

Supporting Information

Theoretical studies on chiral polyoxoanion $[P_2Mo_{18}O_{62}]^{6-}$ and $[PMo_9O_{31}(OH_2)_3]^{3-}$ with histidine: chiral inversion and chiral induction

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Table S1. Experimental and theoretical optimized bond lengths for $[\text{P}_2\text{Mo}_{18}\text{O}_{62}]^{6-}$ (Å)

Bond	Exp	Cal
Mo7-O45	2.36	2.28
O45-Mo11	1.75	1.76
Mo11-O48	2.35	2.27
O48-Mo13	1.77	1.78
Mo13-O69	2.10	2.09
O69-Mo16	1.83	1.84
Mo16-O34	1.77	1.79
O34 - Mo9	2.35	2.26

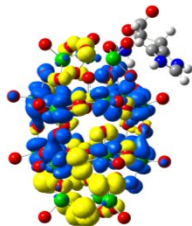
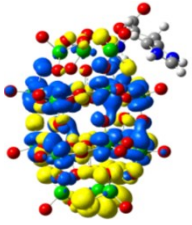
Table S2. Distortion stabilization energy for symmetric $[\text{P}_2\text{Mo}_{18}\text{O}_{62}]^{6-}$ and ${}^L-[\text{P}_2\text{Mo}_{18}\text{O}_{62}]^{6-}$ (kcal mol⁻¹)

	B3LYP	BP86	PBE0
ΔE	-5.88	-4.44	-6.45

$$\Delta E = E(D_3) - E(D_{3h})$$

Undergo $\text{Mo}_{18}^{\text{VI}} \rightarrow \text{Mo}_{18} \text{1e} \rightarrow \text{Mo}_{18}^{\text{VI}}$

Table S3. The EDDMs for crucial transitions contribute to the ECD spectra of **1b**. (Electron densities move from the yellow area to the blue area)

Excitation state	MO	Coefficient	EDDM
18	427→434, 429→434	-0.1585, 0.6464	
19	426→434, 427→434 428→434	-0.1682, 0.1073 0.6329	

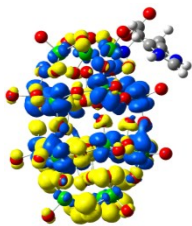
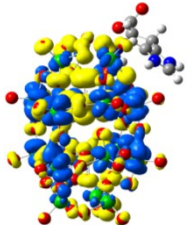
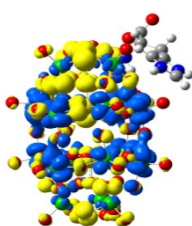
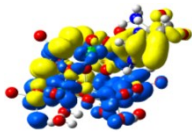
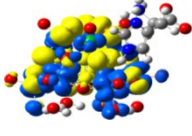
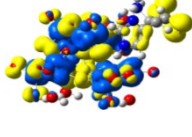
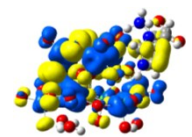
62	408→434, 413→434	-0.2327, 0.2061	
	427→435, 428→435	-0.1420, -0.1143	
	428→436, 429→435	0.3496, 0.3180	
88	403→434, 405→434	-0.1516, 0.1800	
	410→434, 414→434	0.1225, -0.1025	
	421→435, 421→436	0.2013, -0.1847	
	422→435, 424→436	0.2799, -0.1103	
	425→435, 427→435	0.2687, 0.1017	
91	399→434, 400→434	-0.1537, -0.1187	
	402→434, 405→434	-0.1349, -0.1707	
	422→435, 422→436	0.1278, 0.2100	
	423→436, 424→435	0.1342, 0.3647	
	424→436	0.1165	

Table S4. The EDDMs for crucial transitions contribute to the ECD spectra of **2a**.

