Computational Coordinates

$MoO(NH_3)_2(SCH_3)_2Cl$ (**1**)

Mo1	0.385	1.013	0.257
O2	0.314	2.694	0.341
N3	-1.900	0.865	-0.065
S4	0.257	0.730	2.639
Cl5	2.671	0.512	0.273
S6	0.388	0.540	-2.077
N7	-0.155	-1.435	0.531
C8	-1.302	0.884	-2.466
C14	-0.017	-0.977	2.941
H9	-2.127	1.309	-0.814
H20	-2.137	0.001	-0.146
H22	-2.327	1.228	0.639
H15	-0.929	-1.524	0.980
H21	-0.233	-1.818	-0.280
H23	0.506	-1.839	0.990
H10	-1.735	1.144	-1.721
H11	-1.341	1.542	-3.080
H12	-1.691	0.143	-2.796
H16	-0.793	-1.082	3.385
H17	0.658	-1.306	3.436
H18	-0.058	-1.418	2.158

$MoO(NH_3)_2(SCH_3)_3$ (**2**–**4**)

Mo1	0.438	0.997	0.655
O2	0.335	2.559	1.276
N3	-1.812	0.624	1.039
S4	1.146	0.042	2.741
S5	2.635	0.838	-0.218
S6	-0.342	1.203	-1.586
N7	0.119	-1.481	0.307
C8	-2.075	1.400	-1.296
C14	1.058	-1.702	2.567
C24	2.723	1.363	-1.937
H9	-2.299	1.223	0.577
H20	-2.028	-0.208	0.772
H22	-1.985	0.711	1.918
H15	-0.451	-1.800	0.926
H21	-0.218	-1.628	-0.515
H23	0.912	-1.899	0.384
H10	-2.236	1.376	-0.410
H11	-2.347	2.191	-1.628
H12	-2.525	0.734	-1.700
H16	0.486	-2.036	3.176
H17	1.874	-2.058	2.695
H18	0.768	-1.907	1.740
H13	1.905	1.613	-2.217
H25	3.290	2.058	-2.010
H29	3.018	0.681	-2.444

$MoO(S_2C_2(CH_3)_2)(SCH_3)(OH_2)$ (SO_{red} where O=Mo-S-C dihedral angle = 80°)

O1	1.936	-1.007	1.390
C2	4.041	-0.567	0.224
S3	2.777	0.100	-0.860
C4	-3.545	-1.299	0.820
C5	-2.319	-0.798	0.395
S6	-1.106	-0.881	1.518
C7	-2.267	-0.232	-0.951
S8	-0.678	0.383	-1.383
C9	-3.526	-0.192	-1.928
Mo10	0.732	0.262	0.518
O11	0.914	1.713	1.453
H12	1.456	-1.527	2.059
H13	3.797	-1.586	0.558
H14	5.023	-0.618	-0.284
H15	4.162	0.047	1.124
H19	-3.473	-2.324	1.243
H20	-4.002	-0.713	1.648
H21	-4.320	-1.355	0.043
H16	-3.189	0.200	-2.895
H17	-3.957	-1.190	-2.090
H18	-4.322	0.467	-1.548

$MoO(S_2C_2(CH_3)_2)(SCH_3)(OH_2)$ (SO_{red} where O=Mo-S-C dihedral angle = 180°)

O1	1.893	-1.761	0.099
C2	2.687	0.563	-2.117
S3	2.808	0.683	-0.331
C4	-3.554	-1.352	-0.681
C5	-2.320	-0.740	-0.489
S6	-1.153	-1.716	0.162
C7	-2.222	0.675	-0.839
S8	-0.626	1.352	-0.547
C9	-3.440	1.510	-1.439
Mo10	0.706	-0.275	0.547
O11	0.826	-0.157	2.275
H12	1.394	-2.597	0.065
H13	1.864	1.175	-2.513
H14	3.617	0.908	-2.609
H15	2.504	-0.470	-2.438
H19	-3.484	-2.306	-1.245
H20	-4.055	-1.652	0.267
H21	-4.296	-0.745	-1.220
H16	-3.070	2.510	-1.693
H17	-3.848	1.051	-2.351
H18	-4.261	1.619	-0.715

