405
O	2.462731	-3.625109	2.784914
O	2.17486	-3.497537	-0.001395

[Co^{II}Cr^{III}(H₂O)W₁₁O₃₉]⁷⁻, ⁵A-stateE_{tot} = -3913.02939846 a.u.

	X	Y	Z
Co	0.047977	0.001012	-0.12472
W	0.149578	-3.55167	-0.18369
O	-1.1425	-2.89596	-1.46266
O	-0.21122	-5.28915	-0.16742
O	1.553638	-3.58406	-1.5405
O	1.118655	-1.56389	-0.20967
W	2.542044	-1.88744	1.472319
O	1.107342	-1.28943	2.661911
O	3.73995	-2.49499	2.632653
O	1.542487	-3.55806	1.201676
W	2.504119	-1.87467	-1.90192
O	3.017617	-0.00322	-1.73218
O	3.764201	-2.52764	-2.97624
O	3.499749	-2.20321	-0.15614
Cr	-0.23484	-0.00108	-3.30273
O	1.1916	-1.32174	-3.08065
O	-1.61343	-1.39148	-3.70082
O	-1.13804	-0.00214	-1.65914
W	-2.55807	1.682504	-2.10652
O	-1.14622	2.894363	-1.46933
O	-3.81151	2.810136	-2.66307
O	-1.61559	1.38604	-3.70083
W	-2.54998	-1.69386	-2.10467
O	-2.96167	-1.59993	-0.16604
O	-3.80285	-2.82268	-2.66009
O	-3.54149	-0.00478	-2.31651
W	-0.14603	-0.00042	3.358725
O	1.106095	1.293191	2.659675
O	0.230776	0.001935	5.09387
O	-1.5454	1.37429	3.380885
O	-1.12928	0.001149	1.378379
W	-2.52431	-1.66688	1.688468
O	-1.10427	-2.86279	1.124258
O	-3.7387	-2.79385	2.32843
O	-1.54697	-1.36959	3.382906
W	-2.51568	1.67646	1.686476
O	-2.96052	1.597916	-0.16819
O	-3.73294	2.801696	2.324056
O	-3.50404	0.002759	2.019306
W	0.148585	3.553339	-0.20497
O	-1.10223	2.866147	1.117427
O	-0.21304	5.290626	-0.1866
O	1.539086	3.562932	1.193648
O	1.117509	1.564552	-0.2147
W	2.509031	1.861822	-1.90249
O	1.19197	1.318065	-3.08134
O	3.76829	2.516948	-2.97656
O	1.554751	3.581711	-1.54822
W	2.534905	1.900789	1.472468
O	2.958009	0.003276	1.405055
O	3.733518	2.50767	2.632312
O	3.497889	2.203163	-0.15669

[Co^{II}Cr^{III}(H₂O)W₁₁O₃₉]⁷⁻, ⁷A-stateE_{tot} = -3913.06991559 a.u.

	X	Y	Z
Co	0.027302	0.000128	-0.12573
W	0.156571	-3.550675	-0.181048
O	-1.136775	-2.895337	-1.462127
O	-0.205296	-5.288233	-0.164788
O	1.558644	-3.585938	-1.540141
O	1.122013	-1.566837	-0.209139
W	2.54308	-1.88311	1.471236
O	1.105574	-1.287019	2.662767
O	3.740668	-2.487834	2.633394
O	1.546904	-3.558488	1.204993
W	2.503784	-1.873057	-1.899345
O	3.013465	-0.000961	-1.729324
O	3.766567	-2.52338	-2.972244
O	3.504401	-2.200723	-0.154333
Cr	-0.23336	-0.002247	-3.314241
O	1.191979	-1.321748	-3.081321
O	-1.610945	-1.396645	-3.705863
O	-1.135858	-0.003905	-1.672517
W	-2.557656	1.678492	-2.109547
O	-1.146875	2.890114	-1.471406
O	-3.812895	2.805103	-2.663434
O	-1.616418	1.384953	-3.706861
W	-2.544978	-1.698422	-2.106752
O	-2.953323	-1.59778	-0.166445
O	-3.797122	-2.829497	-2.658572
O	-3.538763	-0.009988	-2.319783
W	-0.145796	0.000376	3.362992
O	1.101497	1.29509	2.660166
O	0.230559	0.003629	5.098311
O	-1.549178	1.374721	3.383612
O	-1.12678	0.000568	1.387753
W	-2.522264	-1.669171	1.691029
O	-1.100081	-2.861225	1.125741
O	-3.737307	-2.797804	2.326218
O	-1.547993	-1.370557	3.386489
W	-2.516083	1.67571	1.688096
O	-2.955852	1.589842	-0.169691
O	-3.736616	2.800189	2.320098
O	-3.502812	0.000038	2.018848
W	0.147622	3.552652	-0.207199
O	-1.103632	2.862803	1.116402
O	-0.21877	5.289321	-0.189269
O	1.535572	3.568874	1.194374
O	1.11693	1.570669	-0.214678
W	2.504926	1.862778	-1.900707
O	1.189517	1.318256	-3.08287
O	3.76541	2.51772	-2.973541
O	1.55239	3.585739	-1.550837
W	2.530202	1.905026	1.46987
O	2.954345	0.007203	1.404585
O	3.727368	2.511929	2.631246
O	3.497898	2.207907	-0.156032

[Co^{II}Cr^{III}(H₂O)W₁₁O₃₉]⁷⁻, ¹A-stateE_{tot} = -3913.07126317 a.u.

	X	Y	Z
Co	0.028912	0.000164	-0.13371
W	0.163362	-3.55055	-0.18451
O	-1.13632	-2.89725	-1.4601
O	-0.19526	-5.28881	-0.16607
O	1.561423	-3.5838	-1.54608
O	1.123638	-1.56637	-0.21303
W	2.550167	-1.87995	1.464178
O	1.116771	-1.28534	2.658127
O	3.75302	-2.48131	2.622461
O	1.558159	-3.55685	1.199347
W	2.502689	-1.86656	-1.9056
O	3.008865	0.005953	-1.73765
O	3.761188	-2.51513	-2.98458
O	3.508508	-2.19357	-0.16508
Cr	-0.24509	-0.00254	-3.30354
O	1.183407	-1.31773	-3.08053
O	-1.62175	-1.40186	-3.70082
O	-1.13994	-0.00613	-1.66587
W	-2.56791	1.677793	-2.10237
O	-1.15737	2.88801	-1.4669
O	-3.828	2.80183	-2.64969
O	-1.63205	1.385399	-3.70113
W	-2.55051	-1.70432	-2.10023
O	-2.95286	-1.60529	-0.15832
O	-3.80325	-2.83742	-2.64585
O	-3.54255	-0.01557	-2.30862
W	-0.1359	-0.00008	3.363061
O	1.107618	1.296566	2.655673
O	0.248194	0.003481	5.096613
O	-1.54014	1.37006	3.387744
O	-1.12257	-0.002	1.386959
W	-2.51195	-1.67477	1.69656
O	-1.08976	-2.86287	1.126991
O	-3.7218	-2.80588	2.337632
O	-1.53306	-1.3739	3.389917
W	-2.51444	1.668911	1.694246
O	-2.96165	1.585371	-0.16074
O	-3.734	2.790981	2.332784
O	-3.49614	-0.00786	2.029491
W	0.140813	3.552869	-0.20476
O	-1.10574	2.859822	1.120028
O	-0.22933	5.288726	-0.18514
O	1.533152	3.571456	1.190946
O	1.112653	1.574153	-0.21785
W	2.495171	1.86954	-1.9067
O	1.175479	1.320154	-3.08167
O	3.748923	2.527345	-2.9857
O	1.540302	3.590808	-1.55453
W	2.53194	1.907974	1.463374
O	2.958255	0.012259	1.394037
O	3.731657	2.516724	2.620985
O	3.493241	2.215034	-0.16645

$[\text{Co}^{\text{III}}\text{Cr}^{\text{III}}(\text{H}_2\text{O})\text{W}_{11}\text{O}_{39}]^{6-}$, $^8\text{A-state}$
 $E_{\text{tot}} = -3913.45159928$ a.u.

