New Insights into Solvolysis and Reorganization Energy from Gas-Phase, Electrochemical, and Theoretical Studies of Oxo-Tp*Mo(V) Compounds.

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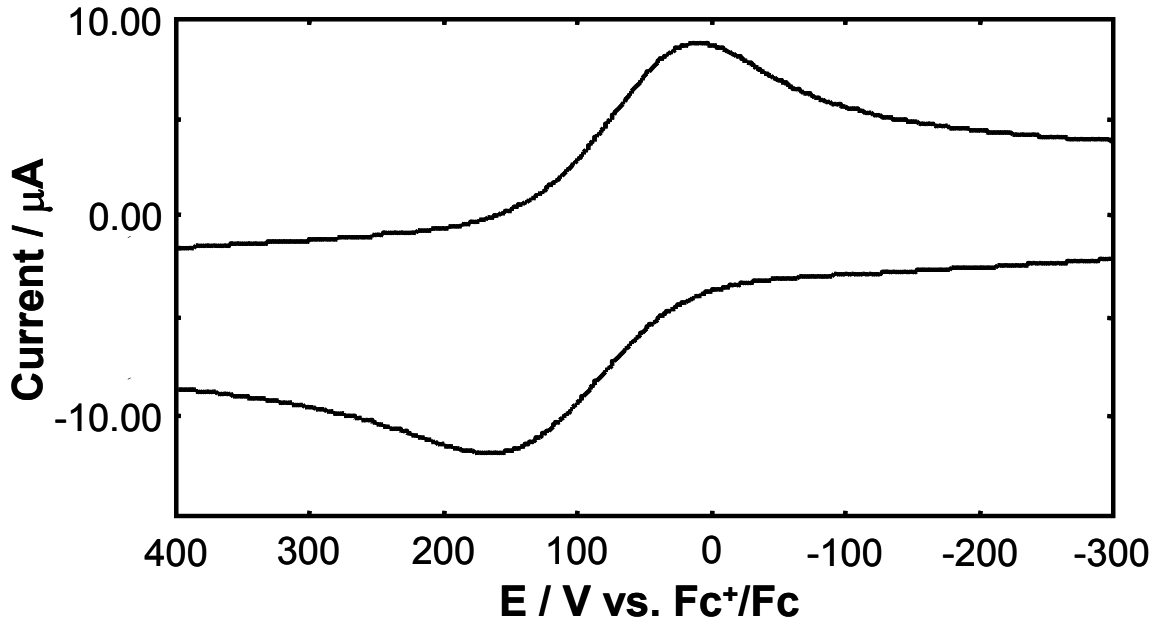

Figure SI-1. Cyclic voltammogram of Tp*MoO(OCH_3)$_2$ (**A**). Experimental conditions in methods section.

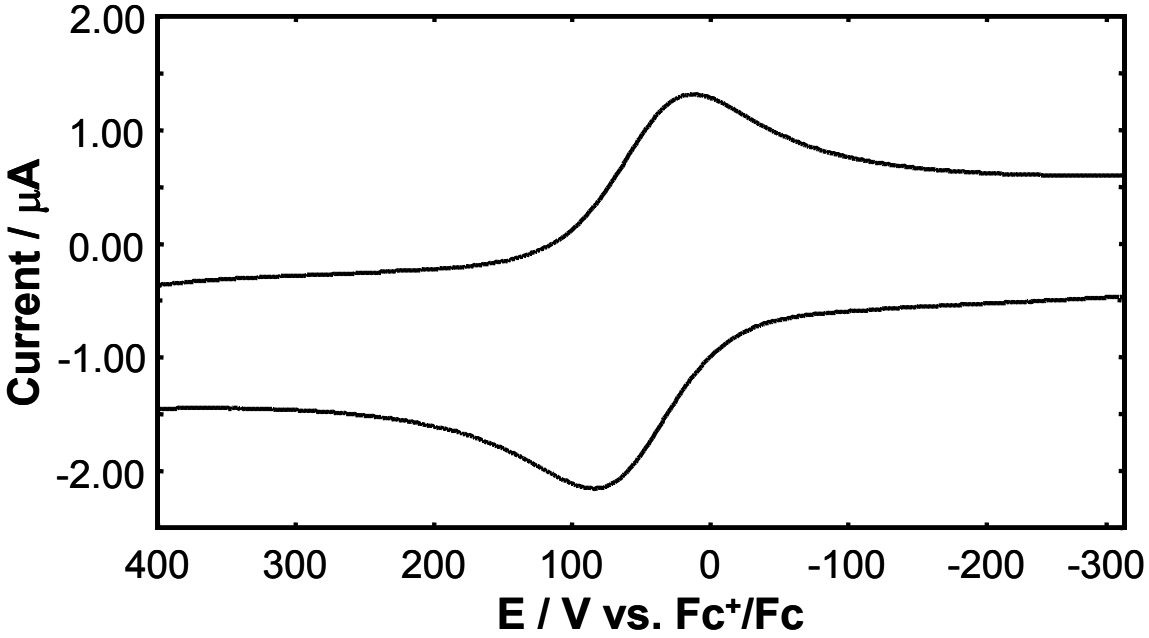

Figure SI-2. Cyclic voltammogram of Tp*MoO(OCH_2CH_3)$_2$ (**B**). Experimental conditions in methods section.

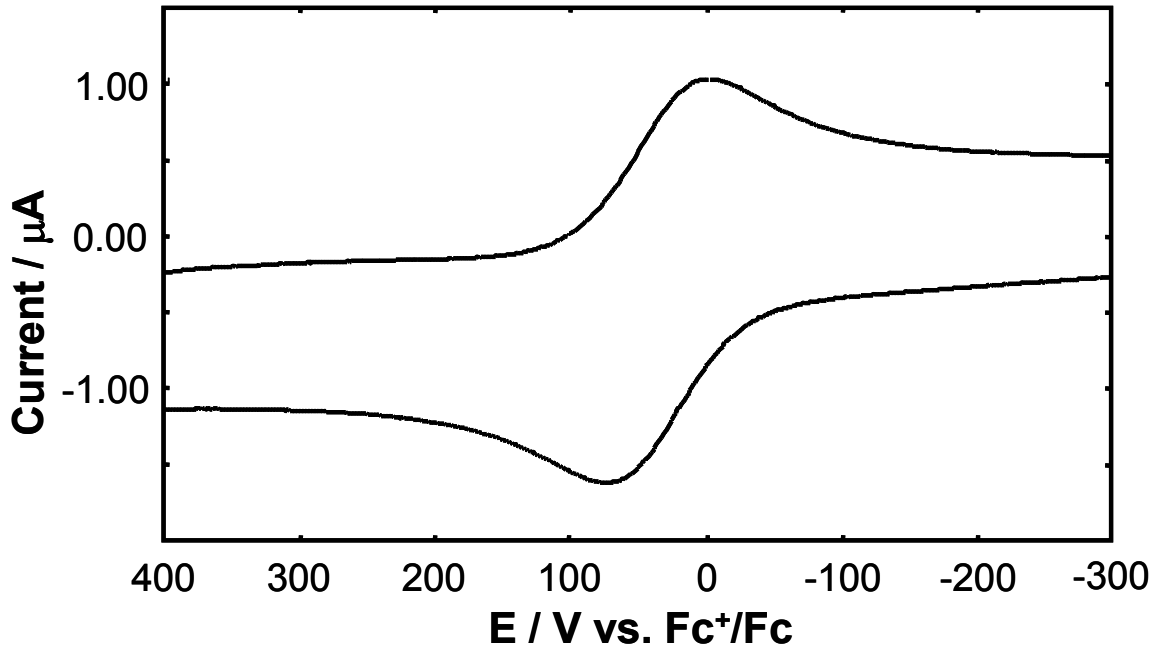

Figure SI-3. Cyclic voltammogram of Tp*MoO($OCH_2CH_2CH_3$)$_2$ (**C**). Experimental conditions in methods section.

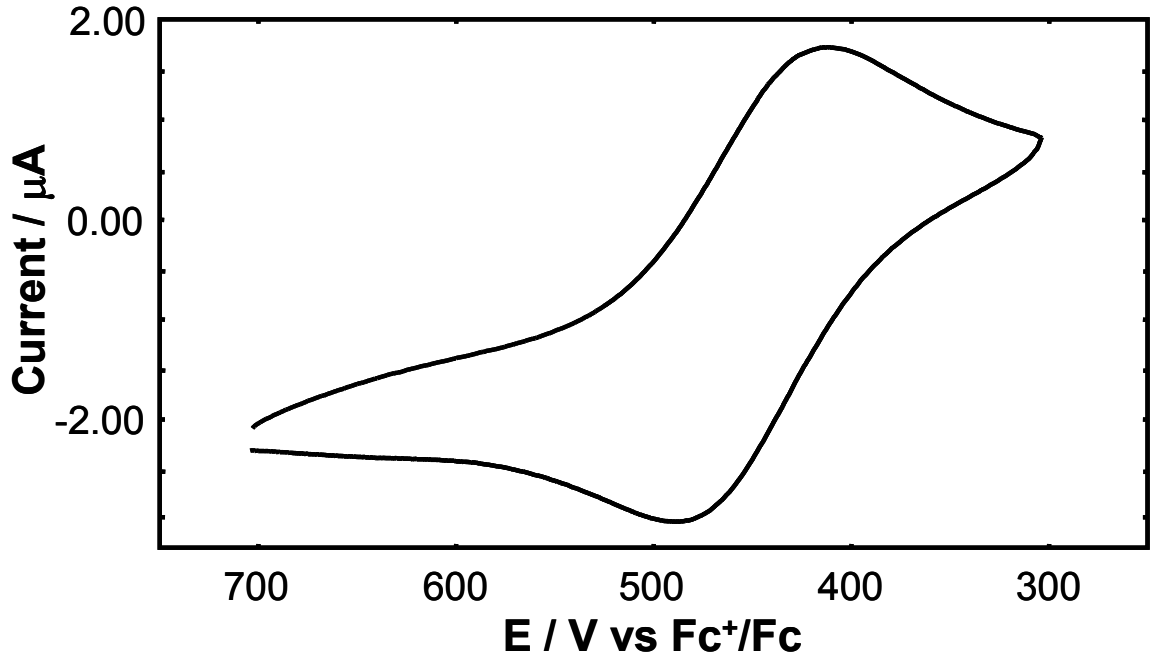

Figure SI-4. Cyclic voltammogram of Tp*MoO($OCH_2CH_2CH_2O$) (**D**). Experimental conditions in methods section.

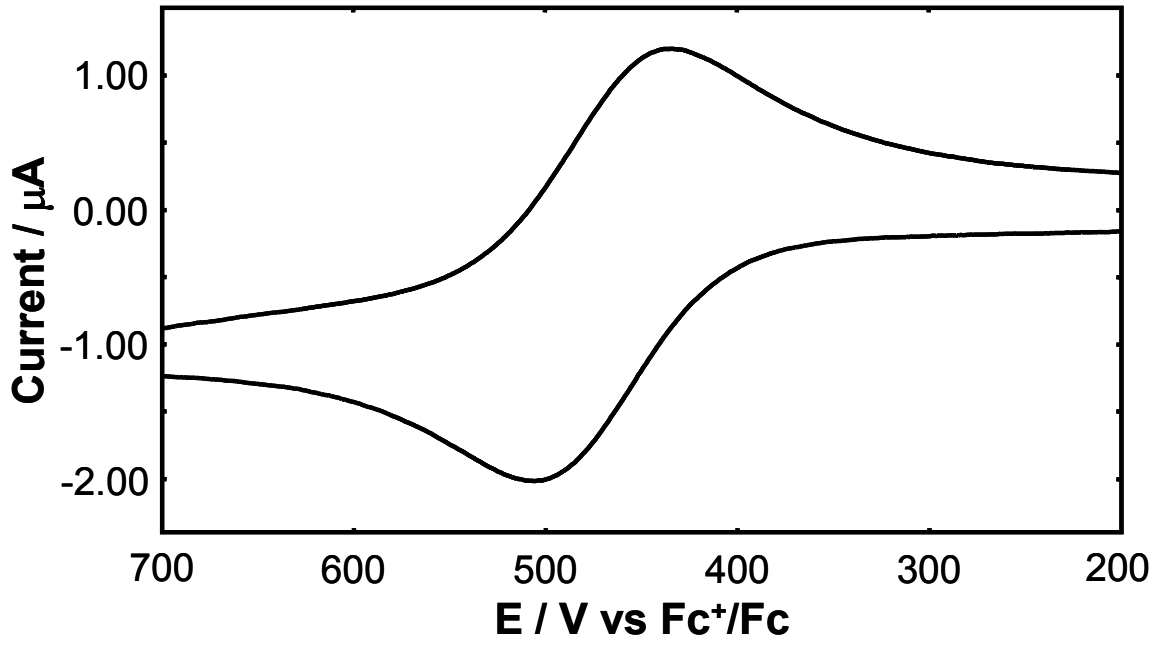

Figure SI-5. Cyclic voltammogram of Tp*MoO[OCH(CH_3)CH_2CH(CH_3)O] (**E**). Experimental conditions in methods section.

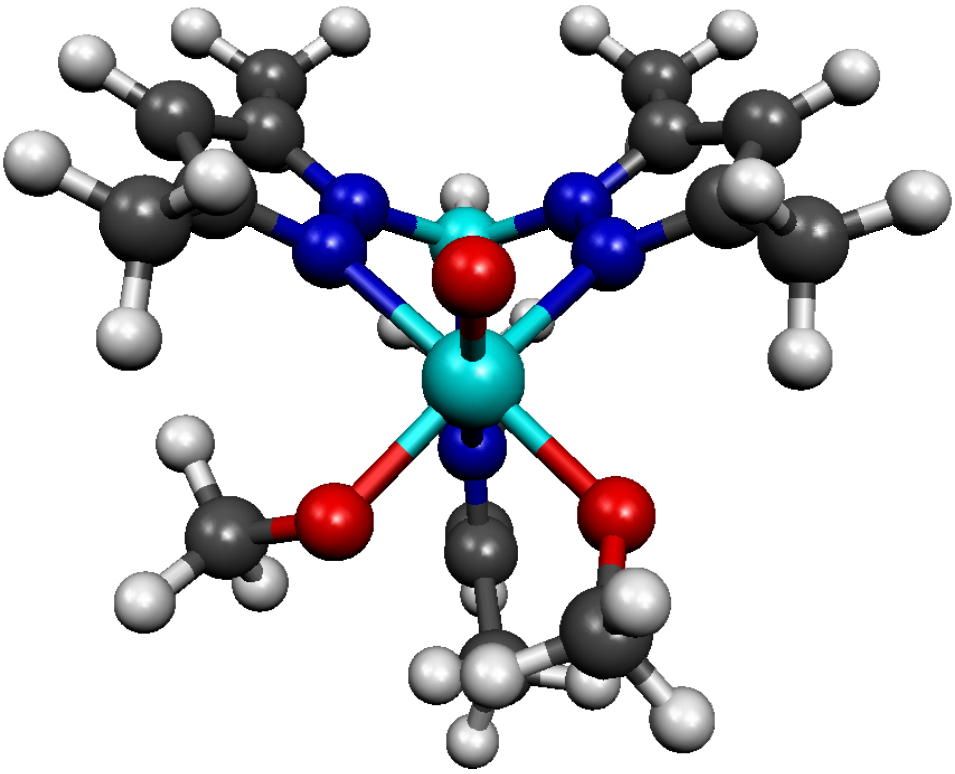

Figure SI-6. Calculated optimized structure for **A**

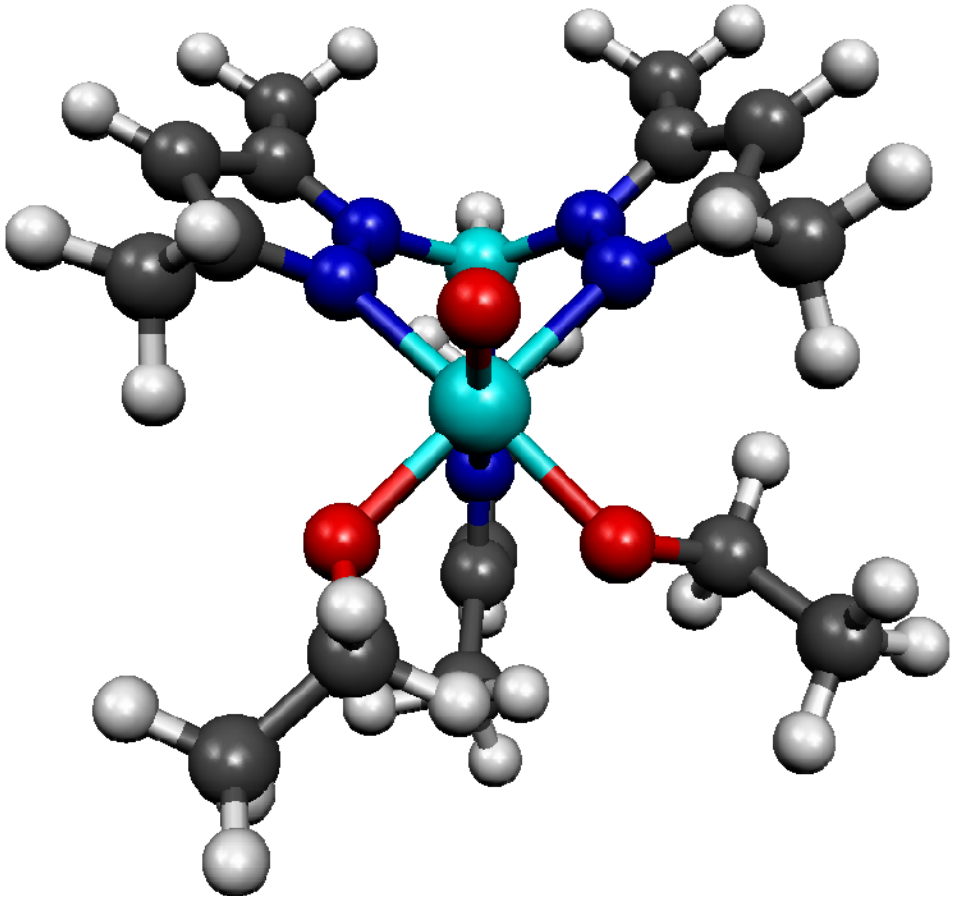

Figure SI-7. Calculated optimized structure for **B**.

