Table S1. ΔG° (25 °C; kcal/mol) between possible spin states in (a) neutral and reduced Co(II)-salen, (b) transition states and intermediates in the IS pathway with methyl acrylate substrate, and (c) transition states and intermediates in the IS pathway with acrylonitrile substrate.

(a)

	neutral Co(II)-salen			**reduced Co(II)-salen**
doublet	+3.25		**singlet**	+4.88
quartet	0.00		**triplet**	0.00

(b)

	IS transition state methyl acrylate, α-carbon	**IS intermediate methyl acrylate, α-carbon**	**IS transition state methyl acrylate, β-carbon**	**IS intermediate methyl acrylate, β-carbon**
open-shell singlet	0.00	+0.09	0.00	0.00
triplet	+0.30	0.00	+1.73	+1.61

(c)

	IS transition state acrylonitrile, α-carbon	**IS intermediate acrylonitrile, α-carbon**	**IS transition state acrylonitrile, β-carbon**	**IS intermediate acrylonitrile, β-carbon**
open-shell singlet	0.00	0.00	0.00	0.00
triplet	+0.32	+0.18	+1.37	+1.09

Cartesian coordinates of optimized geometries from DFT calculations

acrylonitrile

C	-12.134244	0.329739	0.000227
C	-11.038482	1.102427	0.000043
C	-9.708481	0.565127	-0.000095
N	-8.619123	0.150526	-0.000220
H	-12.069049	-0.754454	0.000287
H	-13.124357	0.775810	0.000298
H	-11.110465	2.188225	-0.000040

reduced acrylonitrile

C	-12.185737	0.303101	0.000239
C	-10.986623	1.080345	0.000024
C	-9.680687	0.596373	-0.000105
N	-8.554461	0.200828	-0.000224
H	-12.164191	-0.783906	0.000298
H	-13.157922	0.791203	0.000307
H	-11.074578	2.169456	-0.000040

methyl acrylate

C	-11.738205	-3.175166	0.000033
C	-11.639992	-1.841158	-0.000135
C	-10.356624	-1.088226	0.000033
O	-10.291479	0.125692	-0.000168
O	-9.270869	-1.895115	0.000320
C	-8.011559	-1.209897	0.000433
H	-10.854248	-3.806512	0.000310
H	-12.707713	-3.666573	-0.000102
H	-12.517487	-1.199629	-0.000413
H	-7.250614	-1.992255	0.000670
H	-7.914303	-0.579155	0.889810
H	-7.914006	-0.579407	-0.889090

reduced methyl acrylate

C	-11.766828	-3.226008	-0.000014
C	-11.596308	-1.826870	-0.000201
C	-10.395047	-1.083702	-0.000727
O	-10.231925	0.162088	-0.000237
O	-9.229966	-1.922378	0.000093
C	-8.026712	-1.202574	0.000522
H	-10.918182	-3.904259	-0.000356
H	-12.763634	-3.664694	0.000479
H	-12.483269	-1.190497	0.000200
H	-7.215541	-1.945671	0.001132
H	-7.920289	-0.551184	0.883047
H	-7.919399	-0.551652	-0.882239

Zn(II)-salen

Zn	0.000001	-0.151536	-0.000020
O	-1.500217	-1.288776	-0.448942
O	1.500217	-1.288788	0.448898
N	-1.248696	1.433774	0.475824
N	1.248706	1.433779	-0.475816
C	-2.769486	-1.051271	-0.278732
C	-3.693002	-2.102773	-0.564768
C	-5.058109	-1.936545	-0.416544
C	-5.605043	-0.703979	0.010733
C	-4.743841	0.341368	0.281511
C	-3.332346	0.206769	0.161712
C	-2.545398	1.382264	0.420153
C	2.769487	-1.051279	0.278713
C	3.693000	-2.102791	0.564727

C	5.058109	-1.936555	0.416533
C	5.605049	-0.703974	-0.010692
C	4.743850	0.341381	-0.281450
C	3.332354	0.206776	-0.161682
C	2.545407	1.382274	-0.420107
C	-0.545264	2.707034	0.552223
C	0.545275	2.707042	-0.552194
H	-3.270633	-3.046912	-0.898242
H	-5.722580	-2.770086	-0.637553
H	-6.679190	-0.582239	0.117112
H	-5.141233	1.304240	0.602734
H	-3.112743	2.315373	0.559889
H	3.270627	-3.046942	0.898162
H	5.722578	-2.770102	0.637525
H	6.679198	-0.582228	-0.117046
H	5.141247	1.304264	-0.602635
H	3.112751	2.315391	-0.559799
H	-1.221002	3.566280	0.426553
H	-0.052996	2.792229	1.531759
H	1.221014	3.566285	-0.426511
H	0.053007	2.792252	-1.531728

reduced Zn(II)-salen

Zn	0.000003	-0.090923	0.000005
O	-1.489814	-1.257652	-0.494418
O	1.489819	-1.257663	0.494404
N	-1.245899	1.460253	0.466852
N	1.245906	1.460261	-0.466815
C	-2.768518	-1.039949	-0.302177
C	-3.676194	-2.097275	-0.582567
C	-5.057179	-1.968520	-0.429634
C	-5.609481	-0.752005	0.015402
C	-4.756700	0.306560	0.300234
C	-3.340801	0.216821	0.163334
C	-2.570256	1.391913	0.447642
C	2.768523	-1.039956	0.302171
C	3.676198	-2.097286	0.582544
C	5.057184	-1.968529	0.429616
C	5.609487	-0.752005	-0.015395
C	4.756706	0.306565	-0.300210
C	3.340807	0.216823	-0.163315
C	2.570262	1.391920	-0.447603
C	-0.569921	2.731998	0.534522
C	0.569927	2.732007	-0.534463
H	-3.235877	-3.029383	-0.931484
H	-5.706183	-2.813710	-0.657737
H	-6.685818	-0.640212	0.135329
H	-5.171173	1.256378	0.643362
H	-3.143107	2.309320	0.651395
H	3.235881	-3.029401	0.931443
H	5.706188	-2.813723	0.657706
H	6.685824	-0.640210	-0.135317
H	5.171180	1.256389	-0.643319
H	3.143114	2.309331	-0.651339
H	-1.257190	3.579209	0.354423
H	-0.099900	2.882705	1.521595
H	1.257197	3.579215	-0.354350
H	0.099907	2.882731	-1.521533

inner sphere Zn(II)-salen / acrylonitrile (α-carbon) transition state

Zn	0.437501	0.353935	-0.127961
O	-0.794476	1.627493	0.640472
O	2.193340	1.267789	-0.214419
N	-0.871128	-0.812691	-1.050897

N	1.524017	-1.503743	0.045570
C	-2.014204	1.747088	0.142875
C	-2.673109	2.996199	0.315550
C	-3.959835	3.233059	-0.159420
C	-4.659974	2.223644	-0.834515
C	-4.038075	0.986046	-1.012276
C	-2.737549	0.712156	-0.548342
C	-2.211035	-0.674544	-0.749393
C	3.397227	0.823081	-0.050955
C	4.476718	1.767198	-0.028892
C	5.795617	1.379178	0.130632
C	6.145728	0.016868	0.263842
C	5.131361	-0.926962	0.233657
C	3.767253	-0.570536	0.093917
C	2.804576	-1.649771	0.024156
C	-0.367186	-2.136057	-1.342185
C	0.623734	-2.610456	-0.229829
H	-2.116080	3.770062	0.840267
H	-4.419135	4.209593	-0.003582
H	-5.667361	2.392608	-1.208883
H	-4.578109	0.186398	-1.518007
H	-2.885724	-1.273929	-1.383627
H	4.205300	2.814517	-0.138036
H	6.576241	2.139490	0.148844
H	7.184128	-0.283013	0.380943
H	5.374247	-1.987028	0.323449
H	3.229614	-2.663952	-0.078775
H	-1.170737	-2.885498	-1.447467
H	0.196118	-2.134397	-2.292349
H	1.167669	-3.520814	-0.537957
H	0.056327	-2.835211	0.684588
C	-2.178717	-1.045167	2.102369
C	-2.673309	-1.645271	0.887400
C	-4.108245	-1.818153	0.792585
N	-5.259206	-1.956683	0.642491
H	-1.124697	-1.142354	2.350622
H	-2.726064	-0.231556	2.569058
H	-2.180536	-2.587098	0.622549

inner sphere Zn(II)-salen / acrylonitrile (α-carbon) intermediate

Zn	0.402069	0.322889	-0.154434
O	-0.835367	1.533354	0.737997
O	2.149767	1.251373	-0.215840
N	-0.888652	-0.811910	-1.107920
N	1.512299	-1.537372	0.014488
C	-2.017416	1.718453	0.171010
C	-2.625857	2.997853	0.298068
C	-3.872274	3.286834	-0.252470
C	-4.576107	2.304636	-0.960932
C	-3.999559	1.037300	-1.093751
C	-2.747006	0.711295	-0.549708
C	-2.249137	-0.716292	-0.706156
C	3.357892	0.814715	-0.060092
C	4.427733	1.769422	-0.024729
C	5.751376	1.393877	0.127378
C	6.116296	0.033937	0.238862
C	5.111321	-0.919991	0.194516
C	3.743450	-0.577177	0.062613
C	2.793064	-1.668202	-0.024531
C	-0.373722	-2.129480	-1.398221
C	0.617306	-2.638405	-0.292478
H	-2.065408	3.751966	0.847456
H	-4.295339	4.284464	-0.130769
H	-5.550650	2.515611	-1.396310