$MoOS(S_2C_2H_2)(OH_2)\ (XO_{ox})$

Mo1	1.707	0.455	0.561
O2	1.701	0.448	2.261
S3	0.175	2.062	-0.285
S4	0.159	-1.130	-0.298
O5	2.972	-0.889	0.110
S6	3.416	1.631	-0.002
C7	-1.192	1.198	-0.840
C8	-1.199	-0.248	-0.846
C10	-2.397	1.940	-1.339
C11	-2.421	-0.973	-1.327
H9	3.522	-1.479	0.702
H12	3.279	-1.208	-0.787
H18	-3.095	1.285	-1.631
H19	-2.763	2.513	-0.606
H20	-2.136	2.516	-2.114
H15	-2.606	-0.721	-2.277
H16	-2.267	-1.960	-1.269
H17	-3.203	-0.724	-0.757

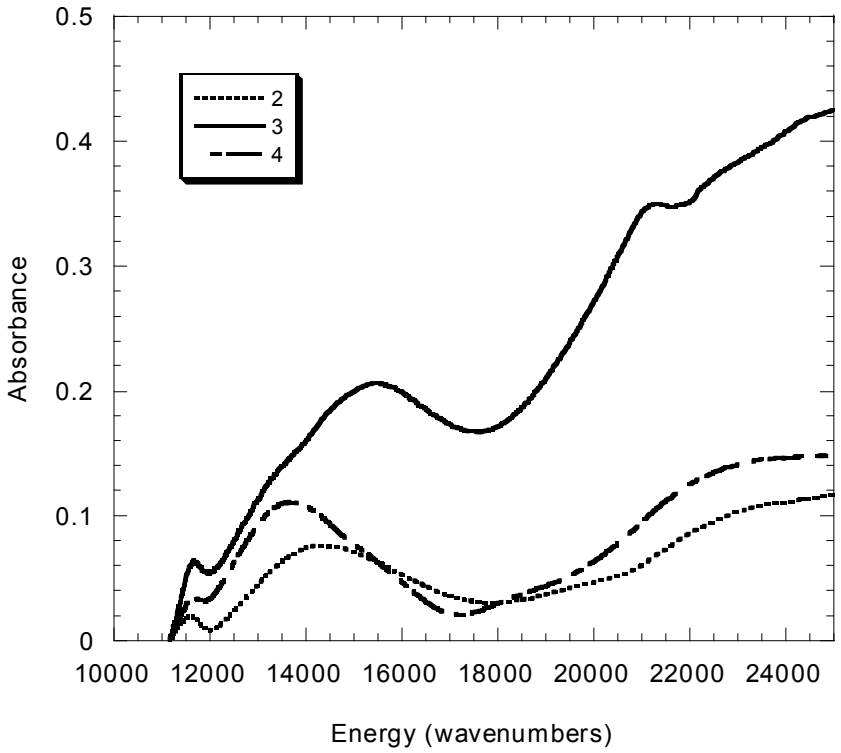

Figure S1. Room temperature PDMS mull absorption spectra of **2**, **3**, and **4**

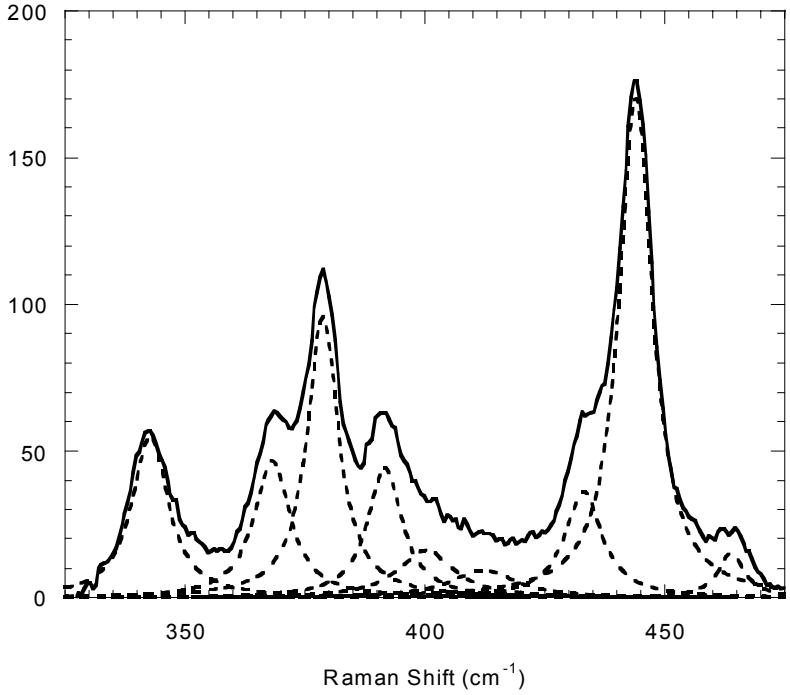

Figure S2. Deconvoluted room temperature resonance Raman spectrum of complex **4**