	X	Y	Z
Co	0.03758	-0.018921	-0.126692
W	0.165411	-3.578944	-0.121682
O	-1.129688	-2.973386	-1.405759
O	-0.162327	-5.309543	-0.054202
O	1.578473	-3.56977	-1.451742
O	1.056484	-1.506827	-0.219832
W	2.561939	-1.827599	1.538004
O	1.126738	-1.210635	2.702721
O	3.767931	-2.390066	2.690475
O	1.558484	-3.470485	1.256029
W	2.537671	-1.887091	-1.891267
O	3.016465	-0.014728	-1.747909
O	3.800693	-2.546883	-2.935459
O	3.463122	-2.144712	-0.113911
Cr	-0.213207	-0.084216	-3.325906
O	1.22003	-1.384004	-3.08616
O	-1.588512	-1.485003	-3.656711
O	-1.064272	-0.083787	-1.64012
W	-2.571675	1.625554	-2.141184
O	-1.179291	2.861106	-1.519818
O	-3.821657	2.719133	-2.729149
O	-1.605871	1.27657	-3.701012
W	-2.534403	-1.779685	-2.073088
O	-2.929001	-1.634268	-0.134082
O	-3.777847	-2.91303	-2.602177
O	-3.496606	-0.085667	-2.2929
W	-0.131558	0.083587	3.387001
O	1.117728	1.371881	2.682466
O	0.2301	0.106961	5.112844
O	-1.546752	1.420759	3.329934
O	-1.057244	0.069061	1.328671
W	-2.51173	-1.678537	1.719254
O	-1.080505	-2.862963	1.179625
O	-3.710068	-2.79535	2.366287
O	-1.515812	-1.290674	3.365309
W	-2.540336	1.71402	1.649038
O	-2.967257	1.576997	-0.199576
O	-3.77483	2.816042	2.259939
O	-3.448849	0.009678	1.997546
W	0.095591	3.565975	-0.27037
O	-1.151537	2.920482	1.070211
O	-0.262571	5.292429	-0.304052
O	1.495812	3.576818	1.111636
O	1.019007	1.524612	-0.198539
W	2.501978	1.845927	-1.960674
O	1.177134	1.251338	-3.10604
O	3.734432	2.471206	-3.058255
O	1.508058	3.516696	-1.600958
W	2.515591	1.954101	1.456509
O	2.94701	0.063526	1.413424
O	3.7267	2.59529	2.56568
O	3.420447	2.202616	-0.215883

$[\text{Co}^{\text{III}}\text{Cr}^{\text{III}}(\text{H}_2\text{O})\text{W}_{11}\text{O}_{39}]^{6-}$, $^2\text{A-state}$
 $E_{\text{tot}} = -3913.43787315$ a.u.

	X	Y	Z
Co	0.020395	0.04421	-0.11128
W	-0.18381	-3.53417	-0.4336
O	-1.38296	-2.65659	-1.6412
O	-0.66094	-5.22299	-0.57865
O	1.229886	-3.47076	-1.74769
O	0.952073	-1.48979	-0.22991
W	2.386673	-2.20112	1.36797
O	1.034734	-1.60476	2.627868
O	3.536224	-3.0263	2.421847
O	1.219013	-3.69842	0.917047
W	2.378916	-1.89701	-2.05201
O	3.081174	-0.11082	-1.78965
O	3.533502	-2.59182	-3.19221
O	3.252866	-2.42681	-0.33151
Cr	-0.21031	0.28685	-3.28007
O	1.091629	-1.14561	-3.14239
O	-1.69066	-0.9571	-3.74749
O	-1.08828	0.262171	-1.62193
W	-2.41009	2.068917	-1.98246
O	-0.90697	3.099038	-1.25855
O	-3.5605	3.32518	-2.44264
O	-1.48354	1.794917	-3.5794
W	-2.68759	-1.3052	-2.20911
O	-3.10263	-1.35149	-0.26322
O	-4.00422	-2.28343	-2.85406
O	-3.50114	0.468163	-2.28438
W	-0.14326	-0.2655	3.364
O	1.199535	0.957103	2.708162
O	0.215262	-0.3722	5.086835
O	-1.41912	1.205969	3.400153
O	-1.09449	-0.11157	1.3052
W	-2.68204	-1.60981	1.571798
O	-1.38653	-2.89451	0.935281
O	-3.99342	-2.64476	2.143947
O	-1.65435	-1.48692	3.263532
W	-2.39773	1.757657	1.795315
O	-2.82821	1.852314	-0.04941
O	-3.48744	2.94067	2.512851
O	-3.46142	0.137972	2.010816
W	0.426097	3.547502	0.048232
O	-0.86216	2.82404	1.302685
O	0.20558	5.28524	0.218292
O	1.793987	3.248027	1.401308
O	1.260732	1.348887	-0.17129
W	2.695467	1.785739	-1.80327
O	1.337093	1.449527	-3.01024
O	3.993054	2.441527	-2.81079
O	1.834637	3.500848	-1.26761
W	2.702962	1.532776	1.602543
O	3.000782	-0.37141	1.443201
O	3.912414	1.985814	2.801786
O	3.655129	1.892842	-0.01272

$[\text{Co}^{\text{II}}\text{Mn}^{\text{II}}(\text{H}_2\text{O})\text{W}_{11}\text{O}_{39}]^{8-}$, ${}^7\text{A}$ -state $E_{\text{tot}} = -4006.62134298$ a.u.

	X	Y	Z
Co	0.01717	0.003892	-0.12124
W	3.323971	1.219737	-0.670158
O	2.843351	-0.160685	-1.925777
O	5.069146	1.409746	-0.958983
O	2.700663	2.579713	-1.949512
O	1.165947	1.533308	-0.338857
W	1.312565	2.969948	1.351625
O	1.389757	1.391546	2.522715
O	1.732331	4.274091	2.488402
O	3.150067	2.53454	0.767068
W	0.766322	2.935301	-1.985992
O	-1.106837	2.840094	-1.455415
O	0.809211	4.393257	-2.999821
O	1.056125	3.99259	-0.229081
Mn	-0.4997	-0.112905	-3.478317
O	0.393025	1.577602	-3.191622
O	-6.125581	0.08006	-2.519405
O	1.144284	-0.989931	-3.963945
O	0.131124	-1.109414	-1.66455
W	-1.114986	-2.832133	-1.975564
O	-2.575136	-1.912101	-1.030342
O	-1.904955	-4.356438	-2.440678
O	-1.396466	-1.813514	-3.534708
W	1.976566	-1.819847	-2.492697
O	2.413774	-2.326722	-0.58217
O	3.31638	-2.655242	-3.314388
O	0.705316	-3.329131	-2.524786
W	0.670134	-0.206525	3.324607
O	-1.040795	0.604231	2.924015
O	0.85132	0.118246	5.066775
O	-0.207683	-1.958222	3.471731
O	0.623237	-1.106699	1.321
W	2.657791	-1.941819	1.250292
O	3.280945	-0.20529	0.628458
O	4.186297	-2.771044	1.634907
O	2.376408	-1.12532	3.043497
W	-0.482782	-2.952161	1.778214
O	-0.613872	-3.298563	-0.078152
O	-1.067772	-4.466392	2.509674
O	1.435755	-3.388902	1.783758
W	-3.357486	-0.945068	0.42747
O	-2.136958	-1.952758	1.526453
O	-4.884725	-1.808845	0.69254
O	-3.561791	0.365853	1.884013
O	-1.80973	0.567969	0.139856
W	-2.732345	1.816114	-1.384992
O	-2.064987	0.777774	-2.770385
O	-3.898085	2.875627	-2.198687
O	-4.072101	0.403567	-0.846571
W	-2.242159	1.813756	1.958924
O	-0.591547	2.789677	1.626438
O	-2.959279	2.74975	3.290605
O	-3.070617	2.659124	0.471826
H	-5.516529	-0.010048	-3.282762
H	-5.480686	0.221901	-1.74096