H	-4.542960	0.259296	-1.630314
H	-2.917126	-1.236183	-1.421376
H	4.144920	2.815334	-0.117877
H	6.523445	2.162664	0.156183
H	7.157991	-0.256971	0.349778
H	5.365914	-1.978767	0.266397
H	3.230677	-2.673821	-0.158414
H	-1.170417	-2.885125	-1.527277
H	0.200924	-2.119018	-2.342706
H	1.164841	-3.538894	-0.624381
H	0.051041	-2.892330	0.615721
C	-2.041583	-1.028343	1.966746
C	-2.604504	-1.578370	0.712088
C	-4.059377	-1.758727	0.795713
N	-5.214715	-1.916058	0.818169
H	-0.993440	-1.197606	2.195426
H	-2.538096	-0.201741	2.464326
H	-2.184999	-2.574518	0.508758

inner sphere Zn(II)-salen / acrylonitrile (β-carbon) transition state

Zn	-0.626120	0.363052	0.047319
O	0.561255	1.635638	-0.790093
O	-2.406038	1.204231	0.199528
N	0.772249	-0.741153	0.934850
N	-1.598091	-1.531621	-0.091881
C	1.776320	1.851347	-0.308664
C	2.382207	3.106121	-0.584328
C	3.673048	3.420559	-0.164054
C	4.427718	2.483959	0.557221
C	3.855999	1.243790	0.845360
C	2.548274	0.895089	0.446340
C	2.093477	-0.479989	0.730795
C	-3.588904	0.697213	0.053173
C	-4.715018	1.583908	0.059540
C	-6.014474	1.129164	-0.082684
C	-6.295131	-0.248131	-0.225396
C	-5.233310	-1.138163	-0.221271
C	-3.887078	-0.712343	-0.098687
C	-2.870288	-1.741616	-0.055828
C	0.363643	-2.096937	1.233615
C	-0.637988	-2.597691	0.147164
H	1.787196	3.819228	-1.151589
H	4.092758	4.398147	-0.401171
H	5.437924	2.714912	0.889040
H	4.433351	0.501392	1.396504
H	2.810177	-1.083200	1.301724
H	-4.496526	2.642795	0.175194
H	-6.833740	1.847711	-0.080020
H	-7.318297	-0.600275	-0.329526
H	-5.422144	-2.208307	-0.318827
H	-3.240874	-2.777092	0.037538
H	1.216734	-2.792357	1.283214
H	-0.155626	-2.140751	2.207044
H	-1.129264	-3.535428	0.458642
H	-0.083297	-2.784212	-0.782975
C	2.713702	-1.456868	-1.092833
C	4.109365	-1.552568	-1.216666
C	4.848479	-2.645629	-0.721700
H	2.163992	-2.377143	-0.900083
H	2.188839	-0.725347	-1.704142
H	4.684125	-0.702298	-1.577532
N	5.471074	-3.565836	-0.330955

inner sphere Zn(II)-salen / acrylonitrile (β-carbon) intermediate

Zn	0.486038	0.335336	-0.017671
O	-0.693096	1.492252	1.025105
O	2.270451	1.179840	-0.101568
N	-0.895230	-0.654460	-1.026391
N	1.461455	-1.574723	0.034644
C	-1.809246	1.870813	0.416371
C	-2.279964	3.196507	0.616473
C	-3.452678	3.663634	0.024276
C	-4.212640	2.823845	-0.799628
C	-3.770504	1.510694	-1.003915
C	-2.598328	1.010361	-0.420849
C	-2.247234	-0.458476	-0.609208
C	3.452557	0.660223	-0.005735
C	4.581840	1.542964	0.030529
C	5.882658	1.078539	0.120945
C	6.162052	-0.305308	0.165450
C	5.096800	-1.191126	0.118731
C	3.750225	-0.757240	0.047937
C	2.730123	-1.782688	-0.048613

C	-0.492735	-2.003774	-1.351729
C	0.486371	-2.603522	-0.281410
H	-1.678618	3.840203	1.255763
H	-3.772884	4.690229	0.204087
H	-5.127172	3.178234	-1.270973
H	-4.357703	0.839720	-1.632349
H	-2.957547	-0.906007	-1.328747
H	4.364223	2.607599	-0.011278
H	6.703418	1.794865	0.152994
H	7.185770	-0.665932	0.228000
H	5.284289	-2.265887	0.140214
H	3.098332	-2.807781	-0.231433
H	-1.350295	-2.690621	-1.461256
H	0.052379	-2.019757	-2.313375
H	0.963511	-3.529425	-0.648558
H	-0.078585	-2.839102	0.631483
C	-2.597226	-1.230816	0.810345
C	-4.027523	-1.181558	1.171712
C	-4.923197	-2.206053	0.863029
H	-2.262028	-2.268297	0.701190
H	-1.979756	-0.716229	1.555888
H	-4.450794	-0.254096	1.551017
N	-5.673511	-3.086383	0.626501

inner sphere Zn(II)-salen / methyl acrylate (α-carbon) transition state

Zn	0.861657	0.374354	-0.135871
O	-0.304368	1.713075	0.646756
O	2.664731	1.198162	-0.094136
N	-0.481437	-0.660898	-1.155104
N	1.878971	-1.553323	-0.105157
C	-1.523000	1.883687	0.168293
C	-2.138523	3.152888	0.358321
C	-3.418274	3.440126	-0.107865
C	-4.155472	2.465065	-0.794089
C	-3.575667	1.208520	-0.986274
C	-2.287279	0.881955	-0.525727
C	-1.802491	-0.518603	-0.756950
C	3.844654	0.689896	0.054734
C	4.960284	1.581864	0.186938
C	6.258191	1.126512	0.341664
C	6.550037	-0.255556	0.359894
C	5.499452	-1.149318	0.220717
C	4.155379	-0.725322	0.080799
C	3.151531	-1.753328	-0.106255
C	-0.034663	-1.980119	-1.542386
C	0.938983	-2.594197	-0.483052
H	-1.553319	3.901907	0.888471
H	-3.842381	4.430211	0.061736
H	-5.154646	2.676897	-1.169829
H	-4.136386	0.437439	-1.516920
H	-2.518677	-1.084939	-1.373567
H	4.733430	2.645235	0.166882
H	7.067614	1.848867	0.446952
H	7.572082	-0.608297	0.474437
H	5.696848	-2.222628	0.221077
H	3.539189	-2.772697	-0.283649
H	-0.872008	-2.682121	-1.700758
H	0.524426	-1.927165	-2.493536
H	1.449983	-3.489080	-0.880871
H	0.364536	-2.889417	0.405822
C	-1.362649	-1.112679	1.980617
C	-2.164955	-1.509009	0.850996
C	-3.631663	-1.370984	1.044065
O	-4.215537	-0.714925	1.887115

O	-4.324745	-2.064994	0.074246
C	-5.736401	-1.880894	0.123999
H	-0.312813	-1.388275	2.039571
H	-1.719648	-0.331707	2.644098
H	-1.921307	-2.486063	0.422628
H	-6.147134	-2.476329	-0.697042
H	-5.998923	-0.824190	-0.003343
H	-6.148011	-2.221903	1.081652

inner sphere Zn(II)-salen / methyl acrylate (α-carbon) intermediate

Zn	0.866742	0.398301	-0.176912
O	-0.275816	1.734379	0.670806
O	2.690250	1.170870	-0.153762
N	-0.484422	-0.613699	-1.178409
N	1.831369	-1.564452	-0.035684
C	-1.445885	1.986152	0.110144
C	-1.977335	3.301032	0.228161
C	-3.199884	3.664565	-0.331476
C	-3.957369	2.726147	-1.044227
C	-3.457678	1.424840	-1.165784
C	-2.234922	1.021425	-0.605777
C	-1.831467	-0.436341	-0.751764
C	3.855186	0.635237	0.018728
C	4.994833	1.501087	0.114620
C	6.280531	1.018543	0.289622
C	6.535150	-0.368492	0.365560
C	5.460172	-1.238500	0.262334
C	4.127959	-0.785743	0.104696
C	3.097579	-1.796015	-0.043476
C	-0.070822	-1.960043	-1.495748
C	0.860199	-2.581636	-0.395161
H	-1.375156	4.022665	0.777142
H	-3.560757	4.687150	-0.216121
H	-4.909772	2.998111	-1.495446
H	-4.035804	0.681396	-1.717351
H	-2.536330	-0.916241	-1.455313
H	4.796695	2.568406	0.049040
H	7.108827	1.723120	0.364947
H	7.547341	-0.743933	0.495022
H	5.628810	-2.315868	0.306383
H	3.460373	-2.828727	-0.197066
H	-0.924794	-2.644007	-1.653614
H	0.515688	-1.968943	-2.432990
H	1.343539	-3.508809	-0.753100
H	0.259928	-2.824806	0.493104
C	-1.461000	-0.888013	1.876575
C	-2.226194	-1.275982	0.678960
C	-3.713386	-1.145544	0.899458
O	-4.279829	-0.526301	1.777530
O	-4.412526	-1.810248	-0.074747
C	-5.825442	-1.622826	-0.014410
H	-0.413010	-1.158163	1.967193
H	-1.847574	-0.114608	2.531208
H	-2.023073	-2.314080	0.378744
H	-6.241150	-2.206196	-0.840809
H	-6.081169	-0.563221	-0.128868
H	-6.230679	-1.974158	0.941638

inner sphere Zn(II)-salen / methyl acrylate (β-carbon) transition state

Zn	1.067608	0.550359	0.013041
O	0.392056	2.158249	0.847607
O	3.009474	0.797481	-0.262119
N	-0.654508	-0.073561	-0.760913
N	1.411653	-1.545044	0.161534

