

P₆Mo₁₈O₇₃ Heteropolyanion and Its Four-Copper Complex: Theoretical and Experimental Investigation

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Table S1. Bond lengths (Å) and angles (°) for **1**.

Cu(1)-O(36)	1.899(4)	Cu(2)-O(34)	1.906(3)
Cu(1)-N(2)	1.969(5)	Cu(2)-N(4)	1.977(5)
Cu(1)-N(1)	2.015(5)	Cu(2)-N(3)	1.994(5)
Cu(1)-O(14)	2.039(4)	Cu(2)-O(1W)	2.007(4)
Cu(1)-O(2W)	2.226(4)		
O(36)-Cu(1)-N(2)	172.83(18)	N(1)-Cu(1)-O(2W)	111.31(19)
O(36)-Cu(1)-N(1)	91.86(18)	O(14)-Cu(1)-O(2W)	96.87(17)
N(2)-Cu(1)-N(1)	81.67(19)	O(34)-Cu(2)-N(4)	176.99(19)
O(36)-Cu(1)-O(14)	93.43(15)	O(34)-Cu(2)-N(3)	96.55(17)
N(2)-Cu(1)-O(14)	93.74(17)	N(4)-Cu(2)-N(3)	81.6(2)
N(1)-Cu(1)-O(14)	151.31(17)	O(34)-Cu(2)-O(1W)	87.33(17)
O(36)-Cu(1)-O(2W)	90.00(16)	N(4)-Cu(2)-O(1W)	95.0(2)
N(2)-Cu(1)-O(2W)	89.47(18)	N(3)-Cu(2)-O(1W)	165.6(2)

Table S2 Comparison of calculated and experimental bond lengths (Å) of [KP₆Mo₁₈O₇₃]¹⁰⁻ anion.

Distances	Calc.	Expt	Distances	Calc.	Expt.
Mo1-O _t	1.743	1.689	Mo4-O31	1.969	2.001
Mo3-O _t	1.767	1.694	Mo8-O15	2.167	2.119
Mo4-O _t	1.748	1.697	Mo8-O16	1.908	1.884
Mo8-O _t	1.748	1.702	Mo8-O19	2.281	2.258
Mo24-O _t	1.756	1.714	Mo8-O20	1.959	1.934
Mo25-O _t	1.747	1.714	Mo24-O12	2.157	2.055
P26-O _t	1.505	1.511	Mo24-O27	1.825	1.827
Mo1-O12	2.100	2.048	Mo24-O30	2.437	2.305
Mo2-O13	1.862	1.804	Mo25-O27	2.197	1.979
Mo2-O14	1.814	1.771	Mo25-O28	1.953	1.891
Mo3-O13	2.103	2.076	P26-O30	1.639	1.578
Mo3-O15	1.826	1.786	P26-O31	1.622	1.538
Mo3-O22	2.399	2.379	P26-O32	1.546	1.526
Mo4-O14	2.111	2.034			
Mo4-O16	1.949	1.885			
Mo4-O17	1.908	1.854			
Mo4-O21	2.160	2.215			

Table S3 Electronic parameters (eV) of $[\text{P}_2\text{Mo}_{18}\text{O}_{62}]^{6-}$, $[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{7-}$ and $[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{10-}$ anions.

	$[\text{P}_2\text{Mo}_{18}\text{O}_{62}]^{6-}$	$[\text{P}_6\text{Mo}_{18}\text{O}_{73}]^{7-}$	$[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{10-}$
$E(\text{LUMO})$	-4.566	-5.980	-4.282xxx
$E(\text{HOMO})$	-5.973	-5.511	-3.759xxx
q/m	0.33	0.39	0.56

Table S4 Bind energies of $[\text{KH}_2\text{P}_6\text{Mo}_{18}\text{O}_{73}]^{8-}$.

	sites ^[a]	VWN/TZP	PW91PW91/TZP
1	27/27	-32.89028	
2	12/12	-32.87245	
3	17/17	-32.86457	
4	20/20	-32.89932	
6	18/18	-32.89266	
7	15/15	-32.90566	
8	14/14	-32.86691	
9	31/31	-32.88453	
10	32/32	-32.91182	-30.255xx
11	30/30	-32.86672	
21	36/36	-32.86797	
26	29/29...33/33 ^[b]	-32.96464	-30.274036
22	29/29...34/34 ^[c]	-32.95712	-30.28003
23	35/35	-32.87660	
24	33/33	-32.91176	-30.247916
25	34/34	-32.900473	

a) Labels are shown in Figure 1 of the paper. b) The hydrogen atom binds to O(29) and form hydrogen bond with O(33). c) The hydrogen atom binds to O(29) and form hydrogen bond with O(34).