 $[\text{Co}^{\text{II}}\text{Mn}^{\text{II}}(\text{H}_2\text{O})\text{W}_{11}\text{O}_{39}]^{8-}$, ${}^1\text{A}$ -state $E_{\text{tot}} = -4006.62158265$ a.u.

	X	Y	Z
Co	0.019322	-0.00119	-0.11696
W	3.329252	1.207521	-0.66955
O	2.845547	-0.17073	-1.92587
O	5.075532	1.3908	-0.956
O	2.71205	2.569623	-1.94725
O	1.170976	1.528063	-0.33938
W	1.3244	2.96468	1.352324
O	1.394334	1.384631	2.52468
O	1.748134	4.265989	2.49075
O	3.15936	2.521607	0.769433
W	0.777304	2.930713	-1.9853
O	-1.09518	2.84372	-1.4554
O	0.827424	4.389778	-2.99745
O	1.071815	3.988522	-0.22659
Mn	-0.49421	-0.11519	-3.47814
O	0.400485	1.576923	-3.19304
O	-6.13033	0.107891	-2.51355
O	1.147694	-0.99557	-3.96807
O	0.122108	-1.09387	-1.67297
W	-1.12851	-2.82443	-1.97749
O	-2.58402	-1.90143	-1.03259
O	-1.92169	-4.34734	-2.44007
O	-1.40517	-1.80935	-3.53935
W	1.971836	-1.82604	-2.49294
O	2.399359	-2.33156	-0.58111
O	3.309861	-2.66905	-3.30884
O	0.691652	-3.3253	-2.5233
W	0.666888	-0.20921	3.325053
O	-1.04006	0.606729	2.924506
O	0.849124	0.111591	5.067922
O	-0.21735	-1.96025	3.471202
O	0.618923	-1.10886	1.324832
W	2.650222	-1.951	1.25222
O	3.279956	-0.2176	0.629907
O	4.175339	-2.78801	1.633131
O	2.37141	-1.1364	3.044851
W	-0.49415	-2.95114	1.777902
O	-0.62455	-3.28917	-0.08054
O	-1.08591	-4.46518	2.504105
O	1.422108	-3.39499	1.783176
W	-3.3617	-0.93199	0.427908
O	-2.14573	-1.9454	1.525298
O	-4.89231	-1.78991	0.692175
O	-3.56101	0.37954	1.883016
O	-1.80695	0.574217	0.138464
W	-2.72394	1.823698	-1.38711
O	-2.05902	0.784296	-2.77126
O	-3.88569	2.887445	-2.20133
O	-4.07072	0.418715	-0.84732
W	-2.23562	1.823237	1.957201
O	-0.58073	2.79068	1.627607
O	-2.94943	2.761318	3.289101
O	-3.06017	2.670821	0.470862
H	-5.52401	0.015496	-3.27878
H	-5.48221	0.245461	-1.73683

[Co^{II}Mn^{II}(H₂O)W₁₁O₃₉]⁸⁻, ⁹A-stateE_{tot} = -4006.62070876 a.u.

	X	Y	Z
Co	0.016931	0.004776	-0.121295
W	3.323204	1.2225	-0.669253
O	2.844441	-0.159161	-1.924538
O	5.068318	1.413605	-0.957083
O	2.699537	2.581464	-1.94929
O	1.164709	1.534466	-0.338996
W	1.309164	2.971879	1.350548
O	1.387009	1.394251	2.522601
O	1.727083	4.277005	2.486759
O	3.147341	2.53777	0.767313
W	0.764826	2.935099	-1.987229
O	-1.10875	2.838173	-1.458395
O	0.806559	4.392101	-3.002279
O	1.05246	3.993522	-0.230829
Mn	-0.496223	-0.117123	-3.474065
O	0.394663	1.575173	-3.191576
O	-6.128413	0.076325	-2.518518
O	1.147358	-0.992275	-3.963261
O	0.132924	-1.108954	-1.664569
W	-1.111439	-2.834955	-1.974565
O	-2.572479	-1.914781	-1.031346
O	-1.899649	-4.360037	-2.438747
O	-1.391501	-1.817122	-3.535113
W	1.980551	-1.820011	-2.490729
O	2.415829	-2.324497	-0.579786
O	3.321849	-2.65469	-3.30994
O	0.709871	-3.329485	-2.521765
W	0.668345	-0.203899	3.324858
O	-1.043123	0.604904	2.923146
O	0.848314	0.121844	5.066896
O	-0.207976	-1.956429	3.472303
O	0.623316	-1.104996	1.321509
W	2.6588	-1.938452	1.252748
O	3.280646	-0.201849	0.630088
O	4.187846	-2.766048	1.638403
O	2.375593	-1.121453	3.045174
W	-0.481177	-2.951362	1.779407
O	-0.6107	-3.298715	-0.077078
O	-1.06506	-4.465849	2.51103
O	1.437742	-3.386298	1.786108
W	-3.356936	-0.947711	0.425844
O	-2.136275	-1.954015	1.525921
O	-4.883376	-1.812823	0.690355
O	-3.563283	0.363556	1.881806
O	-1.810519	0.566395	0.138873
W	-2.733661	1.81306	-1.387514
O	-2.064497	0.772891	-2.770844
O	-3.899586	2.870792	-2.202984
O	-4.072319	0.399848	-0.848738
W	-2.244926	1.812723	1.956573
O	-0.594992	2.789762	1.624356
O	-2.963669	2.748899	3.287145
O	-3.073238	2.656624	0.468392
H	-5.520859	-0.014736	-3.282935
H	-5.482233	0.218371	-1.741372

[Co^{III}Mn^{II}(H₂O)W₁₁O₃₉]⁷⁻, ⁸A-stateE_{tot} = -4007.12690417 a.u.