Excitation state	MO	Coefficient	EDDM
33	247→254, 248→253	-0.1588, 0.4414	
	248→254, 248→255	0.2643, -0.1154	
	249→253, 249→254	-0.1426, -0.2990	
35	246→253, 246→254	0.1443, 0.1218	
	247→253, 248→253	0.4657, 0.1404	
	248→254, 248→255	-0.3253, -0.1670	
64	238→255, 240→253	0.1013, 0.1519	
	242→253, 244→253	-0.1363, 0.1485	
	244→255, 245→255	-0.1423, -0.1103	
	246→254, 246→255	-0.2053, 0.1141	
	246→256, 247→256	-0.1086, 0.2123	
	248→256, 248→257	0.1637, -0.1230	
	249→257, 250→264	-0.1090, 0.2468	
66	241→253, 244→253	0.1254, 0.1124	
	247→256, 247→257	-0.1129, -0.2275	
	248→255, 248→256	0.1065, 0.1640	
	248→257, 248→258	0.2801, -0.2115	
	248→259, 249→258	-0.1002, 0.1593	

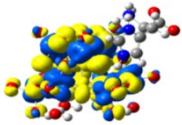
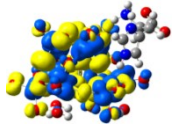
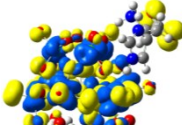
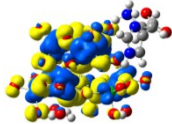
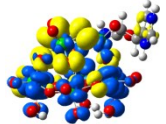
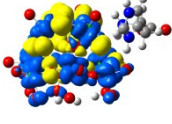
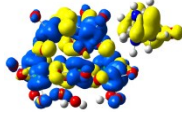
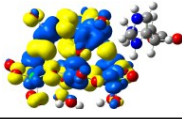
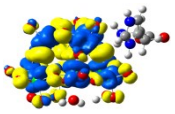
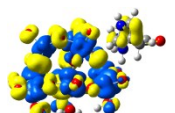
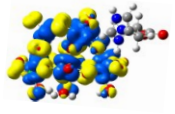
70	231→255, 233→253	-0.1113, 0.1518	
	235→253, 240→253	-0.1044, 0.1072	
	240→254, 242→253	-0.1492, 0.1041	
	245→255, 247→254	0.2079, 0.1149	
	247→257, 248→256	-0.1710, -0.1783	
	248→258	-0.1697	
77	238→253, 239→253	-0.1078, -0.1002	
	240→253, 241→253	0.1465, -0.1077	
	241→255, 244→255	-0.1546, -0.1452	
	245→255, 246→255	0.1760, -0.1076	
	247→256, 247→257	0.1191, -0.1050	
	248→258	0.2796	
88	229→253, 230→253	-0.1069, -0.1702	
	234→255, 236→253	-0.1034, 0.1129	
	238→253, 238→254	-0.1265, -0.1409	
	238→255, 239→253	0.1397, 0.1231	
	239→255, 241→257	-0.1175, 0.1334	
	242→254, 244→255	-0.1501, 0.1580	
90	245→255, 250→265	0.1149, 0.1933	
	237→254, 243→253	0.1421, -0.1758	
	245→256, 246→256	-0.1767, 0.2070	
	246→257, 247→255	0.2356, 0.1153	
	247→257, 248→254	-0.1603, 0.1114	

Table S5. The EDDMs for crucial transitions contribute to the ECD spectra of **2b**.

Excitation state	MO	Coefficient	EDDM
31	247→253, 247→254	0.1765, 0.1936	
	248→253, 248→255	0.5416, 0.2120	
	249→254	-0.1061	
45	245→254, 245→255	0.1140, -0.1012	
	247→253, 247→254	-0.2537, 0.3096	
	248→254, 248→255	0.3036, -0.3009	
	248→257	0.1091	
48	238→253, 239→253	-0.1472, 0.1185	
	245→254, 246→255	0.1581, -0.1331	
	247→254, 247→255	0.2411, 0.1375	
	248→253, 248→255	-0.1786, 0.2165	
	249→256, 249→257	0.1545, 0.1254	
	251→263	0.3189	
64	241→253, 242→253	-0.1009, 0.1023	
	242→257, 243→254	-0.1214, -0.1206	
	244→255, 245→255	0.1905, -0.1343	