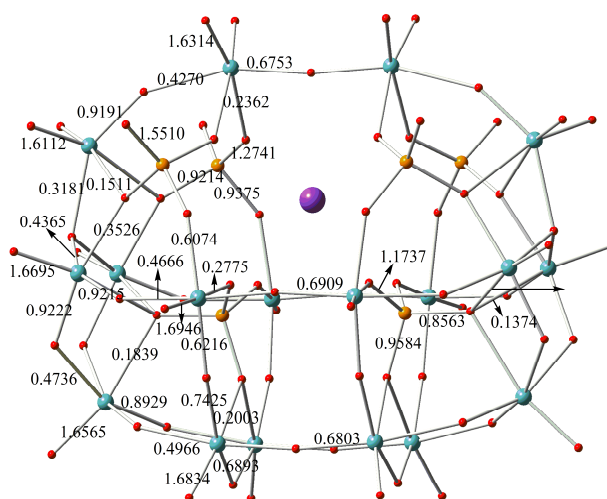


Figure S1. Mayer bond order of $[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{10-}$ anion.

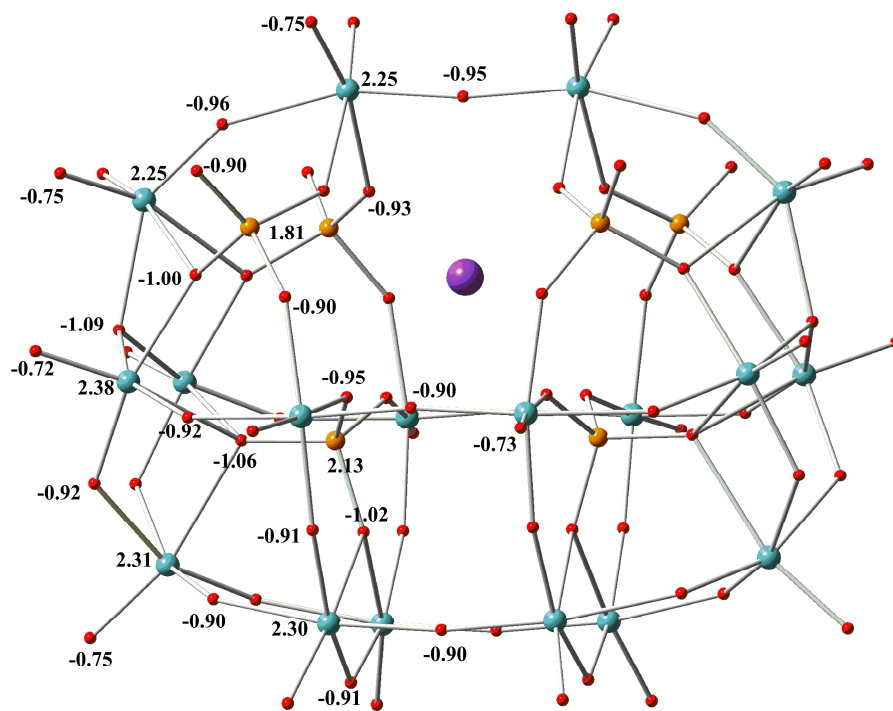


Figure S2. Mulliken charges of $[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{10-}$ anion.

