

Table S1. Electrostatic and Mulliken atomic charges of compound **1** calculated at the PM3 level.

Atom no.	Atoms	Electrostatic	Mulliken
1	Mo1	+2.178	+0.022
2	Mo2	+2.318	+0.121
3	Mo3	+2.240	+0.103
4	Mo4	+2.186	+0.046
5	Mo5	+2.242	+0.037
6	P1	+2.757	+2.218
7	P2	+2.807	+2.234
8	O1	-0.858	-0.300
9	O2	-1.206	-0.857
10	O3	-1.181	-0.746
11	O4	-0.608	-0.096
12	O5	-1.019	-0.658
13	O6	-0.580	-0.062
14	O7	-1.328	-0.867
15	O8	-0.766	-0.275
16	O9	-1.290	-0.909
17	O10	-1.020	-0.167
18	O11	-0.912	-0.116
19	O12	-1.222	-0.762
20	O13	-1.039	-0.244
21	O14	-0.756	-0.248
22	O15	-0.630	-0.089
23	O16	-1.224	-0.757
24	O17	-0.922	-0.332
25	O18	-0.661	-0.155
26	O19	-0.961	-0.134
27	O20	-0.993	-0.651
28	O22	-0.731	-0.198
29	O23	-0.945	-0.397
30	O24	-0.887	-0.104
31	H1o5	+0.432	+0.212
32	H1o20	+0.414	+0.189
33	O21	-0.860	-0.386
34	H1o21	+0.501	+0.208
35	H2o21	+0.369	+0.166
36	O25	-0.890	-0.397
37	H1o25	+0.512	+0.227
38	H2o25	+0.362	+0.178
39	O26	-0.840	-0.347
40	H1o26	+0.375	+0.145
41	H2o26	+0.505	+0.215
42	O27	-0.848	-0.395
43	H1o27	+0.457	+0.224
44	H2o27	+0.386	+0.180
45	O28	-0.921	-0.405

46	H2o28	+0.483	+0.240
47	H1o28	+0.407	+0.171
48	N1	+0.708	+1.084
49	C1	-0.013	-0.370
50	C5	-0.129	-0.075
51	C7	-0.015	+0.014
52	C10	-0.017	-0.035
53	C12	-0.310	-0.049
54	C14	+0.001	-0.081
55	H1c5	+0.107	+0.105
56	H1c7	+0.097	+0.139
57	H1c10	+0.085	+0.096
58	H1c12	+0.144	+0.099
59	H1c14	+0.088	+0.100
60	H1n1	+0.108	-0.026
61	H2n1	+0.181	+0.037
62	H3n1	+0.018	-0.070
63	N2	+0.662	+1.137
64	C6	+0.064	-0.044
65	C11	-0.126	+0.001
66	C16	-0.196	-0.393
67	C19	-0.233	-0.016
68	C21	+0.087	-0.069
69	C24	-0.150	-0.011
70	H1c6	+0.089	+0.106
71	H1c11	+0.111	+0.102
72	H1c19	+0.161	+0.104
73	H1c21	+0.068	+0.099
74	H1c24	+0.117	+0.097
75	H1n2	+0.079	-0.069
76	H2n2	+0.052	-0.073
77	H3n2	+0.250	+0.011
78	N3	+0.330	+1.107
79	C3	-0.228	-0.051
80	C4	-0.057	-0.393
81	C9	+0.046	-0.085
82	C17	-0.154	+0.037
83	C22	-0.182	-0.033
84	C23	+0.107	-0.080
85	H1c3	+0.126	+0.095
86	H1c9	+0.076	+0.100
87	H1c17	+0.123	+0.149
88	H1c22	+0.115	+0.097
89	H1c23	+0.069	+0.108
90	H1n3	+0.237	-0.036
91	H2n3	+0.120	-0.060
92	H3n3	+0.299	+0.025
93	N4	+0.804	+1.118
94	C2	-0.015	-0.070

95	C8	-0.185	-0.019
96	C13	-0.203	+0.012
97	C15	-0.037	-0.085
98	C18	-0.125	-0.373
99	C20	-0.022	-0.037
100	H1c2	+0.085	+0.104
101	H1c8	+0.138	+0.101
102	H1c13	+0.189	+0.127
103	H1c15	+0.087	+0.097
104	H1c20	+0.078	+0.092
105	H1n4	+0.006	-0.067
106	H2n4	+0.043	-0.052
107	H3n4	+0.215	+0.040

Table S2. Electrostatic and Mulliken atomic charges of compound **2** calculated at the PM3 level.