	X	Y	Z
Co	0.003538	0.012264	-0.08723
W	3.469148	0.409093	-0.74085
O	2.669118	-0.87114	-1.94998
O	5.198544	0.182175	-1.0649
O	3.154675	1.842765	-2.06362
O	1.455142	1.227272	-0.39667
W	1.96135	2.636878	1.243375
O	1.710573	1.130509	2.471342
O	2.688618	3.853463	2.309822
O	3.634776	1.776842	0.644325
W	1.373443	2.662472	-2.07204
O	-0.4856	3.019806	-1.55012
O	1.718007	4.00119	-3.18836
O	1.914123	3.650319	-0.3871
Mn	-0.58423	-0.08882	-3.27574
O	0.661475	1.359758	-3.19728
O	-3.53933	-0.09125	-4.92572
O	0.786568	-1.33322	-3.90141
O	-0.17878	-1.18612	-1.57007
W	-1.78061	-2.6034	-1.80024
O	-2.98075	-1.30311	-0.92345
O	-2.92122	-3.88741	-2.25134
O	-1.89134	-1.53676	-3.40868
W	1.455507	-2.31318	-2.42937
O	1.785193	-2.84769	-0.53146
O	2.533779	-3.446	-3.27383
O	-0.15053	-3.48295	-2.41413
W	0.670636	-0.23977	3.337422
O	-0.82304	0.927675	2.926738
O	0.952098	0.091657	5.058001
O	-0.59809	-1.73366	3.564081
O	0.356748	-1.16799	1.372239
W	2.128655	-2.46347	1.29855
O	3.11493	-0.92794	0.597488
O	3.434254	-3.60016	1.688863
O	2.097251	-1.53958	3.06263
W	-1.15251	-2.66505	1.926108
O	-1.38827	-3.08827	0.05706
O	-2.05492	-3.97606	2.710089
O	0.619923	-3.55393	1.887559
W	-3.50582	-0.10446	0.466398
O	-2.50348	-1.34027	1.613374
O	-5.17914	-0.59626	0.786343
O	-3.35624	1.236785	1.913215
O	-1.62411	0.998415	0.148659
W	-2.29915	2.419053	-1.38669
O	-1.93776	1.179677	-2.75867
O	-3.22041	3.666141	-2.25324
O	-3.86749	1.329335	-0.78881
W	-1.74293	2.328052	1.933845
O	0.079037	2.90593	1.53664
O	-2.20193	3.452008	3.226477
O	-2.39108	3.323079	0.418884
H	-3.03709	-0.83606	-4.46162
H	-3.37522	0.664645	-4.31175

[Co^{III}Mn^{II}(H₂O)W₁₁O₃₉]⁷⁻, ²A-stateE_{tot} = -4007.12739418 a.u.

	X	Y	Z
Co	0.005525	0.006515	-0.084577
W	3.482736	0.284465	-0.735439
O	2.640124	-0.966951	-1.948267
O	5.203536	-0.006091	-1.056027
O	3.223561	1.726972	-2.058955
O	1.498172	1.173874	-0.395616
W	2.053521	2.564477	1.245613
O	1.748173	1.068165	2.475744
O	2.82391	3.753073	2.313142
O	3.695797	1.644007	0.649388
W	1.471865	2.610085	-2.070612
O	-0.373029	3.035375	-1.551602
O	1.866806	3.933951	-3.187891
O	2.046493	3.578391	-0.384403
Mn	-0.583055	-0.071246	-3.272645
O	0.714929	1.333469	-3.194933
O	-3.537489	0.034707	-4.930782
O	0.74621	-1.363146	-3.905882
O	-0.221113	-1.163212	-1.576975
W	-1.873337	-2.535276	-1.802912
O	-3.026614	-1.193062	-0.92847
O	-3.057367	-3.779149	-2.252489
O	-1.944139	-1.468914	-3.413844
W	1.375935	-2.361426	-2.431344
O	1.678944	-2.906957	-0.529909
O	2.413138	-3.535931	-3.269495
O	-0.273103	-3.468022	-2.413223
W	0.659088	-0.26464	3.338729
O	-0.791892	0.954944	2.925729
O	0.948313	0.054105	5.060334
O	-0.665878	-1.712903	3.56369
O	0.312958	-1.179285	1.376144
W	2.034914	-2.539093	1.299932
O	3.076903	-1.0398	0.601289
O	3.296975	-3.723352	1.691727
O	2.036843	-1.615716	3.065762
W	-1.251827	-2.621137	1.926313
O	-1.496664	-3.030632	0.053533
O	-2.203564	-3.900341	2.704237
O	0.48675	-3.57375	1.887915
W	-3.508648	0.023546	0.461873
O	-2.554083	-1.249271	1.609701
O	-5.198649	-0.407236	0.779911
O	-3.311756	1.357178	1.909791
O	-1.586608	1.055184	0.145624
W	-2.206911	2.499178	-1.388485
O	-1.891019	1.247206	-2.759454
O	-3.08257	3.778135	-2.255951
O	-3.817109	1.469859	-0.79171
W	-1.659641	2.387788	1.931833
O	0.182865	2.900548	1.537841
O	-2.079294	3.527102	3.224235
O	-2.268569	3.407191	0.417101
H	-3.061741	-0.727026	-4.465546
H	-3.347528	0.785035	-4.317512

[Co^{III}Fe^{II}(H₂O)W₁₁O₃₉]⁷⁻, ⁹A-stateE_{tot} = -4028.68168 a.u.

	X	Y	Z
Co	-0.024376	0.013148	-0.149747
W	-0.132819	-3.471798	-0.816362
O	-1.350322	-2.493933	-1.924776
O	-0.606457	-5.146798	-1.135309
O	1.308664	-3.319845	-2.121295
O	0.987735	-1.504177	-0.460175
W	2.389999	-2.344992	1.156781
O	0.989694	-1.890191	2.435533
O	3.513053	-3.269633	2.168545
O	1.246602	-3.802949	0.533902
W	2.428024	-1.691303	-2.209541
O	3.059066	0.087147	-1.69577
O	3.696064	-2.261673	-3.315082
O	3.311181	-2.391961	-0.505172
Fe	-0.091205	0.624566	-3.245047
O	1.240144	-0.876226	-3.333207
O	0.250923	3.538322	-4.874666
O	-1.758571	-0.643093	-3.87711
O	-1.222736	0.354778	-1.515795
W	-2.449071	2.200258	-1.698028
O	-0.923965	3.145845	-0.824094
O	-3.628209	3.502896	-1.944501
O	-1.518719	2.259167	-3.297929
W	-2.674509	-1.093978	-2.368236
O	-3.118634	-1.375877	-0.390068
O	-4.036747	-2.020346	-3.036407
O	-3.547395	0.679358	-2.231316
W	-0.178531	-0.676625	3.374085
O	1.170583	0.629218	2.920613
O	0.184751	-1.031075	5.070924
O	-1.458983	0.764546	3.606528
O	-1.120993	-0.193369	1.322725
W	-2.687867	-1.809751	1.376879
O	-1.33104	-2.970674	0.614449
O	-3.966223	-2.951276	1.834144
O	-1.65801	-1.88035	3.087437
W	-2.419439	1.498977	2.036808
O	-2.873636	1.809619	0.230092
O	-3.540203	2.558499	2.912103
O	-3.485604	-0.15502	2.055011
W	0.3917	3.472436	0.51329
O	-0.909853	2.646916	1.707728
O	0.16464	5.191169	0.863606
O	1.749797	3.0659	1.876076
O	1.207168	1.36913	0.0831
W	2.724113	1.974334	-1.491567
O	1.471088	1.895083	-2.840068
O	4.107144	2.730264	-2.307394
O	1.838283	3.609482	-0.765574
W	2.655346	1.344877	1.88323
O	2.963086	-0.527515	1.470556
O	3.862342	1.648931	3.14394
O	3.629457	1.871563	0.340324
H	-0.574629	3.210266	-4.402435
H	0.968801	3.201031	-4.279402

[Co^{III}Fe^{III}(H₂O)W₁₁O₃₉]⁶⁻, ¹⁰A-stateE_{tot} = -4028.522199 a.u.