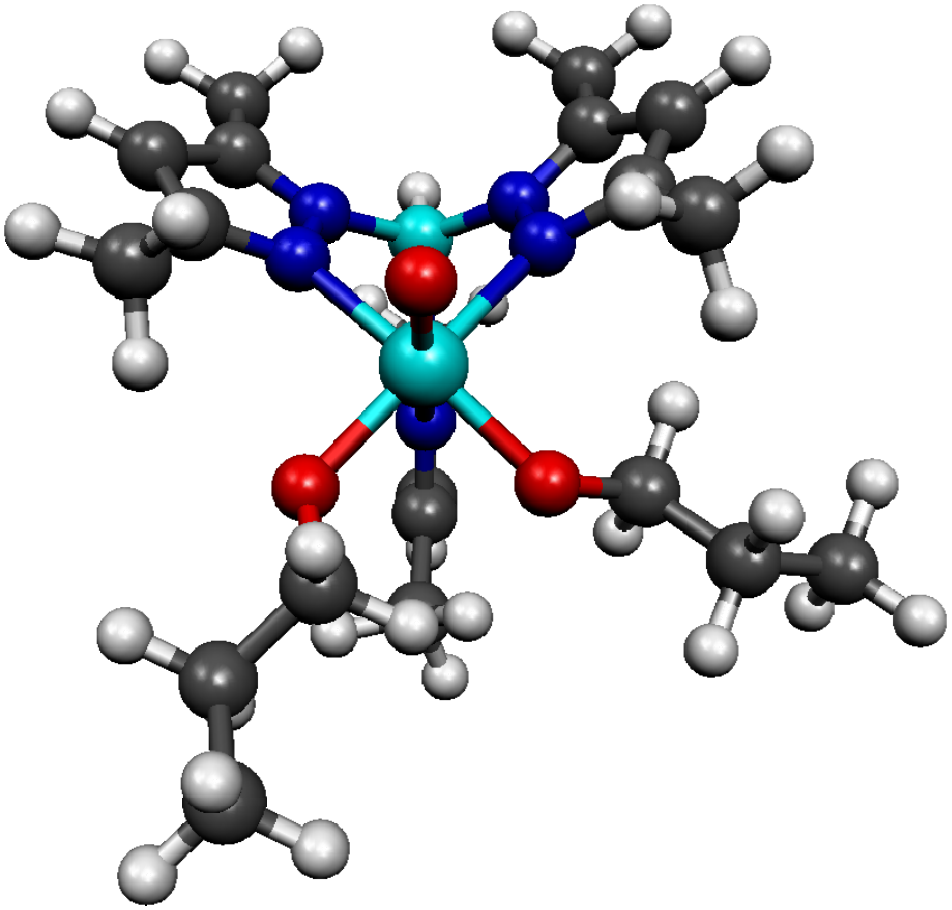

Figure SI-8. Calculated optimized structure for **C**.

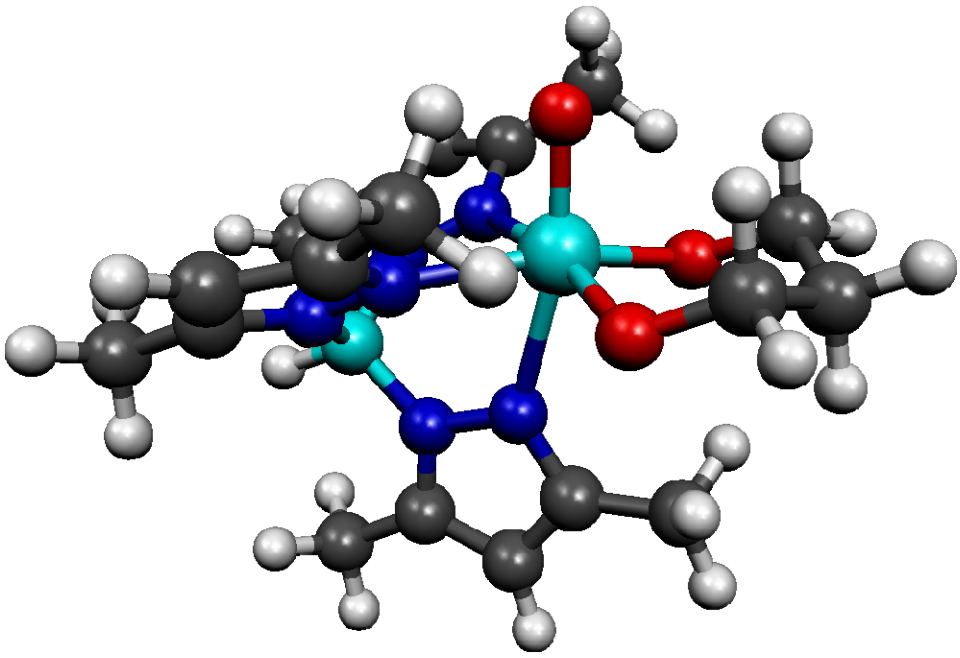

Figure SI-9. Calculated optimized structure of **D** in the chair conformation.

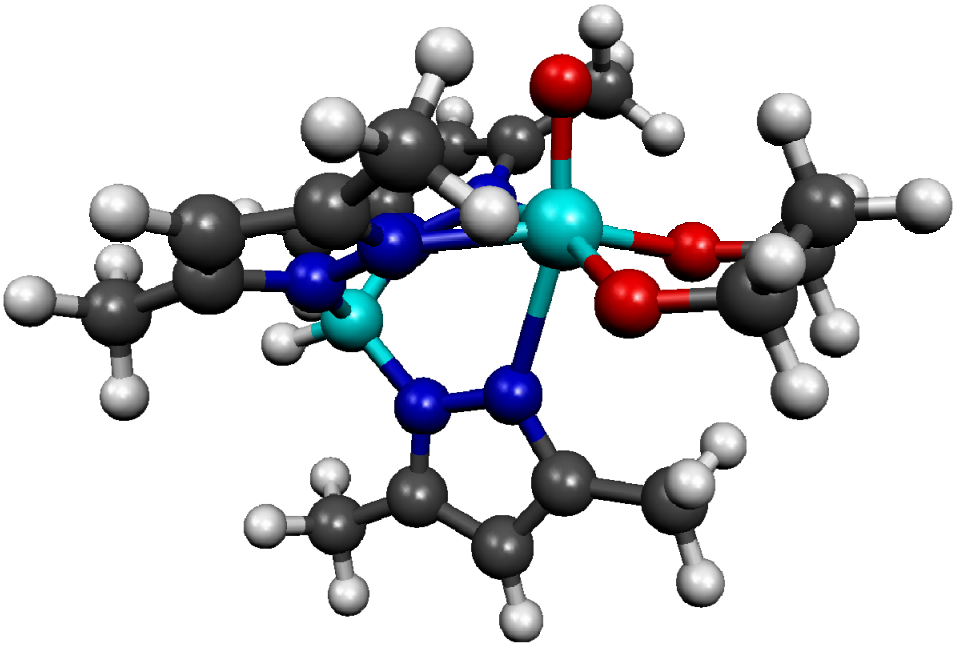

Figure SI-10. Calculated optimized structure of **D** in the boat conformation.

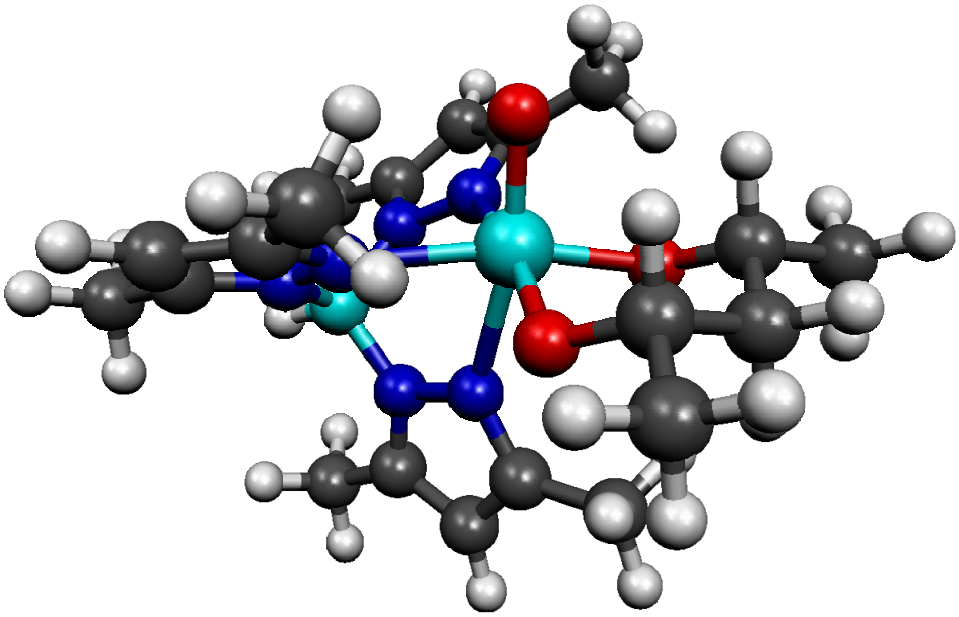

Figure SI-11. Calculated optimized structure of **E** in the chair conformation.

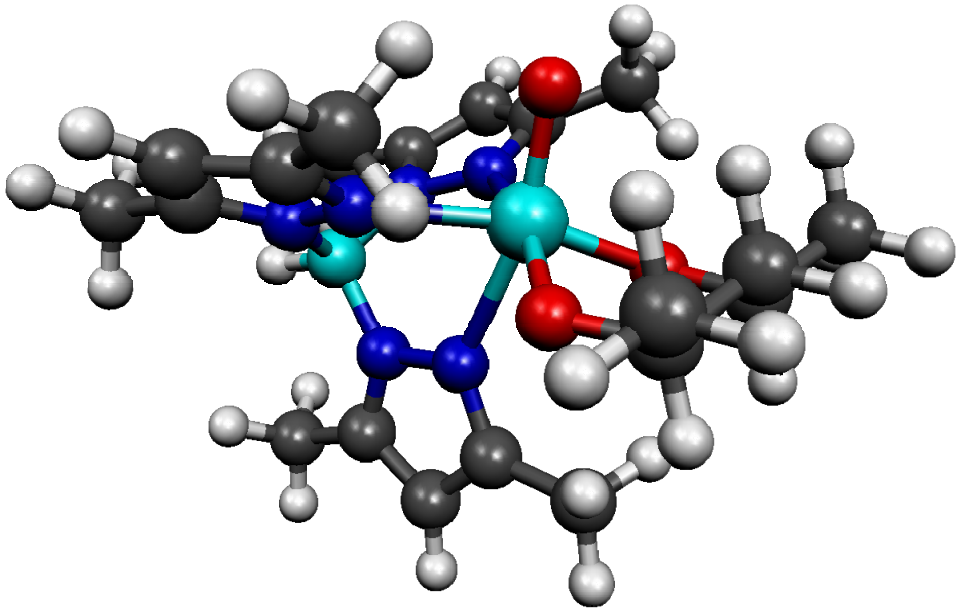

Figure SI-12. Calculated optimized structure of **E** in the boat conformation.

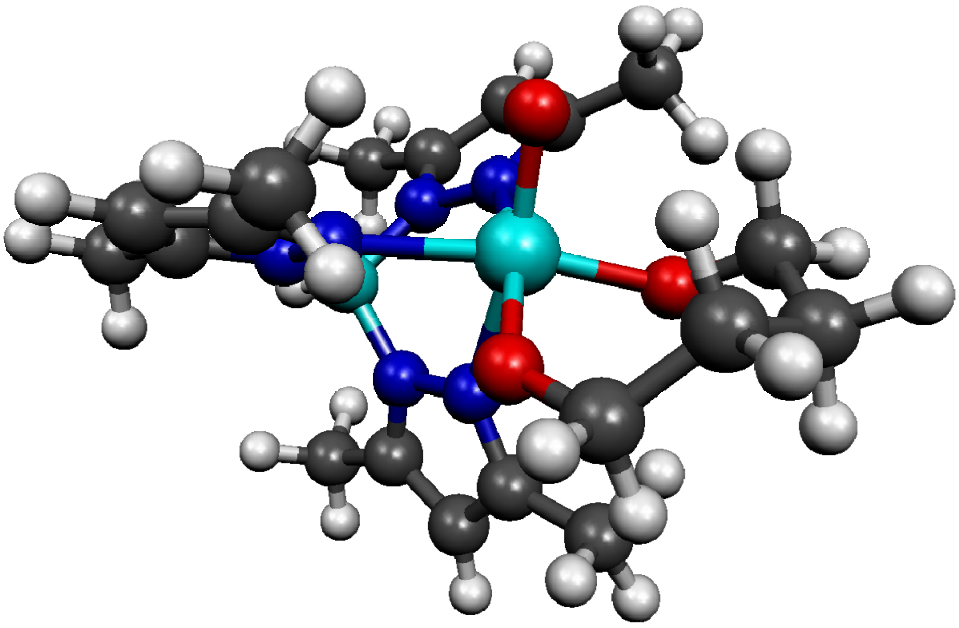

Figure SI-13. Calculated optimized structure for **F** in the boat-twist conformation.

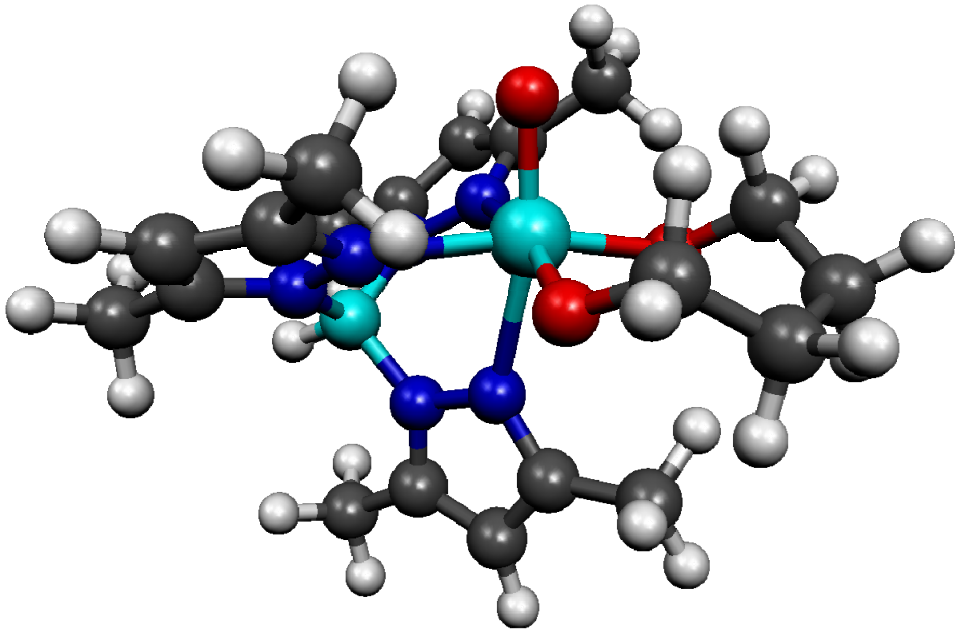

Figure SI-14. Calculated optimized structure of **F** in the chair conformation.