C	-0.700376	2.742926	0.382039
C	-0.845818	4.139640	0.606376
C	-1.965197	4.851912	0.184195
C	-3.007643	4.194871	-0.487008
C	-2.892296	2.824076	-0.718336
C	-1.768952	2.072131	-0.315270
C	-1.816792	0.606734	-0.545245
C	3.982824	-0.052748	-0.177232
C	5.325990	0.436582	-0.284301
C	6.425810	-0.400768	-0.212106
C	6.272517	-1.794943	-0.044088
C	4.988249	-2.307596	0.048483
C	3.836941	-1.483211	-0.000580
C	2.548679	-2.142747	0.052290
C	-0.710775	-1.493743	-1.034898
C	0.151503	-2.257139	0.014526
H	-0.031089	4.633855	1.132116
H	-2.027114	5.922496	0.379943
H	-3.889668	4.737985	-0.820196
H	-3.701528	2.294230	-1.222132
H	-2.692471	0.276756	-1.119051
H	5.440761	1.509444	-0.419362
H	7.425879	0.025069	-0.290709
H	7.139441	-2.449064	0.004854
H	4.840557	-3.382165	0.166858
H	2.570174	-3.243098	-0.033323
H	-1.737261	-1.885971	-1.001060
H	-0.294337	-1.714389	-2.034604
H	0.303305	-3.309547	-0.280054
H	-0.379072	-2.233146	0.975706
C	-2.762290	0.009413	1.210345
C	-3.194639	-1.331841	1.202051
C	-4.422032	-1.710885	0.563050
O	-5.227819	-0.984344	-0.023543
O	-4.653585	-3.082519	0.663479
C	-5.856018	-3.510388	0.047822
H	-1.948505	0.286507	1.880127
H	-3.537110	0.766239	1.100249
H	-2.581240	-2.132208	1.609365
H	-5.907035	-4.594161	0.198598
H	-5.866033	-3.281782	-1.026038
H	-6.735519	-3.029647	0.496016

inner sphere Zn(II)-salen / methyl acrylate (β-carbon) intermediate

Zn	1.017052	0.499917	0.133463
O	0.263965	2.008082	1.105184
O	2.959099	0.836878	-0.064419
N	-0.654007	-0.102123	-0.730726
N	1.447935	-1.591103	0.090024
C	-0.701661	2.675329	0.487531
C	-0.746282	4.088052	0.644158
C	-1.730074	4.872334	0.046087
C	-2.723513	4.277945	-0.743425
C	-2.703617	2.888824	-0.905729
C	-1.726198	2.069864	-0.318707
C	-1.870617	0.565072	-0.479829
C	3.961785	0.018353	-0.071296
C	5.287149	0.564048	-0.115407
C	6.416586	-0.236030	-0.132745
C	6.313882	-1.644857	-0.122726
C	5.048549	-2.210124	-0.093175
C	3.868309	-1.427660	-0.055747
C	2.604337	-2.135325	-0.074204
C	-0.700922	-1.500422	-1.075535

C	0.212531	-2.326764	-0.114525
H	0.033315	4.535644	1.257749
H	-1.719845	5.952660	0.193270
H	-3.496110	4.878508	-1.219510
H	-3.480743	2.408487	-1.501760
H	-2.643630	0.353132	-1.239410
H	5.363158	1.648752	-0.129101
H	7.400665	0.231677	-0.158857
H	7.203870	-2.268947	-0.143724
H	4.939693	-3.295895	-0.095077
H	2.666061	-3.220961	-0.266518
H	-1.721776	-1.912563	-1.012522
H	-0.347336	-1.675778	-2.110231
H	0.394291	-3.342751	-0.505732
H	-0.301256	-2.412248	0.853711
C	-2.662218	0.047182	0.932795
C	-3.143785	-1.327896	0.943997
C	-4.386822	-1.678940	0.325541
O	-5.173901	-0.927896	-0.254696
O	-4.656827	-3.038723	0.438391
C	-5.880476	-3.436473	-0.158577
H	-1.941632	0.261253	1.728224
H	-3.502152	0.748594	0.978987
H	-2.553281	-2.135655	1.369496
H	-5.967270	-4.513994	0.015455
H	-5.890462	-3.229662	-1.236573
H	-6.736714	-2.914496	0.287716

Ni(II)-salen

Ni	0.000011	0.226905	0.000190
O	-1.271192	-1.128636	0.062369
O	1.271187	-1.128647	-0.061803
N	-1.268874	1.598365	0.154903
N	1.268829	1.598392	-0.154647
C	-2.560745	-1.019039	0.017991
C	-3.349463	-2.210719	-0.043682
C	-4.728938	-2.154702	-0.093424
C	-5.422568	-0.917528	-0.079342
C	-4.693266	0.251731	-0.012212
C	-3.271161	0.234744	0.036286
C	-2.567049	1.469763	0.138019
C	2.560761	-1.019048	-0.017901
C	3.349504	-2.210705	0.043720
C	4.728990	-2.154653	0.093187
C	5.422595	-0.917474	0.078835
C	4.693268	0.251762	0.011703
C	3.271151	0.234746	-0.036511
C	2.567008	1.469740	-0.138314
C	-0.665694	2.916818	0.375955
C	0.665621	2.916817	-0.375892
H	-2.817031	-3.157725	-0.053757
H	-5.296054	-3.082578	-0.143639
H	-6.507868	-0.895060	-0.117368
H	-5.201113	1.215772	0.006129
H	-3.170278	2.381464	0.221628
H	2.817111	-3.157733	0.053954
H	5.296129	-3.082522	0.143274
H	6.507893	-0.894982	0.116811
H	5.201097	1.215805	-0.006868
H	3.170234	2.381390	-0.222427
H	-1.324933	3.727496	0.037040
H	-0.479819	3.047683	1.451987
H	1.324789	3.727527	-0.036977
H	0.479813	3.047583	-1.451942

reduced Ni(II)-salen

Ni	0.000000	0.225753	0.000060
O	-1.290357	-1.141405	0.051496
O	1.290360	-1.141391	-0.051238
N	-1.260677	1.602176	0.114216
N	1.260648	1.602188	-0.114236
C	-2.587462	-1.028938	0.014023
C	-3.379277	-2.209824	-0.043963
C	-4.772913	-2.167510	-0.081365
C	-5.453766	-0.933020	-0.059971
C	-4.714720	0.241806	-0.000263
C	-3.291468	0.238676	0.038567
C	-2.584189	1.471156	0.121723
C	2.587473	-1.028913	-0.013991
C	3.379301	-2.209787	0.043990
C	4.772945	-2.167463	0.081167
C	5.453785	-0.932972	0.059541
C	4.714724	0.241845	-0.000166
C	3.291465	0.238705	-0.038771
C	2.584166	1.471172	-0.121916
C	-0.690265	2.922696	0.330631
C	0.690221	2.922699	-0.330662
H	-2.844223	-3.156999	-0.059230
H	-5.336982	-3.098897	-0.127872
H	-6.541520	-0.899118	-0.088816
H	-5.225588	1.206090	0.020240
H	-3.180341	2.387996	0.198946
H	2.844255	-3.156963	0.059438
H	5.337026	-3.098843	0.127677
H	6.541544	-0.899060	0.088211
H	5.225584	1.206129	-0.020846
H	3.180300	2.388011	-0.199278
H	-1.334958	3.713190	-0.092892
H	-0.579234	3.130180	1.409674
H	1.334904	3.713205	0.092856
H	0.579183	3.130182	-1.409705

inner sphere Ni(II)-salen / acrylonitrile (*α*-carbon) transition state

Ni	0.538545	-0.016260	-0.021112
O	-0.505396	1.483872	0.290933
O	2.065777	1.069576	0.400080
N	-0.894480	-1.098147	-0.522795
N	1.620907	-1.553905	-0.302888
C	-1.759227	1.658190	-0.059664
C	-2.270466	2.988452	-0.038188
C	-3.582369	3.280588	-0.394475
C	-4.453747	2.256527	-0.798842
C	-3.975273	0.945301	-0.824422
C	-2.656455	0.618350	-0.459332
C	-2.244589	-0.815419	-0.468958
C	3.310837	0.781745	0.253723
C	4.298750	1.795856	0.497917
C	5.650070	1.546485	0.350452
C	6.127668	0.271465	-0.042080
C	5.206224	-0.734543	-0.275613
C	3.811455	-0.517166	-0.139595
C	2.916220	-1.616741	-0.360692
C	-0.508766	-2.375744	-1.087494
C	0.822124	-2.775357	-0.442444
H	-1.581605	3.772677	0.269145
H	-3.928883	4.314025	-0.364599
H	-5.479545	2.474781	-1.088294
H	-4.642198	0.136800	-1.122516

