

Supplementary Information

On the Electronic Structure of Giant Polyoxometalates: Mo₁₃₂ vs W₇₂Mo₆₀

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Optimized Cartessian coordinates of Mo₁₃₂ and W₇₂Mo₆₀

Cartesian coordinates of Mo₁₃₂

MO	-1.952587362	10.051581199	8.032679305	MO	-4.692280066	6.458269448	10.439171952	MO	10.881227547	4.743674705	4.144800390	MO	-3.720357218	-14.275924034	-1.394310155	MO	10.97518239	-3.566227036	-5.776799988
MO	0.000000000	0.000000000	12.883468886	MO	-1.203616589	11.128631058	-6.878186881	MO	11.591343992	2.558137313	4.144800390	MO	-7.873961007	-8.882794701	4.144800390	MO	10.16300477	-1.249088746	-8.033675035
MO	-1.517470041	-1.795310054	-1.795310054	MO	-1.795310054	-1.795310054	-6.878186881	MO	-12.146825891	-6.878186881	-1.394310155	MO	-7.873961007	-8.882794701	4.144800390	MO	8.955239129	-1.932373025	-1.032367305
MO	1.951424187	2.685094970	12.569513198	MO	0.000000000	14.377837755	3.100196033	MO	11.414100679	1.543466596	1.543466596	MO	-9.781595000	-7.43125065	2.942381078	MO	12.08622505	-6.48047793	-4.713595325
MO	0.000000000	3.319961124	12.569513198	MO	-1.404446955	12.07828154	1.543466596	MO	12.820966621	2.5013972184	1.543466596	MO	-9.786907734	-5.94968795	5.338202558	MO	10.98679676	2.199120370	-6.878186881
MO	-1.286469522	-4.600925232	-4.600925232	MO	-8.920582951	9.427812481	-5.429184642	MO	-12.820966621	2.5013972184	1.543466596	MO	-8.920582951	9.427812481	-5.429184642	MO	7.159593149	-1.217050149	-6.878186881
MO	0.000000000	5.761303314	11.803174143	MO	-9.570999425	13.0986167	1.543466596	MO	-10.05960633	7.008401671	2.942381078	MO	-8.456797139	-5.94968795	1.543466596	MO	5.486579240	-9.768982026	-6.878186881
MO	0.000000000	7.982983662	10.439171952	MO	-6.014852019	10.23351645	-4.144800390	MO	8.68209209	7.469348044	5.338202558	MO	-6.186306210	-10.90417087	1.543466596	MO	12.105452396	-3.932298826	-2.659682370
MO	-1.517470041	-1.795310054	-1.795310054	MO	-1.795310054	-1.795310054	-6.878186881	MO	-12.146825891	-6.878186881	-1.394310155	MO	-7.873961007	-8.882794701	4.144800390	MO	8.955239129	-1.932373025	-1.032367305
MO	-1.951424187	2.685094970	12.569513198	MO	-6.78533846	10.77073920	-6.102344145	MO	12.287792760	2.942381078	2.942381078	MO	-8.478135978	-5.927743809	7.598195659	MO	13.059612130	-6.136722382	-1.088175005
MO	-3.38409122	-4.660925232	11.803174143	MO	-4.660925232	11.803174143	-6.533139311	MO	8.167650490	7.060997500	5.367043967	MO	-11.43488879	-5.439262966	7.741385783	MO	10.971979467	-7.115670560	-1.088175005
MO	-1.517470041	-1.795310054	-1.795310054	MO	-1.795310054	-1.795310054	-6.878186881	MO	-12.146825891	-6.878186881	-1.394310155	MO	-7.873961007	-8.882794701	4.144800390	MO	8.955239129	-1.932373025	-1.032367305
MO	-7.572268631	2.466877617	10.439171952	MO	-9.786407734	5.949686795	-5.338202558	MO	7.876748952	9.193988885	5.743035747	MO	-9.44488879	-8.369323047	-6.72030547	MO	0.000000000	-13.059826314	-6.533139311
MO	-2.144456042	11.421503688	9.033810921	MO	-10.65868959	8.047482245	-5.367043967	MO	6.149295547	9.289863675	5.492188462	MO	-10.90955456	-6.491550565	6.72303547	MO	3.448301442	-13.24845644	-5.367043967