Atom no.	Atoms	Electrostatic	Mulliken
1	Mo1	+1.686	+0.022
2	Mo2	+1.620	-0.074
3	Mo3	+1.735	+0.006
4	Mo4	+1.572	-0.061
5	Mo5	+1.748	+0.000
6	P1	+2.842	+2.109
7	P2	+2.239	+2.068
8	O1	-0.705	-0.601
9	O2	-0.717	-0.148
10	O3	-0.852	-0.581
11	O4	-1.280	-0.590
12	O5	-0.574	-0.277
13	O6	-1.306	-0.623
14	O7	-1.127	-0.611
15	O8	-1.008	-0.597
16	O9	-0.793	-0.504
17	O10	-1.199	-0.694
18	O11	-0.988	-0.643
19	O12	-0.572	-0.274
20	O13	-0.745	-0.185
21	O14	-0.724	-0.304
22	O15	-0.659	-0.291
23	O16	-0.775	-0.225
24	O17	-0.554	-0.281
25	O18	-0.350	-0.001
26	O20	-0.784	-0.550
27	O21	-0.788	-0.221
28	O22	-0.812	-0.188
29	O23	-0.287	+0.049
30	O24	-0.601	-0.331
31	H1o1	+0.295	+0.263
32	H1o3	+0.359	+0.253
33	O19	-0.718	-0.422
34	H1o19	+0.377	+0.235
35	H2o19	+0.381	+0.189
36	N1	+0.836	+0.256
37	C7	-0.511	-0.160
38	C9	-0.688	-0.190
39	H1c7	+0.146	+0.069
40	H2c7	+0.141	+0.062
41	H3c7	+0.202	+0.085
42	H1c9	+0.182	+0.081
43	H2c9	+0.197	+0.103
44	H3c9	+0.183	+0.066
45	H1n1	-0.012	+0.193

46	H2n1	-0.044	+0.194
47	N2	+0.955	+0.209
48	C2	-0.815	-0.167
49	C3	-0.785	-0.161
50	H1c2	+0.246	+0.084
51	H2c2	+0.194	+0.065
52	H3c2	+0.229	+0.069
53	H1c3	+0.207	+0.095
54	H2c3	+0.212	+0.064
55	H3c3	+0.217	+0.062
56	H1n2	-0.021	+0.202
57	H2n2	+0.070	+0.203
58	N3	+0.785	+0.232
59	C1	-0.800	-0.169
60	C10	-0.712	-0.167
61	H1c1	+0.221	+0.071
62	H2c1	+0.229	+0.058
63	H3c1	+0.189	+0.086
64	H1c10	+0.211	+0.104
65	H2c10	+0.202	+0.070
66	H3c10	+0.211	+0.062
67	H1n3	+0.031	+0.201
68	H2n3	+0.114	+0.202
69	N4	+0.471	+0.145
70	C4	-0.431	-0.141
71	C6	-0.781	-0.156
72	H1c4	+0.108	+0.046
73	H2c4	+0.136	+0.050
74	H3c4	+0.185	+0.101
75	H1c6	+0.231	+0.109
76	H2c6	+0.223	+0.072
77	H3c6	+0.212	+0.047
78	H1n4	+0.264	+0.205
79	H2n4	+0.191	+0.222
80	N5	+1.002	+0.346
81	C5	-0.810	-0.190
82	C8	-0.721	-0.191
83	H1c5	+0.211	+0.075
84	H2c5	+0.246	+0.095
85	H3c5	+0.196	+0.066
86	H1c8	+0.227	+0.110
87	H2c8	+0.192	+0.069
88	H3c8	+0.198	+0.081
89	H1n5	+0.144	+0.195
90	H2n5	-0.019	+0.166
91	O1d	-0.276	-0.215
92	O1w	-0.334	-0.212
93	O2w	-0.534	-0.404
94	C2d	-0.140	-0.113