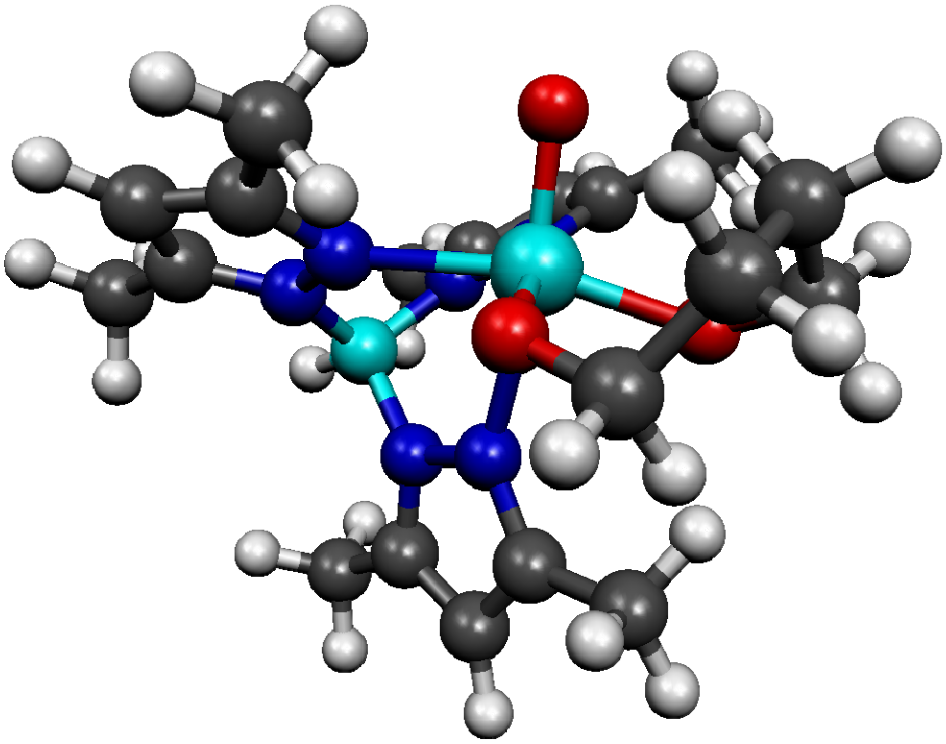

Figure SI-15. Calculated optimized structure of **F** in the boat conformation.

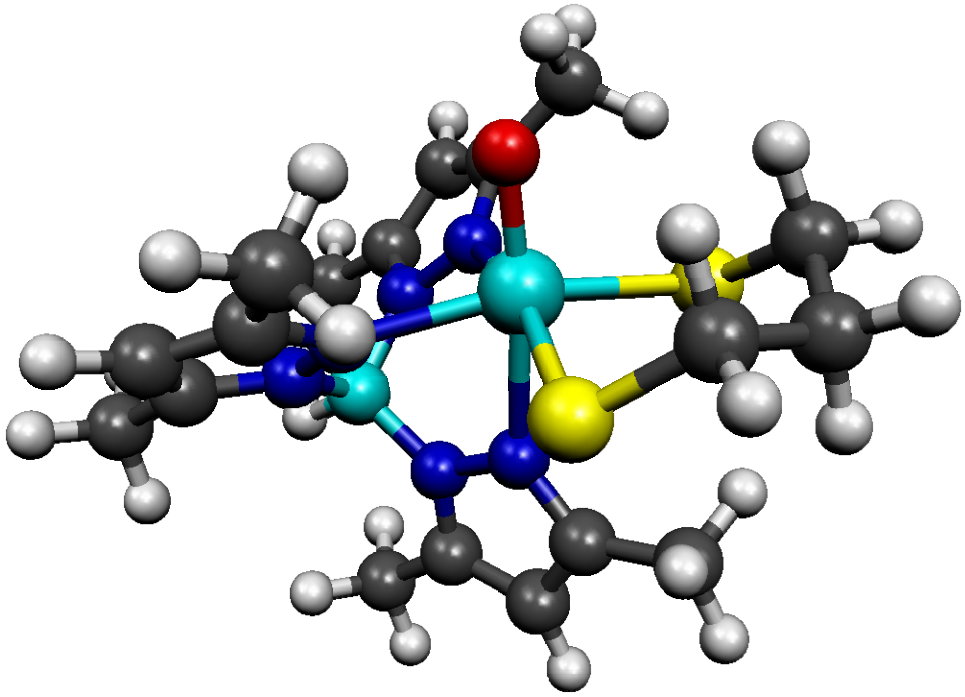

Figure SI-16. Calculated optimized structure of Tp*MoO[S$(CH_2)_3$S] in the chair conformation.

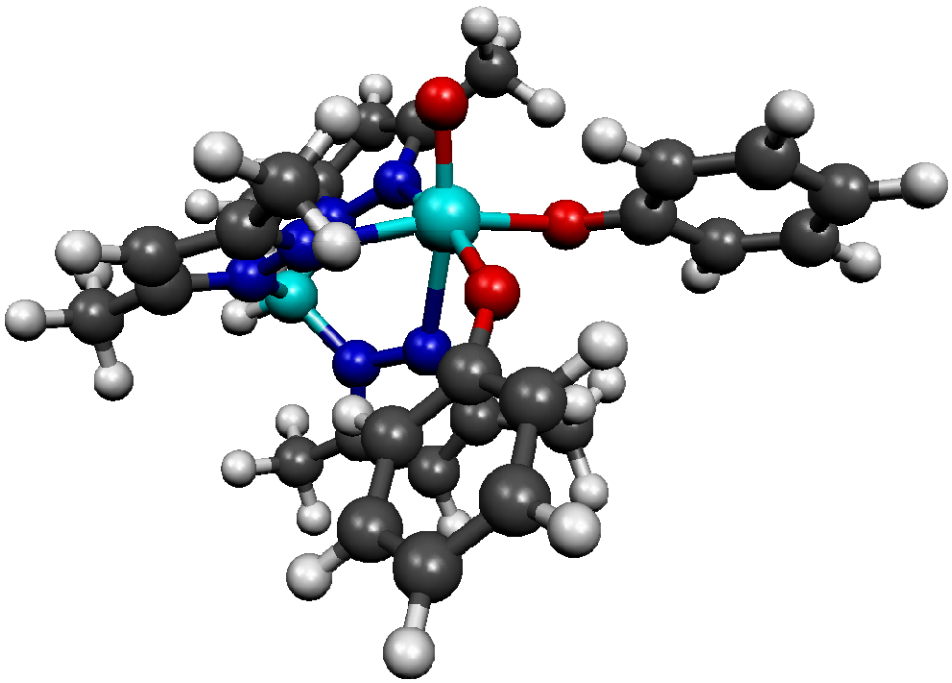

Figure SI-17. Calculated optimized structure of Tp*MoO(OC_6H_5)$_2$.

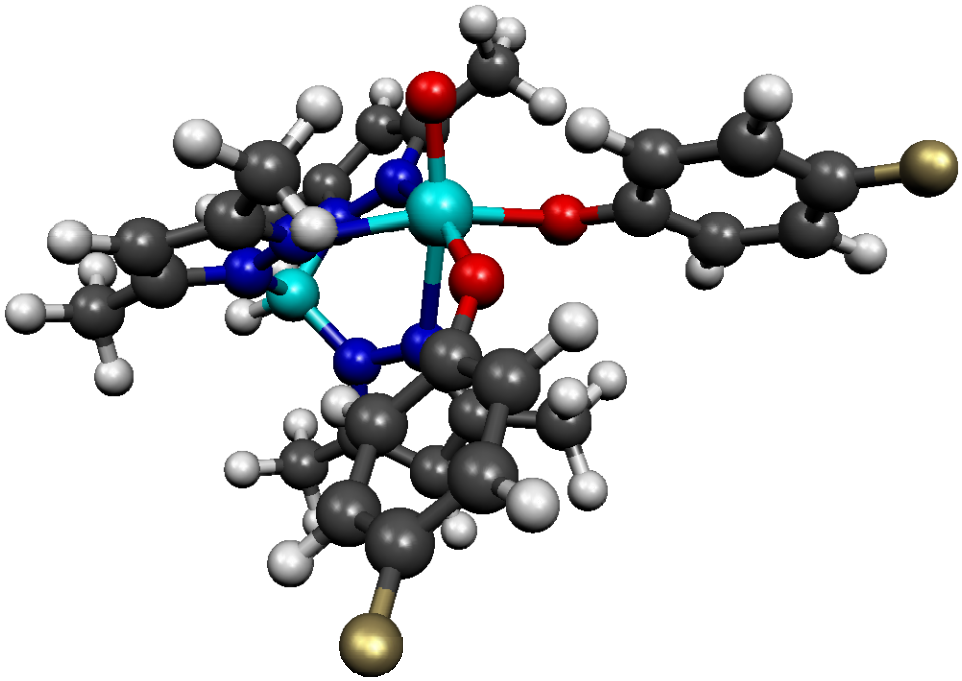

Figure SI-18. Calculated optimized structure of Tp*MoO(*p*-$OC_6H_4F)_2$.

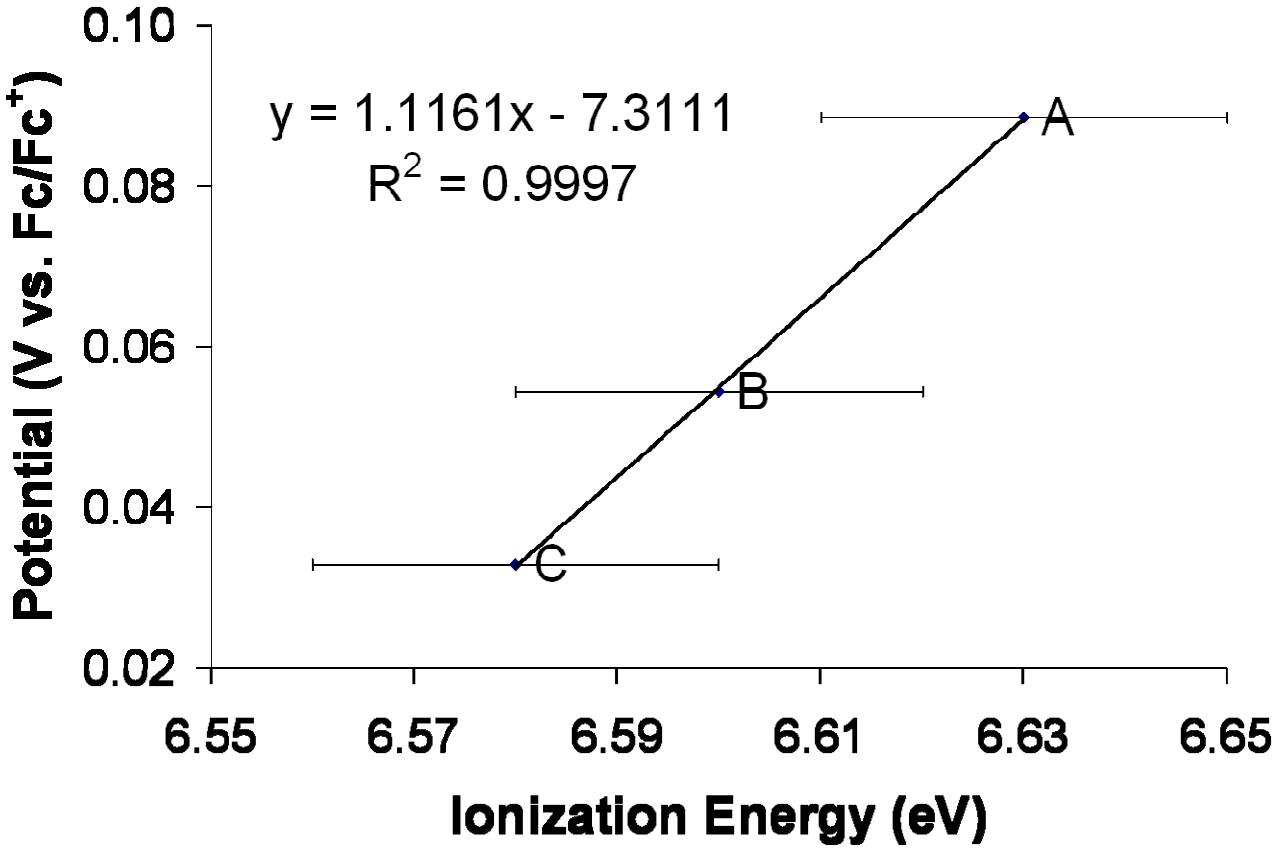

Figure SI-19. Correlation between experimental oxidation potentials (V vs. Fc/Fc^{+}) and ionization energies (eV) for alkoxide containing $Tp^{*}MoO(OX)_2$ molecules.

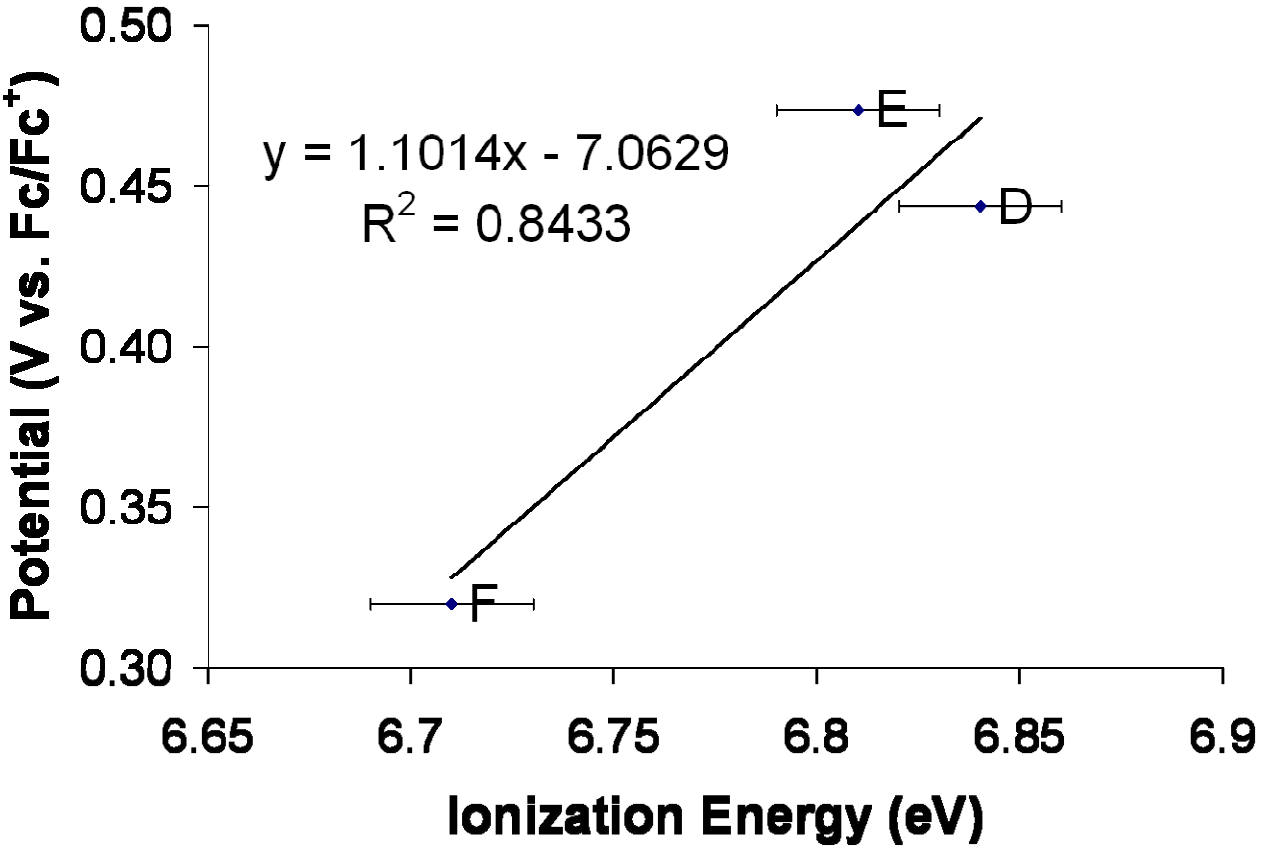

Figure SI-20. Correlation between experimental oxidation potentials (V vs. Fc/Fc^{+}) and ionization energies (eV) for diolato containing $Tp^{*}MoO(OX)_2$ molecules.