	X	Y	Z
Co	-0.008418	-0.024987	-0.126524
W	-3.51516	0.000772	-0.731294
O	-2.635261	1.2659	-1.873001
O	-5.201193	0.410213	-0.978818
O	-3.336842	-1.403611	-2.065872
O	-1.522588	-0.970146	-0.457165
W	-2.220322	-2.474468	1.17443
O	-1.795644	-1.093301	2.48068
O	-3.024744	-3.656722	2.183045
O	-3.745382	-1.406647	0.617099
W	-1.644923	-2.413253	-2.189375
O	0.150371	-2.975637	-1.720123
O	-2.140438	-3.654132	-3.325583
O	-2.257573	-3.358181	-0.513075
Fe	0.54124	0.212416	-3.365014
O	-0.887029	-1.12471	-3.275774
O	3.764397	-0.087857	-4.610347
O	-0.761604	1.699067	-3.831142
O	0.252947	1.095574	-1.588725
W	2.058322	2.50156	-1.707457
O	3.109885	1.053812	-0.892616
O	3.291746	3.712164	-1.990694
O	2.046154	1.594229	-3.342416
W	-1.269609	2.601689	-2.292404
O	-1.469598	2.994088	-0.346437
O	-2.238314	3.913347	-2.93853
O	0.468671	3.51376	-2.180813
W	-0.587855	0.105407	3.376961
O	0.762012	-1.192713	2.928058
O	-0.89357	-0.2662	5.063481
O	0.807877	1.453069	3.606447
O	-0.167709	1.023458	1.3756
W	-1.875203	2.564779	1.447226
O	-3.022182	1.200884	0.696437
O	-3.036521	3.801733	1.880865
O	-1.865586	1.549636	3.131827
W	1.444485	2.429214	2.025161
O	1.663397	2.878697	0.19287
O	2.467118	3.604185	2.831527
O	-0.242188	3.426407	2.064084
W	3.504538	-0.254488	0.443865
O	2.694672	1.006269	1.671748
O	5.21008	0.022801	0.738594
O	3.201887	-1.6594	1.790375
O	1.460196	-1.080684	0.121029
W	2.02858	-2.560764	-1.558858
O	1.767944	-1.216489	-2.817181
O	2.775029	-3.832489	-2.503908
O	3.65083	-1.658773	-0.889789
W	1.49763	-2.59523	1.804211
O	-0.36423	-2.948102	1.403313
O	1.851457	-3.82995	2.996208
O	2.012018	-3.513904	0.203188
H	3.280905	0.705194	-4.255801
H	3.354526	-0.856749	-4.155872

[Co^{II}Co^{II}(H₂O)W₁₁O₃₉]⁸⁻, ⁷A-stateE_{tot} = -4047.75595145 a.u.

	X	Y	Z
Co	-0.023375	0.005539	-0.127111
W	0.06009	-3.457862	-0.828624
O	-1.212748	-2.529622	-1.945736
O	-0.333195	-5.164495	-1.170955
O	1.476043	-3.275794	-2.185645
O	1.077857	-1.542652	-0.491577
W	2.509261	-2.233528	1.109455
O	1.083332	-1.860772	2.401162
O	3.683806	-3.10307	2.132945
O	1.459582	-3.790096	0.511341
W	2.461318	-1.556128	-2.219994
O	2.9953	-2.50103	-1.665449
O	3.77385	-2.03881	-3.337697
O	3.45843	-2.241326	-0.534635
Co	-0.174825	0.655072	-3.250134
O	1.244119	-0.780671	-3.332634
O	0.035081	3.569977	-4.854835
O	-1.749948	-0.6853	-3.925885
O	-1.264329	0.325938	-1.576065
W	-2.539192	2.068614	-1.678496
O	-1.074082	3.095355	-0.796785
O	-3.810593	3.309109	-1.879972
O	-1.667292	2.236134	-3.315539
W	-2.585419	-1.185172	-2.374973
O	-3.022449	-1.507391	-0.379174
O	-3.928203	-2.175863	-3.025798
O	-3.608045	0.522723	-2.22629
W	-0.145341	-0.716226	3.356737
O	1.133993	0.667195	2.902831
O	0.254375	-1.063931	5.062351
O	-1.493965	0.669141	3.670473
O	-1.129333	-0.283063	1.423687
W	-2.57927	-1.934895	1.384106
O	-1.165224	-3.032485	0.599415
O	-3.804249	-3.156317	1.831261
O	-1.562293	-2.021263	3.120797
W	-2.469773	1.336303	2.068445
O	-2.934829	1.635978	0.262053
O	-3.64965	2.340594	2.956935
O	-3.502152	-0.353136	2.092792
W	0.234275	3.468559	0.547207
O	-1.022705	2.573622	1.741033
O	-0.077976	5.184959	0.917235
O	1.621534	3.172921	1.928675
O	1.155802	1.520078	0.111307
W	2.574216	2.122546	-1.466326
O	1.336934	1.985247	-2.825668
O	3.936638	2.943624	-2.282779
O	1.661535	3.755565	-0.752716
W	2.585082	1.474249	1.87251
O	2.974705	-0.385748	1.433593
O	3.782863	1.806878	3.151638
O	3.563328	2.067138	0.358527
H	-0.770629	3.187946	-4.369905
H	0.766933	3.252924	-4.261624

$[\text{Co}^{\text{II}}\text{Co}^{\text{II}}(\text{H}_2\text{O})\text{W}_{11}\text{O}_{39}]^{8-}$, ¹A-state $E_{\text{tot}} = -4047.75615006$ a.u.

	X	Y	Z
Co	-0.02697	0.005298	-0.12478
W	0.069531	-3.45905	-0.82052
O	-1.20219	-2.53629	-1.94511
O	-0.31778	-5.16721	-1.16285
O	1.489497	-3.27736	-2.17767
O	1.079972	-1.54141	-0.48919
W	2.512192	-2.22405	1.117301
O	1.081993	-1.85516	2.406413
O	3.687648	-3.08832	2.14403
O	1.46822	-3.78554	0.520678
W	2.468668	-1.55743	-2.21483
O	2.997667	0.253919	-1.65986
O	3.785405	-2.03584	-3.32962
O	3.464087	-2.23259	-0.52501
Co	-0.17147	0.649773	-3.24934
O	1.253613	-0.78425	-3.33018
O	0.038489	3.562834	-4.8602
O	-1.74059	-0.69687	-3.92939
O	-1.25329	0.322228	-1.58221
W	-2.5409	2.061396	-1.68695
O	-1.08055	3.093829	-0.80363
O	-3.81625	3.297173	-1.89113
O	-1.66734	2.23103	-3.3224
W	-2.57607	-1.19692	-2.37877
O	-3.01437	-1.51357	-0.38308
O	-3.91572	-2.19145	-3.02963
O	-3.60062	0.510081	-2.23302
W	-0.15026	-0.71174	3.357489
O	1.12565	0.673898	2.906335
O	0.244193	-1.05773	5.064775
O	-1.50433	0.670683	3.667018
O	-1.13039	-0.28383	1.424186
W	-2.57924	-1.93817	1.383528
O	-1.15991	-3.03574	0.60186
O	-3.80357	-3.16166	1.826516
O	-1.56545	-2.0213	3.119709
W	-2.47516	1.335271	2.061699
O	-2.93657	1.627553	0.252617
O	-3.66104	2.337791	2.944111
O	-3.50545	-0.35798	2.085588
W	0.226118	3.471724	0.54002
O	-1.03182	2.573933	1.734919
O	-0.09189	5.187321	0.9092
O	1.60912	3.18005	1.928271
O	1.151451	1.52315	0.110726
W	2.573037	2.123033	-1.46485
O	1.338371	1.986526	-2.82593
O	3.935114	2.947468	-2.2786
O	1.65446	3.758915	-0.75385
W	2.576401	1.48503	1.875777
O	2.970592	-0.37556	1.440389
O	3.770389	1.821277	3.157462
O	3.557649	2.076278	0.363922
H	-0.76784	3.18121	-4.37597
H	0.769629	3.247611	-4.26491

 $[\text{Co}^{\text{III}}\text{Co}^{\text{II}}(\text{H}_2\text{O})\text{W}_{11}\text{O}_{39}]^{7-}$, ⁸A-state $E_{\text{tot}} = -4048.23100993$ a.u.