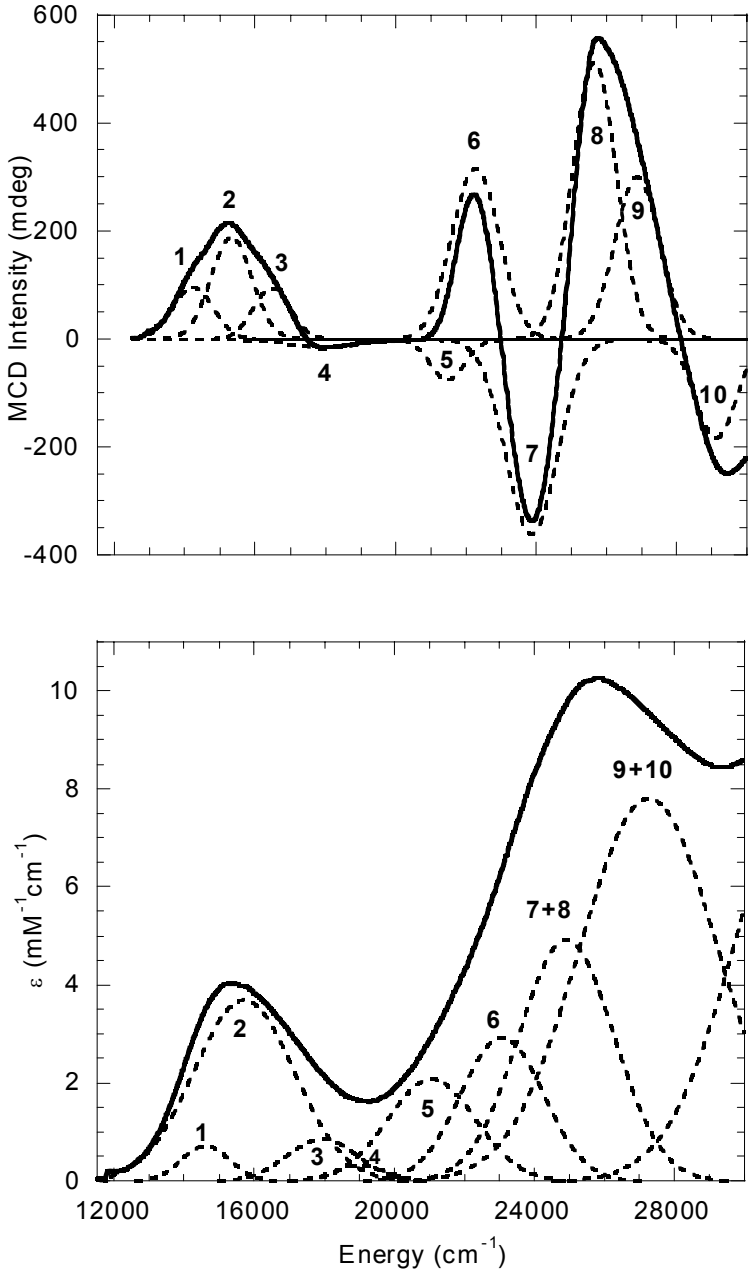

Figure S3. Gaussian resolved (top) MCD spectra and (bottom) electronic absorbance spectra of complex **2**

