Electronic Supporting Information for

A tripodal tris(aminophenolate) ligand and its seven-coordinate molybdenum(VI) complex

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Table S1. Energy and Cartesian Coordinates of (Clamp)Mo.

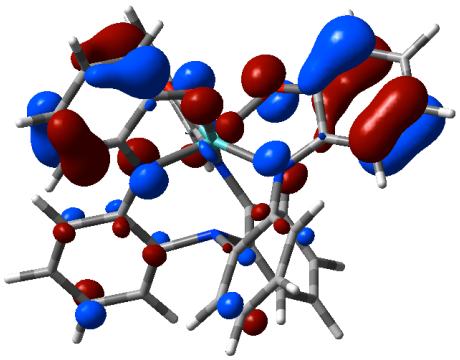
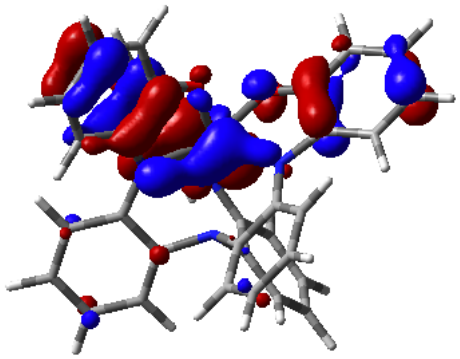
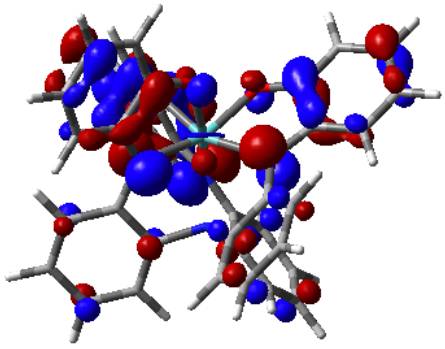
Energy of optimized structure = –1899.29327247 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	42	0.000000	0.000000	0.698498
2	8	-1.184460	1.011809	1.978371
3	8	-0.284023	-1.531677	1.978371
4	8	1.468482	0.519867	1.978371
5	7	0.000000	1.986297	0.010714
6	7	-1.720184	-0.993148	0.010714
7	7	1.720184	-0.993148	0.010714
8	7	0.000000	0.000000	-1.641692
9	6	-1.195008	2.335404	1.954874
10	6	-0.595855	2.937366	0.811314
11	6	-0.736780	4.327313	0.619034
12	1	-0.370628	4.804409	-0.281676
13	6	-1.378416	5.086667	1.591349
14	1	-1.477425	6.158795	1.445814
15	6	-1.898761	4.491457	2.754872
16	1	-2.387584	5.108827	3.503288
17	6	-1.812999	3.117702	2.942221
18	1	-2.236250	2.626067	3.812439
19	6	-1.425015	-2.202609	1.954874
20	6	-2.245906	-1.984709	0.811314
21	6	-3.379173	-2.801727	0.619034
22	1	-3.975426	-2.723178	-0.281676
23	6	-3.715974	-3.737077	1.591349
24	1	-4.594960	-4.358885	1.445814
25	6	-2.940336	-3.890103	2.754872
26	1	-3.230582	-4.622122	3.503288
27	6	-1.793510	-3.128955	2.942221
28	1	-1.156116	-3.249683	3.812439
29	6	2.620023	-0.132795	1.954874
30	6	2.841761	-0.952657	0.811314
31	6	4.115953	-1.525586	0.619034
32	1	4.346054	-2.081231	-0.281676
33	6	5.094391	-1.349590	1.591349
34	1	6.072385	-1.799910	1.445814
35	6	4.839096	-0.601354	2.754872
36	1	5.618166	-0.486705	3.503288
37	6	3.606509	0.011252	2.942221