	X	Y	Z
Co	-0.024788	0.007571	-0.131209
W	0.052282	-3.475815	-0.834062
O	-1.212752	-2.546774	-1.940672
O	-0.340308	-5.169296	-1.165303
O	1.473091	-3.234686	-2.136571
O	1.066567	-1.44715	-0.459183
W	2.513635	-2.227265	1.14219
O	1.088861	-1.851413	2.424978
O	3.680407	-3.102018	2.149331
O	1.442028	-3.740844	0.514972
W	2.499603	-1.536972	-2.219292
O	3.05376	0.255663	-1.683629
O	3.784107	-2.038231	-3.340384
O	3.428975	-2.216891	-0.51806
Co	-0.157774	0.648458	-3.25925
O	1.264025	-0.772943	-3.314294
O	0.067984	3.529205	-4.873021
O	-1.704791	-0.674102	-3.875909
O	-1.220806	0.308531	-1.50721
W	-2.546016	2.082883	-1.6818
O	-1.086428	3.10179	-0.798327
O	-3.7943	3.321024	-1.92199
O	-1.634864	2.189199	-3.29228
W	-2.59262	-1.211286	-2.372612
O	-3.036632	-1.530119	-0.398698
O	-3.900829	-2.195661	-3.064542
O	-3.56395	0.508334	-2.212913
W	-0.140421	-0.708952	3.372065
O	1.136576	0.669447	2.923911
O	0.241027	-1.054802	5.066659
O	-1.495759	0.661772	3.613713
O	-1.112687	-0.263354	1.327554
W	-2.589852	-1.959018	1.36613
O	-1.176416	-3.043239	0.595217
O	-3.809661	-3.167326	1.811772
O	-1.557307	-1.987056	3.075997
W	-2.498582	1.354986	2.050774
O	-2.960369	1.656473	0.248113
O	-3.671846	2.348715	2.934469
O	-3.474542	-0.352314	2.056767
W	0.20852	3.485544	0.549642
O	-1.047531	2.585774	1.731966
O	-0.108017	5.187908	0.910167
O	1.590011	3.140855	1.900096
O	1.132576	1.425346	0.101304
W	2.600778	2.121053	-1.479092
O	1.34869	1.954993	-2.814887
O	3.930556	2.960844	-2.302253
O	1.63743	3.702044	-0.739062
W	2.585633	1.466011	1.892013
O	2.993144	-0.384583	1.473358
O	3.775233	1.827491	3.154253
O	3.522964	2.055452	0.351151
H	-0.738911	3.167467	-4.390767
H	0.803263	3.228836	-4.28005

[Co^{III}Co^{II}(H₂O)W₁₁O₃₉]⁷⁻, ²A-stateE_{tot} = -4048.19184852 a.u.

	X	Y	Z
Co	-0.0053	-0.00803	-0.11277
W	3.346971	-0.86109	-0.9382
O	2.064325	-1.79521	-2.02157
O	4.860615	-1.68534	-1.35069
O	3.449395	0.582753	-2.23529
O	1.719451	0.626301	-0.45543
W	2.867879	1.79579	1.072509
O	2.174144	0.494436	2.367975
O	4.046532	2.680551	2.059864
O	4.048477	0.374538	0.409283
W	2.064851	2.003551	-2.22642
O	0.518037	3.037011	-1.61265
O	2.818112	3.097938	-3.40815
O	3.048744	2.722055	-0.57646
Co	-0.78839	0.099047	-3.2054
O	0.908119	1.021159	-3.22792
O	-3.52444	1.10316	-4.7652
O	0.020534	-1.6013	-3.80694
O	-0.71324	-1.02591	-1.39865
W	-2.7608	-1.8221	-1.61996
O	-3.3634	-0.19794	-0.68881
O	-4.29185	-2.66144	-1.93871
O	-2.55376	-0.84271	-3.1945
W	0.392427	-2.74039	-2.4156
O	0.660517	-3.34761	-0.51125
O	0.955699	-4.18832	-3.2735
O	-1.51372	-3.20589	-2.21914
W	0.764484	-0.39216	3.320972
O	-0.23674	1.201328	2.935212
O	1.24104	-0.16627	5.01181
O	-0.91029	-1.34774	3.573988
O	0.027308	-1.19317	1.261833
W	1.244326	-3.06384	1.257475
O	2.657491	-1.9941	0.47853
O	2.072111	-4.58399	1.650125
O	1.588528	-2.11361	2.965158
W	-1.91511	-2.0922	2.048804
O	-2.43347	-2.42978	0.259444
O	-3.1519	-2.9668	2.969342
O	-0.53493	-3.49125	1.967689
W	-3.28541	1.141001	0.67682
O	-2.6961	-0.35621	1.791406
O	-4.98946	1.289319	1.137605
O	-2.52785	2.336822	2.039648
O	-1.1196	1.470522	0.132483
W	-1.39184	3.065859	-1.37372
O	-1.58305	1.816815	-2.70737
O	-1.8879	4.572629	-2.17711
O	-3.18546	2.5901	-0.59105
W	-0.6532	2.84647	1.952705
O	1.220507	2.728552	1.467143
O	-0.61873	4.0559	3.245851
O	-1.02929	3.941307	0.458174
H	-3.34185	0.232274	-4.29356
H	-3.02371	1.735755	-4.19196

[Co^{II}Ni^{II}(H₂O)W₁₁O₃₉]⁸⁻, ⁶A-stateE_{tot} = -4071.97606114 a.u.