MO	-1.286469522	-4.600925232	-4.600925232	MO	-8.920582951	9.427812481	-5.429184642	MO	-12.820966621	2.5013972184	1.543466596	MO	-8.920582951	9.427812481	-5.429184642	MO	4.420536526	-10.548977560	-5.338202558
MO	0.518052224	-1.51519844	10.765012143	MO	-6.186306210	10.90417087	-1.543466596	MO	4.420436526	10.565997760	5.338202558	MO	-12.47536434	-11.394310155	5.7239411880	MO	-5.119305665	-6.102344145	-6.102344145
MO	2.803767717	-6.187291708	10.765012143	MO	-8.450192464	11.631871415	-3.100196033	MO	6.053422095	11.21639367	7.741385783	MO	-1.952587362	-10.051581199	-8.032679305	MO	9.730513139	-3.16165373	-7.307577378
MO	0.000000000	5.761303314	11.803174143	MO	-6.014852019	10.23351645	-4.144800390	MO	-12.146825891	-6.878186881	-1.394310155	MO	-7.873961007	-8.882794701	4.144800390	MO	8.955239129	-1.932373025	-1.032367305
MO	1.860657854	1.860654385	12.405804729	MO	-4.49910842	9.73081939	-9.033810921	MO	9.92058995	-3.548314654	5.492188462	MO	-12.105452396	-2.659682370	-5.927743809	MO	12.16165373	-4.03472207	-6.533139311
MO	-1.149949795	-1.582770108	12.405804729	MO	-5.439262966	5.439262966	-7.741385783	MO	9.730513139	3.16165373	7.307577378	MO	-10.158185067	-6.618675068	-4.713595325	MO	8.682058083	-1.492828743	-9.072702596
MO	0.000000000	5.761303314	11.803174143	MO	-1.795310054	-1.795310054	-6.878186881	MO	-12.146825891	-6.878186881	-1.394310155	MO	-7.873961007	-8.882794701	4.144800390	MO	8.955239129	-1.932373025	-1.032367305
MO	4.424056803	0.044321144	11.831996777	MO	-5.009892668	11.831996777	0.72303547	MO	8.682058083	1.492828743	9.072702596	MO	-12.108622350	-6.618675068	-4.713595325	MO	10.16300477	-1.249088746	-8.033675035
MO	-1.517470041	-1.795310054	-1.795310054	MO	-1.448802090	-1.448802090	-6.878186881	MO	-10.158185067	-6.618675068	-4.713595325	MO	-7.598195659	-8.23705045	-6.878186881	MO	7.666657286	-3.948746440	-9.072702596
MO	3.484244790	-1.13514903	14.242279965	MO	-3.484244790	11.768033012	2.942381078	MO	-11.252576903	9.033810921	9.033810921	MO	-5.439262966	-7.741385783	9.033810921	MO	7.877773282	-6.350246927	-7.598195659
MO	3.605188455	2.564528785	11.831996777	MO	-3.720357218	14.275924034	1.394310155	MO	7.866657286	3.948746440	9.072702596	MO	-10.16300477	-1.249088746	-8.033675035	MO	10.192004114	-5.57039747	-9.033810921
MO	1.242656023	4.221224038	11.831996777	MO	-2.803767717	16.87291708	-10.765012143	MO	-7.877773282	6.350246927	7.598195659	MO	-8.955239129	-1.932373025	-1.032367305	MO	11.414912933	-0.939232303	-5.338202558
MO	2.152269244	2.962344476	14.242279965	MO	-2.152269244	10.765012143	-4.144800390	MO	-10.192004114	-5.57039747	9.033810921	MO	-10.98679676	2.199120370	-6.878186881	MO	12.675649000	-7.906897700	-5.367043967
MO	1.409260649	-4.193822064	11.831996777	MO	-4.05846250	9.862757114	-6.102344145	MO	11.414912933	-0.939232303	5.338202558	MO	-7.592266352	-2.466877617	-10.439171952	MO	12.447969955	2.320354174	-7.741385783