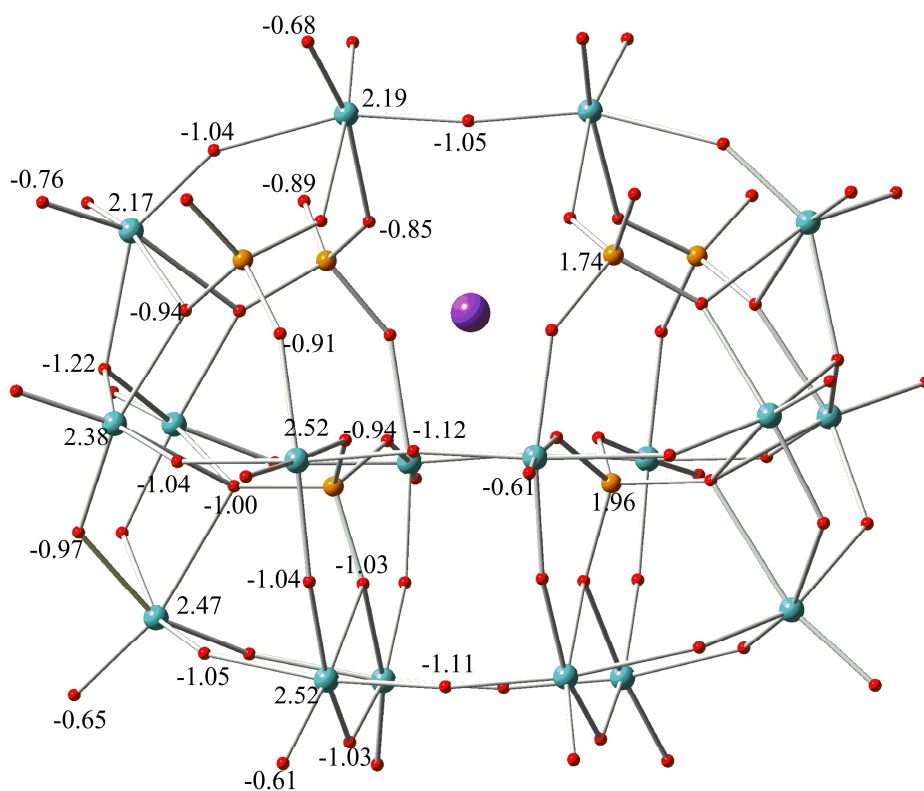


Figure S3. Multipolar charges of $[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{10-}$ anion.

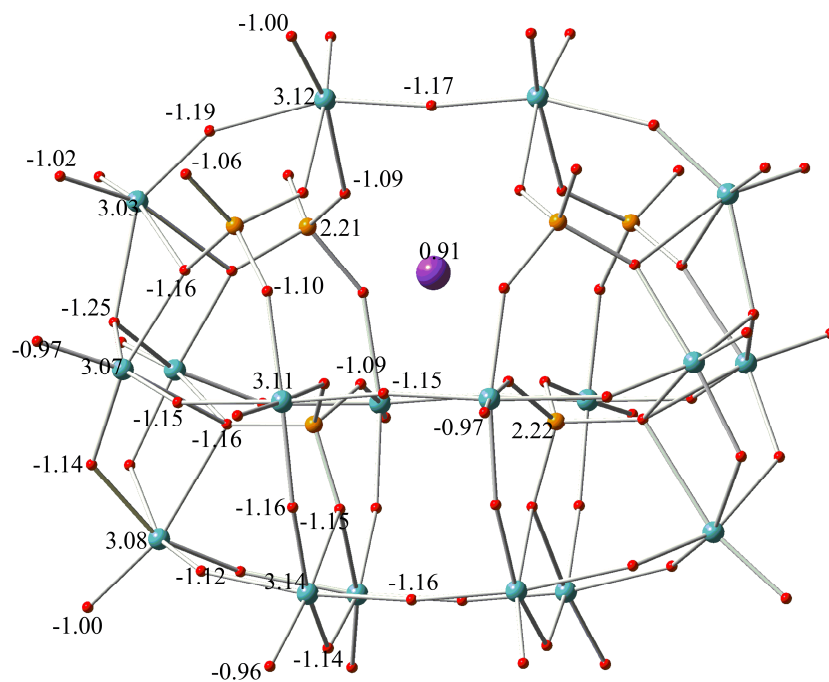


Figure S4. Voronoi charges of $[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{10-}$ anion.

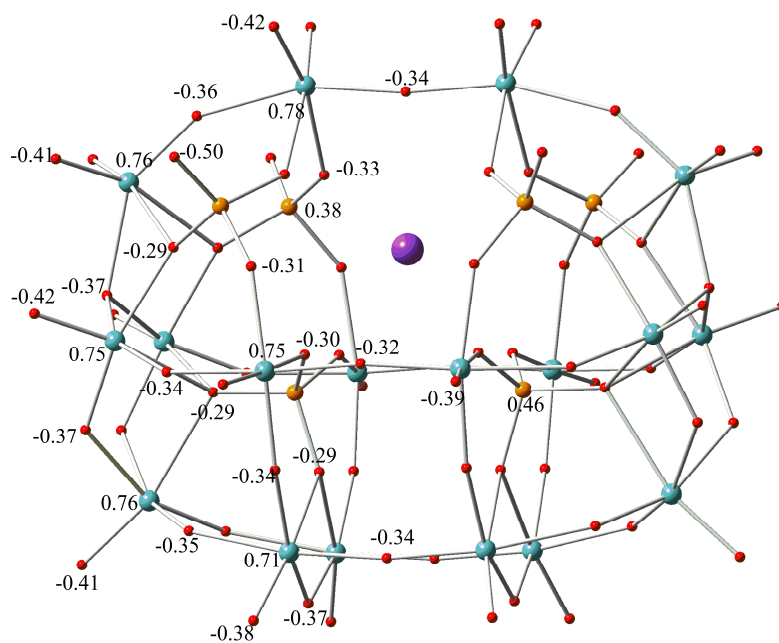


Figure S5. Hirshfeld charges of $[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{10-}$ anion.