Calculated geometries of the complexes under study. (Cartesian coordinates in Angstroms)

A – Tp*MoO$(OCH_3)_2$

1.Mo	-0.000633	-0.002586	-0.006573
2.O	1.733009	-0.063914	0.026677
3.O	-0.479885	1.903928	-0.070041
4.C	-1.193160	2.591555	-1.059996
5.H	-0.956417	2.224293	-2.086056
6.H	-0.948518	3.676643	-1.002133
7.H	-2.295294	2.475712	-0.919313
8.O	-0.473941	-0.031315	1.891410
9.C	-0.158021	1.055723	2.721672
10.H	-0.355215	2.023842	2.199305
11.H	0.923349	1.038591	3.001087
12.H	-0.766735	1.011678	3.653347
13.N	-0.013230	-0.108345	-2.214080
14.C	0.760889	0.542486	-3.104091
15.C	0.483202	0.049568	-4.387351
16.C	-0.484796	-0.938796	-4.219995
17.N	-0.761804	-1.014753	-2.896822
18.N	-0.196379	-2.158310	-0.129438
19.N	-0.879246	-2.783268	-1.126427
20.C	-0.738291	-4.124300	-1.000116
21.C	0.072004	-4.359607	0.108662
22.C	0.395546	-3.098918	0.630136
23.N	-2.295585	-0.294886	-0.424369
24.C	-3.377731	0.233005	0.173018
25.C	-4.534056	-0.296566	-0.427285
26.C	-4.088345	-1.181135	-1.404682
27.N	-2.734271	-1.153349	-1.376560
28.B	-1.696634	-1.968257	-2.141362
29.H	0.939650	0.367522	-5.333268
30.H	0.389098	-5.336734	0.494111
31.H	-5.577316	-0.069106	-0.173513
32.C	-1.380448	-5.095270	-1.923393
33.H	-1.058548	-4.940039	-2.974914
34.H	-1.107573	-6.126288	-1.627190
35.H	-2.487870	-5.011047	-1.903924
36.C	1.244775	-2.721947	1.784392
37.H	0.709643	-1.982571	2.419486
38.H	1.517777	-3.612692	2.380868
39.H	2.171095	-2.218576	1.430347
40.C	-3.266416	1.174489	1.315429
41.H	-4.211480	1.734759	1.453322
42.H	-3.039224	0.617669	2.250314
43.H	-2.423033	1.881433	1.165107
44.C	-4.860613	-2.040421	-2.340008
45.H	-4.647527	-3.118866	-2.178459
46.H	-5.945190	-1.879107	-2.188111
47.H	-4.623238	-1.815364	-3.401469
48.C	1.743822	1.563083	-2.666578
49.H	2.266809	1.999931	-3.538103
50.H	1.251980	2.376876	-2.091825
51.H	2.484394	1.104320	-1.975953
52.C	-1.144032	-1.801175	-5.235052
53.H	-0.943420	-2.878280	-5.052419
54.H	-2.246710	-1.670016	-5.233781
55.H	-0.766393	-1.546311	-6.243800
56.H	-2.238356	-2.717755	-2.927649

$\mathbf{A}^{+}$ – Tp*MoO$(OCH_3)_2^{+}$

1.Mo	-0.105813	0.036623	0.019428
2.O	1.608182	0.099639	0.233906
3.O	-0.474318	1.842015	-0.434752
4.C	-1.283248	2.467068	-1.394443
5.H	-0.959409	2.159738	-2.416895
6.H	-1.168732	3.566154	-1.288222
7.H	-2.350198	2.177434	-1.264180
8.O	-0.569420	0.031925	1.854477
9.C	0.201951	0.344760	2.990962
10.H	-0.080716	1.359063	3.349847
11.H	1.287920	0.335667	2.740158
12.H	-0.014005	-0.383600	3.800780
13.N	0.032618	-0.206326	-2.160478
14.C	0.842493	0.436889	-3.036790
15.C	0.527028	-0.000656	-4.326257
16.C	-0.496551	-0.938538	-4.186854
17.N	-0.775240	-1.041066	-2.866259
18.N	-0.157867	-2.088456	-0.160042
19.N	-0.890537	-2.752722	-1.095607
20.C	-0.669145	-4.080013	-0.980090
21.C	0.238799	-4.268042	0.063895
22.C	0.548743	-3.002792	0.557073
23.N	-2.319514	-0.279339	-0.408998
24.C	-3.403089	0.313882	0.143714
25.C	-4.553443	-0.194215	-0.470312
26.C	-4.116369	-1.124793	-1.412687
27.N	-2.764054	-1.150690	-1.350780
28.B	-1.733736	-1.974051	-2.116607
29.H	1.001043	0.318049	-5.263181
30.H	0.629547	-5.225676	0.429883
31.H	-5.594102	0.075490	-0.250029
32.C	-1.320261	-5.087831	-1.850925
33.H	-1.045660	-4.944533	-2.916995
34.H	-1.005421	-6.103737	-1.546991
35.H	-2.426705	-5.032276	-1.783442
36.C	1.454960	-2.633436	1.666593
37.H	0.885462	-2.226692	2.529770
38.H	2.012101	-3.523509	2.012824
39.H	2.179895	-1.853527	1.348928
40.C	-3.291163	1.300399	1.246980
41.H	-4.233446	1.870015	1.352690
42.H	-3.082663	0.788660	2.210340
43.H	-2.456468	2.012637	1.077842
44.C	-4.900057	-1.972241	-2.345384
45.H	-4.736031	-3.053145	-2.151304
46.H	-5.979856	-1.763797	-2.226592
47.H	-4.626574	-1.781837	-3.404353
48.C	1.880398	1.397578	-2.593651
49.H	2.430276	1.798253	-3.465030
50.H	1.440446	2.246543	-2.027182
51.H	2.604698	0.907078	-1.908294
52.C	-1.204025	-1.728701	-5.224452
53.H	-1.046672	-2.819033	-5.085751
54.H	-2.298985	-1.547913	-5.203101
55.H	-0.828566	-1.453027	-6.227697
56.H	-2.273422	-2.735975	-2.885634

B – Tp*MoO(OCH_2CH_3)$_2$

1.Mo	-2.937612	-1.502465	3.241754
2.N	-2.816631	0.040222	1.722071
3.C	-3.818899	0.720520	1.134712
4.C	-3.262151	1.695039	0.294506
5.C	-1.879946	1.564199	0.411388
6.N	-1.637220	0.559346	1.286245
7.N	-1.247165	-2.304147	1.826321
8.N	-0.245070	-1.496740	1.401763
9.C	0.624544	-2.187159	0.625469
10.C	0.153601	-3.494398	0.549444
11.C	-1.029167	-3.525653	1.309621
12.N	-1.166667	-0.478797	4.089847
13.N	-0.228347	0.115377	3.305200
14.C	0.637387	0.818861	4.072147
15.C	0.235104	0.670657	5.398010
16.C	-0.905433	-0.144509	5.368691
17.B	-0.301879	-0.019991	1.778798
18.C	-1.975340	-4.649833	1.520566
19.C	1.831719	-1.570084	0.016119
20.C	-5.234829	0.402855	1.433981
21.C	-0.798792	2.328933	-0.262260
22.C	-1.781449	-0.596213	6.476617
23.C	1.773821	1.591930	3.506816
24.O	-2.531144	-3.138007	4.248780
25.O	-4.195310	-2.517273	2.140634
26.C	-1.292234	-3.596889	4.732644
27.C	-1.513357	-4.506219	5.920722
28.C	-5.057490	-3.456947	2.741051
29.C	-5.837041	-4.201075	1.682182
30.O	-4.007188	-0.573402	4.245210
31.H	2.518997	-1.159989	0.786544
32.H	2.385661	-2.329472	-0.568644
33.H	1.568151	-0.734016	-0.666209
34.H	0.612025	-4.326773	0.000247
35.H	0.619531	0.584443	1.269917
36.H	-5.915178	0.984974	0.784526
37.H	-5.460293	0.626041	2.499867
38.H	-5.412234	-0.686720	1.299998
39.H	-3.802553	2.416305	-0.331315
40.H	-1.242845	3.116167	-0.901263
41.H	-0.171485	1.675030	-0.904749
42.H	-0.120668	2.817131	0.469299
43.H	2.457442	0.948560	2.913904
44.H	1.422805	2.402682	2.833108
45.H	2.356020	2.054351	4.326779
46.H	0.712186	1.112189	6.282083
47.H	-1.425205	-0.194196	7.443719
48.H	-1.814463	-1.705770	6.539416
49.H	-2.826479	-0.264383	6.292597
50.H	-2.023682	-3.960388	6.743333
51.H	-0.545044	-4.894224	6.302164
52.H	-0.753498	-4.147143	3.920635
53.H	-0.634322	-2.737609	5.007697
54.H	-1.482827	-5.620040	1.315347
55.H	-2.377509	-4.635931	2.556542
56.H	-2.853165	-4.544509	0.845946
57.H	-4.453165	-4.156633	3.372693
58.H	-6.533415	-4.932829	2.144645
59.H	-5.148440	-4.750383	1.004840
60.H	-6.430374	-3.493192	1.065562
61.H	-5.750691	-2.926458	3.443091
62.H	-2.153263	-5.368492	5.637894

B^+ – $Tp^*MoO(OCH_2CH_3)_2^+$

1.Mo	-2.903479	-1.602547	3.222202
2.N	-2.818586	-0.017313	1.800564
3.C	-3.863750	0.671770	1.269720
4.C	-3.347188	1.639710	0.410998
5.C	-1.957358	1.511623	0.452910
6.N	-1.664679	0.502525	1.302101
7.N	-1.223033	-2.346615	1.871389
8.N	-0.247505	-1.528098	1.400170
9.C	0.619785	-2.227055	0.629896
10.C	0.178768	-3.549651	0.610623
11.C	-0.980714	-3.588623	1.393877
12.N	-1.263336	-0.388249	4.045746
13.N	-0.253632	0.113918	3.287624
14.C	0.625271	0.775240	4.076331
15.C	0.156920	0.687984	5.387607
16.C	-1.032739	-0.044141	5.336098
17.B	-0.306281	-0.047532	1.764456
18.C	-1.879952	-4.736158	1.673452
19.C	1.795126	-1.607856	-0.031660
20.C	-5.273785	0.359611	1.587687
21.C	-0.919746	2.289215	-0.265998
22.C	-1.964088	-0.408154	6.430203
23.C	1.837953	1.446675	3.547041
24.O	-2.256803	-2.902046	4.439232
25.O	-4.046756	-2.662403	2.148524
26.C	-0.981599	-3.393596	4.802760
27.C	-1.120617	-4.424356	5.894656
28.C	-5.351950	-3.129725	2.480659
29.C	-6.127864	-3.471465	1.238603
30.O	-4.125914	-0.853414	4.188110
31.H	2.482530	-1.139253	0.703501
32.H	2.361482	-2.377026	-0.589535
33.H	1.491203	-0.817398	-0.749838
34.H	0.645919	-4.388144	0.078718
35.H	0.596370	0.563887	1.240278
36.H	-5.944394	1.102454	1.118028
37.H	-5.446225	0.356594	2.685599
38.H	-5.549341	-0.649685	1.209103
39.H	-3.922515	2.359105	-0.184972
40.H	-1.400760	3.046199	-0.913421
41.H	-0.289456	1.635947	-0.904803
42.H	-0.242749	2.815610	0.438932
43.H	2.497755	0.736589	3.006219
44.H	1.577849	2.260997	2.838490
45.H	2.416159	1.888732	4.379985
46.H	0.623596	1.121957	6.280908
47.H	-1.611109	0.011021	7.390367
48.H	-2.061031	-1.510796	6.536549
49.H	-2.985985	-0.023302	6.224355
50.H	-1.605096	-3.993513	6.795392
51.H	-0.115488	-4.793936	6.184486
52.H	-0.482034	-3.806216	3.895134
53.H	-0.370083	-2.519785	5.137079
54.H	-1.370815	-5.691096	1.444457
55.H	-2.212261	-4.749155	2.733178
56.H	-2.799801	-4.670596	1.053967
57.H	-5.221807	-4.027157	3.130721
58.H	-7.129934	-3.860349	1.516410
59.H	-5.606352	-4.250541	0.645378
60.H	-6.270497	-2.579152	0.593224
61.H	-5.855416	-2.346738	3.099260
62.H	-1.722873	-5.291059	5.552432

C – Tp*MoO($OCH_2CH_2CH_3$)$_2$

1.Mo	-0.001288	0.001172	0.011123
2.N	2.167471	0.002324	0.008399
3.C	3.006158	1.055255	-0.003894
4.C	4.320122	0.578017	0.102606
5.C	4.223548	-0.809679	0.181355
6.N	2.909115	-1.131369	0.129342
7.N	0.510243	-1.753749	-1.463055
8.N	1.451568	-2.678762	-1.155721
9.C	1.572182	-3.584586	-2.155845
10.C	0.665716	-3.220466	-3.146697
11.C	0.023874	-2.060215	-2.677978
12.N	0.234012	-1.681544	1.429095
13.N	1.252655	-2.576917	1.328074
14.C	1.251537	-3.400954	2.402222
15.C	0.194738	-3.013816	3.223634
16.C	-0.416445	-1.926319	2.583385
17.B	2.227943	-2.508791	0.145680
18.C	-0.988266	-1.213906	-3.357705
19.C	2.528554	-4.721388	-2.107248
20.C	2.489806	2.440923	-0.097267
21.C	5.301293	-1.826405	0.291484
22.C	-1.559742	-1.087246	3.016940
23.C	2.246657	-4.489027	2.587750
24.O	-1.847956	-0.527280	-0.389468
25.O	-0.017839	1.167475	-1.558333
26.C	-2.454411	-1.789136	-0.287762
27.C	-3.949139	-1.645643	-0.084143
28.C	-1.149217	1.944252	-1.864809
29.C	-0.981799	2.641696	-3.197749
30.O	-0.100373	1.141135	1.316323
31.H	2.330202	-5.392031	-1.244160
32.H	2.445048	-5.320673	-3.034249
33.H	3.579272	-4.372231	-2.016067
34.H	0.495433	-3.733362	-4.101962
35.H	3.066785	-3.378867	0.257380
36.H	3.318814	3.163340	-0.217228
37.H	1.907603	2.695593	0.815316
38.H	1.781771	2.520890	-0.951068
39.H	5.241346	1.173816	0.119073
40.H	6.285133	-1.321490	0.339637
41.H	5.307886	-2.514318	-0.580670
42.H	5.187523	-2.452377	1.201707
43.H	2.223572	-5.216703	1.749303
44.H	3.282592	-4.092405	2.646976
45.H	2.032584	-5.035011	3.526479
46.H	-0.091657	-3.465823	4.181670
47.H	-1.909543	-1.395005	4.020345
48.H	-2.410395	-1.161130	2.304097
49.H	-1.259387	-0.017061	3.034362
50.H	-4.126488	-1.045143	0.837537
51.H	-2.259874	-2.383168	-1.218719
52.H	-2.008620	-2.383618	0.548552
53.H	-1.506795	-1.784678	-4.152280
54.H	-1.725825	-0.818909	-2.626455
55.H	-0.500773	-0.325793	-3.816712
56.H	-2.061683	1.291788	-1.868853
57.H	-0.815447	1.868836	-3.982764
58.H	-0.053211	3.254931	-3.161932
59.H	-1.318055	2.703076	-1.055372
60.H	-4.366034	-1.049756	-0.926937
61.C	-2.185227	3.505094	-3.538412
62.H	-2.351655	4.283567	-2.761641
63.H	-2.061623	4.022986	-4.511299
64.H	-3.113309	2.894971	-3.596482
65.C	-4.632447	-2.999369	0.013612
66.H	-5.727485	-2.900519	0.158626
67.H	-4.467077	-3.598460	-0.908636
68.H	-4.230777	-3.590452	0.865910