	X	Y	Z
Co	-0.013807	0.002442	-0.123125
W	0.362904	-3.452486	-0.795154
O	-0.991115	-2.644802	-1.913454
O	0.120577	-5.189352	-1.125554
O	1.741689	-3.152033	-2.172967
O	1.210536	-1.448951	-0.482642
W	2.714066	-1.989141	1.098594
O	1.26373	-1.739388	2.402688
O	3.968204	-2.74472	2.118704
O	1.799519	-3.644718	0.528448
W	2.5548	-1.34935	-2.233713
O	2.945841	0.500448	-1.686539
O	3.887262	-1.713598	-3.373443
O	3.642604	-1.928127	-0.551723
Ni	-0.292533	0.611123	-3.247828
O	1.256167	-0.681514	-3.314892
O	-0.310127	3.487982	-4.887439
O	-1.692577	-0.851401	-3.889909
O	-1.27382	0.209194	-1.566085
W	-2.721122	1.824739	-1.66377
O	-1.354326	2.991605	-0.801157
O	-4.095995	2.946555	-1.878168
O	-1.876977	2.039511	-3.310586
W	-2.478291	-1.431702	-2.338469
O	-2.865914	-1.767106	-0.345738
O	-3.722449	-2.540312	-2.993041
O	-3.643997	0.179624	-2.187228
W	-0.047484	-0.702436	3.359165
O	1.093837	0.787974	2.894065
O	0.387915	-1.005698	5.064674
O	-1.518672	0.557732	3.679128
O	-1.083822	-0.371547	1.436149
W	-2.385517	-2.14584	1.424254
O	-0.887142	-3.129592	0.634151
O	-3.500673	-3.465981	1.877697
O	-1.355115	-2.130439	3.144375
W	-2.554958	1.127776	2.083817
O	-3.057372	1.368	0.274688
O	-3.817724	2.027273	2.97071
O	-3.439178	-0.648204	2.121091
W	-0.070054	3.48933	0.526259
O	-1.232418	2.486446	1.73764
O	-0.535533	5.171028	0.895322
O	1.34783	3.324068	1.902282
O	1.017432	1.621276	0.104303
W	2.348722	2.318676	-1.501043
O	1.105326	2.054534	-2.828828
O	3.613853	3.259062	-2.345756
O	1.307094	3.885221	-0.785207
W	2.459191	1.719094	1.843142
O	3.008436	-0.107085	1.415027
O	3.633404	2.162814	3.110757
O	3.366979	2.380712	0.318351
H	-1.077092	3.04489	-4.39218
H	0.447359	3.244984	-4.291397

[Co^{III}Ni^{II}(H₂O)W₁₁O₃₉]⁷⁻, ⁷A-stateE_{tot} = -4072.45067686 a.u.

	X	Y	Z
Co	-0.01394	0.004897	-0.12199
W	0.162992	-3.48156	-0.81788
O	-1.14204	-2.59965	-1.91458
O	-0.17567	-5.18908	-1.13598
O	1.560169	-3.1976	-2.13313
O	1.113193	-1.41671	-0.45559
W	2.600209	-2.13725	1.126722
O	1.17565	-1.80239	2.424266
O	3.806949	-2.96688	2.125213
O	1.57389	-3.69074	0.520702
W	2.518042	-1.45879	-2.23543
O	3.028055	0.351048	-1.70848
O	3.797154	-1.91276	-3.3832
O	3.496433	-2.10238	-0.54277
Ni	-0.23947	0.619815	-3.2339
O	1.23343	-0.73775	-3.29496
O	-0.07886	3.451403	-4.90704
O	-1.70643	-0.73931	-3.84465
O	-1.22117	0.268673	-1.50144
W	-2.62385	1.994821	-1.66325
O	-1.19903	3.066646	-0.79544
O	-3.91319	3.188966	-1.90741
O	-1.73409	2.104996	-3.28378
W	-2.57012	-1.30886	-2.33815
O	-2.97679	-1.63063	-0.36341
O	-3.84416	-2.33818	-3.02662
O	-3.59075	0.37643	-2.16935
W	-0.079	-0.69561	3.377858
O	1.14295	0.721678	2.912932
O	0.326799	-1.02222	5.070476
O	-1.48182	0.626283	3.624244
O	-1.08783	-0.2957	1.337211
W	-2.50396	-2.04199	1.402004
O	-1.0665	-3.08475	0.623601
O	-3.68358	-3.28532	1.858898
O	-1.45874	-2.02311	3.098883
W	-2.52247	1.277887	2.069568
O	-3.00595	1.556024	0.26833
O	-3.72314	2.234608	2.957014
O	-3.4383	-0.46074	2.089879
W	0.097176	3.498142	0.541508
O	-1.1176	2.5572	1.735442
O	-0.27532	5.189458	0.90077
O	1.501683	3.203299	1.878734
O	1.089065	1.465169	0.094133
W	2.500085	2.194723	-1.51289
O	1.228148	1.968144	-2.81472
O	3.780284	3.07944	-2.36768
O	1.498807	3.753561	-0.76369
W	2.557009	1.563132	1.860427
O	3.018516	-0.27609	1.447997
O	3.747003	1.96845	3.109148
O	3.455196	2.17897	0.309749
H	-0.87495	3.079207	-4.41595
H	0.663266	3.181616	-4.30735

[Co^{II}Cu^{II}(H₂O)W₁₁O₃₉]⁸⁻, ⁵A-stateE_{tot} = -4098.77241532 a.u.

	X	Y	Z
Co	0.016708	-0.013734	-0.112239
W	1.316912	3.197579	-0.843856
O	2.069756	1.830099	-1.979369
O	2.352693	4.600907	-1.221246
O	-0.080397	3.577695	-2.189414
O	-0.378744	1.845148	-0.470885
W	-1.38255	3.044356	1.137131
O	-0.189131	2.143057	2.398045
O	-2.090352	4.31912	2.165938
O	0.192265	4.063461	0.502848
W	-1.662011	2.39611	-2.180528
O	-2.878908	0.966541	-1.586091
O	-2.68839	3.346628	-3.297528
O	-2.278936	3.43069	-0.497445
Cu	-0.211512	-0.692203	-3.292214
O	-0.891999	1.163718	-3.287907
O	-1.587969	-3.278542	-4.812155
O	1.695641	-0.08744	-3.934078
O	1.051057	-0.817179	-1.514257
W	1.445794	-2.872043	-1.698996
O	-0.277486	-3.261723	-0.7725
O	2.073236	-4.522757	-1.992285
O	0.503524	-2.62043	-3.312315
W	2.749524	0.047874	-2.432258
O	3.396584	0.183084	-0.457089
O	4.336622	0.420755	-3.17883
O	3.050711	-1.928492	-2.311482
W	0.508765	0.605962	3.347851
O	-1.23571	-0.149082	2.936518
O	0.317171	1.093033	5.055315
O	1.189874	-1.201303	3.652063
O	1.193796	-0.191075	1.402117
W	3.183961	0.736628	1.310154
O	2.308307	2.317338	0.553106
O	4.801306	1.366299	1.735736
O	2.318244	1.23316	3.069828
W	1.778905	-2.21351	2.035654
O	2.054099	-2.704156	0.228837
O	2.473101	-3.59757	2.925966
O	3.405571	-1.080412	2.017387
W	-1.591632	-3.086382	0.597467
O	-0.048804	-2.756835	1.753095
O	-1.978077	-4.784057	0.98487
O	-2.709648	-2.257605	2.007281
O	-1.663718	-0.929901	0.161758
W	-3.229578	-0.911304	-1.380684
O	-2.070628	-1.276023	-2.772371
O	-4.822432	-1.127537	-2.164254
O	-3.035207	-2.780363	-0.672078
W	-2.910905	-0.317447	1.951025
O	-2.53971	1.545663	1.490054
O	-4.111662	-0.135689	3.257533
O	-4.080199	-0.471203	0.461825
H	-0.686642	-3.217929	-4.349167
H	-2.125911	-2.692357	-4.217644

[Co^{III}Cu^{II}(H₂O)W₁₁O₃₉]⁷⁻, ⁶A-stateE_{tot} = -4099.25346242 a.u.