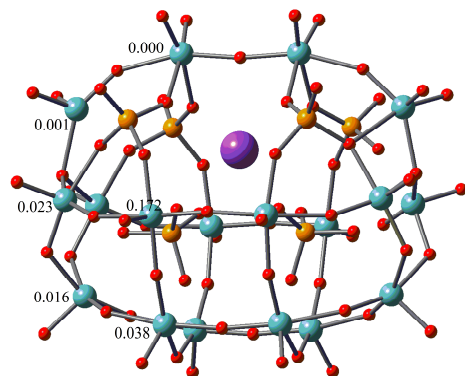


Figure S6. Spin densities of $[\text{KP}_6\text{Mo}_{18}\text{O}_{73}]^{10-}$ anion.

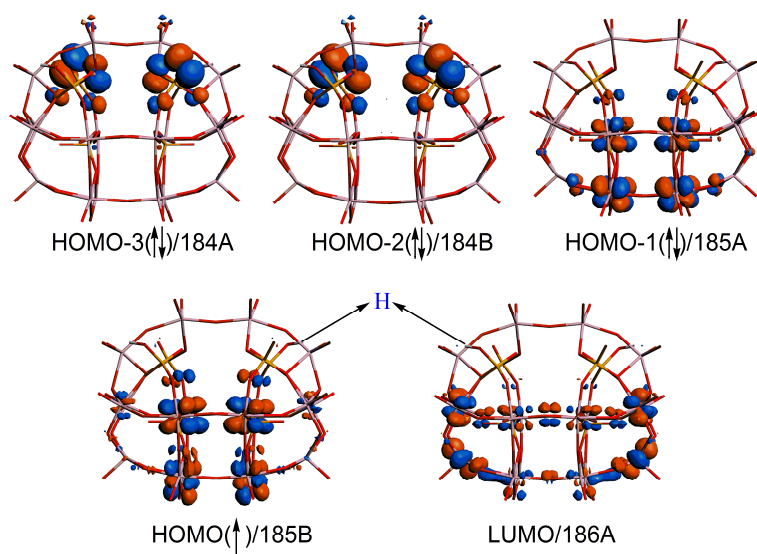


Figure S7. Schematic view of the frontier orbitals of protonated $\text{H}_2\text{KP}_6\text{Mo}_{18}\text{O}_{73}^{8-}$ anion under C_2 symmetry

Coordinates of KP_6Mo_{18} (7 \square) at PW91PW91/TZP level:

1 P	2.160298	0.000000	0.958039
2 P	2.872127	2.448790	-2.487069
3 P	2.872127	-2.448790	-2.487069
4 Mo	5.162962	-1.771551	0.008264
5 Mo	5.162962	1.771551	0.008264
6 Mo	1.915893	0.000000	-4.759539
7 Mo	5.286845	0.000000	-2.944040
8 Mo	5.037688	0.000000	2.969266
9 Mo	1.913153	1.700684	3.970683
10 Mo	-1.913153	1.700684	3.970683
11 Mo	1.897042	3.396624	0.585911
12 Mo	-1.897042	3.396624	0.585911
13 Mo	-5.162962	1.771551	0.008264
14 Mo	-5.162962	-1.771551	0.008264
15 Mo	-1.915893	0.000000	-4.759539
16 Mo	-5.286845	0.000000	-2.944040
17 Mo	-5.037688	0.000000	2.969266
18 Mo	-1.913153	-1.700684	3.970683
19 Mo	1.913153	-1.700684	3.970683
20 Mo	-1.897042	-3.396624	0.585911
21 Mo	1.897042	-3.396624	0.585911
22 P	-2.160298	0.000000	0.958039
23 P	-2.872127	-2.448790	-2.487069
24 P	-2.872127	2.448790	-2.487069
25 K	0.000000	0.000000	-1.620371
26 O	5.781109	0.000000	-0.862775
27 O	3.962529	-1.545520	-1.688624
28 O	3.757568	0.000000	0.948322
29 O	3.878526	-2.930286	0.624521
30 O	6.363456	-2.829961	-0.614969
31 O	5.903434	-1.307099	1.649789
32 O	6.363456	2.829961	-0.614969
33 O	5.903434	1.307099	1.649789
34 O	3.878526	2.930286	0.624521
35 O	3.962529	1.545520	-1.688624
36 O	1.800912	-1.489376	-3.022349
37 O	1.800912	1.489376	-3.022349
38 O	2.106209	1.346040	-5.846639
39 O	2.106209	-1.346040	-5.846639
40 O	-5.781109	0.000000	-0.862775
41 O	-3.962529	1.545520	-1.688624
42 O	-3.757568	0.000000	0.948322
43 O	-3.878526	2.930286	0.624521