38	1	3.392366	0.623616	3.812439
39	6	0.823613	1.155027	-2.031768
40	6	0.762310	2.237424	-1.131101
41	6	1.529918	3.378805	-1.412713
42	1	1.564599	4.196540	-0.704576
43	6	2.310175	3.425540	-2.570681
44	1	2.911963	4.308850	-2.765695
45	6	2.346829	2.350070	-3.457095
46	1	2.962449	2.391801	-4.350236
47	6	1.598693	1.198734	-3.180844
48	1	1.633509	0.342659	-3.846454
49	6	-1.412090	0.135757	-2.031768
50	6	-2.318821	-0.458532	-1.131101
51	6	-3.691090	-0.364455	-1.412713
52	1	-4.416609	-0.743288	-0.704576
53	6	-4.121692	0.287900	-2.570681
54	1	-5.187555	0.367409	-2.765695
55	6	-3.208635	0.857379	-3.457095
56	1	-3.552585	1.369656	-4.350236
57	6	-1.837481	0.785142	-3.180844
58	1	-1.113506	1.243330	-3.846454
59	6	0.588476	-1.290784	-2.031768
60	6	1.556511	-1.778892	-1.131101
61	6	2.161172	-3.014350	-1.412713
62	1	2.852011	-3.453252	-0.704576
63	6	1.811518	-3.713440	-2.570681
64	1	2.275592	-4.676259	-2.765695
65	6	0.861806	-3.207449	-3.457095
66	1	0.590136	-3.761457	-4.350236
67	6	0.238788	-1.983876	-3.180844
68	1	-0.520003	-1.585989	-3.846454

Table S2. Frontier orbitals of (Clamp)Mo (B3LYP/6-31G* except SDD for Mo). Only one component of each *E* set is depicted.

Orbital Number	Energy, eV	Designation	Depiction (isovalue = 0.04)
149, 150	–5.92	*E*, amidophenoxide SJO	
151, 152	–5.47	*E* π_b, amidophenoxide RAO	
153 [HOMO]	–4.58	*A* π_{nb} amidophenoxide RAO	

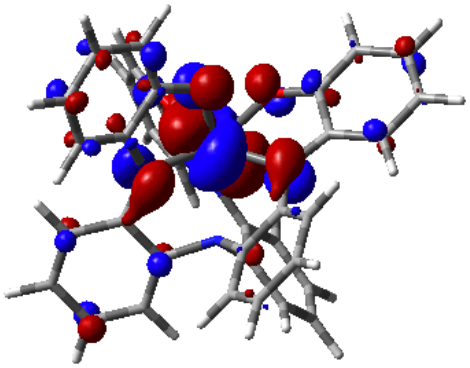
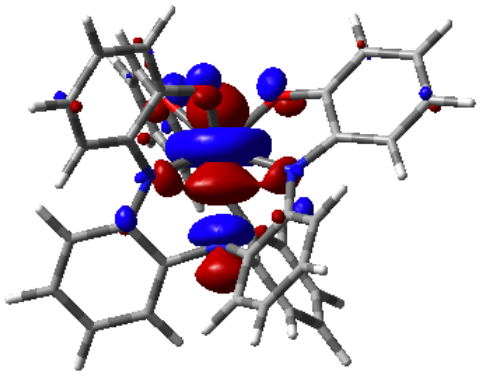
154, 155 [LUMO]	–2.58	*E* π*, Mo *d*π	
156	–1.79	*A* σ*, Mo d_{z^2}	

Table S3. TDDFT calculated excited states for (Clamp)Mo. In cases where a single excitation is major, it is indicated in boldface. Multiple boldface entries involve separate components of *E*-symmetry orbitals.

Excitation Number	Symmetry	Energy, λ [exptl λ]	Oscillator strength (*f*)	Component excitations	Coefficients
1	^1E	1.41 eV, 881 nm [985 nm]	0.0554	151 → 154 152 → 155 **153 → 154** **153 → 155**	0.10045 –0.10045 **0.29211** **0.61930**
2	^1E	1.41 eV, 881 nm [985 nm]	0.0554	151 → 155 152 → 154 **153 → 154** **153 → 155**	0.10045 0.10045 **0.61930** **–0.29211**
3	^1A	1.84 eV, 672 nm	0.0001	**151 → 154** **151 → 155** **152 → 154** **152 → 155**	**0.42852** **0.24127** **–0.24128** **0.42853**
4	^1A	1.94 eV, 640 nm	0.0027	**153 → 156**	**0.68466**
5	^1E	2.24 eV, 554 nm [563 nm]	0.1161	**151 → 154** **152 → 155** 152 → 156 153 → 154	**0.46842** **–0.46842** –0.11886 –0.12339
6	^1E	2.24 eV, 554 nm [563 nm]	0.1161	**151 → 155** 151 → 156 **152 → 154** 153 → 155	**0.46842** –0.11886 **0.46842** 0.12339
7	^1A	2.52 eV, 491 nm	0.0000	149 → 154 149 → 155 150 → 154 150 → 155 151 → 154 151 → 155 152 → 154 152 → 155	–0.15481 0.31263 0.31264 0.15482 –0.15487 0.31049 –0.31049 –0.15487
8	^1E	2.61 eV, 475 nm	0.0228	**151 → 156** **152 → 156**	**0.50744** **–0.41479**
9	^1E	2.61 eV, 475 nm	0.0228	**151 → 156** **152 → 156**	**0.41480** **0.50745**