	245→257, 247→256	-0.1248, 0.2361	
	247→257, 248→255	0.1893, -0.1015	
	248→256	0.2622	
65	232→253, 239→253	0.1318, 0.1328	
	240→254, 241→253	0.1709, 0.1454	
	242→254, 243→254	-0.1586, -0.1587	
	247→257, 248→256	0.2654, -0.2343	
80	231→253, 233→255	0.1936, 0.1161	
	237→253, 241→255	-0.1490, -0.1510	
	242→254, 242→255	-0.1291, 0.1143	
	243→255, 244→254	-0.1310, 0.1194	
	246→253, 246→257	0.1296, 0.1185	
	247→258, 249→259	-0.1933, -0.1270	
84	229→253, 230→253	0.1208, -0.1102	
	236→254, 237→254	0.1077, -0.1332	
	238→254, 244→253	0.1783, 0.2066	
	245→256, 246→257	0.1928, 0.1083	
	247→254, 248→254	0.1026, -0.1085	
	248→256	0.1534	

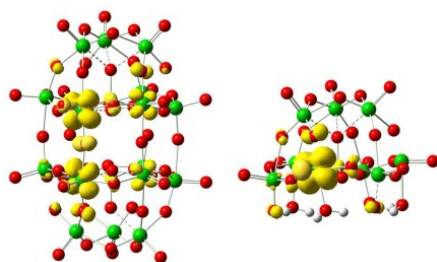


Fig. S1 Spin density distribution computed for $[\text{P}_2\text{Mo}_{18}\text{O}_{62}]^{7-}$ (left) and $[\text{PMo}_9\text{O}_{31}(\text{OH}_2)_3]^{4-}$ (right).

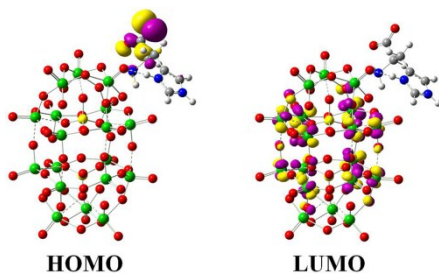


Fig. S2 Frontier molecular orbitals for **1a**.

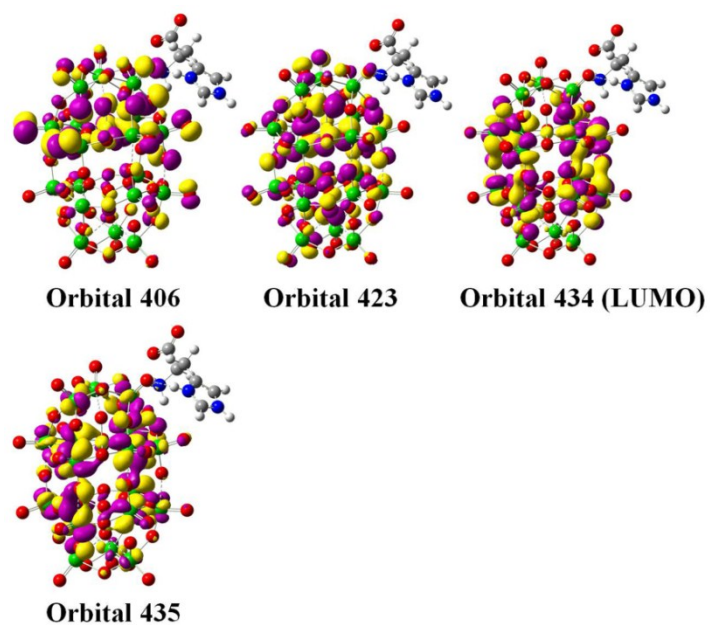


Fig. S3 Molecular orbitals involved in main transitions in the calculated ECD of **1a**.

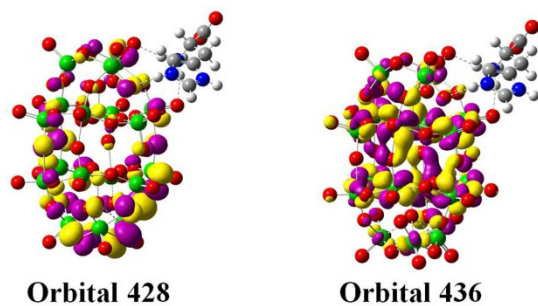


Fig. S4 Molecular orbitals involved in main transitions in the calculated ECD of **1b**.