44 O	-6.363456	2.829961	-0.614969
45 O	-5.903434	1.307099	1.649789
46 O	-6.363456	-2.829961	-0.614969
47 O	-5.903434	-1.307099	1.649789
48 O	-3.878526	-2.930286	0.624521
49 O	-3.962529	-1.545520	-1.688624
50 O	-1.800912	1.489376	-3.022349
51 O	-1.800912	-1.489376	-3.022349
52 O	-2.106209	-1.346040	-5.846639
53 O	-2.106209	1.346040	-5.846639
54 O	0.000000	0.000000	-4.552057
55 O	6.275203	1.354647	-3.401283
56 O	3.892310	0.000000	-4.151438
57 O	6.275203	-1.354647	-3.401283
58 O	6.294765	0.000000	4.148392
59 O	3.882815	-1.334140	3.564087
60 O	3.882815	1.334140	3.564087
61 O	2.277661	2.781821	5.261890
62 O	2.014875	0.000000	4.924225
63 O	1.690947	0.000000	2.459599
64 O	1.882536	2.871855	2.464814
65 O	0.000000	1.698919	4.095289
66 O	-2.277661	2.781821	5.261890
67 O	-1.882536	2.871855	2.464814
68 O	2.143193	3.349129	-1.332454
69 O	2.208867	5.076681	0.852995
70 O	0.000000	3.500087	0.479293
71 O	1.634322	1.258003	0.250141
72 O	1.634322	-1.258003	0.250141
73 O	2.143193	-3.349129	-1.332454
74 O	-2.208867	5.076681	0.852995
75 O	3.529366	3.415264	-3.428918
76 O	3.529366	-3.415264	-3.428918
77 O	-6.275203	-1.354647	-3.401283
78 O	-3.892310	0.000000	-4.151438
79 O	-6.275203	1.354647	-3.401283
80 O	-6.294765	0.000000	4.148392
81 O	-3.882815	1.334140	3.564087
82 O	-3.882815	-1.334140	3.564087
83 O	-2.277661	-2.781821	5.261890
84 O	-2.014875	0.000000	4.924225
85 O	-1.690947	0.000000	2.459599
86 O	-1.882536	-2.871855	2.464814
87 O	0.000000	-1.698919	4.095289

88 O	2.277661	-2.781821	5.261890
89 O	1.882536	-2.871855	2.464814
90 O	-2.143193	-3.349129	-1.332454
91 O	-2.208867	-5.076681	0.852995
92 O	0.000000	-3.500087	0.479293
93 O	-1.634322	-1.258003	0.250141
94 O	-1.634322	1.258003	0.250141
95 O	-2.143193	3.349129	-1.332454
96 O	2.208867	-5.076681	0.852995
97 O	-3.529366	-3.415264	-3.428918
98 O	-3.529366	3.415264	-3.428918

Coordinates of $\text{KP}_6\text{Mo}_{18}\text{-3e}$ (10 □) at PW91PW91/TZP level:

1 P	2.182712	0.000000	0.980618
2 P	2.867994	2.438748	-2.477754
3 P	2.867994	-2.438748	-2.477754
4 Mo	5.183906	-1.782196	-0.001746
5 Mo	5.183906	1.782196	-0.001746
6 Mo	1.922045	0.000000	-4.738837
7 Mo	5.300501	0.000000	-2.944635
8 Mo	5.032546	0.000000	2.975787
9 Mo	1.900023	1.700785	4.001776
10 Mo	-1.900023	1.700785	4.001776
11 Mo	1.888238	3.382492	0.622283
12 Mo	-1.888238	3.382492	0.622283
13 Mo	-5.183906	1.782196	-0.001746
14 Mo	-5.183906	-1.782196	-0.001746
15 Mo	-1.922045	0.000000	-4.738837
16 Mo	-5.300501	0.000000	-2.944635
17 Mo	-5.032546	0.000000	2.975787
18 Mo	-1.900023	-1.700785	4.001776
19 Mo	1.900023	-1.700785	4.001776
20 Mo	-1.888238	-3.382492	0.622283
21 Mo	1.888238	-3.382492	0.622283
22 P	-2.182712	0.000000	0.980618
23 P	-2.867994	-2.438748	-2.477754
24 P	-2.867994	2.438748	-2.477754
25.K	0.000000	0.000000	-1.602250
26 O	5.807096	0.000000	-0.884169
27 O	3.989799	-1.533430	-1.715104
28 O	3.780621	0.000000	0.958122
29 O	3.903115	-2.922077	0.607973
30 O	6.393602	-2.850916	-0.622897
31 O	5.940568	-1.309358	1.623321
32 O	6.393602	2.850916	-0.622897
33 O	5.940568	1.309358	1.623321
34 O	3.903115	2.922077	0.607973
35 O	3.989799	1.533430	-1.715104
36 O	1.827943	-1.443443	-3.038396
37 O	1.827943	1.443443	-3.038396
38 O	2.136595	1.348091	-5.834568
39 O	2.136595	-1.348091	-5.834568
40 O	-5.807096	0.000000	-0.884169
41 O	-3.989799	1.533430	-1.715104
42 O	-3.780621	0.000000	0.958122