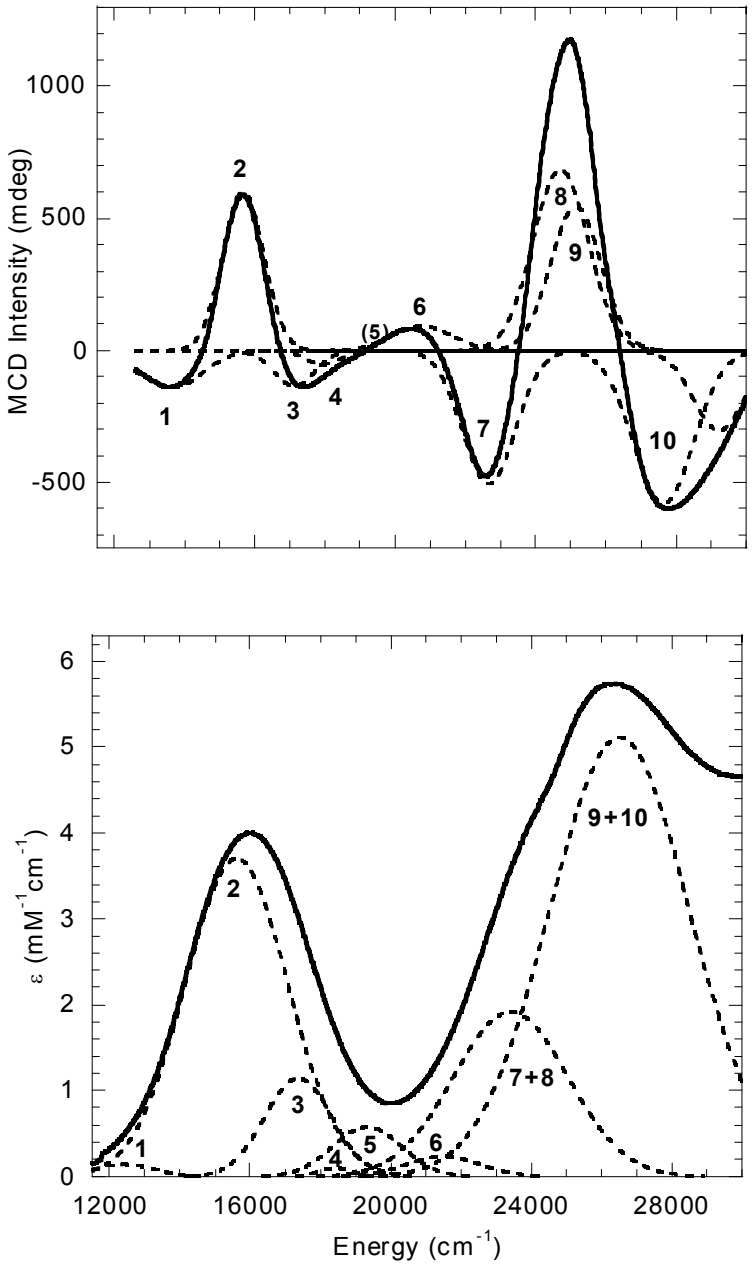

Figure S4. Gaussian resolved (top) MCD spectra and (bottom) electronic absorbance spectra of complex **3**

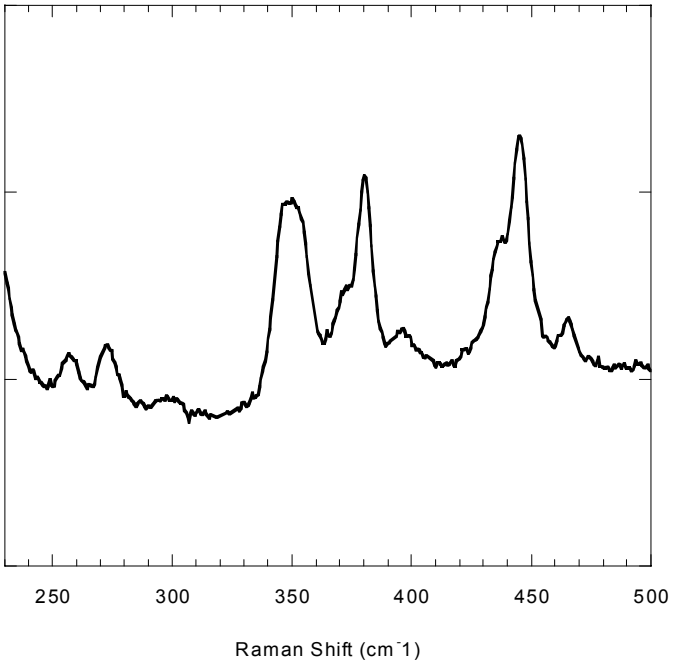

Figure S5. Room temperature resonance Raman spectra of (L-N_2S_2)MoO(SePh)