H	-2.842216	-1.391799	-1.192569
H	3.930794	2.773772	0.798521
H	6.362973	2.348501	0.541295
H	7.193645	0.088866	-0.152783
H	5.545808	-1.728278	-0.571784
H	3.377325	-2.590245	-0.578358
H	-1.257904	-3.163153	-0.893337
H	-0.380243	-2.325620	-2.188049
H	1.361747	-3.544778	-1.017009
H	0.626110	-3.166932	0.567018
C	-2.781452	-0.818626	2.295958
C	-2.958699	-1.625808	1.106982
C	-4.328448	-1.979363	0.784750
N	-5.411532	-2.254949	0.441198
H	-1.777972	-0.705589	2.698278
H	-3.507903	-0.046919	2.535111
H	-2.332311	-2.524887	1.085433

inner sphere Ni(II)-salen / acrylonitrile (α-carbon) intermediate

Ni	0.529070	-0.074623	0.104545
O	-0.551771	1.381298	0.534141
O	2.051149	1.028173	0.533628
N	-0.893099	-1.188067	-0.351601
N	1.642614	-1.558689	-0.327998
C	-1.742842	1.607422	0.026532
C	-2.202882	2.954855	-0.024396
C	-3.446574	3.291134	-0.551071
C	-4.293887	2.296972	-1.061435
C	-3.865372	0.966657	-1.011197
C	-2.624119	0.596454	-0.469287
C	-2.273980	-0.873798	-0.379810
C	3.294895	0.785731	0.315331
C	4.268570	1.806919	0.587978
C	5.617986	1.605756	0.366369
C	6.108683	0.374942	-0.135059
C	5.201857	-0.637123	-0.399953
C	3.809899	-0.468707	-0.189834
C	2.934190	-1.576797	-0.449889
C	-0.506528	-2.391643	-1.050612
C	0.872504	-2.791675	-0.517689
H	-1.529884	3.717377	0.362703
H	-3.754207	4.337096	-0.574138
H	-5.263013	2.548759	-1.487012
H	-4.519408	0.181389	-1.390435
H	-2.784741	-1.396438	-1.209647
H	3.890700	2.751461	0.971843
H	6.318789	2.412026	0.582923
H	7.172850	0.229572	-0.303775
H	5.552150	-1.598341	-0.779662
H	3.411585	-2.517449	-0.759132
H	-1.209133	-3.229908	-0.876087
H	-0.449492	-2.262813	-2.154545
H	1.400392	-3.496977	-1.179132
H	0.747435	-3.262810	0.468854
C	-2.727887	-0.822636	2.230228
C	-3.006360	-1.563192	0.977985
C	-4.441267	-1.766503	0.746799
N	-5.568821	-1.945690	0.507584
H	-1.696822	-0.782816	2.569480
H	-3.399158	-0.028613	2.544260
H	-2.542039	-2.560251	1.001415

inner sphere Ni(II)-salen / acrylonitrile (β-carbon) transition state

Ni	0.616756	0.075759	0.034836

O	-0.288989	1.665209	0.353730
O	2.240487	1.028647	0.406030
N	-0.918092	-0.886815	-0.412930
N	1.551345	-1.561927	-0.230925
C	-1.536452	1.946204	0.055871
C	-1.950407	3.305896	0.145445
C	-3.252393	3.700544	-0.144560
C	-4.208415	2.754285	-0.552691
C	-3.826890	1.417302	-0.652543
C	-2.518040	0.983310	-0.352350
C	-2.209295	-0.449850	-0.448604
C	3.452948	0.623410	0.255008
C	4.531300	1.548265	0.465897
C	5.852484	1.172690	0.312627
C	6.207256	-0.149485	-0.052886
C	5.195786	-1.072093	-0.253833
C	3.827913	-0.724328	-0.111293
C	2.835225	-1.743284	-0.296424
C	-0.650610	-2.200690	-0.973651
C	0.642715	-2.708401	-0.332106
H	-1.197228	4.028290	0.453052
H	-3.525944	4.752310	-0.060140
H	-5.225731	3.056589	-0.792691
H	-4.554045	0.667908	-0.963872
H	-2.881154	-1.006422	-1.111644
H	4.257583	2.562350	0.746368
H	6.637791	1.910059	0.477727
H	7.250769	-0.431432	-0.168167
H	5.439903	-2.099435	-0.528212
H	3.204158	-2.759781	-0.491092
H	-1.474066	-2.904934	-0.773612
H	-0.522027	-2.154433	-2.072060
H	1.098935	-3.535578	-0.897147
H	0.423596	-3.060993	0.686417
C	-3.098556	-1.259691	1.280604
C	-4.505553	-1.283195	1.262840
C	-5.246319	-2.353385	0.722445
H	-2.576981	-2.212927	1.198825
H	-2.610087	-0.534436	1.928254
H	-5.069284	-0.395829	1.542869
N	-5.872995	-3.253087	0.292787

inner sphere Ni(II)-salen / acrylonitrile (β-carbon) intermediate

Ni	0.568368	0.015902	0.071190
O	-0.382549	1.549306	0.536262
O	2.170450	0.953251	0.568515
N	-0.929341	-0.904296	-0.527471
N	1.536147	-1.564177	-0.352290
C	-1.573799	1.879408	0.087517
C	-1.936524	3.256482	0.095876
C	-3.182793	3.692585	-0.346048
C	-4.127826	2.774524	-0.827136
C	-3.790605	1.416476	-0.840385
C	-2.547473	0.948508	-0.390144
C	-2.286137	-0.540756	-0.355798
C	3.391170	0.592660	0.379164
C	4.450599	1.508480	0.698810
C	5.779804	1.179304	0.510546
C	6.162132	-0.085281	-0.001010
C	5.169311	-0.999098	-0.309835
C	3.794839	-0.697658	-0.135083
C	2.822792	-1.710404	-0.435726
C	-0.658262	-2.173481	-1.165231
C	0.650620	-2.711982	-0.574396

H	-1.191867	3.959143	0.464488
H	-3.417426	4.757106	-0.323123
H	-5.099423	3.106414	-1.187460
H	-4.515058	0.686619	-1.204508
H	-2.921379	-1.028330	-1.113934
H	4.155793	2.478823	1.090766
H	6.549426	1.908810	0.762187
H	7.211390	-0.331911	-0.142799
H	5.434976	-1.983910	-0.697224
H	3.212685	-2.691506	-0.740868
H	-1.462792	-2.910120	-0.994117
H	-0.548621	-2.076954	-2.265861
H	1.130165	-3.470633	-1.213324
H	0.438286	-3.164398	0.405644
C	-2.842174	-1.156457	1.090459
C	-4.301962	-1.084233	1.263821
C	-5.154897	-2.136062	0.923458
H	-2.486741	-2.192976	1.119629
H	-2.306137	-0.567304	1.842840
H	-4.767531	-0.129516	1.498460
N	-5.873699	-3.035564	0.661941

inner sphere Ni(II)-salen / methyl acrylate (α-carbon) transition state

Ni	0.945993	0.175558	-0.286413
O	0.068224	1.790596	-0.029683
O	2.555649	1.057024	0.294868
N	-0.547230	-0.669727	-1.028075
N	1.829103	-1.494251	-0.443704
C	-1.199302	2.047207	-0.254097
C	-1.623262	3.405298	-0.175672
C	-2.944472	3.779713	-0.398262
C	-3.913386	2.815842	-0.717329
C	-3.518620	1.478522	-0.795777
C	-2.194219	1.067661	-0.570675
C	-1.855201	-0.383000	-0.671434
C	3.754326	0.592441	0.309575
C	4.841242	1.463128	0.664438
C	6.149792	1.019485	0.696742
C	6.482997	-0.322011	0.385441
C	5.461916	-1.193058	0.046140
C	4.107669	-0.775750	-0.002060
C	3.098616	-1.741765	-0.332008
C	-0.261006	-2.003413	-1.527219
C	0.887869	-2.591090	-0.695394
H	-0.861611	4.143811	0.066338
H	-3.222706	4.831776	-0.328256
H	-4.948322	3.098821	-0.897958
H	-4.258337	0.716730	-1.045069
H	-2.590486	-0.921197	-1.286839
H	4.583985	2.491970	0.904214
H	6.941738	1.717157	0.969023
H	7.516468	-0.658219	0.416431
H	5.688365	-2.233492	-0.192614
H	3.438087	-2.775644	-0.485490
H	-1.137378	-2.669777	-1.475011
H	0.055906	-1.968849	-2.586782
H	1.387609	-3.442445	-1.187001
H	0.495049	-2.929553	0.275060
C	-1.636536	-0.628431	2.104610
C	-2.285690	-1.234812	0.964644
C	-3.769133	-1.261309	1.020947
O	-4.508929	-0.569160	1.697568
O	-4.279287	-2.168029	0.111554
C	-5.700488	-2.183272	0.033960

H	-0.559998	-0.720767	2.223129
H	-2.141754	0.171223	2.638429
H	-1.899316	-2.217895	0.678005
H	-5.954282	-2.939992	-0.714429
H	-6.092758	-1.205195	-0.269762
H	-6.149135	-2.441791	1.000779

inner sphere Ni(II)-salen / methyl acrylate (α-carbon) intermediate

Ni	0.937414	0.149613	-0.262142
O	0.027251	1.742654	0.054991
O	2.539731	1.043522	0.338055
N	-0.537298	-0.693648	-1.038184
N	1.846939	-1.502165	-0.454622
C	-1.222281	2.009110	-0.245819
C	-1.640638	3.370668	-0.210290
C	-2.945288	3.751042	-0.511941
C	-3.900505	2.790273	-0.874253
C	-3.509100	1.447966	-0.911225
C	-2.206389	1.032547	-0.599196
C	-1.869803	-0.438489	-0.641281
C	3.745712	0.599119	0.328342
C	4.823111	1.478048	0.693041
C	6.139145	1.055370	0.700002
C	6.490361	-0.272338	0.352316
C	5.478997	-1.151383	0.003192
C	4.118071	-0.755532	-0.020447
C	3.120890	-1.731445	-0.360409
C	-0.240534	-2.023116	-1.538431
C	0.918938	-2.607568	-0.716997
H	-0.888688	4.108386	0.062972
H	-3.218740	4.806057	-0.472578
H	-4.920424	3.077286	-1.122415
H	-4.237430	0.687160	-1.198209
H	-2.578163	-0.941416	-1.320563
H	4.552337	2.496608	0.960503
H	6.922778	1.759316	0.980390
H	7.529393	-0.592424	0.363392
H	5.719365	-2.182034	-0.263153
H	3.475315	-2.756795	-0.536845
H	-1.107844	-2.702970	-1.481950
H	0.068887	-1.992955	-2.601832
H	1.429737	-3.448093	-1.217148
H	0.533404	-2.960401	0.251764
C	-1.562694	-0.643261	2.012393
C	-2.263404	-1.202055	0.846553
C	-3.758710	-1.192004	1.014123
O	-4.416274	-0.536555	1.798389
O	-4.358220	-2.019790	0.095808
C	-5.783320	-1.989350	0.118014
H	-0.482375	-0.735181	2.079790
H	-2.050635	0.126710	2.602114
H	-1.955742	-2.233414	0.622331
H	-6.111301	-2.682613	-0.661650
H	-6.157549	-0.979919	-0.088775
H	-6.170950	-2.303968	1.094153