43 O	-3.903115	2.922077	0.607973
44 O	-6.393602	2.850916	-0.622897
45 O	-5.940568	1.309358	1.623321
46 O	-6.393602	-2.850916	-0.622897
47 O	-5.940568	-1.309358	1.623321
48 O	-3.903115	-2.922077	0.607973
49 O	-3.989799	-1.533430	-1.715104
50 O	-1.827943	1.443443	-3.038396
51 O	-1.827943	-1.443443	-3.038396
52 O	-2.136595	-1.348091	-5.834568
53 O	-2.136595	1.348091	-5.834568
54 O	0.000000	0.000000	-4.595321
55 O	6.302267	1.354702	-3.406647
56 O	3.932732	0.000000	-4.177298
57 O	6.302267	-1.354702	-3.406647
58 O	6.342796	0.000000	4.122735
59 O	3.936854	-1.354297	3.552051
60 O	3.936854	1.354297	3.552051
61 O	2.316806	2.802761	5.272243
62 O	2.012064	0.000000	4.953852
63 O	1.722896	0.000000	2.487270
64 O	1.838822	2.865686	2.471854
65 O	0.000000	1.738986	4.151848
66 O	-2.316806	2.802761	5.272243
67 O	-1.838822	2.865686	2.471854
68 O	2.125206	3.322704	-1.363958
69 O	2.257395	5.068007	0.855592
70 O	0.000000	3.532765	0.491512
71 O	1.651273	1.254813	0.271126
72 O	1.651273	-1.254813	0.271126
73 O	2.125206	-3.322704	-1.363958
74 O	-2.257395	5.068007	0.855592
75 O	3.516077	3.388933	-3.456156
76 O	3.516077	-3.388933	-3.456156
77 O	-6.302267	-1.354702	-3.406647
78 O	-3.932732	0.000000	-4.177298
79 O	-6.302267	1.354702	-3.406647
80 O	-6.342796	0.000000	4.122735
81 O	-3.936854	1.354297	3.552051
82 O	-3.936854	-1.354297	3.552051
83 O	-2.316806	-2.802761	5.272243
84 O	-2.012064	0.000000	4.953852
85 O	-1.722896	0.000000	2.487270
86 O	-1.838822	-2.865686	2.471854

87 O	0.000000	-1.738986	4.151848
88 O	2.316806	-2.802761	5.272243
89 O	1.838822	-2.865686	2.471854
90 O	-2.125206	-3.322704	-1.363958
91 O	-2.257395	-5.068007	0.855592
92 O	0.000000	-3.532765	0.491512
93 O	-1.651273	-1.254813	0.271126
94 O	-1.651273	1.254813	0.271126
95 O	-2.125206	3.322704	-1.363958
96 O	2.257395	-5.068007	0.855592
97 O	-3.516077	-3.388933	-3.456156
98 O	-3.516077	3.388933	-3.456156

Coordinates of $\text{KH}_2\text{P}_6\text{Mo}_{18}\text{-3e}$ (8 □) at PW91PW91/TZP level:

1	P	-2.186328	-0.025131	-1.042642
2	P	-2.882533	2.432744	2.428570
3	P	-2.810295	-2.369036	2.292996
4	Mo	-5.164741	-1.777423	-0.118424
5	Mo	-5.205152	1.760649	-0.075981
6	Mo	-1.912224	0.106025	4.719491
7	Mo	-5.250156	-0.014079	2.869916
8	Mo	-5.031061	-0.006884	-3.071013
9	Mo	-1.897724	1.697846	-4.067343
10	Mo	1.902667	1.703710	-4.088892
11	Mo	-1.902095	3.366624	-0.680631
12	Mo	1.878809	3.403884	-0.736118
13	Mo	5.164741	1.777423	-0.118424
14	Mo	5.205152	-1.760649	-0.075981
15	Mo	1.912224	-0.106025	4.719491
16	Mo	5.250156	0.014079	2.869916
17	Mo	5.031061	0.006884	-3.071013
18	Mo	1.897724	-1.697846	-4.067343
19	Mo	-1.902667	-1.703710	-4.088892
20	Mo	1.902095	-3.366624	-0.680631
21	Mo	-1.878809	-3.403884	-0.736118
22	P	2.186328	0.025131	-1.042642
23	P	2.882533	-2.432744	2.428570
24	P	2.810295	2.369036	2.292996
25	K	0.000000	0.000000	1.533570
26	O	-5.798147	-0.025839	0.820804
27	O	-3.855432	-1.432205	1.553536
28	O	-3.786956	-0.027756	-1.032181
29	O	-3.879810	-2.930845	-0.707714
30	O	-6.325488	-2.841992	0.587292
31	O	-5.951729	-1.343482	-1.720550
32	O	-6.415653	2.817699	0.552462
33	O	-5.947834	1.278997	-1.699598
34	O	-3.916465	2.896094	-0.670827
35	O	-4.029626	1.532904	1.681894
36	O	-1.772579	-1.545478	3.033014
37	O	-1.829766	1.425081	2.967920
38	O	-2.050725	1.452003	5.810683
39	O	-2.212636	-1.240022	5.793582
40	O	5.798147	0.025839	0.820804
41	O	3.855432	1.432205	1.553536
42	O	3.786956	0.027756	-1.032181
43	O	3.879810	2.930845	-0.707714

44	O	6.325488	2.841992	0.587292
45	O	5.951729	1.343482	-1.720550
46	O	6.415653	-2.817699	0.552462
47	O	5.947834	-1.278997	-1.699598
48	O	3.916465	-2.896094	-0.670827
49	O	4.029626	-1.532904	1.681894
50	O	1.772579	1.545478	3.033014
51	O	1.829766	-1.425081	2.967920
52	O	2.050725	-1.452003	5.810683
53	O	2.212636	1.240022	5.793582
54	O	0.000000	0.000000	4.546883
55	O	-6.435327	1.142279	3.392726
56	O	-3.889798	0.115899	4.098096
57	O	-5.955802	-1.569393	3.326519
58	O	-6.331136	-0.010763	-4.220249
59	O	-3.930064	-1.361655	-3.639084
60	O	-3.935423	1.346096	-3.633477
61	O	-2.302511	2.809016	-5.326117
62	O	-2.009953	-0.000871	-5.022035
63	O	-1.721313	-0.020859	-2.543261
64	O	-1.852537	2.852767	-2.525625
65	O	-0.000471	1.726812	-4.206082
66	O	2.295501	2.802971	-5.361135
67	O	1.836078	2.906734	-2.563004
68	O	-2.148306	3.302841	1.309769
69	O	-2.269917	5.048698	-0.893256
70	O	-0.008188	3.513639	-0.566556
71	O	-1.669048	1.225645	-0.318093
72	O	-1.650708	-1.284116	-0.331106
73	O	-2.157672	-3.413620	1.341001
74	O	2.226093	5.094045	-0.898816
75	O	-3.515289	3.365061	3.428238
76	O	-3.724539	-3.255558	3.295449
77	O	6.435327	-1.142279	3.392726
78	O	3.889798	-0.115899	4.098096
79	O	5.955802	1.569393	3.326519
80	O	6.331136	0.010763	-4.220249
81	O	3.930064	1.361655	-3.639084
82	O	3.935423	-1.346096	-3.633477
83	O	2.302511	-2.809016	-5.326117
84	O	2.009953	0.000871	-5.022035
85	O	1.721313	0.020859	-2.543261
86	O	1.852537	-2.852767	-2.525625
87	O	0.000471	-1.726812	-4.206082

88	O	-2.295501	-2.802971	-5.361135
89	O	-1.836078	-2.906734	-2.563004
90	O	2.148306	-3.302841	1.309769
91	O	2.269917	-5.048698	-0.893256
92	O	0.008188	-3.513639	-0.566556
93	O	1.669048	-1.225645	-0.318093
94	O	1.650708	1.284116	-0.331106
95	O	2.157672	3.413620	1.341001
96	O	-2.226093	-5.094045	-0.898816
97	O	3.515289	-3.365061	3.428238
98	O	3.724539	3.255558	3.295449
99	H	4.593876	2.770355	3.415623
100	H	-4.593876	-2.770355	3.415623