	X	Y	Z
Co	-0.01863	0.009032	-0.12374
W	-0.3043	-3.46679	-0.83417
O	-1.43002	-2.39783	-1.96504
O	-0.87118	-5.10615	-1.18757
O	1.15249	-3.36961	-2.12399
O	0.909311	-1.56452	-0.43583
W	2.234274	-2.48443	1.179797
O	0.823404	-1.96396	2.42953
O	3.280974	-3.47958	2.20734
O	1.021819	-3.88697	0.530999
W	2.340731	-1.78766	-2.1728
O	3.076607	-0.07179	-1.60009
O	3.590469	-2.41079	-3.27182
O	3.176967	-2.57236	-0.46221
Cu	0.006464	0.679647	-3.31285
O	1.229627	-0.87347	-3.29198
O	0.554614	3.542862	-4.83652
O	-1.60269	-0.43955	-3.86515
O	-1.17924	0.434157	-1.44502
W	-2.24637	2.332321	-1.71087
O	-0.72515	3.20756	-0.79279
O	-3.32097	3.70794	-2.03357
O	-1.25771	2.289844	-3.29452
W	-2.62851	-0.91192	-2.41376
O	-3.17937	-1.20134	-0.47373
O	-3.99024	-1.74076	-3.2006
O	-3.43247	0.893806	-2.28616
W	-0.29404	-0.69949	3.359937
O	1.138587	0.53538	2.958493
O	0.009218	-1.0957	5.060084
O	-1.50206	0.808125	3.5951
O	-1.16847	-0.15162	1.325157
W	-2.81745	-1.67142	1.308447
O	-1.5152	-2.90601	0.563294
O	-4.17315	-2.73984	1.718043
O	-1.83986	-1.82176	3.03873
W	-2.38338	1.606171	2.010235
O	-2.77735	1.977196	0.196155
O	-3.46307	2.71699	2.873884
O	-3.54605	0.019282	1.979033
W	0.572696	3.443067	0.586578
O	-0.80213	2.671714	1.729131
O	0.430623	5.168188	0.953097
O	1.879674	2.95215	1.96312
O	1.275024	1.30369	0.151403
W	2.820042	1.826489	-1.40522
O	1.579033	1.784872	-2.76627
O	4.242295	2.518438	-2.21175
O	2.032428	3.511037	-0.68218
W	2.684672	1.175538	1.956374
O	2.897594	-0.70646	1.532043
O	3.883622	1.397917	3.2422
O	3.711806	1.667893	0.436876
H	-0.28791	3.237853	-4.37844
H	1.245635	3.158012	-4.24017

[Co^{II}Zn^{II}(H₂O)W₁₁O₃₉]⁸⁻, ⁴A-stateE_{tot} = -3891.79250681 a.u.

	X	Y	Z
Co	0.029524	0.000507	-0.148431
W	-0.162371	3.518889	-0.178308
O	1.137698	2.864931	-1.435906
O	0.182555	5.270986	-0.174307
O	-1.586663	3.577667	-1.531331
O	-1.132422	1.549846	-0.22694
W	-2.561144	1.8776	1.496842
O	-1.122842	1.278732	2.674959
O	-3.750397	2.488611	2.679818
O	-1.558238	3.543547	1.214904
W	-2.543494	1.87059	-1.905256
O	-3.029408	-0.009369	-1.717609
O	-3.882409	2.539693	-2.892572
O	-3.528636	2.192602	-0.107357
Zn	0.184441	0.004799	-3.322208
O	-1.321033	1.38847	-3.171481
O	1.750285	1.500133	-3.742239
O	1.278501	0.006071	-1.625761
W	2.590919	-1.650589	-2.113474
O	1.163605	-2.854052	-1.440517
O	3.907698	-2.791565	-2.536563
O	1.76598	-1.481005	-3.74464
W	2.574966	1.677084	-2.111143
O	2.987619	1.620597	-0.089067
O	3.880546	2.830661	-2.534514
O	3.632184	0.018244	-2.30387
W	0.141887	-0.000047	3.404444
O	-1.111873	-1.293265	2.674112
O	-0.27697	-0.003016	5.141855
O	1.518024	-1.370009	3.436867
O	1.135202	0.003049	1.424424
W	2.520944	1.678029	1.720943
O	1.077395	2.85792	1.157222
O	3.707465	2.821878	2.414508
O	1.507957	1.378646	3.438573
W	2.527486	-1.665653	1.71719
O	3.001235	-1.594639	-0.090659
O	3.726493	-2.796288	2.411104
O	3.498782	0.012905	2.107013
W	-0.13587	-3.523041	-0.192445
O	1.100156	-2.852663	1.1517
O	0.226674	-5.271609	-0.188319
O	-1.526609	-3.561007	1.207626
O	-1.118047	-1.559462	-0.229246
W	-2.530148	-1.879953	-1.906129
O	-1.306203	-1.392506	-3.168979
O	-3.860756	-2.561038	-2.896563
O	-1.556281	-3.588438	-1.538311
W	-2.540978	-1.90504	1.495745
O	-2.985213	-0.01474	1.432774
O	-3.726008	-2.528869	2.676262
O	-3.507677	-2.221653	-0.110507

[Co^{III}Zn^{II}(H₂O)W₁₁O₃₉]⁷⁻, ⁵A-stateE_{tot} = -3892.27788872 a.u.

	X	Y	Z
Co	0.02566	-0.00015	-0.15246
W	-0.1345	3.543146	-0.17952
O	1.156211	2.880919	-1.43117
O	0.217086	5.278671	-0.16971
O	-1.55681	3.536463	-1.50129
O	-1.10575	1.461036	-0.21737
W	-2.56115	1.880802	1.515112
O	-1.12758	1.281803	2.696912
O	-3.74349	2.509649	2.677345
O	-1.52465	3.508427	1.199462
W	-2.55614	1.865861	-1.92077
O	-3.06796	-0.00031	-1.74016
O	-3.8652	2.551907	-2.91176
O	-3.48438	2.184502	-0.11167
Zn	0.182854	0.001953	-3.34067
O	-1.31826	1.379053	-3.16251
O	1.720004	1.463806	-3.69732
O	1.218802	0.002052	-1.55526
W	2.592491	-1.6825	-2.10353
O	1.160843	-2.8771	-1.43503
O	3.878911	-2.8202	-2.56617
O	1.722826	-1.45652	-3.69877
W	2.58848	1.690705	-2.10166
O	2.998996	1.626725	-0.1027
O	3.87306	2.830956	-2.56309
O	3.582792	0.004778	-2.27572
W	0.125718	-0.00138	3.412896
O	-1.12514	-1.2868	2.69534
O	-0.26791	-0.00279	5.140898
O	1.509745	-1.35429	3.384866
O	1.112722	-8.6E-05	1.330646
W	2.537387	1.691666	1.711312
O	1.102818	2.870638	1.154342
O	3.72893	2.816808	2.393297
O	1.508084	1.352419	3.386456
W	2.537088	-1.69266	1.708972
O	3.001039	-1.62178	-0.10463
O	3.731018	-2.81618	2.389432
O	3.467404	0.000809	2.074085
W	-0.13002	-3.54427	-0.188
O	1.106125	-2.87094	1.150108
O	0.225191	-5.27903	-0.17993
O	-1.51866	-3.51402	1.194661
O	-1.10455	-1.46237	-0.21747
W	-2.55508	-1.86322	-1.92227
O	-1.31592	-1.37683	-3.16291
O	-3.86276	-2.55085	-2.9139
O	-1.55181	-3.53612	-1.50606
W	-2.55621	-1.88897	1.513163
O	-3.00021	-0.00366	1.464915
O	-3.73745	-2.5211	2.674801
O	-3.48106	-2.18973	-0.11364