inner sphere Ni(II)-salen / methyl acrylate (β-carbon) transition state

Ni	0.924877	0.401753	0.051060
O	0.567415	2.200551	0.338773
O	2.771320	0.809036	0.373886
N	-0.839265	-0.042937	-0.360644
N	1.295203	-1.450678	-0.173261
C	-0.544645	2.845599	0.075986
C	-0.521794	4.267756	0.155835
C	-1.648437	5.039716	-0.106317
C	-2.860314	4.428063	-0.473419
C	-2.908308	3.038565	-0.559579
C	-1.785142	2.225776	-0.291077
C	-1.932628	0.767626	-0.385664
C	3.793984	0.044003	0.210370
C	5.111480	0.593050	0.368008
C	6.246353	-0.178174	0.200362
C	6.162658	-1.553773	-0.127597
C	4.909063	-2.120982	-0.277341
C	3.721722	-1.361946	-0.119083
C	2.455908	-2.025322	-0.253513
C	-1.016265	-1.394295	-0.864237
C	0.070154	-2.257101	-0.220845
H	0.424928	4.727457	0.431911
H	-1.585213	6.125265	-0.030092
H	-3.744303	5.024827	-0.688614
H	-3.839490	2.545229	-0.841051
H	-2.755739	0.440697	-1.030537
H	5.174097	1.648819	0.619934
H	7.226023	0.282957	0.324405
H	7.063334	-2.149105	-0.254699
H	4.814488	-3.179832	-0.522647
H	2.484521	-3.110899	-0.420714
H	-2.012141	-1.784015	-0.604256
H	-0.914883	-1.430930	-1.966342
H	0.233430	-3.204694	-0.756426
H	-0.225393	-2.486791	0.813300
C	-3.092610	0.317781	1.323650
C	-3.558729	-1.006200	1.335852
C	-4.766579	-1.371590	0.650459
O	-5.530565	-0.640360	0.016281
O	-5.034122	-2.734759	0.769875
C	-6.223937	-3.148073	0.120526
H	-2.306454	0.600761	2.021238
H	-3.822332	1.095912	1.107136
H	-2.983818	-1.804786	1.799240
H	-6.306496	-4.226648	0.292962
H	-6.190347	-2.943588	-0.957673
H	-7.106808	-2.636823	0.526283

inner sphere Ni(II)-salen / methyl acrylate (β-carbon) intermediate

Ni	1.051951	0.216408	0.144389
O	0.611686	1.977944	0.525633
O	2.880140	0.690313	0.496596
N	-0.680398	-0.285595	-0.299033
N	1.518241	-1.590527	-0.219777
C	-0.472140	2.608920	0.131239
C	-0.445961	4.034300	0.137561
C	-1.540722	4.794423	-0.259618
C	-2.720300	4.167604	-0.691992
C	-2.767182	2.771869	-0.700539
C	-1.679801	1.978391	-0.296849
C	-1.864158	0.478748	-0.286708
C	3.939454	0.002591	0.247833
C	5.228433	0.606972	0.437007
C	6.399780	-0.080017	0.178185
C	6.384000	-1.420687	-0.278847
C	5.159870	-2.041040	-0.460919
C	3.936995	-1.368570	-0.211018
C	2.705789	-2.088244	-0.378446
C	-0.829371	-1.620160	-0.821962
C	0.340409	-2.461005	-0.302668
H	0.477583	4.505409	0.467917
H	-1.474536	5.882537	-0.239774
H	-3.579324	4.751531	-1.016157
H	-3.677620	2.264509	-1.023815
H	-2.535149	0.197827	-1.116438
H	5.238919	1.636421	0.786598
H	7.355393	0.421730	0.329584
H	7.312748	-1.949677	-0.477582
H	5.117807	-3.076108	-0.803418
H	2.789224	-3.151402	-0.643740
H	-1.788430	-2.062700	-0.481326
H	-0.852542	-1.634504	-1.931008
H	0.538650	-3.346658	-0.925893
H	0.106302	-2.802605	0.716476
C	-2.817013	0.094992	1.056069
C	-3.350735	-1.263495	1.088325
C	-4.528067	-1.595338	0.350385
O	-5.204480	-0.846005	-0.361107
O	-4.883015	-2.933696	0.503250
C	-6.049444	-3.307071	-0.210475
H	-2.176664	0.329286	1.912002
H	-3.627772	0.827035	0.977960
H	-2.850610	-2.058647	1.635412
H	-6.211303	-4.368547	0.005415
H	-5.928205	-3.160191	-1.291713
H	-6.923825	-2.723895	0.106878

Co(II)-salen – doublet

Co	0.000003	0.210274	-0.000098
O	-1.293828	-1.130763	0.011634
O	1.293830	-1.130759	-0.011086
N	-1.275502	1.592137	0.158664
N	1.275458	1.592177	-0.158591
C	-2.586787	-1.016442	-0.008127
C	-3.379641	-2.203082	-0.086207
C	-4.759398	-2.141506	-0.113121
C	-5.445064	-0.900828	-0.059898
C	-4.710822	0.264082	0.021650
C	-3.287456	0.241515	0.048498
C	-2.578226	1.472732	0.154381
C	2.586793	-1.016464	0.008317
C	3.379664	-2.203081	0.086479
C	4.759424	-2.141474	0.113089
C	5.445066	-0.900807	0.059496
C	4.710813	0.264074	-0.022159
C	3.287436	0.241489	-0.048735
C	2.578188	1.472693	-0.154589
C	-0.667923	2.911023	0.373176
C	0.667944	2.911179	-0.372673
H	-2.850274	-3.151089	-0.126595
H	-5.332280	-3.064940	-0.175973
H	-6.530837	-0.872424	-0.080957
H	-5.214848	1.229132	0.067895
H	-3.177239	2.386212	0.248590
H	2.850337	-3.151102	0.127096
H	5.332329	-3.064897	0.175906
H	6.530835	-0.872382	0.080507
H	5.214832	1.229111	-0.068684
H	3.177220	2.386135	-0.248964
H	-1.323436	3.721908	0.026878
H	-0.488473	3.047884	1.449268
H	1.323408	3.721889	-0.025951
H	0.488584	3.048503	-1.448722

Co(II)-salen – quartet

Co	0.000000	-0.041386	0.000009
O	1.511241	-1.212247	0.347957
O	-1.511242	-1.212245	-0.347941
N	1.290922	1.529542	-0.322313
N	-1.290920	1.529544	0.322332
C	2.787258	-1.001629	0.210384
C	3.688482	-2.089702	0.418469
C	5.057427	-1.931543	0.298271
C	5.626334	-0.677271	-0.026947
C	4.785242	0.400006	-0.227697
C	3.371840	0.276892	-0.125388
C	2.589789	1.463583	-0.330014
C	-2.787259	-1.001625	-0.210368
C	-3.688484	-2.089698	-0.418451
C	-5.057429	-1.931538	-0.298249
C	-5.626334	-0.677266	0.026968
C	-4.785241	0.400011	0.227718
C	-3.371840	0.276896	0.125407
C	-2.589787	1.463585	0.330033
C	0.606443	2.811486	-0.476731
C	-0.606440	2.811486	0.476751
H	3.249142	-3.050661	0.672511
H	5.708531	-2.788889	0.459833
H	6.703348	-0.565475	-0.114076
H	5.200351	1.376975	-0.475207
H	3.159524	2.389934	-0.495157

H	-3.249145	-3.050658	-0.672493
H	-5.708533	-2.788884	-0.459811
H	-6.703348	-0.565469	0.114099
H	-5.200348	1.376980	0.475229
H	-3.159521	2.389937	0.495177
H	1.268340	3.664598	-0.266504
H	0.244651	2.903174	-1.511495
H	-1.268336	3.664599	0.266524
H	-0.244647	2.903174	1.511515

reduced Co(II)-salen – singlet

Co	0.000005	0.230232	0.000069
O	-1.319088	-1.164999	0.019578
O	1.319099	-1.164994	-0.019458
N	-1.268745	1.579393	0.128134
N	1.268744	1.579401	-0.128000
C	-2.600408	-1.035756	-0.004097
C	-3.426308	-2.208385	-0.075681
C	-4.808825	-2.137594	-0.100997
C	-5.475797	-0.890136	-0.053105
C	-4.712727	0.266045	0.020143
C	-3.295512	0.237265	0.044945
C	-2.576026	1.475255	0.139811
C	2.600421	-1.035749	0.004134
C	3.426326	-2.208377	0.075657
C	4.808844	-2.137584	0.100900
C	5.475812	-0.890124	0.052989
C	4.712735	0.266057	-0.020198
C	3.295518	0.237274	-0.044925
C	2.576026	1.475264	-0.139736
C	-0.684768	2.905408	0.341309
C	0.684762	2.905421	-0.341133
H	-2.908797	-3.164940	-0.110741
H	-5.391564	-3.057644	-0.157580
H	-6.562613	-0.839822	-0.071263
H	-5.205701	1.239627	0.061752
H	-3.172676	2.391702	0.240826
H	2.908819	-3.164934	0.110731
H	5.391588	-3.057633	0.157435
H	6.562628	-0.839808	0.071089
H	5.205705	1.239640	-0.061819
H	3.172670	2.391713	-0.240761
H	-1.329796	3.708667	-0.051615
H	-0.553760	3.071754	1.421795
H	1.329787	3.708669	0.051817
H	0.553753	3.071803	-1.421613

reduced Co(II)-salen – triplet

Co	0.000000	0.045807	0.000010
O	1.497216	-1.258190	0.164681
O	-1.497217	-1.258189	-0.164661
N	1.289974	1.551720	-0.286663
N	-1.289972	1.551721	0.286682
C	2.772123	-1.026699	0.112657
C	3.679925	-2.116775	0.307035
C	5.057698	-1.964750	0.251113
C	5.631192	-0.696993	0.003375
C	4.788705	0.388413	-0.181282
C	3.371640	0.278121	-0.136200
C	2.604522	1.479626	-0.311199
C	-2.772124	-1.026696	-0.112638
C	-3.679927	-2.116772	-0.307015
C	-5.057700	-1.964745	-0.251094
C	-5.631193	-0.696988	-0.003355