MO	0.000000000	-6.352619615	14.242279965	MO	-6.352619615	14.242279965	-7.307577378	MO	-12.477469955	-2.320354174	7.741385783	MO	-5.473926352	-11.803174143	-6.533139311	MO	8.705748952	-1.193938885	-7.741385783
MO	0.000000000	-1.393920102	13.397187244	MO	-4.63231652	9.773379383	-5.598195659	MO	8.689139878	2.826196967	11.684228405	MO	-2.145460402	-11.42310921	-9.033810921	MO	5.915208480	-8.145178244	-4.713595325
MO	0.000000000	6.352619615	13.397187244	MO	-4.043233813	8.183228388	-7.307579256	MO	9.950954498	3.67610826	10.765012143	MO	-3.610072102	-9.405537368	-7.598195659	MO	1.660954794	-10.838975668	-6.102344145
MO	-1.393920102	-1.393920102	-1.393920102	MO	-6.352619615	-6.352619615	-7.307579256	MO	-7.307579256	-7.307579256	-7.307579256	MO	-9.730513139	-3.16165373	-7.598195659	MO	3.610072102	-9.405537368	-7.598195659
MO	0.000000000	10.231266988	7.307577378	MO	-4.231647584	11.146447078	-5.338202558	MO	9.951020480	3.610178244	7.307579256	MO	-10.881227547	-4.743447405	-6.144800390	MO	6.053422095	-11.12163967	-7.741385783
MO	1.242656023	8.701871053	9.072702596	MO	-0.69345677	11.404377339	-9.423810178	MO	5.001444882	1.963049420	13.397187244	MO	-11.593133952	-2.508132713	-4.144800390	MO	10.881227547	-4.743447405	-6.144800390
MO	0.000000000	10.231266988	7.307577378	MO	-1.393920102	-1.393920102	-7.307579256	MO	-12.165074098	-12.165074098	-12.165074098	MO	-12.165074098	-12.165074098	-12.165074098	MO	11.593133952	-2.508132713	-4.144800390
MO	-5.018052224	-4.578519844	10.765012143	MO	-6.186306210	10.90417087	-1.543466596	MO	-6.186306210	10.90417087	-1.543466596	MO	-11.41100667	-5.154346596	9.033810921	MO	11.41100667	-5.154346596	9.033810921
MO	-8.033767717	-6.187291708	10.765012143	MO	-8.450192464	11.631871415	-3.100196033	MO	9.433977453	-7.61566277	4.713595325	MO	-12.280706621	-2.519731184	-1.543466596	MO	12.280706621	-2.519731184	-1.543466596
MO	-1.860657854	1.860654385	12.405804729	MO	-4.49910842	9.73081939	-9.033810921	MO	-12.405804729	-4.49910842	5.492188462	MO	-12.280706621	-2.519731184	-1.543466596	MO	12.280706621	-2.519731184	-1.543466596
MO	-1.149949795	-1.582770108	12.405804729	MO	-5.439262966	5.439262966	-7.741385783	MO	7.488175105	-6.984197955	8.033675035	MO	-10.0960633	-7.008401671	-2.942381078	MO	10.96969629	-7.008401671	-2.942381078
MO	4.424056803	0.044321144	11.831996777	MO	0.000000000	10.63044154	-7.834207007	MO	10.187117405	-6.476794713	6.678186881	MO	-8.68209209	-7.469348044	-5.338202558	MO	8.68209209	-7.469348044	-5.338202558
MO	-1.517470041	-1.795310054	-1.795310054	MO	-1.448802090	-1.448802090	-6.878186881	MO	-12.146825891	-6.878186881	-1.394310155	MO	-7.873961007	-8.882794701	4.144800390	MO	8.955239129	-1.932373025	-1.032367305
MO	-3.484244790	-1.13514903	14.242279965	MO	-3.484244790	11.768033012	2.942381078	MO	-12.146825891	-6.878186881	-1.394310155	MO	-7.873961007	-8.882794701	4.144800390	MO	8.955239129	-1.932373025	-1.032367305
MO	3.605188455	2.564528785	11.831996777	MO	-3.720357218	14.275924034	1.394310155	MO	4.428494832	-9.27960266	8.033675035	MO	-13.676364900	-5.367043967	6.72303547	MO	12.287792760	-2.6518821	-2.942381078