C^+ – Tp*MoO($OCH_2CH_2CH_3$)$_2^+$

1.Mo	-0.046807	-0.037426	-0.059552
2.N	2.074549	-0.005664	0.026157
3.C	2.872617	1.095797	0.048338
4.C	4.194230	0.663107	0.128800
5.C	4.157592	-0.733283	0.161218
6.N	2.862172	-1.111237	0.098268
7.N	0.448091	-1.786772	-1.448634
8.N	1.425062	-2.687126	-1.167831
9.C	1.532941	-3.591303	-2.170725
10.C	0.580894	-3.254597	-3.131297
11.C	-0.075446	-2.114628	-2.650977
12.N	0.320795	-1.591218	1.452755
13.N	1.273251	-2.551451	1.321482
14.C	1.239464	-3.378670	2.391792
15.C	0.224725	-2.927420	3.236146
16.C	-0.330954	-1.801033	2.622684
17.B	2.223219	-2.510137	0.120102
18.C	-1.137335	-1.309075	-3.305308
19.C	2.519039	-4.700464	-2.158328
20.C	2.332220	2.469836	-0.033831
21.C	5.277570	-1.701067	0.242179
22.C	-1.416745	-0.910517	3.097419
23.C	2.163275	-4.528703	2.551865
24.O	-1.802049	-0.741984	-0.063225
25.O	-0.094444	0.972158	-1.662791
26.C	-2.398478	-2.017617	-0.098988
27.C	-3.904346	-1.897127	-0.016840
28.C	-0.955129	2.087981	-1.869719
29.C	-0.631582	2.789858	-3.163914
30.O	-0.258163	1.248591	1.076660
31.H	2.382168	-5.364411	-1.279118
32.H	2.406993	-5.313495	-3.072281
33.H	3.562043	-4.320729	-2.126258
34.H	0.393022	-3.776438	-4.078183
35.H	3.077620	-3.360355	0.222763
36.H	3.150651	3.209035	0.040700
37.H	1.595487	2.658526	0.776858
38.H	1.799284	2.623497	-0.998847
39.H	5.089594	1.296617	0.155393
40.H	6.240353	-1.157863	0.279907
41.H	5.295315	-2.378155	-0.637355
42.H	5.202095	-2.337776	1.148272
43.H	2.085562	-5.238999	1.702492
44.H	3.221514	-4.197671	2.609793
45.H	1.923951	-5.076120	3.482765
46.H	-0.068309	-3.362512	4.199974
47.H	-1.730438	-1.200257	4.117219
48.H	-2.305498	-0.952360	2.430055
49.H	-1.083156	0.149160	3.110453
50.H	-4.173138	-1.345664	0.911981
51.H	-2.077224	-2.553462	-1.024788
52.H	-1.995951	-2.605565	0.764809
53.H	-1.641524	-1.900256	-4.092901
54.H	-1.898061	-0.956823	-2.577099
55.H	-0.702292	-0.400062	-3.774131
56.H	-2.007756	1.707693	-1.883021
57.H	-0.664138	2.044859	-3.990488
58.H	0.413283	3.171203	-3.120885
59.H	-0.873605	2.775628	-0.990192
60.H	-4.262395	-1.276993	-0.868606
61.C	-1.613681	3.922499	-3.422380
62.H	-1.586405	4.678988	-2.608916
63.H	-1.385377	4.444837	-4.372068
64.H	-2.656421	3.543654	-3.491253
65.C	-4.557806	-3.269122	-0.038465
66.H	-5.661161	-3.187684	0.017800
67.H	-4.309546	-3.820891	-0.970382
68.H	-4.222611	-3.890884	0.819283

D – Tp*MoO($OCH_2CH_2CH_2O$) in chair conformation

1.B	0.001199	0.021144	-0.003487
2.N	1.528292	0.031906	0.001550
3.N	2.175725	1.224699	0.005119
4.C	3.494491	0.963955	-0.002085
5.C	3.688934	-0.425965	-0.009323
6.C	2.416330	-0.989657	-0.006031
7.N	-0.494550	0.730536	1.262366
8.C	-1.240119	0.258079	2.288948
9.C	-1.357229	1.282473	3.226447
10.C	-0.644578	2.370775	2.702042
11.N	-0.125887	2.014593	1.512811
12.N	-0.488482	0.764301	-1.253175
13.N	-0.122959	2.055922	-1.465465
14.C	-0.651663	2.451090	-2.637592
15.C	-1.367264	1.379854	-3.191740
16.C	-1.241567	0.325011	-2.289332
17.H	-0.411709	-1.119963	-0.018746
18.Mo	0.974895	3.234088	0.037734
19.O	-0.234720	4.475415	0.044487
20.C	-1.786253	-1.055656	-2.364119
21.C	-0.453597	3.834934	-3.132260
22.C	4.505029	2.048697	-0.002137
23.C	2.008615	-2.419012	-0.008495
24.C	-1.787191	-1.123473	2.322263
25.C	-0.442474	3.736141	3.244008
26.H	4.646976	-0.961079	-0.016753
27.H	2.908478	-3.063840	0.000407
28.H	1.393101	-2.673437	0.880430
29.H	1.408562	-2.676091	-0.907235
30.H	4.399039	2.671119	0.912431
31.H	4.337604	2.723588	-0.868834
32.H	5.528451	1.629989	-0.048392
33.H	-0.993199	4.557122	-2.480927
34.H	-0.818679	3.939931	-4.171505
35.H	0.623285	4.104106	-3.075844
36.H	-1.916561	1.370108	-4.141650
37.H	-2.376710	-1.174304	-3.293074
38.H	-2.446926	-1.285224	-1.501384
39.H	-0.977570	-1.816959	-2.368335
40.H	-0.816526	3.807364	4.282961
41.H	0.636347	4.000265	3.206617
42.H	-0.972568	4.483414	2.613639
43.H	-2.400131	-1.260795	3.233920
44.H	-2.427150	-1.334105	1.439548
45.H	-0.979626	-1.886296	2.330032
46.H	-1.900918	1.241995	4.178837
47.O	2.176295	3.883814	1.451867
48.O	2.186240	3.933016	-1.344961
49.C	2.659031	5.254288	-1.189063
50.C	2.659328	5.206157	1.353483
51.C	3.457541	5.464874	0.086963
52.H	3.294781	5.503199	-2.071384
53.H	1.782196	5.957199	-1.189958
54.H	4.355397	4.808997	0.074411
55.H	3.815432	6.520064	0.107155
56.H	3.297408	5.411480	2.245483
57.H	1.788349	5.915520	1.386327

D^{+} – Tp*MoO($OCH_2CH_2CH_2O$)$^{+}$ in chair conformation

1.B	0.031028	-0.023040	-0.005462
2.N	1.554650	0.003165	-0.004678
3.N	2.183498	1.208963	0.007059
4.C	3.519226	0.970469	0.006225
5.C	3.727586	-0.410097	-0.005792
6.C	2.462330	-0.998788	-0.012219
7.N	-0.467147	0.708007	1.249615
8.C	-1.269032	0.286843	2.253797
9.C	-1.470593	1.369408	3.114954
10.C	-0.766344	2.442416	2.572250
11.N	-0.152533	2.017963	1.435871
12.N	-0.466973	0.745704	-1.237679
13.N	-0.159260	2.062689	-1.380553
14.C	-0.772225	2.520200	-2.504214
15.C	-1.469114	1.461465	-3.083529
16.C	-1.263550	0.352683	-2.257542
17.H	-0.383409	-1.159135	-0.022478
18.Mo	1.062486	3.163370	0.043113
19.O	-0.010769	4.525844	0.066142
20.C	-1.782260	-1.029669	-2.391429
21.C	-0.631798	3.923049	-2.955623
22.C	4.522067	2.061037	0.017078
23.C	2.084437	-2.433268	-0.024446
24.C	-1.796558	-1.095900	2.341145
25.C	-0.620131	3.829191	3.069170
26.H	4.693522	-0.930710	-0.009620
27.H	2.994257	-3.062175	-0.025568
28.H	1.478859	-2.704923	0.865568
29.H	1.485752	-2.691724	-0.923038
30.H	4.401457	2.694453	0.921905
31.H	4.393752	2.719126	-0.868808
32.H	5.545078	1.642104	0.007161
33.H	-0.955713	4.630094	-2.161063
34.H	-1.238465	4.100053	-3.862565
35.H	0.430758	4.156540	-3.186052
36.H	-2.059328	1.488541	-4.008171
37.H	-2.360279	-1.125803	-3.329458
38.H	-2.449711	-1.299061	-1.545838
39.H	-0.959218	-1.774061	-2.411404
40.H	-1.224083	3.978047	3.982966
41.H	0.443626	4.051930	3.304497
42.H	-0.943979	4.563013	2.299193
43.H	-2.383549	-1.217021	3.270663
44.H	-2.457669	-1.335604	1.481801
45.H	-0.977896	-1.845420	2.345892
46.H	-2.063034	1.369711	4.038593
47.O	2.217028	3.835206	1.407814
48.O	2.207465	3.870613	-1.312175
49.C	2.561286	5.252830	-1.217437
50.C	2.570513	5.219093	1.350497
51.C	3.324310	5.537263	0.067782
52.H	3.180956	5.505149	-2.103426
53.H	1.612841	5.848265	-1.250030
54.H	4.290653	4.987316	0.057247
55.H	3.565992	6.624177	0.081067
56.H	3.196438	5.446571	2.238796
57.H	1.622417	5.813421	1.406099

D – Tp*MoO($OCH_2CH_2CH_2O$) in boat conformation

1.H	0.047540	-0.049269	0.031104
2.C	1.168280	-0.020234	0.002299
3.C	1.629654	1.425336	0.016740
4.H	2.743034	1.453517	0.020072
5.H	1.274324	1.912256	0.953623
6.C	1.112491	2.209043	-1.175148
7.H	-0.008599	2.232832	-1.141683
8.O	1.627625	-0.748607	-1.114100
9.O	1.532101	1.691821	-2.417593
10.Mo	2.573148	0.043228	-2.639492
11.O	4.143713	0.438019	-2.022834
12.N	0.814896	-0.762613	-3.991137
13.N	1.069072	-1.384402	-5.168569
14.N	3.171126	0.683684	-4.654085
15.N	3.290082	-1.941810	-3.255757
16.N	3.144104	-0.146647	-5.729316
17.N	3.258238	-2.365647	-4.546505
18.C	3.724855	1.847657	-5.039023
19.C	3.666154	0.484346	-6.807692
20.C	4.049669	1.760798	-6.400443
21.H	4.512125	2.537312	-7.022784
22.C	3.877307	-3.565598	-4.649256
23.C	3.943045	-2.866093	-2.528767
24.C	4.328653	-3.913803	-3.377568
25.H	4.874775	-4.824633	-3.101361
26.C	-0.517521	-0.757141	-3.822189
27.C	-0.084085	-1.778552	-5.758402
28.C	-1.124300	-1.389478	-4.919483
29.H	-2.197991	-1.545629	-5.084389
30.B	2.520484	-1.542628	-5.610255
31.H	1.527929	-0.539995	0.923843
32.H	1.457406	3.270182	-1.107952
33.C	3.929225	2.952666	-4.071555
34.H	4.277358	3.867916	-4.586260
35.H	2.983498	3.156506	-3.524434
36.H	4.678657	2.655805	-3.305315
37.C	3.760893	-0.149844	-8.148220
38.H	4.241141	0.550212	-8.858458
39.H	4.361256	-1.083571	-8.121476
40.H	2.759417	-0.416126	-8.548204
41.C	3.998070	-4.305641	-5.932257
42.H	4.553832	-3.720071	-6.694902
43.H	4.539900	-5.256160	-5.764625
44.H	3.003294	-4.544732	-6.364491
45.C	4.176573	-2.669219	-1.077682
46.H	4.582114	-3.588716	-0.615078
47.H	4.891525	-1.832914	-0.915395
48.H	3.228341	-2.374911	-0.578194
49.C	-0.125082	-2.490591	-7.062421
50.H	0.329897	-1.887707	-7.876983
51.H	0.423876	-3.455614	-7.022704
52.H	-1.175630	-2.704365	-7.338317
53.C	-1.153341	-0.159336	-2.623603
54.H	-2.255400	-0.161230	-2.724385
55.H	-0.871153	-0.727451	-1.711455
56.H	-0.798283	0.883032	-2.480671
57.H	2.581507	-2.110116	-6.681419

D^{+} – Tp*MoO($OCH_2CH_2CH_2O$)$^{+}$ in boat conformation

1.H	0.071180	-0.035182	0.099276
2.C	1.183724	0.021413	0.034146
3.C	1.657853	1.463638	0.027955
4.H	2.767889	1.495142	0.095621
5.H	1.259983	1.959841	0.942014
6.C	1.187091	2.258533	-1.177558
7.H	0.079155	2.391416	-1.158504
8.O	1.583166	-0.677953	-1.142567
9.O	1.518354	1.632634	-2.416868
10.Mo	2.477926	0.006537	-2.672089
11.O	4.000234	0.436013	-1.959984
12.N	0.808671	-0.784831	-3.995629
13.N	1.034656	-1.402540	-5.183207
14.N	3.201209	0.619497	-4.622485
15.N	3.321671	-1.888124	-3.296446
16.N	3.102891	-0.161181	-5.732315
17.N	3.221609	-2.371459	-4.564223
18.C	3.863399	1.757361	-4.962274
19.C	3.690851	0.464333	-6.777623
20.C	4.175154	1.693478	-6.317965
21.H	4.695520	2.455061	-6.912168
22.C	3.913992	-3.528106	-4.662524
23.C	4.096488	-2.744679	-2.576096
24.C	4.471257	-3.796493	-3.406857
25.H	5.078565	-4.668554	-3.133667
26.C	-0.531581	-0.756406	-3.802682
27.C	-0.135437	-1.770289	-5.755159
28.C	-1.154900	-1.368570	-4.894229
29.H	-2.233619	-1.504721	-5.043804
30.B	2.474309	-1.561505	-5.637311
31.H	1.601688	-0.526404	0.907824
32.H	1.645245	3.273169	-1.180856
33.C	4.128875	2.825160	-3.972813
34.H	4.709018	3.645930	-4.432581
35.H	3.175329	3.236737	-3.575555
36.H	4.693093	2.421242	-3.103918
37.C	3.771138	-0.128043	-8.133830
38.H	4.237016	0.591902	-8.832270
39.H	4.380190	-1.056574	-8.138668
40.H	2.765757	-0.392520	-8.522789
41.C	4.020375	-4.303908	-5.920480
42.H	4.586994	-3.746044	-6.695968
43.H	4.547081	-5.257911	-5.731597
44.H	3.020629	-4.532332	-6.344548
45.C	4.396669	-2.508283	-1.146308
46.H	5.030745	-3.319360	-0.744134
47.H	4.919141	-1.536284	-1.011661
48.H	3.459791	-2.456115	-0.550101
49.C	-0.211351	-2.468107	-7.062238
50.H	0.229145	-1.859155	-7.879510
51.H	0.329736	-3.437408	-7.042064
52.H	-1.268086	-2.671486	-7.318534
53.C	-1.159064	-0.162512	-2.599415
54.H	-2.259529	-0.153096	-2.706724
55.H	-0.899441	-0.746376	-1.690737
56.H	-0.806507	0.878841	-2.444700
57.H	2.540601	-2.123072	-6.706652

E – Tp*MoO[OCH(CH_3)CH_2CH(CH_3)O] in chair conformation

1.C	-0.007924	0.039577	-0.248665
2.C	2.557167	0.045570	-0.209734
3.O	-0.116833	1.409768	0.099477
4.O	2.649718	1.415081	0.145658
5.Mo	1.274835	2.647499	-0.520596
6.O	1.304575	2.281883	-2.214953
7.N	1.233412	3.643340	1.598546
8.N	1.225323	4.994500	1.724805
9.N	2.764876	4.250820	-0.736311
10.N	-0.211107	4.247091	-0.791403
11.N	2.527736	5.523778	-0.323729
12.N	0.010879	5.522110	-0.376703
13.C	3.964523	4.226296	-1.344494
14.C	3.576194	6.314705	-0.653467
15.C	4.511214	5.517234	-1.311024
16.H	5.477954	5.839602	-1.718118
17.C	-1.022757	6.312193	-0.752091
18.C	-1.385820	4.220302	-1.446262
19.C	-1.931985	5.511953	-1.441673
20.H	-2.881595	5.832912	-1.888290
21.C	1.204452	3.125189	2.839084
22.C	1.190913	5.348856	3.030918
23.C	1.177013	4.172084	3.774222
24.H	1.150074	4.083855	4.867811
25.B	1.252043	5.852978	0.461938
26.C	-1.239594	-0.675769	0.263874
27.H	-2.157213	-0.186162	-0.122942
28.H	-1.266259	-0.628570	1.374710
29.H	-1.244516	-1.742100	-0.047021
30.C	3.776501	-0.666194	0.336137
31.H	4.702818	-0.172062	-0.023336
32.H	3.794609	-1.731670	0.022791
33.H	3.771421	-0.621588	1.447355
34.C	4.492989	2.972465	-1.934180
35.H	5.533432	3.108458	-2.284486
36.H	4.445015	2.153809	-1.183345
37.H	3.858488	2.651608	-2.789356
38.C	3.633733	7.761926	-0.321218
39.H	4.572118	8.197790	-0.714408
40.H	2.780630	8.320361	-0.760922
41.H	3.605894	7.932834	0.776028
42.C	-1.090937	7.761481	-0.430976
43.H	-0.223194	8.316836	-0.845300
44.H	-2.015179	8.195207	-0.858510
45.H	-1.099847	7.939446	0.665447
46.C	-1.891653	2.963532	-2.049413
47.H	-2.922489	3.094310	-2.428947
48.H	-1.232161	2.644942	-2.886329
49.H	-1.861021	2.145898	-1.296568
50.C	1.172377	6.763286	3.487003
51.H	2.070425	7.319621	3.143550
52.H	0.283131	7.308316	3.104515
53.H	1.147778	6.798711	4.593133
54.C	1.203985	1.661984	3.076181
55.H	1.182023	1.441441	4.160348
56.H	0.324659	1.195406	2.581439
57.H	2.105922	1.200619	2.618765
58.H	1.245287	7.031482	0.751865
59.H	2.556246	-0.017453	-1.333279
60.H	0.025947	-0.026706	-1.371480
61.C	1.268277	-0.588360	0.290699
62.H	1.251565	-0.546054	1.405252
63.H	1.274991	-1.664607	-0.001171