C	-4.788704	0.388418	0.181302
C	-3.371639	0.278124	0.136220
C	-2.604520	1.479628	0.311219
C	0.641550	2.845120	-0.430205
C	-0.641547	2.845121	0.430225
H	3.228698	-3.088772	0.497134
H	5.701776	-2.831718	0.399838
H	6.711755	-0.573975	-0.039618
H	5.214319	1.376359	-0.368980
H	3.183170	2.406755	-0.450102
H	-3.228701	-3.088769	-0.497114
H	-5.701778	-2.831712	-0.399818
H	-6.711755	-0.573968	0.039638
H	-5.214317	1.376364	0.369000
H	-3.183167	2.406758	0.450122
H	1.302454	3.678984	-0.130377
H	0.357542	3.007951	-1.483068
H	-1.302450	3.678985	0.130397
H	-0.357538	3.007952	1.483088

inner sphere Co(II)-salen / acrylonitrile (α-carbon) transition state – singlet

Co	0.539353	-0.022855	-0.011658
O	-0.530431	1.491028	0.325372
O	2.072057	1.084782	0.357104
N	-0.878493	-1.081009	-0.556734
N	1.630680	-1.554912	-0.302261
C	-1.775120	1.664715	-0.043570
C	-2.306756	2.988130	-0.003145
C	-3.612771	3.271549	-0.385401
C	-4.462968	2.246963	-0.833999
C	-3.968549	0.942313	-0.875630
C	-2.654026	0.623449	-0.487874
C	-2.233626	-0.803875	-0.500821
C	3.323320	0.788145	0.226105
C	4.307836	1.803859	0.456747
C	5.662251	1.551871	0.325368
C	6.138491	0.270513	-0.039136
C	5.215834	-0.738704	-0.262137
C	3.821252	-0.517948	-0.140129
C	2.926660	-1.623023	-0.358041
C	-0.505370	-2.384962	-1.083125
C	0.832914	-2.777502	-0.444995
H	-1.635973	3.774088	0.338210
H	-3.973090	4.299863	-0.341394
H	-5.483974	2.460532	-1.143104
H	-4.619165	0.132307	-1.205219
H	-2.834332	-1.394841	-1.208214
H	3.937991	2.787446	0.735993
H	6.374286	2.356694	0.507002
H	7.204781	0.082600	-0.138736
H	5.556551	-1.737684	-0.538697
H	3.388698	-2.596787	-0.571010
H	-1.257576	-3.160840	-0.857935
H	-0.396781	-2.358460	-2.184182
H	1.369541	-3.544985	-1.025013
H	0.644361	-3.175094	0.563304
C	-2.765296	-0.792472	2.272528
C	-2.924986	-1.620611	1.101897
C	-4.286707	-1.997117	0.773054
N	-5.364247	-2.294929	0.431928
H	-1.866905	-0.807168	2.583982
H	-3.573168	-0.066417	2.500759
H	-2.642463	-2.565157	0.950622

inner sphere Co(II)-salen / acrylonitrile (α-carbon) transition state – triplet

Co	0.560918	0.003502	-0.010846
O	-0.506111	1.515356	0.311284
O	2.094690	1.098649	0.350279
N	-0.876189	-1.062312	-0.551449
N	1.634907	-1.542116	-0.283302
C	-1.753811	1.692766	-0.047425
C	-2.280877	3.017257	0.012433
C	-3.587341	3.308892	-0.359500
C	-4.442769	2.290914	-0.816113
C	-3.953651	0.986643	-0.877303
C	-2.635981	0.658108	-0.501401
C	-2.222951	-0.762402	-0.538762
C	3.345387	0.790312	0.230545
C	4.335294	1.801265	0.455160
C	5.688498	1.536717	0.336364
C	6.156446	0.246932	-0.008640
C	5.227578	-0.757600	-0.225774
C	3.833894	-0.523715	-0.116461
C	2.930909	-1.622772	-0.328216
C	-0.499963	-2.363103	-1.078466
C	0.826686	-2.759483	-0.420329
H	-1.605703	3.796620	0.360002
H	-3.944928	4.337346	-0.301202
H	-5.464924	2.511389	-1.116477
H	-4.608152	0.182219	-1.212105
H	-2.826128	-1.353539	-1.242110
H	3.971359	2.791088	0.719584
H	6.405849	2.337888	0.512716
H	7.221820	0.049208	-0.098303
H	5.562021	-1.762549	-0.487611
H	3.385092	-2.603078	-0.526572
H	-1.256702	-3.138197	-0.866902
H	-0.372413	-2.335867	-2.178318
H	1.364050	-3.538002	-0.984400
H	0.622560	-3.141721	0.590784
C	-2.881776	-0.801359	2.266486
C	-2.997491	-1.626364	1.094429
C	-4.329876	-2.006319	0.685917
N	-5.383720	-2.297199	0.268752
H	-1.898893	-0.659604	2.708275
H	-3.642721	-0.056610	2.482515
H	-2.322663	-2.487644	1.070527

inner sphere Co(II)-salen / acrylonitrile (α-carbon) intermediate – singlet

Co	0.515611	-0.076144	0.073336
O	-0.581424	1.401133	0.519657
O	2.042479	1.034544	0.479725
N	-0.892433	-1.130251	-0.477881
N	1.623239	-1.566906	-0.337314
C	-1.766395	1.635034	0.008951
C	-2.236614	2.980673	-0.023691
C	-3.478358	3.317278	-0.554450
C	-4.317649	2.327419	-1.087116
C	-3.881607	0.998781	-1.055388
C	-2.641416	0.628490	-0.512857
C	-2.284972	-0.839875	-0.437638
C	3.293587	0.768358	0.296032
C	4.269619	1.783142	0.565450
C	5.623674	1.562984	0.381597
C	6.108564	0.316123	-0.077762
C	5.194552	-0.691782	-0.341109
C	3.801038	-0.502944	-0.167991
C	2.917639	-1.607906	-0.432624

C	-0.530452	-2.395502	-1.085335
C	0.842804	-2.794395	-0.529032
H	-1.572018	3.741583	0.380951
H	-3.792251	4.361720	-0.562793
H	-5.285482	2.581242	-1.514374
H	-4.528678	0.215148	-1.450721
H	-2.819369	-1.366240	-1.249292
H	3.893236	2.740669	0.917407
H	6.328335	2.366449	0.595617
H	7.174349	0.152638	-0.218169
H	5.542277	-1.665167	-0.690939
H	3.389403	-2.557928	-0.719391
H	-1.251296	-3.204066	-0.856598
H	-0.479738	-2.332059	-2.192160
H	1.372422	-3.511988	-1.175954
H	0.703786	-3.256862	0.459535
C	-2.630019	-0.787302	2.182688
C	-2.942871	-1.533559	0.939534
C	-4.384481	-1.751909	0.763052
N	-5.519008	-1.943842	0.573969
H	-1.589950	-0.738405	2.490829
H	-3.298923	0.000195	2.517099
H	-2.472600	-2.528598	0.956158

inner sphere Co(II)-salen / acrylonitrile (α-carbon) intermediate – triplet

Co	0.519676	-0.084670	0.100202
O	-0.583863	1.384142	0.561099
O	2.045071	1.031968	0.493488
N	-0.893494	-1.155559	-0.414342
N	1.629448	-1.568581	-0.329102
C	-1.760023	1.624624	0.032871
C	-2.221652	2.973087	-0.007536
C	-3.452477	3.317406	-0.558470
C	-4.288518	2.332612	-1.105182
C	-3.861158	1.001299	-1.065381
C	-2.633117	0.622929	-0.501124
C	-2.291416	-0.851139	-0.416113
C	3.295612	0.772218	0.296182
C	4.269719	1.790047	0.560705
C	5.622911	1.576730	0.362661
C	6.108655	0.334137	-0.107122
C	5.196463	-0.676579	-0.366141
C	3.803933	-0.494695	-0.178541
C	2.922920	-1.602827	-0.438359
C	-0.529815	-2.405560	-1.049424
C	0.853294	-2.799678	-0.516476
H	-1.558649	3.729946	0.407201
H	-3.759645	4.363795	-0.572267
H	-5.247313	2.592094	-1.549113
H	-4.506571	0.221753	-1.471400
H	-2.799298	-1.364563	-1.253778
H	3.892626	2.744291	0.920753
H	6.326131	2.382303	0.573492
H	7.173719	0.175964	-0.258714
H	5.544968	-1.646896	-0.723649
H	3.396256	-2.549455	-0.733659
H	-1.238685	-3.226606	-0.824461
H	-0.494075	-2.326474	-2.156758
H	1.377569	-3.510159	-1.175355
H	0.731208	-3.268191	0.471450
C	-2.666612	-0.804361	2.180975
C	-2.979973	-1.536533	0.922098
C	-4.424805	-1.732108	0.733590
N	-5.560824	-1.908119	0.539350