Excitation Number	Symmetry	Energy, λ [exptl λ]	Oscillator strength (*f*)	Component excitations	Coefficients
10	^1E	2.66 eV, 465 nm	0.0190	148 → 155 **149 → 154** **150 → 155** 152 → 156	–0.13394 **0.46267** **0.46268** –0.15974
11	^1E	2.66 eV, 465 nm	0.0190	148 → 154 **149 → 155** **150 → 154** 151 → 156	–0.13394 **0.46268** **–0.46267** –0.15974
12	^1A	2.74 eV, 453 nm	0.0635	**149 → 154** **149 → 155** **150 → 154** **150 → 155**	**0.43746** **0.21182** **0.21182** **–0.43745**

II. Calculations on [(Clamp)Mo]$^+$

Table S4. Energy and Cartesian coordinates of [(Clamp)Mo]$^+$

Energy of optimized structure = –1899.09067122 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	42	0.000000	0.000000	0.723803
2	8	-1.230835	1.008046	1.987826
3	8	-0.257576	-1.569957	1.987826
4	8	1.488411	0.561912	1.987826
5	7	0.000000	1.997414	0.040801
6	7	-1.729811	-0.998707	0.040801
7	7	1.729811	-0.998707	0.040801
8	7	0.000000	0.000000	-1.620001
9	6	-1.275651	2.318731	1.937836
10	6	-0.643745	2.928449	0.799020
11	6	-0.801449	4.321775	0.583249
12	1	-0.413232	4.793514	-0.310535
13	6	-1.487311	5.068477	1.520574
14	1	-1.610966	6.135659	1.364962
15	6	-2.038589	4.468854	2.682089
16	1	-2.561496	5.090878	3.402149
17	6	-1.941945	3.106375	2.896052
18	1	-2.383863	2.622816	3.760678
19	6	-1.370254	-2.264112	1.937836
20	6	-2.214239	-2.021724	0.799020
21	6	-3.342043	-2.854963	0.583249
22	1	-3.944689	-2.754627	-0.310535
23	6	-3.645775	-3.822288	1.520574
24	1	-4.508153	-4.462967	1.364962
25	6	-2.850847	-3.999897	2.682089
26	1	-3.128082	-4.763759	3.402149
27	6	-1.719227	-3.234961	2.896052
28	1	-1.079493	-3.375894	3.760678
29	6	2.645906	-0.054619	1.937836
30	6	2.857984	-0.906725	0.799020
31	6	4.143492	-1.466813	0.583249
32	1	4.357921	-2.038888	-0.310535
33	6	5.133085	-1.246190	1.520574
34	1	6.119119	-1.672692	1.364962
35	6	4.889436	-0.468958	2.682089
36	1	5.689577	-0.327119	3.402149
37	6	3.661172	0.128586	2.896052
38	1	3.463356	0.753078	3.760678
39	6	0.811150	1.166937	-2.010318
40	6	0.767486	2.246684	-1.105201
41	6	1.540451	3.386198	-1.370899
42	1	1.586949	4.192150	-0.649278
43	6	2.310152	3.443143	-2.534327
44	1	2.917576	4.322146	-2.726373
45	6	2.325822	2.375628	-3.432420

46	1	2.930927	2.425577	-4.331892
47	6	1.576585	1.222702	-3.166431
48	1	1.606827	0.378250	-3.846515
49	6	-1.416172	0.119008	-2.010318
50	6	-2.329429	-0.458680	-1.105201
51	6	-3.702759	-0.359029	-1.370899
52	1	-4.423983	-0.721736	-0.649278
53	6	-4.136925	0.279079	-2.534327
54	1	-5.201876	0.365623	-2.726373
55	6	-3.220265	0.826407	-3.432420
56	1	-3.566075	1.325469	-4.331892
57	6	-1.847183	0.754012	-3.166431
58	1	-1.130988	1.202428	-3.846515
59	6	0.605022	-1.285945	-2.010318
60	6	1.561943	-1.788004	-1.105201
61	6	2.162308	-3.027169	-1.370899
62	1	2.837033	-3.470413	-0.649278
63	6	1.826773	-3.722222	-2.534327
64	1	2.284300	-4.687768	-2.726373
65	6	0.894443	-3.202035	-3.432420
66	1	0.635147	-3.751046	-4.331892
67	6	0.270598	-1.976713	-3.166431
68	1	-0.475840	-1.580678	-3.846515