E^+ – Tp*MoO[$OCH(CH_3)CH_2CH(CH_3)O$]$^+$ in chair conformation

1.C	-0.022164	0.078288	-0.320517
2.C	2.574310	0.085123	-0.279011
3.O	-0.081046	1.435649	0.159099
4.O	2.611089	1.442264	0.203442
5.Mo	1.271547	2.651699	-0.400845
6.O	1.299758	2.108627	-2.048230
7.N	1.231203	3.660498	1.615920
8.N	1.224083	5.012894	1.757826
9.N	2.689464	4.261635	-0.759088
10.N	-0.134851	4.258344	-0.813638
11.N	2.513222	5.528428	-0.298259
12.N	0.022770	5.526841	-0.350809
13.C	3.851613	4.224632	-1.461144
14.C	3.549996	6.302487	-0.692134
15.C	4.421114	5.496696	-1.430470
16.H	5.368015	5.806185	-1.890480
17.C	-0.996519	6.299630	-0.790032
18.C	-1.267304	4.218843	-1.562679
19.C	-1.836893	5.491112	-1.560464
20.H	-2.764497	5.798787	-2.059400
21.C	1.204949	3.121162	2.860147
22.C	1.193373	5.346437	3.067954
23.C	1.180658	4.156935	3.797017
24.H	1.156606	4.057215	4.889549
25.B	1.250424	5.877612	0.501885
26.C	-1.252725	-0.649654	0.152803
27.H	-2.169181	-0.115043	-0.169855
28.H	-1.259861	-0.720337	1.261353
29.H	-1.282399	-1.677542	-0.264750
30.C	3.793246	-0.637046	0.231845
31.H	4.716462	-0.097450	-0.061850
32.H	3.841202	-1.664254	-0.185528
33.H	3.766398	-0.708836	1.340024
34.C	4.344797	2.977488	-2.088939
35.H	5.285838	3.165459	-2.637448
36.H	4.529591	2.197863	-1.317185
37.H	3.592228	2.563004	-2.794624
38.C	3.657743	7.742021	-0.353953
39.H	4.603712	8.152640	-0.753670
40.H	2.817870	8.326942	-0.784210
41.H	3.644449	7.904807	0.744014
42.C	-1.117133	7.740600	-0.462526
43.H	-0.261810	8.323746	-0.863838
44.H	-2.047447	8.149256	-0.899281
45.H	-1.144796	7.908479	0.634391
46.C	-1.735386	2.969168	-2.204550
47.H	-2.659148	3.152980	-2.782951
48.H	-0.959193	2.556914	-2.885442
49.H	-1.941689	2.189551	-1.438300
50.C	1.177995	6.751090	3.545117
51.H	2.078959	7.307381	3.211089
52.H	0.290847	7.302177	3.168239
53.H	1.151421	6.772817	4.650635
54.C	1.204821	1.657791	3.092902
55.H	1.185578	1.440911	4.176808
56.H	0.320189	1.185509	2.613760
57.H	2.109200	1.190731	2.646612
58.H	1.243814	7.053504	0.784753
59.H	2.587821	0.156323	-1.399054
60.H	-0.000764	0.148426	-1.440463
61.C	1.270513	-0.572081	0.159185
62.H	1.252954	-0.646771	1.271912
63.H	1.279434	-1.613182	-0.237421

E – Tp*MoO[OCH(CH_3)CH_2CH(CH_3)O] in boat conformation

1.H	0.033620	-0.052982	0.012552
2.C	1.156355	-0.035435	0.012806
3.C	1.603348	1.416299	0.008746
4.H	2.720322	1.446336	0.009978
5.H	1.250612	1.902541	0.947634
6.C	1.094690	2.219703	-1.175776
7.H	-0.028231	2.205183	-1.147629
8.O	1.608712	-0.742721	-1.129242
9.O	1.510715	1.676385	-2.417152
10.Mo	2.572538	0.045825	-2.639564
11.O	4.140730	0.445079	-2.018022
12.N	0.813352	-0.759067	-3.991227
13.N	1.066051	-1.382784	-5.167731
14.N	3.179064	0.683161	-4.654188
15.N	3.295692	-1.937661	-3.256819
16.N	3.141998	-0.146241	-5.730034
17.N	3.256024	-2.363831	-4.546713
18.C	3.744132	1.841469	-5.040366
19.C	3.668003	0.479796	-6.809314
20.C	4.064802	1.752069	-6.402496
21.H	4.534296	2.524204	-7.025016
22.C	3.875865	-3.563074	-4.652069
23.C	3.955271	-2.860245	-2.533317
24.C	4.336337	-3.908671	-3.383119
25.H	4.885859	-4.818050	-3.108875
26.C	-0.518764	-0.754913	-3.819930
27.C	-0.087487	-1.779680	-5.754882
28.C	-1.126606	-1.390160	-4.915053
29.H	-2.200447	-1.547736	-5.077541
30.B	2.516707	-1.541150	-5.609617
31.C	1.657794	-0.769081	1.241136
32.H	2.769092	-0.736284	1.266053
33.H	1.338713	-1.831140	1.209970
34.H	1.268598	-0.306086	2.173186
35.C	1.565211	3.659621	-1.115724
36.H	2.676902	3.687478	-1.120525
37.H	1.202035	4.163319	-0.194323
38.H	1.195689	4.221044	-1.998373
39.C	3.964375	2.945769	-4.075893
40.H	4.357618	3.843591	-4.588943
41.H	3.016166	3.192079	-3.551587
42.H	4.683857	2.627563	-3.289526
43.C	3.755081	-0.155041	-8.149986
44.H	4.237080	0.542379	-8.861630
45.H	4.350313	-1.092114	-8.125042
46.H	2.750945	-0.415749	-8.546852
47.C	3.990583	-4.303941	-5.935137
48.H	4.552885	-3.723628	-6.697089
49.H	4.523165	-5.259615	-5.767294
50.H	2.994019	-4.533062	-6.368437
51.C	4.201077	-2.664775	-1.084195
52.H	4.643280	-3.573595	-0.634101
53.H	4.889908	-1.805885	-0.925902
54.H	3.252522	-2.406158	-0.566249
55.C	-0.129636	-2.494890	-7.057044
56.H	0.325508	-1.894465	-7.873313
57.H	0.418476	-3.460335	-7.015082
58.H	-1.180506	-2.708489	-7.331810
59.C	-1.153943	-0.156210	-2.622085
60.H	-2.255956	-0.156327	-2.722613
61.H	-0.871330	-0.723754	-1.709901
62.H	-0.795398	0.884625	-2.478738
63.H	2.577014	-2.109064	-6.680494

E^{+} – Tp*MoO[OCH(CH$_3$)CH$_2$CH(CH$_3$)O]$^{+}$ in boat conformation

1.H	0.049439	-0.096791	0.099658
2.C	1.163548	-0.025373	0.051760
3.C	1.583001	1.436423	0.028101
4.H	2.695297	1.498727	0.101003
5.H	1.168290	1.916612	0.944181
6.C	1.113353	2.254527	-1.165374
7.H	-0.002755	2.313351	-1.164099
8.O	1.548781	-0.686963	-1.165640
9.O	1.470462	1.615738	-2.404798
10.Mo	2.459512	0.018540	-2.668995
11.O	3.975081	0.458744	-1.947982
12.N	0.794109	-0.776967	-3.997503
13.N	1.022184	-1.397196	-5.182932
14.N	3.199507	0.622809	-4.621618
15.N	3.318890	-1.877957	-3.292184
16.N	3.096363	-0.159759	-5.730078
17.N	3.212794	-2.363649	-4.558881
18.C	3.893620	1.742315	-4.958062
19.C	3.710451	0.447854	-6.771169
20.C	4.217942	1.666387	-6.310662
21.H	4.762786	2.413741	-6.901017
22.C	3.919721	-3.511816	-4.663566
23.C	4.109622	-2.724541	-2.579736
24.C	4.491431	-3.772350	-3.414096
25.H	5.115508	-4.634301	-3.146633
26.C	-0.546233	-0.755239	-3.804872
27.C	-0.144276	-1.772682	-5.753903
28.C	-1.166634	-1.373429	-4.894408
29.H	-2.244426	-1.515316	-5.043747
30.B	2.463744	-1.557266	-5.632599
31.C	1.779360	-0.779891	1.205646
32.H	2.887627	-0.722098	1.147859
33.H	1.472223	-1.844799	1.185282
34.H	1.456543	-0.340386	2.172477
35.C	1.699482	3.645983	-1.170254
36.H	2.809150	3.589995	-1.189138
37.H	1.393397	4.197846	-0.257004
38.H	1.351028	4.214661	-2.055724
39.C	4.184111	2.807591	-3.973018
40.H	4.797990	3.603406	-4.433191
41.H	3.243657	3.257539	-3.586393
42.H	4.725266	2.390337	-3.095704
43.C	3.792411	-0.152295	-8.123960
44.H	4.283475	0.553567	-8.819566
45.H	4.379092	-1.095085	-8.117928
46.H	2.785707	-0.394234	-8.523845
47.C	4.026551	-4.283936	-5.924168
48.H	4.571817	-3.713808	-6.705973
49.H	4.575317	-5.226946	-5.742766
50.H	3.026797	-4.533243	-6.336250
51.C	4.428268	-2.484759	-1.154407
52.H	5.092495	-3.279279	-0.767777
53.H	4.926280	-1.498914	-1.026422
54.H	3.502422	-2.459622	-0.538923
55.C	-0.218163	-2.476337	-7.058174
56.H	0.232164	-1.875020	-7.875644
57.H	0.315008	-3.449881	-7.029786
58.H	-1.274939	-2.672740	-7.319420
59.C	-1.178393	-0.161450	-2.603999
60.H	-2.279265	-0.172223	-2.705899
61.H	-0.902299	-0.731050	-1.691466
62.H	-0.842367	0.886313	-2.459533
63.H	2.530138	-2.121155	-6.700632

F – Tp*MoO[O(CH$_2$)$_4$O] in boat-twist conformation

1.O	-0.119530	0.082737	0.043156
2.O	2.728345	-0.140106	0.227218
3.Mo	1.426840	1.303353	0.068547
4.O	1.415068	1.773563	-1.600635
5.N	1.300435	1.248138	2.403497
6.N	1.425182	2.384537	3.132512
7.N	3.047996	2.694045	0.601078
8.N	0.098469	3.007536	0.539567
9.N	2.908169	3.638547	1.568438
10.N	0.416120	3.933153	1.481872
11.C	4.269505	2.835034	0.055768
12.C	4.038721	4.378530	1.653087
13.C	4.929023	3.893444	0.696414
14.H	5.939859	4.268078	0.491081
15.C	-0.509657	4.921523	1.488337
16.C	-1.031901	3.408166	-0.069038
17.C	-1.448320	4.618545	0.504991
18.C	1.133094	0.231742	3.265991
19.C	1.333864	2.110214	4.455656
20.C	1.143637	0.736839	4.576927
21.B	1.621464	3.710579	2.400826
22.C	-0.426161	-0.720004	-1.069073
23.H	-1.502164	-1.012925	-0.995344
24.H	-0.299948	-0.113757	-2.007056
25.C	2.756489	-1.461877	-0.245647
26.H	3.822635	-1.695985	-0.488693
27.H	2.462258	-2.159535	0.581434
28.C	0.413167	-1.979337	-1.194628
29.H	-0.030410	-2.572311	-2.028186
30.H	0.289834	-2.593733	-0.270697
31.C	1.899473	-1.758912	-1.465565
32.H	2.037233	-0.936046	-2.207804
33.H	2.318370	-2.679556	-1.932708
34.H	-2.333404	5.209305	0.236983
35.H	1.026163	0.168857	5.508624
36.C	-1.638182	2.618589	-1.167793
37.H	-2.567531	3.098485	-1.528186
38.H	-0.921165	2.520661	-2.012011
39.H	-1.860378	1.587398	-0.819978
40.C	-0.451437	6.077969	2.419966
41.H	0.482401	6.665078	2.290774
42.H	-1.310374	6.750681	2.233142
43.H	-0.489629	5.753856	3.481652
44.C	4.210743	5.485541	2.629567
45.H	5.211455	5.941518	2.503639
46.H	3.447441	6.280166	2.491190
47.H	4.122790	5.126939	3.677080
48.C	4.712283	1.956269	-1.053346
49.H	4.073032	2.113626	-1.949531
50.H	5.766988	2.156905	-1.319704
51.H	4.586209	0.891703	-0.760278
52.C	1.428752	3.155670	5.507911
53.H	2.400705	3.692229	5.470325
54.H	0.628680	3.919367	5.403995
55.H	1.331626	2.689676	6.507304
56.C	0.993598	-1.170316	2.801647
57.H	0.502450	-1.792205	3.575047
58.H	0.400885	-1.199137	1.861532
59.H	1.990736	-1.610639	2.582687
60.H	1.704795	4.623114	3.196727

F^{+} – Tp*MoO[O(CH$_2$)$_4$O]$^{+}$ in boat-twist conformation

1.O	-0.121356	0.114576	0.075718
2.O	2.630312	-0.190929	0.336068
3.Mo	1.404637	1.245173	0.179808
4.O	1.473055	1.546431	-1.524692
5.N	1.303664	1.252201	2.427031
6.N	1.406905	2.380623	3.175460
7.N	2.968342	2.705487	0.607015
8.N	0.179035	3.024377	0.514161
9.N	2.881231	3.625652	1.604947
10.N	0.420898	3.922034	1.506298
11.C	4.148032	2.891974	-0.036117
12.C	3.993025	4.395491	1.611009
13.C	4.821191	3.947074	0.578857
14.H	5.808012	4.344964	0.310728
15.C	-0.472236	4.934719	1.434040
16.C	-0.882888	3.471411	-0.204918
17.C	-1.318298	4.671823	0.355007
18.C	1.169294	0.205939	3.278402
19.C	1.337265	2.076639	4.491176
20.C	1.179405	0.693038	4.587608
21.B	1.605894	3.709594	2.455091
22.C	-0.466413	-0.659825	-1.062830
23.H	-1.527799	-0.971154	-0.952235
24.H	-0.369044	-0.004104	-1.965514
25.C	2.830243	-1.384057	-0.408153
26.H	3.889849	-1.381485	-0.755083
27.H	2.733662	-2.225778	0.320872
28.C	0.427410	-1.881062	-1.225242
29.H	-0.037846	-2.484457	-2.037412
30.H	0.365300	-2.507219	-0.304545
31.C	1.894411	-1.598247	-1.580268
32.H	1.964117	-0.735963	-2.283850
33.H	2.306432	-2.472155	-2.133548
34.H	-2.162104	5.286763	0.017782
35.H	1.082148	0.106926	5.510216
36.C	-1.434085	2.723021	-1.357240
37.H	-2.216223	3.318976	-1.862651
38.H	-0.637090	2.477831	-2.092185
39.H	-1.886313	1.763605	-1.024657
40.C	-0.473248	6.080543	2.375339
41.H	0.463364	6.672084	2.299832
42.H	-1.322702	6.751725	2.148862
43.H	-0.566984	5.744081	3.428800
44.C	4.207344	5.498760	2.578533
45.H	5.201567	5.954741	2.414362
46.H	3.440343	6.293956	2.468251
47.H	4.159680	5.137721	3.627036
48.C	4.561020	2.042092	-1.176976
49.H	3.799529	2.064187	-1.986421
50.H	5.528520	2.386844	-1.585791
51.H	4.669121	0.982207	-0.858833
52.C	1.425446	3.098361	5.563061
53.H	2.394198	3.640094	5.533637
54.H	0.619770	3.856865	5.473155
55.H	1.333157	2.614305	6.553281
56.C	1.054811	-1.194201	2.804595
57.H	0.749861	-1.858117	3.634634
58.H	0.312124	-1.275545	1.982803
59.H	2.029887	-1.552795	2.409375
60.H	1.685269	4.622562	3.244420