MO	1.242656023	4.221224038	11.831996777	MO	-2.803767717	16.87291708	-10.765012143	MO	-12.477469955	-2.320354174	7.741385783	MO	-12.477469955	-2.320354174	7.741385783	MO	12.287792760	-2.6518821	-2.942381078
MO	-2.152269244	2.962344476	14.242279965	MO	-2.152269244	10.765012143	-4.144800390	MO	4.692										

Cartesian coordinates of W₇₂Mo₆₀

W	6.73902645	9.27547416	5.72276760	W	0.00000000	12.73930335	-2.65051771	Mo	-11.06375577	-7.18794158	1.10962543	O	-3.42097532	13.24209126	-5.37251818
W	9.62724222	9.61437608	4.69623144	W	3.51518039	-1.70135301	4.69623144	W	-4.72808038	-12.31827937	-1.10962543	O	-6.79214151	3.14496791	-7.72127782
W	7.48268239	7.28952013	4.69623144	W	-4.32277815	9.26103779	8.20820808	W	4.72808038	-12.31827937	-1.10962543	O	-12.38452008	4.01897701	-6.48741825
W	4.62824224	11.31881080	4.69623144	W	-4.42802424	11.31881080	4.69623144	W	-8.78618988	8.85028280	4.10435760	O	-6.68860435	-1.41602749	-6.08843911
W	4.32379515	12.10241632	4.69623144	W	5.39942295	4.69623144	8.20820808	W	-5.39942295	4.69623144	8.20820808	O	-12.32647057	3.14496791	-7.72127782
W	7.47164329	6.97398782	8.00347057	W	1.94754673	-2.68958122	12.55406185	W	-7.62933297	10.50897597	6.48761985	O	-11.52403267	1.51471184	-6.97157160
W	10.24106876	4.70120519	6.90828805	W	0.00000000	-1.96073355	12.36059672	W	-8.82494384	5.95218049	5.33122038	O	-6.90711403	-3.12514707	-7.87169510
W	10.25052272	6.30160595	6.90828805	W	1.88441660	6.90828805	12.36059672	W	8.82494384	5.95218049	5.33122038	O	-11.09890325	-1.51471184	-6.97157160
W	4.72508038	12.31827937	1.10962543	W	1.23523368	-4.24668612	11.84716465	W	-10.59811008	8.69729290	5.72518181	O	-12.48364935	-2.33237873	-7.78194230
W	11.32615235	6.90828805	1.10962543	W	0.00000000	-2.92498310	11.84716465	W	-11.47042239	10.50897597	6.48761985	O	-6.11943210	-3.12514707	-7.87169510
W	4.71896031	-5.49510227	10.49504689	W	0.00000000	0.00000000	12.81218432	W	-4.40497466	11.84716465	2.92722281	O	-5.51307946	-7.59797592	-6.08843911
W	10.90397384	-3.54291587	5.72276760	W	-1.94754673	-2.68958122	12.55406185	W	-5.00837640	12.73930335	5.72518181	O	-6.83324846	-7.99916658	-6.97157160
W	10.43895928	-5.49510227	10.49504689	W	3.15119681587	-0.02386951	12.36059672	W	-11.47042239	10.50897597	6.48761985	O	-6.11943210	-3.12514707	-7.87169510
W	8.84152196	-3.54291587	5.72276760	W	0.00000000	-5.80661825	11.87197146	W	-11.49596092	-5.90387619	5.72518181	O	-6.20924872	-6.23084872	-6.08131888
W	10.13487974	-6.61286799	4.69623144	W	-1.15248959	1.58625515	12.36059672	W	-11.68253584	-5.90387619	5.72518181	O	-6.35895319	-6.23084872	-6.08131888
W	12.10272365	-6.61286799	4.69623144	W	-1.52681571	1.58625515	12.36059672	W	-12.10848545	-5.90387619	5.72518181	O	-6.35895319	-6.23084872	-6.08131888
W	12.12041632	-6.61286799	4.69623144	W	-1.68416652	-0.60589937	12.36059672	W	-12.55884545	-1.18584859	-0.73617629	O	-6.25156579	-6.90828805	-6.08843911
W	11.54854476	-1.251613957	6.90828805	W	0.00000000	0.00000000	14.50873508	W	-14.82554651	-0.86319167	1.38081632	O	-6.43331468	-6.97157160	-7.87169510