H	-1.624243	-0.750279	2.479883
H	-3.345460	-0.036622	2.540209
H	-2.529879	-2.541718	0.947264

inner sphere Co(II)-salen / acrylonitrile (β-carbon) transition state – singlet

Co	0.648279	0.075687	-0.013307
O	-0.281712	1.685510	0.302104
O	2.269146	1.040729	0.354113
N	-0.852687	-0.846383	-0.578445
N	1.590765	-1.560432	-0.258632
C	-1.523417	1.958163	-0.008581
C	-1.966562	3.308226	0.114269
C	-3.267021	3.689051	-0.196100
C	-4.199573	2.739985	-0.651825
C	-3.793834	1.412191	-0.778021
C	-2.483880	0.992355	-0.465695
C	-2.158731	-0.437406	-0.567547
C	3.489065	0.620906	0.261342
C	4.561114	1.542023	0.496620
C	5.887354	1.156919	0.406960
C	6.245558	-0.172525	0.081745
C	5.235307	-1.092658	-0.145155
C	3.866087	-0.734934	-0.064725
C	2.874896	-1.753627	-0.282730
C	-0.591283	-2.187284	-1.088936
C	0.679737	-2.701136	-0.403589
H	-1.233761	4.033876	0.461231
H	-3.560220	4.733592	-0.089095
H	-5.216102	3.033247	-0.905701
H	-4.503436	0.660161	-1.123091
H	-2.836791	-1.007717	-1.211325
H	4.282085	2.562803	0.746140
H	6.669734	1.892742	0.591341
H	7.290594	-0.464823	0.014806
H	5.483780	-2.125990	-0.391775
H	3.245235	-2.771325	-0.466429
H	-1.429512	-2.874565	-0.891994
H	-0.438932	-2.164146	-2.182857
H	1.150841	-3.528088	-0.957313
H	0.422989	-3.060441	0.603449
C	-2.956466	-1.245903	1.174845
C	-4.363743	-1.280718	1.203509
C	-5.110166	-2.364678	0.699467
H	-2.435025	-2.199454	1.094117
H	-2.455205	-0.513318	1.804502
H	-4.925569	-0.392235	1.483366
N	-5.739536	-3.275588	0.299331

inner sphere Co(II)-salen / acrylonitrile (β-carbon) transition state – triplet

Co	0.654477	0.114761	-0.071431
O	-0.297543	1.685542	0.279706
O	2.281390	1.074782	0.276556
N	-0.857474	-0.818955	-0.688267
N	1.576066	-1.542221	-0.256414
C	-1.552940	1.951898	-0.007567
C	-2.004332	3.290966	0.158973
C	-3.317647	3.664009	-0.110173
C	-4.248148	2.712489	-0.562316
C	-3.831614	1.392808	-0.731419
C	-2.507316	0.982632	-0.465732
C	-2.163899	-0.436524	-0.600641
C	3.495047	0.632579	0.242549
C	4.575823	1.549467	0.459330
C	5.895920	1.138384	0.434585
C	6.240664	-0.213310	0.191727
C	5.223548	-1.127063	-0.023131
C	3.857642	-0.744179	-0.004890
C	2.859342	-1.750718	-0.233484
C	-0.571136	-2.154225	-1.184507
C	0.655452	-2.673786	-0.425055
H	-1.271463	4.016301	0.506396
H	-3.620694	4.701898	0.027720
H	-5.275173	2.997949	-0.780974
H	-4.541280	0.639803	-1.073007
H	-2.873174	-1.023655	-1.191976
H	4.307010	2.586336	0.645525
H	6.685376	1.869584	0.606357
H	7.282043	-0.525033	0.175491
H	5.461728	-2.174685	-0.212412
H	3.220597	-2.775549	-0.392902
H	-1.419745	-2.842050	-1.044076
H	-0.342877	-2.131833	-2.267015
H	1.144222	-3.517568	-0.936844
H	0.342373	-3.005727	0.575833
C	-2.916678	-1.271947	1.202518
C	-4.321184	-1.336230	1.275082
C	-5.063769	-2.422933	0.773140
H	-2.373429	-2.209342	1.082695
H	-2.409482	-0.532450	1.819613
H	-4.890725	-0.466906	1.596736
N	-5.689394	-3.337986	0.374319

inner sphere Co(II)-salen / acrylonitrile (β-carbon) intermediate – singlet

Co	0.563339	-0.012532	0.121697
O	-0.416645	1.527308	0.634382
O	2.170531	0.959090	0.552079
N	-0.918754	-0.911766	-0.499067
N	1.544552	-1.575669	-0.336483
C	-1.585605	1.871402	0.150431
C	-1.957694	3.247448	0.177857
C	-3.181432	3.690684	-0.315740
C	-4.099065	2.783552	-0.867303
C	-3.757867	1.426472	-0.894512
C	-2.537237	0.950727	-0.394449
C	-2.284601	-0.539631	-0.358370
C	3.397010	0.596874	0.361244
C	4.451016	1.519427	0.664278
C	5.783174	1.195557	0.474236
C	6.166183	-0.071130	-0.025469
C	5.174250	-0.992376	-0.321126
C	3.800190	-0.696184	-0.142012
C	2.831117	-1.718186	-0.436768

C	-0.665600	-2.200197	-1.117113
C	0.664224	-2.728029	-0.560928
H	-1.235079	3.943361	0.599629
H	-3.420930	4.753860	-0.278453
H	-5.051895	3.122980	-1.268345
H	-4.462329	0.703822	-1.309802
H	-2.904107	-1.024389	-1.131040
H	4.152856	2.492408	1.047264
H	6.550315	1.931229	0.715038
H	7.215450	-0.316506	-0.170496
H	5.442646	-1.979373	-0.701047
H	3.224328	-2.694768	-0.750997
H	-1.462103	-2.935208	-0.903983
H	-0.600298	-2.118539	-2.220599
H	1.135962	-3.473324	-1.220954
H	0.478136	-3.198893	0.415500
C	-2.857586	-1.149811	1.071049
C	-4.321018	-1.065300	1.224129
C	-5.176436	-2.121525	0.905303
H	-2.513083	-2.189448	1.115622
H	-2.331454	-0.560540	1.830344
H	-4.783033	-0.102513	1.431677
N	-5.897428	-3.023765	0.661300

inner sphere Co(II)-salen / acrylonitrile (β-carbon) intermediate – triplet

Co	0.571671	-0.025327	0.143372
O	-0.419348	1.505357	0.667762
O	2.174433	0.945161	0.589173
N	-0.920598	-0.952029	-0.435758
N	1.556518	-1.573900	-0.351408
C	-1.580229	1.852541	0.168888
C	-1.945746	3.231097	0.187321
C	-3.157429	3.680634	-0.329163
C	-4.069692	2.777398	-0.896068
C	-3.736041	1.418077	-0.912246
C	-2.529089	0.934496	-0.386390
C	-2.292470	-0.560473	-0.330875
C	3.401619	0.596089	0.378705
C	4.452275	1.518851	0.692456
C	5.784847	1.208614	0.482923
C	6.171427	-0.044248	-0.047669
C	5.182710	-0.965659	-0.354052
C	3.808444	-0.682905	-0.156529
C	2.843499	-1.706071	-0.462041
C	-0.663679	-2.214263	-1.097150
C	0.684886	-2.733064	-0.580248
H	-1.225932	3.923722	0.619194
H	-3.391209	4.745311	-0.298958
H	-5.012211	3.121399	-1.317181
H	-4.436949	0.699339	-1.340607
H	-2.892853	-1.034960	-1.126507
H	4.151238	2.481170	1.099471
H	6.549272	1.944235	0.732493
H	7.220905	-0.279381	-0.207660
H	5.454152	-1.942509	-0.757380
H	3.241203	-2.675186	-0.793375
H	-1.440118	-2.972918	-0.885476
H	-0.622721	-2.111372	-2.201810
H	1.153464	-3.459139	-1.263596
H	0.526148	-3.223643	0.391304
C	-2.897902	-1.152846	1.065289
C	-4.368517	-1.034612	1.199604
C	-5.243623	-2.090552	0.946449
H	-2.583372	-2.201566	1.121976

H	-2.379809	-0.582988	1.846015
H	-4.812426	-0.056385	1.373011
N	-5.982750	-2.990895	0.754739

inner sphere Co(II)-salen / methyl acrylate (α-carbon) transition state – singlet