95	C3d	-0.398	-0.115
96	N1d	-0.068	+0.030
97	C1d	+0.733	+0.517
98	H1c2d	+0.051	+0.085
99	H2c2d	+0.115	+0.063
100	H3c2d	+0.170	+0.082
101	H1c3d	+0.224	+0.113
102	H2c3d	+0.172	+0.073
103	H3c3d	+0.229	+0.097
104	H1c1d	+0.378	+0.286
105	H2c1d	+0.050	+0.037

Table S3. Electrostatic and Mulliken atomic charges of compound **3** calculated at the PM3 level.

Atom no.	Atoms	Electrostatic	Mulliken
1	Mo1	+2.488	+0.190
2	O2	-0.853	-0.249
3	O3	-0.866	-0.120
4	O4	-0.977	-0.162
5	O5	-0.900	-0.139
6	O6	-0.958	-0.170
7	O7	-1.189	-0.721
8	Mo8	+2.330	+0.077
9	Mo9	+2.317	+0.113
10	Mo10	+2.351	+0.128
11	Mo11	+2.318	+0.070
12	P12	+2.511	+2.297
13	O13	-0.621	-0.051
14	O14	-0.927	-0.112
15	O15	-0.805	-0.016
16	O16	-0.847	-0.095
17	O17	-0.615	-0.057
18	O18	-0.829	-0.093
19	O19	-0.923	-0.145
20	O20	-0.854	-0.104
21	O21	-1.152	-0.701
22	O22	-0.598	-0.035
23	O23	-0.929	-0.147
24	O24	-0.905	-0.131
25	O25	-0.610	-0.033
26	O26	-0.769	-0.037
27	O27	-0.727	+0.013
28	O28	-1.204	-0.718
29	O29	-1.170	-0.712
30	Mo30	+2.420	+0.149
31	Mo31	+2.324	+0.053
32	Mo32	+2.444	+0.160
33	Mo33	+2.347	+0.104
34	Mo34	+2.350	+0.109
35	Mo35	+2.341	+0.116
36	Mo36	+2.359	+0.128
37	O37	-0.834	-0.247
38	O38	-0.825	-0.091
39	O39	-0.897	-0.132
40	O40	-0.961	-0.160
41	O41	-0.607	-0.028
42	O42	-0.850	-0.120
43	O43	-0.842	-0.249
44	O44	-0.977	-0.156
45	O45	-0.850	-0.081

46	O46	-0.956	-0.165
47	O47	-0.596	-0.031
48	O48	-0.893	-0.102
49	O49	-0.602	-0.036
50	O50	-0.834	-0.081
51	O51	-0.609	-0.040
52	O52	-0.942	-0.174
53	O53	-0.622	-0.055
54	N54	+0.807	+0.902
55	C55	-0.332	-0.190
56	C56	-0.579	-0.192
57	H57	+0.040	-0.042
58	H58	+0.139	+0.012
59	H59	+0.142	+0.064
60	H60	+0.153	+0.105
61	H61	+0.114	+0.079
62	H62	+0.179	+0.082
63	H63	+0.206	+0.111
64	H64	+0.172	+0.065
65	O65	-0.024	+0.003
66	O66	-0.008	-0.003
67	H67	+0.062	+0.011
68	N69	+1.140	+0.900
69	C70	-0.684	-0.186
70	C71	-0.755	-0.192
71	H72	-0.024	-0.042
72	H73	+0.196	+0.064
73	H74	+0.227	+0.105
74	H75	+0.185	+0.080
75	H76	+0.201	+0.081
76	H77	+0.238	+0.110
77	H78	+0.220	+0.066
78	H68	+0.060	+0.012
79	N79	+1.156	+0.900
80	C80	-0.711	-0.186
81	C81	-0.748	-0.192
82	H82	-0.027	-0.042
83	H83	+0.204	+0.064
84	H84	+0.231	+0.104
85	H85	+0.191	+0.080
86	H86	+0.197	+0.081
87	H87	+0.238	+0.110
88	H88	+0.216	+0.065