W	7.63545066	-4.24668612	10.49504689	W	-3.62591341	-2.58131095	11.84716465	W	-8.62522357	-0.49877270	0.73617629	O	-6.48553276	-5.51307946	-7.59797592
W	7.63505220	-4.24668612	10.49504689	W	-1.26232368	-4.24668612	11.84716465	W	-11.01390828	-6.34024114	-0.73617629	O	-11.09890325	-1.51471184	-6.97157160
W	11.36817037	-1.251613957	6.90828805	W	-2.12317416	-6.92496330	11.84716465	W	-12.30149042	-8.01590986	-0.73617629	O	-6.97134032	-7.87169510	-7.87169510
W	13.17573249	-0.68794558	1.10962543	W	3.43852449	1.11724420	14.23469272	W	-6.20628667	-10.95394874	-1.52369107	O	-11.70422365	-4.50777101	-7.78194230
W	7.85424846	6.90828805	1.10962543	W	1.39531586	-6.69811749	10.83181588	W	-4.40597466	-11.65397987	-2.92722281	O	-2.89024025	2.33040472	-10.81615988
W	5.98208311	8.23631311	1.72137782	W	-1.39531586	-6.69811749	10.83181588	W	-5.40228989	-11.83191372	-1.39591632	O	5.69059510	-4.59873304	-10.81615988
W	5.98942284	10.20604637	4.10435760	W	0.00000000	-6.39181244	13.44923170	W	6.20628667	-10.95394874	-1.52369107	O	-3.97012290	-7.42830599	-11.70422365
W	4.83547658	4.80523865	1.31338441	W	0.00000000	3.11338441	12.55406185	W	6.40297466	-11.65397987	-2.92722281	O	-8.94132194	4.90878429	-8.02847057
W	7.85020787	7.63505220	1.60615121	W	-3.15119681	1.02288951	12.55406185	W	5.40228989	-11.83191372	-1.39591632	O	-7.63505220	8.28750816	-6.90828805
W	7.62933297	10.50897597	6.48761985	W	-5.52242213	-1.79434372	11.87197146	W	-7.48268239	10.29930313	2.65051771	W	0.00000000	11.44511659	-5.72276760
W	9.82948924	5.95218049	5.33122038	W	0.00000000	-8.02838793	10.49504689	W	-10.2502723	8.30130691	1.10962543	W	-1.94548911	10.63979163	-6.03047057
W	9.93486374	7.44447314	2.92722281	W	-1.14509754	4.21071144	11.84716465	W	-12.7280038	12.31827937	-1.10962543	W	-5.51307946	9.62296879	-6.90828805
W	10.59811008	8.69729290	5.72518181	W	3.61547819	14.23469272	14.23469272	W	-13.71732429	9.68734874	-1.10962543	W	-12.48364935	-2.33237873	-7.78194230
W	6.20628667	10.95394874	1.52369107	W	-5.37719140	2.65021103	11.84716465	W	-10.2502723	8.30130691	-1.10962543	W	-4.21304358	-4.69756285	-11.87197146
W	6.49979528	10.50897597	6.48761985	W	-4.63172847	-6.61445451	11.84716465	W	-7.48268239	10.29930313	2.65051771	W	-12.48364935	-2.33237873	-7.78194230
W	8.44398522	11.62214959	3.13972755	W	-3.42852424	-1.11724420	14.23469272	W	-4.32852424	-11.31881080	-4.69623144	W	6.31304358	-4.69756285	-11.87197146
W	2.62327940	11.18772939	5.33122038	W	-6.80147078	-4.72478887	10.83181588	W	7.48268239	-10.29930313	-2.65051771	W	-7.86054297	3.96038519	-6.08843911
W	5.08827640	-5.89851038	1.31338441	W	-5.89851038	1.31338441	12.55406185	W	-8.20820808	-12.31827937	-1.10962543	W	-8.85418181	-4.01897701	-6.48741825
W	4.04074666	11.65397987	2.92722281	W	-6.17987487	-1.97512787	10.95394874	W	-6.20628667	10.95394874	-1.52369107	O	-10.21703329	5.54889696	-6.97157160
W	2.62327940	11.18772939	5.33122038	W	-1.37849167	-4.99976231	12.36059672	W	-1.37849167	-4.99976231	12.36059672	O	-12.37512329	5.54889696	-6.97157160