F – Tp*MoO[O(CH_2)$_4$O] in chair conformation

1.O	-0.005204	0.051267	-0.056003
2.O	2.823621	0.004666	-0.194269
3.Mo	1.441524	1.386219	-0.033075
4.O	1.360461	1.987977	-1.655751
5.N	1.493054	1.148196	2.296265
6.N	1.569620	2.241849	3.097017
7.N	2.996853	2.842468	0.524733
8.N	0.021129	2.940682	0.639182
9.N	2.833263	3.721185	1.548751
10.N	0.320868	3.812478	1.637124
11.C	4.165162	3.123382	-0.080739
12.C	3.897259	4.555732	1.611904
13.C	4.766829	4.202951	0.581348
14.H	5.726424	4.677851	0.340870
15.C	-0.679960	4.714543	1.775505
16.C	-1.170687	3.291776	0.125227
17.C	-1.648723	4.412297	0.820695
18.C	1.447231	0.069037	3.097823
19.C	1.570927	1.876377	4.400465
20.C	1.493888	0.487530	4.437019
21.B	1.602183	3.627876	2.458084
22.C	-0.125430	-0.845193	-1.139662
23.H	-1.216409	-1.002085	-1.329754
24.H	0.296543	-0.383671	-2.069606
25.C	2.814568	-1.002672	-1.183465
26.H	3.877692	-1.292498	-1.368314
27.C	0.506264	-2.204113	-0.902154
28.H	-2.592935	4.945521	0.652045
29.H	1.471879	-0.148040	5.331409
30.C	-1.761537	2.542407	-1.009647
31.H	-2.782743	2.904593	-1.232668
32.H	-1.126997	2.653762	-1.915970
33.H	-1.785458	1.456921	-0.772885
34.C	-0.662617	5.791081	2.799962
35.H	0.218578	6.456977	2.684603
36.H	-1.576666	6.408538	2.707691
37.H	-0.627199	5.377439	3.830340
38.C	4.030471	5.621596	2.638910
39.H	4.972550	6.179719	2.477095
40.H	3.187732	6.343489	2.596239
41.H	4.049139	5.201395	3.666957
42.C	4.613871	2.355901	-1.267179
43.H	3.918373	2.523135	-2.118705
44.H	5.635217	2.656223	-1.567781
45.H	4.582459	1.267743	-1.045089
46.C	1.639345	2.854715	5.517199
47.H	2.563486	3.469266	5.471420
48.H	0.778198	3.556362	5.504238
49.H	1.630839	2.317255	6.484886
50.C	1.373434	-1.306808	2.554341
51.H	1.076019	-2.023798	3.343460
52.H	0.645279	-1.341322	1.715469
53.H	2.360111	-1.614802	2.145800
54.H	1.664863	4.485334	3.314759
55.H	2.420350	-0.590965	-2.149405
56.C	2.046759	-2.250750	-0.778362
57.H	0.180592	-2.846641	-1.753003
58.H	0.039444	-2.650220	0.004971
59.H	2.343440	-2.476821	0.268419
60.H	2.434557	-3.096144	-1.390808

F^{+} – Tp*MoO[O(CH$_2$)$_4$O]$^{+}$ in chair conformation

1.O	0.086508	-0.040740	-0.023798
2.O	2.848271	0.032004	-0.077301
3.Mo	1.435579	1.293021	0.115619
4.O	1.329439	1.689432	-1.571279
5.N	1.489568	1.145478	2.355535
6.N	1.561384	2.241955	3.157593
7.N	2.905612	2.854538	0.514463
8.N	0.090882	2.936528	0.640596
9.N	2.812470	3.702243	1.575163
10.N	0.334018	3.795321	1.666727
11.C	4.012121	3.190791	-0.195479
12.C	3.846813	4.574033	1.552470
13.C	4.630381	4.269004	0.437211
14.H	5.550062	4.778837	0.123899
15.C	-0.625177	4.746953	1.703545
16.C	-1.037490	3.350037	0.007281
17.C	-1.517521	4.483875	0.661106
18.C	1.467844	0.053011	3.161877
19.C	1.585298	1.869960	4.456923
20.C	1.524731	0.475886	4.490343
21.B	1.600972	3.623813	2.513048
22.C	-0.221303	-0.701189	-1.245074
23.H	-1.321861	-0.858851	-1.293997
24.H	0.070355	0.000601	-2.069796
25.C	2.889273	-0.890973	-1.170078
26.H	3.942858	-1.233852	-1.254088
27.C	0.501214	-2.031087	-1.376834
28.H	-2.420573	5.055060	0.411553
29.H	1.522477	-0.159665	5.384912
30.C	-1.596989	2.631109	-1.160243
31.H	-2.492614	3.155725	-1.540880
32.H	-0.848472	2.557121	-1.978279
33.H	-1.888520	1.594239	-0.885585
34.C	-0.643876	5.837710	2.707997
35.H	0.256744	6.482169	2.628163
36.H	-1.536322	6.473341	2.556922
37.H	-0.673077	5.438908	3.743541
38.C	4.031750	5.635442	2.571549
39.H	4.954203	6.206542	2.356441
40.H	3.179356	6.346878	2.580962
41.H	4.117454	5.210265	3.593387
42.C	4.407855	2.455702	-1.417830
43.H	3.566806	2.411718	-2.143643
44.H	5.274222	2.944126	-1.900480
45.H	4.680246	1.406263	-1.172460
46.C	1.663169	2.839623	5.576567
47.H	2.583151	3.458339	5.518954
48.H	0.797307	3.534478	5.577338
49.H	1.671874	2.299549	6.541760
50.C	1.412475	-1.327524	2.628950
51.H	1.252422	-2.050652	3.449842
52.H	0.595546	-1.435176	1.884624
53.H	2.366810	-1.583706	2.118699
54.H	1.665346	4.488405	3.356132
55.H	2.620125	-0.336726	-2.106128
56.C	1.974767	-2.087587	-0.922419
57.H	0.412852	-2.315474	-2.450850
58.H	-0.051136	-2.817690	-0.816681
59.H	2.018571	-2.287642	0.170267
60.H	2.442641	-2.976867	-1.398498

F – Tp*MoO[O(CH_2)$_4$O] in boat conformation

1.O	1.290975	1.358369	-0.258508
2.O	1.248436	-1.421489	-0.270807
3.Mo	-0.063823	-0.020729	0.098166
4.O	-0.233498	0.020750	1.820914
5.N	-0.564317	0.135154	-2.229823
6.N	-1.858264	0.052637	-2.636516
7.N	-1.624898	-1.551816	-0.090910
8.N	-1.721111	1.435013	-0.021297
9.N	-2.773441	-1.343876	-0.787015
10.N	-2.877358	1.170172	-0.681094
11.C	-1.711323	-2.755998	0.504256
12.C	-3.590911	-2.414356	-0.653543
13.C	-2.942800	-3.335194	0.167426
14.H	-3.324202	-4.313705	0.485597
15.C	-3.764654	2.172748	-0.474034
16.C	-1.867774	2.604792	0.623397
17.C	-3.151544	3.105921	0.359430
18.C	0.179023	0.355612	-3.328893
19.C	-1.950365	0.218461	-3.977549
20.C	-0.659316	0.411633	-4.454369
21.B	-2.967791	-0.058320	-1.594765
22.C	2.534045	1.557178	0.387050
23.H	2.489630	2.548764	0.903891
24.H	3.333156	1.645440	-0.394652
25.C	2.634353	-1.249301	-0.454504
26.H	3.055007	-2.211855	-0.832432
27.H	2.816324	-0.485351	-1.245697
28.C	2.904121	0.490782	1.405899
29.H	2.012538	0.323971	2.049621
30.H	3.697088	0.901773	2.070681
31.C	3.381309	-0.831586	0.801077
32.H	3.316445	-1.639669	1.563905
33.H	4.457210	-0.751694	0.514191
34.H	-3.587922	4.041865	0.730629
35.H	-0.358642	0.578216	-5.496676
36.C	-0.777323	3.155395	1.464861
37.H	-1.017073	4.182730	1.798282
38.H	-0.615576	2.509344	2.355169
39.H	0.177171	3.156405	0.895226
40.C	-5.121441	2.189307	-1.080192
41.H	-5.714163	1.296568	-0.788909
42.H	-5.668601	3.091331	-0.745139
43.H	-5.076362	2.204412	-2.190180
44.C	-4.921466	-2.504183	-1.309295
45.H	-5.404380	-3.463550	-1.041739
46.H	-5.593041	-1.677825	-0.994401
47.H	-4.838669	-2.454472	-2.415745
48.C	-0.627925	-3.257256	1.383043
49.H	-0.565893	-2.637680	2.304616
50.H	-0.808845	-4.310801	1.667863
51.H	0.352583	-3.157117	0.870701
52.C	-3.242218	0.196638	-4.712532
53.H	-3.790381	-0.756717	-4.557579
54.H	-3.915910	1.018275	-4.387224
55.H	-3.055576	0.314818	-5.797346
56.C	1.653495	0.513115	-3.282978
57.H	2.008997	1.056709	-4.179969
58.H	1.938405	1.074705	-2.367107
59.H	2.163909	-0.473510	-3.258246
60.H	-4.053241	-0.083888	-2.136879

F^{+} – Tp*MoO[O(CH$_2$)$_4$O]$^{+}$ in boat conformation

1.O	1.272668	1.317964	-0.309201
2.O	1.317635	-1.333724	-0.379201
3.Mo	-0.034525	-0.038887	-0.046619
4.O	-0.078434	-0.082621	1.683753
5.N	-0.582945	0.077019	-2.254190
6.N	-1.871557	0.095379	-2.685531
7.N	-1.653983	-1.473715	-0.115658
8.N	-1.711958	1.374311	0.009667
9.N	-2.782503	-1.303143	-0.855332
10.N	-2.857819	1.187319	-0.700141
11.C	-1.780681	-2.629042	0.591156
12.C	-3.625836	-2.337289	-0.637979
13.C	-3.007746	-3.204038	0.269181
14.H	-3.412166	-4.150294	0.649997
15.C	-3.764478	2.131947	-0.359702
16.C	-1.889763	2.452097	0.812792
17.C	-3.170971	2.958179	0.597867
18.C	0.207057	0.194228	-3.349989
19.C	-1.920493	0.227068	-4.029763
20.C	-0.604170	0.295037	-4.482787
21.B	-2.983326	-0.007250	-1.654525
22.C	2.436659	1.699134	0.427579
23.H	2.231228	2.692950	0.888621
24.H	3.250646	1.852610	-0.318937
25.C	2.724469	-1.168508	-0.328557
26.H	3.189764	-2.143533	-0.595830
27.H	2.990138	-0.447975	-1.138549
28.C	2.813289	0.698553	1.499452
29.H	1.942173	0.579014	2.179224
30.H	3.613427	1.161577	2.118542
31.C	3.286462	-0.679004	0.995656
32.H	3.104672	-1.438857	1.787312
33.H	4.390798	-0.667616	0.840415
34.H	-3.624652	3.833047	1.080223
35.H	-0.270729	0.403687	-5.522572
36.C	-0.823676	2.939765	1.718209
37.H	-1.191121	3.785906	2.327605
38.H	-0.482020	2.127566	2.395973
39.H	0.059869	3.284585	1.138351
40.C	-5.126595	2.194850	-0.942688
41.H	-5.722129	1.292807	-0.688006
42.H	-5.662092	3.079963	-0.551168
43.H	-5.095572	2.267505	-2.049806
44.C	-4.956079	-2.444379	-1.283007
45.H	-5.442579	-3.392733	-0.987868
46.H	-5.622171	-1.606987	-0.986149
47.H	-4.874932	-2.423118	-2.389793
48.C	-0.720063	-3.103935	1.507493
49.H	-0.528863	-2.352961	2.304947
50.H	-1.013658	-4.060739	1.976466
51.H	0.238974	-3.245434	0.963968
52.C	-3.191532	0.282692	-4.793253
53.H	-3.798422	-0.635578	-4.648634
54.H	-3.817730	1.145814	-4.483891
55.H	-2.976285	0.385392	-5.873369
56.C	1.686969	0.192311	-3.286850
57.H	2.109999	0.477232	-4.268095
58.H	2.050075	0.908166	-2.519020
59.H	2.071041	-0.817102	-3.027654
60.H	-4.070240	-0.008966	-2.185065

Tp*MoO[S(CH2)3S] in chair conformation

1.B	0.034588	-0.015788	-0.005308
2.N	1.549653	0.007041	-0.004076
3.N	2.208720	1.203548	0.006973
4.C	3.530663	0.916571	0.003661
5.C	3.703060	-0.478584	-0.008473
6.C	2.424662	-1.026444	-0.012899
7.N	-0.488702	0.678020	1.252905
8.C	-1.280935	0.193639	2.238103
9.C	-1.513982	1.234124	3.136502
10.C	-0.824111	2.347928	2.635305
11.N	-0.195494	1.987778	1.492277
12.N	-0.487460	0.714204	-1.243287
13.N	-0.197842	2.032304	-1.441283
14.C	-0.826315	2.425840	-2.573678
15.C	-1.512434	1.325795	-3.109677
16.C	-1.277260	0.258314	-2.243924
17.H	-0.365908	-1.163366	-0.022241
18.Mo	0.904229	3.218419	0.042438
19.O	-0.212067	4.537418	0.063057
20.C	-1.760497	-1.141931	-2.319005
21.C	-0.779839	3.818533	-3.066898
22.C	4.596335	1.941105	0.011723
23.C	2.000634	-2.448934	-0.023105
24.C	-1.769435	-1.207044	2.268156
25.C	-0.774003	3.725031	3.171883
26.H	4.653701	-1.023046	-0.013300
27.H	2.893123	-3.104428	-0.027444
28.H	1.389377	-2.705495	0.869009
29.H	1.389395	-2.693527	-0.918502
30.H	4.497077	2.597070	0.905962
31.H	4.501937	2.607490	-0.875129
32.H	5.591679	1.455073	0.011532
33.H	-1.179711	4.517555	-2.299875
34.H	-1.373023	3.916291	-3.996919
35.H	0.271437	4.133808	-3.255043
36.H	-2.115231	1.308438	-4.024985
37.H	-2.358568	-1.281491	-3.240595
38.H	-2.400324	-1.405290	-1.449151
39.H	-0.920190	-1.868314	-2.337146
40.H	-1.379597	3.798930	4.095806
41.H	0.276525	4.026110	3.384254
42.H	-1.157464	4.449662	2.420602
43.H	-2.372518	-1.372601	3.181881
44.H	-2.405550	-1.441113	1.387464
45.H	-0.931745	-1.936590	2.267984
46.H	-2.118050	1.190223	4.050002
47.S	2.396434	3.876443	1.800760
48.S	2.392307	3.933270	-1.696785
49.C	2.899300	5.630659	-1.203807
50.C	2.907677	5.586101	1.364620
51.C	3.708218	5.728546	0.078662
52.H	3.499803	6.007121	-2.058260
53.H	1.981858	6.255475	-1.126169
54.H	4.542008	4.992595	0.063119
55.H	4.176240	6.741913	0.095494
56.H	3.517876	5.930896	2.225165
57.H	1.993717	6.217806	1.315369