Coordinates of P₂Mo₁₈ at PW91PW91/TZP level:

1	P	0.000000	0.000000	2.036936
2	P	0.000000	0.000000	-2.036936
3	O	0.000000	0.000000	3.641108
4	O	0.741595	1.291832	1.577131
5	O	-1.489557	-0.003676	1.577131
6	O	0.747962	-1.288156	1.577131
7	O	0.000000	0.000000	-3.641108
8	O	0.747962	1.288156	-1.577131
9	O	0.741595	-1.291832	-1.577131
10	O	-1.489557	0.003676	-1.577131
11	Mo	-3.122469	1.711582	-1.897638
12	Mo	3.030933	-1.878659	-1.902313
13	Mo	0.078962	-3.559928	-1.897638
14	Mo	-3.142433	-1.685535	-1.902313
15	Mo	3.043508	1.848347	-1.897638
16	Mo	0.111500	3.564194	-1.902313
17	Mo	-0.990061	-1.715618	-4.984084
18	Mo	-0.990739	1.715227	-4.984084
19	Mo	1.980799	0.000391	-4.984084
20	Mo	3.043508	-1.848347	1.897638
21	Mo	-3.142433	1.685535	1.902313
22	Mo	-3.122469	-1.711582	1.897638
23	Mo	0.111500	-3.564194	1.902313
24	Mo	0.078962	3.559928	1.897638
25	Mo	3.030933	1.878659	1.902313
26	Mo	-0.990739	-1.715227	4.984084
27	Mo	1.980799	-0.000391	4.984084
28	Mo	-0.990061	1.715618	4.984084
29	O	0.777697	-1.346864	-5.729214
30	O	-0.194015	-2.940461	-3.733749
31	O	2.017430	3.479217	-2.184391
32	O	2.004375	-3.486754	-2.184391
33	O	0.777570	1.346938	-5.729214
34	O	-2.447348	-1.638390	-3.732693
35	O	-4.021805	0.007537	-2.184391
36	O	-1.555268	-0.000073	-5.729214
37	O	3.384484	-0.006361	-1.569747
38	O	-1.697751	-2.927868	-1.569747
39	O	-3.373183	1.529808	0.002103
40	O	-2.449507	1.638252	-3.733749
41	O	2.643522	1.302209	-3.733749
42	O	3.011445	2.156358	0.002103
43	O	2.642561	-1.300270	-3.732693

44 O	-0.195213	2.938660	-3.732693
45 O	-3.373183	-1.529808	-0.002103
46 O	-1.686733	2.934229	-1.569747
47 O	-4.443815	2.779724	-2.217197
48 O	-1.608308	2.787815	-6.193374
49 O	-1.610164	-2.786743	-6.193374
50 O	3.218473	-0.001072	-6.193374
51 O	-0.158227	5.240859	-2.225274
52 O	4.629219	2.458594	-2.217197
53 O	4.617831	-2.483401	-2.225274
54 O	-0.185404	-5.238319	-2.217197
55 O	-4.459604	-2.757458	-2.225274
56 O	-1.555268	0.000073	5.729214
57 O	-2.449507	-1.638252	3.733749
58 O	2.004375	3.486754	2.184391
59 O	-4.021805	-0.007537	2.184391
60 O	0.777697	1.346864	5.729214
61 O	-0.195213	-2.938660	3.732693
62 O	2.017430	-3.479217	2.184391
63 O	0.777570	-1.346938	5.729214
64 O	-1.697751	2.927868	1.569747
65 O	-1.686733	-2.934229	1.569747
66 O	3.011445	-2.156358	-0.002103
67 O	2.643522	-1.302209	3.733749
68 O	-0.194015	2.940461	3.733749
69 O	0.361739	3.686167	-0.002103
70 O	-2.447348	1.638390	3.732693
71 O	2.642561	1.300270	3.732693
72 O	0.361739	-3.686167	0.002103
73 O	3.384484	0.006361	1.569747
74 O	4.629219	-2.458594	2.217197
75 O	3.218473	0.001072	6.193374
76 O	-1.608308	-2.787815	6.193374
77 O	-1.610164	2.786743	6.193374
78 O	4.617831	2.483401	2.225274
79 O	-0.185404	5.238319	2.217197
80 O	-4.459604	2.757458	2.225274
81 O	-4.443815	-2.779724	2.217197
82 O	-0.158227	-5.240859	2.225274