W	4.04074666	11.65397987	2.92722281	W	1.37849167	4.99976231	12.36059672	W	-8.44398522	11.62214959	3.13972755	W	-6.80448465	3.96552173	-5.50358899
W	4.03192324	7.82405533	9.08439111	W	1.37849167	4.99976231	12.36059672	W	-11.0390828	6.62214959	3.13972755	W	-6.80448465	3.96552173	-5.50358899
W	5.01615171	10.49504689	5.72276760	W	0.00000000	-9.18194768	11.72043968	W	-11.0390828	6.62214959	3.13972755	W	-6.80448465	3.96552173	-5.50358899
W	11.19542227	-6.61286799	4.69623144	W	-3.11301450	-9.18194768	11.72043968	W	-9.62223235	-9.18194768	-1.10962543	W	-6.80448465	3.96552173	-5.50358899
W	8.85032376	5.51307946	7.59797592	W	-7.63545066	-2.48099311	10.49504689	W	-11.48677474	9.41257433	1.38081632	W	1.86324030	10.79187737	-6.06115121
W	9.43316486	8.97157160	6.90828805	W	-1.94548911	10.63979163	8.02347057	W	-11.48677474	9.41257433	1.38081632	W	-3.00050892	12.97996528	-6.90828805
W	9.40713463	3.12514707	7.87169510	W	1.94548911	-10.63979163	8.02347057	W	-5.07036996	-11.76802250	-0.73617629	W	0.59362365	10.59304669	-6.33122038
W	11.09890325	-1.51373023	5.50358899	W	-2.80924025	6.23904872	10.83181588	W	-5.40228989	-11.83191372	-1.39591632	W	4.20973324	13.24209126	-5.37251818
W	11.47022281	5.40710710	7.87169510	W	-5.40680510	-1.51373023	5.50358899	W	-6.34232230	10.29930313	2.65051771	W	-6.64443361	-6.97157160	-7.87169510
W	9.65222357	8.63877270	2.92722281	W	-3.75701309	5.71108489	13.44923170	W	-12.30323243	0.24191742	-2.92722281	W	-1.32764800	8.69921844	-6.08843911
W	11.31985828	-4.69623144	1.10962543	W	-4.69623144	1.10962543	12.55406185	W	-14.82554651	-0.86319167	1.38081632	W	-1.42841597	6.92296879	-6.90828805
W	11.48674774	9.41257433	1.38081632	W	-7.86054297	-3.96358159	9.08439111	W	-7.86054297	-3.96358159	9.08439111	W	-6.48553276	-5.51307946	-7.59797592
W	5.07036996	11.76802250	-0.73617629	W	-8.73255032	-2.83737760	11.72043968	W	-8.73255032	-2.83737760	11.72043968	W	-5.93910759	3.96874829	-10.81615988
W	4.81054044	6.90828805	1.10962543	W	0.00000000	-8.02838793	10.49504689	W	-11.48677474	9.41257433	1.38081632	W	-6.80448465	3.96552173	-5.50358899
W	5.40228989	11.83191372	-1.39591632	W	-6.82620460	-10.79108773	6.06115121	W	-7.86054297	-3.96358159	9.08439111	W	-7.86054297	-3.96358159	9.08439111
W	10.10200000	10.10200000	1.31338441	W	-3.84243340	-4.4784599	7.59797592	W	-8.20820808	-12.31827937	-1.10962543	W	-7.86054297	-3.96358159	9.08439111
W	0.00000000	0.00000000	5.72276760	W	-2.20017868	-11.42846156	8.97157160	W	-4.4398522	-11.62214959	-3.13972755	W	-4.21304358	-4.69756285	-11.87197146
W	1.63943384	12.59345082	7.78194230	W	1.86324030	-10.79108773	6.06115121	W	-4.83047658	-9.82933861	-6.06115121	W	-7.70701309	-5.51307946	-7.59797592
W	5.19712058	12.42838468	6.90828805	W	2.12001863	-4.24668612	10.49504689	W	-2.62337940	-11.8772939	-5.33122038	W	-5.51307946	9.62296879	-6.90828805
W	10.44481571	7.82405533	4.10435760	Mo	-4.71896803	6.49510227	10.49504689	W	-5.00837640	-12.73930335	-5.72518181	W	-11.49596092	-5.90387619	5.72518181
W	9.94717186	-5.10664409	6.061												