Tp*MoO[S(CH2)3S]$^{+}$ in chair conformation

1.B	0.055279	-0.038700	-0.005306
2.N	1.573931	0.017913	-0.002198
3.N	2.228504	1.219238	0.010201
4.C	3.556794	0.937357	0.005704
5.C	3.732197	-0.450030	-0.008680
6.C	2.458918	-1.007076	-0.013423
7.N	-0.485227	0.677817	1.235518
8.C	-1.286263	0.233429	2.229082
9.C	-1.549327	1.315797	3.071552
10.C	-0.876727	2.412887	2.534630
11.N	-0.223870	1.998574	1.410764
12.N	-0.481677	0.713651	-1.226273
13.N	-0.224590	2.040163	-1.360066
14.C	-0.877765	2.487064	-2.471180
15.C	-1.545781	1.404939	-3.043000
16.C	-1.279887	0.297755	-2.234321
17.H	-0.329901	-1.184068	-0.022496
18.Mo	0.951170	3.178275	0.042565
19.O	0.124483	4.690332	0.068322
20.C	-1.746089	-1.103044	-2.368389
21.C	-0.831348	3.893140	-2.924742
22.C	4.630150	1.957855	0.013421
23.C	2.054872	-2.434946	-0.027076
24.C	-1.757654	-1.169125	2.318399
25.C	-0.824775	3.803684	3.032438
26.H	4.686966	-0.990735	-0.015211
27.H	2.956150	-3.076442	-0.033028
28.H	1.449691	-2.701437	0.864938
29.H	1.449696	-2.684704	-0.923916
30.H	4.559574	2.608020	0.913207
31.H	4.565291	2.615681	-0.881043
32.H	5.620027	1.463431	0.014386
33.H	-1.161304	4.591253	-2.125408
34.H	-1.478957	4.029088	-3.810612
35.H	0.210713	4.183555	-3.195202
36.H	-2.161493	1.421240	-3.951218
37.H	-2.337344	-1.216056	-3.296254
38.H	-2.386652	-1.402705	-1.512029
39.H	-0.895263	-1.814747	-2.407787
40.H	-1.472460	3.914358	3.921735
41.H	0.218328	4.080823	3.312566
42.H	-1.150989	4.528155	2.255359
43.H	-2.352599	-1.308624	3.240306
44.H	-2.396191	-1.439920	1.450968
45.H	-0.909489	-1.884840	2.338732
46.H	-2.166037	1.305941	3.979208
47.S	2.408212	3.761890	1.804813
48.S	2.401098	3.818392	-1.705893
49.C	2.681759	5.579731	-1.227080
50.C	2.688580	5.537955	1.381284
51.C	3.444015	5.759325	0.079442
52.H	3.275561	6.000328	-2.064549
53.H	1.691595	6.085297	-1.197073
54.H	4.373186	5.144960	0.066458
55.H	3.787476	6.820963	0.095041
56.H	3.287054	5.930170	2.229808
57.H	1.698600	6.045188	1.373908

Tp*MoO(OC_6H_5)$_2$

1.Mo	0.005813	0.063155	0.020990
2.O	1.737346	0.011484	0.036930
3.O	-0.401178	1.989603	0.049280
4.O	-0.417799	-0.014498	1.965550
5.N	-0.087419	0.046363	-2.155326
6.C	0.580907	0.800283	-3.051274
7.C	0.237635	0.369613	-4.339813
8.C	-0.663354	-0.679617	-4.173000
9.N	-0.836660	-0.858343	-2.842500
10.N	-0.134716	-2.078606	-0.142775
11.N	-0.835971	-2.692415	-1.133233
12.C	-0.666686	-4.032839	-1.043652
13.C	0.181671	-4.278629	0.034538
14.C	0.497296	-3.025910	0.577478
15.N	-2.289497	-0.273100	-0.283604
16.C	-3.367423	0.241940	0.335976
17.C	-4.526898	-0.265839	-0.274304
18.C	-4.092024	-1.120196	-1.282696
19.N	-2.737794	-1.102252	-1.261482
20.B	-1.710718	-1.867704	-2.088230
21.H	0.606324	0.773624	-5.290877
22.H	0.529112	-5.257811	0.386232
23.H	-5.566923	-0.037017	-0.008751
24.C	-1.319146	-4.993517	-1.970407
25.H	-1.037762	-4.802321	-3.027290
26.H	-1.013439	-6.025423	-1.712413
27.H	-2.426523	-4.935009	-1.909651
28.C	1.370329	-2.665216	1.719075
29.H	0.831795	-1.990662	2.418476
30.H	1.707271	-3.571095	2.256395
31.H	2.257768	-2.099147	1.362131
32.C	-3.257971	1.161358	1.493028
33.H	-4.223232	1.672902	1.671417
34.H	-2.974064	0.604395	2.411604
35.H	-2.467697	1.924663	1.335389
36.C	-4.873833	-1.943419	-2.242062
37.H	-4.680724	-3.028981	-2.105163
38.H	-5.956023	-1.766205	-2.092143
39.H	-4.626253	-1.697767	-3.296670
40.C	1.512128	1.871087	-2.625253
41.H	2.127641	2.209335	-3.480096
42.H	0.953179	2.746752	-2.225730
43.H	2.174952	1.502484	-1.813615
44.C	-1.351293	-1.510248	-5.194903
45.H	-1.074900	-2.582326	-5.107420
46.H	-2.456003	-1.449340	-5.099957
47.H	-1.071299	-1.163087	-6.207894
48.H	-2.261641	-2.603347	-2.880198
49.C	-0.089030	0.891739	2.904336
50.C	0.944319	1.827645	2.722912
51.C	-0.790825	0.875586	4.121577
52.C	1.257218	2.723287	3.741187
53.H	1.498831	1.829152	1.770956
54.C	-0.472809	1.779813	5.129453
55.H	-1.587952	0.122916	4.250393
56.C	0.551728	2.711860	4.945605
57.H	2.075007	3.447740	3.589273
58.H	-1.033997	1.756494	6.078229
59.H	0.803298	3.427902	5.744782
60.C	-1.072987	2.942384	-0.612346
61.C	-0.868215	4.275861	-0.215273
62.C	-1.969518	2.663933	-1.658600
63.C	-1.543143	5.309003	-0.856571
64.H	-0.175397	4.461826	0.622493
65.C	-2.637736	3.709683	-2.290505
66.H	-2.133073	1.615283	-1.955839
67.C	-2.432545	5.033919	-1.899318
68.H	-1.377674	6.348910	-0.530696
69.H	-3.340069	3.479522	-3.108265
70.H	-2.970783	5.853032	-2.402358

$Tp^*MoO(OC_6H_5)_2^+$

1.Mo	-0.069517	0.160912	0.024568
2.O	1.649137	0.236624	0.187397
3.O	-0.392770	2.033661	-0.225792
4.O	-0.543982	0.112098	1.894742
5.N	-0.074163	0.009310	-2.142264
6.C	0.666446	0.699931	-3.044167
7.C	0.333352	0.244084	-4.321680
8.C	-0.630714	-0.749181	-4.151041
9.N	-0.859046	-0.870317	-2.823008
10.N	-0.110023	-1.951939	-0.155535
11.N	-0.852511	-2.624344	-1.075854
12.C	-0.619550	-3.950054	-0.956511
13.C	0.304432	-4.126495	0.076850
14.C	0.612500	-2.856019	0.559186
15.N	-2.310981	-0.190838	-0.293756
16.C	-3.388047	0.346699	0.322524
17.C	-4.547288	-0.188011	-0.253199
18.C	-4.123462	-1.080673	-1.235461
19.N	-2.769113	-1.057733	-1.236891
20.B	-1.750943	-1.848190	-2.050996
21.H	0.754378	0.593060	-5.272872
22.H	0.705677	-5.080117	0.442289
23.H	-5.584798	0.043914	0.018757
24.C	-1.276762	-4.965256	-1.814324
25.H	-1.031046	-4.814327	-2.886352
26.H	-0.940382	-5.977693	-1.522329
27.H	-2.382044	-4.925763	-1.719936
28.C	1.522686	-2.455264	1.653404
29.H	0.970737	-1.921468	2.457272
30.H	2.011081	-3.345274	2.090668
31.H	2.304664	-1.756261	1.285980
32.C	-3.274593	1.315897	1.438618
33.H	-4.249370	1.806374	1.619107
34.H	-2.959895	0.808741	2.375585
35.H	-2.519659	2.102287	1.230909
36.C	-4.918267	-1.945349	-2.143373
37.H	-4.734355	-3.022620	-1.945241
38.H	-5.997708	-1.752301	-1.997798
39.H	-4.674530	-1.761161	-3.210549
40.C	1.651539	1.731447	-2.644556
41.H	2.312078	1.975657	-3.497174
42.H	1.146990	2.668821	-2.321662
43.H	2.274229	1.378387	-1.795222
44.C	-1.321118	-1.581575	-5.166933
45.H	-1.067138	-2.656633	-5.053738
46.H	-2.424825	-1.494387	-5.090498
47.H	-1.017742	-1.263274	-6.181893
48.H	-2.300583	-2.610092	-2.813047
49.C	-0.092706	0.781402	2.978803
50.C	0.940216	1.727736	2.888982
51.C	-0.713611	0.516453	4.208901
52.C	1.340653	2.404662	4.035581
53.H	1.417232	1.925108	1.914887
54.C	-0.301348	1.202376	5.344672
55.H	-1.515887	-0.238789	4.242286
56.C	0.724246	2.148640	5.261748
57.H	2.147052	3.152219	3.969907
58.H	-0.787786	0.998899	6.311736
59.H	1.044833	2.694584	6.163049
60.C	-1.108294	2.973635	-0.866672
61.C	-0.805479	4.315755	-0.581282
62.C	-2.110348	2.640609	-1.791955
63.C	-1.526238	5.323139	-1.208242
64.H	-0.014338	4.533163	0.154448
65.C	-2.807888	3.664821	-2.421605
66.H	-2.314132	1.579041	-2.006150
67.C	-2.527490	5.001837	-2.130052
68.H	-1.305148	6.376806	-0.975208
69.H	-3.590195	3.413621	-3.154767
70.H	-3.094249	5.804466	-2.627807

Tp*MoO(p-C_6H_4F)$_2$

1.Mo	0.856391	-0.095121	0.360974
2.O	2.588095	-0.144212	0.379808
3.O	0.450785	1.833269	0.390800
4.O	0.432946	-0.173931	2.306228
5.N	0.762922	-0.111044	-1.814843
6.C	1.431859	0.641636	-2.711766
7.C	1.088885	0.209826	-3.999733
8.C	0.187979	-0.839616	-3.832156
9.N	0.013968	-1.016954	-2.501694
10.N	0.718086	-2.236313	0.196947
11.N	0.015609	-2.850922	-0.792828
12.C	0.185254	-4.191283	-0.702281
13.C	1.034552	-4.435920	0.375346
14.C	1.350881	-3.183201	0.917356
15.N	-1.438630	-0.429931	0.055003
16.C	-2.516985	0.083906	0.674951
17.C	-3.676338	-0.425704	0.066364
18.C	-3.241109	-1.280754	-0.941222
19.N	-1.886899	-1.260617	-0.921289
20.B	-0.859091	-2.027011	-1.747618
21.H	1.458341	0.612222	-4.951266
22.H	1.382866	-5.415193	0.727105
23.H	-4.716347	-0.198450	0.332890
24.C	-0.467235	-5.153105	-1.627469
25.H	-0.185853	-4.963767	-2.684715
26.H	-0.161451	-6.184625	-1.367955
27.H	-1.574651	-5.094856	-1.566698
28.C	2.224816	-2.822481	2.057479
29.H	1.686893	-2.148576	2.758102
30.H	2.562940	-3.728277	2.594474
31.H	3.112030	-2.256147	1.699894
32.C	-2.407514	1.003340	1.832739
33.H	-3.374053	1.510558	2.014914
34.H	-2.119268	0.445780	2.749331
35.H	-1.620440	1.769323	1.673331
36.C	-4.022849	-2.106441	-1.898389
37.H	-3.827976	-3.191454	-1.759858
38.H	-5.105075	-1.930529	-1.747406
39.H	-3.776990	-1.862165	-2.953661
40.C	2.364760	1.711357	-2.286950
41.H	2.979301	2.049309	-3.142474
42.H	1.808044	2.587947	-1.886176
43.H	3.028701	1.341832	-1.476560
44.C	-0.498938	-1.671627	-4.853781
45.H	-0.222431	-2.743483	-4.764358
46.H	-1.603714	-1.610772	-4.759817
47.H	-0.218245	-1.325906	-5.866892
48.H	-1.409994	-2.762679	-2.539189
49.C	0.761412	0.731815	3.243787
50.C	1.793239	1.671206	3.062241
51.C	0.062210	0.714500	4.463461
52.C	2.113396	2.569621	4.076375
53.H	2.347312	1.675960	2.110423
54.C	0.375868	1.614153	5.477667
55.H	-0.732487	-0.037904	4.596169
56.C	1.397094	2.529596	5.263161
57.H	2.922466	3.307706	3.958442
58.H	-0.161181	1.616364	6.439211
59.C	-0.222006	2.784148	-0.272340
60.C	-0.018622	4.119457	0.121823
61.C	-1.119203	2.504681	-1.318243
62.C	-0.689487	5.157551	-0.516625
63.H	0.674680	4.311232	0.957101
64.C	-1.791304	3.543882	-1.957815
65.H	-1.284603	1.456568	-1.615528
66.C	-1.565715	4.849361	-1.548377
67.H	-0.547704	6.208346	-0.218438
68.H	-2.500180	3.348856	-2.777608
69.F	1.707400	3.411692	6.249732
70.F	-2.227675	5.859168	-2.173164

$Tp^*MoO(p\text{-}C_6H_4F)_2^+$

1.Mo	0.775846	0.018385	0.362730
2.O	2.491957	0.109585	0.537569
3.O	0.444136	1.896139	0.114658
4.O	0.298641	-0.036860	2.237971
5.N	0.768880	-0.134380	-1.800789
6.C	1.507238	0.555803	-2.705611
7.C	1.176726	0.093556	-3.981273
8.C	0.216919	-0.903450	-3.807311
9.N	-0.011764	-1.020395	-2.479050
10.N	0.738356	-2.095063	0.190893
11.N	-0.003020	-2.770800	-0.728331
12.C	0.230525	-4.096237	-0.605040
13.C	1.154505	-4.268927	0.428780
14.C	1.460737	-2.996913	0.908281
15.N	-1.467930	-0.334893	0.045133
16.C	-2.547040	0.199647	0.660051
17.C	-3.704507	-0.341059	0.086577
18.C	-3.277454	-1.235823	-0.892611
19.N	-1.923098	-1.207155	-0.894825
20.B	-0.902059	-1.998626	-1.705298
21.H	1.597377	0.439787	-4.933679
22.H	1.557096	-5.221152	0.796343
23.H	-4.742954	-0.112888	0.358289
24.C	-0.426473	-5.114942	-1.458861
25.H	-0.182771	-4.967335	-2.531796
26.H	-0.087937	-6.125904	-1.164205
27.H	-1.531687	-5.077408	-1.362653
28.C	2.371800	-2.593148	2.000788
29.H	1.819780	-2.060498	2.805231
30.H	2.862965	-3.481675	2.437949
31.H	3.152062	-1.893147	1.631616
32.C	-2.435508	1.171753	1.774046
33.H	-3.409990	1.663794	1.951810
34.H	-2.123916	0.665692	2.712585
35.H	-1.678284	1.955908	1.566528
36.C	-4.069562	-2.107808	-1.795867
37.H	-3.881657	-3.183336	-1.592098
38.H	-5.149657	-1.918092	-1.650784
39.H	-3.827103	-1.928551	-2.864137
40.C	2.490320	1.590900	-2.309973
41.H	3.149928	1.833300	-3.163810
42.H	1.984668	2.528701	-1.990244
43.H	3.114373	1.242143	-1.459877
44.C	-0.468142	-1.743704	-4.820328
45.H	-0.209500	-2.816990	-4.701029
46.H	-1.572374	-1.661352	-4.746382
47.H	-0.164397	-1.429417	-5.836394
48.H	-1.449819	-2.762881	-2.466180
49.C	0.755568	0.617281	3.324363
50.C	1.796517	1.559111	3.246053
51.C	0.138210	0.342269	4.556767
52.C	2.211652	2.221871	4.393395
53.H	2.274065	1.765220	2.274241
54.C	0.553274	1.003635	5.703648
55.H	-0.668793	-0.407500	4.586257
56.C	1.582817	1.934828	5.599827
57.H	3.018721	2.970492	4.371486
58.H	0.092040	0.814794	6.685540
59.C	-0.269044	2.825300	-0.538456
60.C	0.037677	4.173993	-0.279128
61.C	-1.276998	2.482639	-1.457230
62.C	-0.675044	5.178651	-0.915413
63.H	0.831318	4.404658	0.449369
64.C	-1.975630	3.490566	-2.107045
65.H	-1.486650	1.419246	-1.654789
66.C	-1.669911	4.817107	-1.820331
67.H	-0.476345	6.244706	-0.724033
68.H	-2.764744	3.266317	-2.840919
69.F	-2.358815	5.786854	-2.442931
70.F	1.981368	2.584474	6.705989