Co	0.952097	0.122000	0.022529
O	0.123946	1.777618	0.377424
O	2.646000	0.994633	0.339474
N	-0.615439	-0.715835	-0.482696
N	1.797795	-1.556057	-0.276939
C	-1.082007	2.135127	0.011395
C	-1.398556	3.526231	0.022533
C	-2.647836	4.003775	-0.357317
C	-3.652819	3.115917	-0.773912
C	-3.368365	1.748851	-0.785356
C	-2.117662	1.234580	-0.401657
C	-1.924858	-0.247259	-0.394490
C	3.834478	0.513156	0.180105
C	4.966865	1.370988	0.373102
C	6.264515	0.917290	0.211524
C	6.533484	-0.424004	-0.148303
C	5.463647	-1.284769	-0.335558
C	4.121979	-0.856159	-0.182390
C	3.066760	-1.817658	-0.362913
C	-0.458595	-2.069512	-0.992461
C	0.823200	-2.647753	-0.381213
H	-0.608351	4.204171	0.339291
H	-2.841263	5.076932	-0.336073
H	-4.632420	3.479246	-1.077686
H	-4.145194	1.046017	-1.086501
H	-2.591427	-0.729700	-1.126155
H	4.756498	2.401395	0.649483
H	7.093832	1.607554	0.365448
H	7.556500	-0.771242	-0.271787
H	5.643123	-2.326324	-0.607192
H	3.372870	-2.852066	-0.571913
H	-1.313161	-2.716270	-0.731542
H	-0.377798	-2.078328	-2.097254
H	1.226297	-3.494179	-0.960140
H	0.603924	-2.998471	0.638077
C	-2.552199	-0.046922	2.302942
C	-2.684401	-0.942835	1.176153
C	-4.083395	-1.281926	0.800460
O	-5.091435	-0.623711	0.988844
O	-4.128554	-2.463431	0.092228
C	-5.419387	-2.806404	-0.402303
H	-1.572841	0.107408	2.747805
H	-3.319352	0.702031	2.476917
H	-2.072649	-1.845739	1.233885
H	-5.297464	-3.756341	-0.930669
H	-5.798240	-2.038865	-1.087721
H	-6.141541	-2.917363	0.415320

inner sphere Co(II)-salen / methyl acrylate (α-carbon) transition state - triplet

Co	0.962462	0.148686	0.011835
O	0.153524	1.813586	0.339601
O	2.664719	1.002065	0.293939
N	-0.633766	-0.689059	-0.461614
N	1.778140	-1.548340	-0.260245
C	-1.063093	2.173723	0.012271
C	-1.372956	3.566245	0.042669
C	-2.630844	4.051225	-0.294270
C	-3.652761	3.169018	-0.683744
C	-3.375293	1.802276	-0.715466

C	-2.112690	1.279393	-0.378523
C	-1.929365	-0.196148	-0.398232
C	3.846456	0.501325	0.135916
C	4.990175	1.349118	0.300044
C	6.280576	0.874959	0.138915
C	6.529197	-0.477777	-0.191381
C	5.447298	-1.328849	-0.350293
C	4.112460	-0.879049	-0.196966
C	3.042909	-1.829440	-0.348322
C	-0.486001	-2.046085	-0.962660
C	0.786781	-2.628065	-0.337913
H	-0.570261	4.238260	0.339851
H	-2.819342	5.124828	-0.259606
H	-4.640603	3.538396	-0.951312
H	-4.164645	1.103745	-0.991454
H	-2.608259	-0.676049	-1.118278
H	4.795060	2.388285	0.553736
H	7.119843	1.557764	0.269968
H	7.546659	-0.840963	-0.314595
H	5.611227	-2.378560	-0.599039
H	3.332995	-2.872332	-0.535990
H	-1.347123	-2.683231	-0.702545
H	-0.395447	-2.064919	-2.067242
H	1.178234	-3.493428	-0.896092
H	0.562480	-2.949728	0.689813
C	-2.697810	0.001764	2.322316
C	-2.750809	-0.921977	1.217831
C	-4.101087	-1.318990	0.765515
O	-5.145711	-0.697125	0.878847
O	-4.059711	-2.508766	0.064203
C	-5.303493	-2.899238	-0.506699
H	-1.742577	0.213779	2.795469
H	-3.509608	0.709251	2.464228
H	-2.079570	-1.779331	1.288925
H	-5.114685	-3.844127	-1.024820
H	-5.669777	-2.146804	-1.215450
H	-6.070309	-3.038209	0.265059

inner sphere Co(II)-salen / methyl acrylate (α-carbon) intermediate - singlet

Co	0.985672	-0.001597	0.102287
O	0.022018	1.564743	0.557948
O	2.608514	0.981096	0.487881
N	-0.509223	-0.939052	-0.423170
N	1.963688	-1.576900	-0.322434
C	-1.143316	1.893874	0.056913
C	-1.498107	3.274689	0.014745
C	-2.703198	3.713704	-0.525690
C	-3.619949	2.796536	-1.060317
C	-3.298583	1.435870	-1.012549
C	-2.102020	0.961044	-0.454946
C	-1.878196	-0.534816	-0.375615
C	3.830226	0.611259	0.290202
C	4.892135	1.538748	0.551903
C	6.220938	1.206149	0.352467
C	6.593963	-0.075107	-0.116347
C	5.594752	-1.001272	-0.372037
C	4.224352	-0.696966	-0.182466
C	3.248603	-1.724639	-0.435855
C	-0.261467	-2.227377	-1.035573
C	1.082866	-2.736834	-0.500309
H	-0.771756	3.978959	0.415983
H	-2.925920	4.781286	-0.542611
H	-4.557780	3.129919	-1.500240
H	-4.001160	0.707334	-1.422442

H	-2.445400	-1.005949	-1.197165
H	4.601773	2.523058	0.911477
H	6.993216	1.946377	0.561672
H	7.640527	-0.327884	-0.269002
H	5.855327	-1.999566	-0.727746
H	3.636418	-2.710445	-0.728236
H	-1.042518	-2.974369	-0.794695
H	-0.222763	-2.169535	-2.144033
H	1.543294	-3.495586	-1.153637
H	0.921433	-3.184882	0.491377
C	-2.100361	-0.596037	2.241457
C	-2.599231	-1.180762	0.979452
C	-4.105403	-1.097743	0.869389
O	-4.862989	-0.431686	1.545455
O	-4.563445	-1.885590	-0.153936
C	-5.968931	-1.800509	-0.381818
H	-1.033956	-0.626761	2.441140
H	-2.714091	0.126805	2.769751
H	-2.328025	-2.244051	0.881862
H	-6.178947	-2.474059	-1.217139
H	-6.262612	-0.775664	-0.636525
H	-6.532443	-2.107986	0.506768

inner sphere Co(II)-salen / methyl acrylate (α-carbon) intermediate – triplet

Co	0.992764	-0.015798	0.137411
O	0.020706	1.541582	0.607419
O	2.613359	0.978977	0.498820
N	-0.506144	-0.971305	-0.351000
N	1.975771	-1.583967	-0.302458
C	-1.136980	1.873861	0.090630
C	-1.486671	3.255818	0.041840
C	-2.681515	3.698550	-0.518004
C	-3.592206	2.783910	-1.066883
C	-3.276468	1.422062	-1.011716
C	-2.091559	0.943330	-0.432765
C	-1.879546	-0.556120	-0.342346
C	3.834795	0.618440	0.282426
C	4.893350	1.554021	0.528142
C	6.221505	1.231730	0.308388
C	6.597083	-0.046603	-0.166255
C	5.601183	-0.980365	-0.406939
C	4.231537	-0.686636	-0.196525
C	3.259859	-1.721728	-0.435547
C	-0.254629	-2.248674	-0.982778
C	1.100686	-2.749953	-0.469362
H	-0.763952	3.957983	0.453201
H	-2.900177	4.766887	-0.539714
H	-4.521135	3.119939	-1.523435
H	-3.974609	0.695566	-1.432521
H	-2.420335	-1.019924	-1.186378
H	4.600891	2.536072	0.892183
H	6.991165	1.977903	0.505824
H	7.643095	-0.291353	-0.334985
H	5.863981	-1.976563	-0.766862
H	3.650786	-2.704299	-0.734638
H	-1.024029	-3.008150	-0.740880
H	-0.230340	-2.179989	-2.091812
H	1.556550	-3.503858	-1.131322
H	0.957307	-3.200844	0.523769
C	-2.142098	-0.612078	2.255936
C	-2.629605	-1.188183	0.979536
C	-4.135558	-1.093355	0.853703
O	-4.897088	-0.447208	1.544500
O	-4.586215	-1.848090	-0.196395

C	-5.989160	-1.750661	-0.435649
H	-1.074464	-0.618077	2.450102
H	-2.779094	0.070517	2.809431
H	-2.373423	-2.257701	0.895281
H	-6.192956	-2.398298	-1.292652
H	-6.275847	-0.717445	-0.662900
H	-6.562648	-2.082094	0.437777

inner sphere Co(II)-salen / methyl acrylate (β-carbon) transition state – singlet

Co	1.065073	0.286056	-0.001586
O	0.630973	2.086628	0.354717
O	2.897502	0.751608	0.350489
N	-0.637174	-0.166995	-0.563571
N	1.508260	-1.542149	-0.288057
C	-0.486502	2.701888	0.066487
C	-0.533445	4.119661	0.220365
C	-1.674755	4.856812	-0.071508
C	-2.838659	4.217335	-0.536509
C	-2.822295	2.832789	-0.689458
C	-1.680853	2.054279	-0.400832
C	-1.774007	0.594047	-0.543705
C	3.950391	0.013031	0.212756
C	5.241892	0.595259	0.427281
C	6.406557	-0.139745	0.288749
C	6.372748	-1.508382	-0.066880
C	5.140611	-2.107166	-0.274293
C	3.927571	-1.386195	-0.145080
C	2.686177	-2.084528	-0.348398
C	-0.784442	-1.526597	-1.069356
C	0.310960	-2.380075	-0.422571
H	0.374811	4.603000	0.574557
H	-1.662406	5.939154	0.058703
H	-3.733733	4.788888	-0.773019
H	-3.717009	2.316572	-1.040604
H	-2.581713	0.257740	-1.202943
H	5.264064	1.647543	0.700076
H	7.367070	0.346623	0.457667
H	7.293328	-2.077211	-0.172189
H	5.085870	-3.162940	-0.543946
H	2.753748	-3.161368	-0.554779
H	-1.774228	-1.938492	-0.821393
H	-0.676521	-1.545381	-2.169044
H	0.522044	-3.297837	-0.993052
H	-0.015231	-2.667876	0.587238
C	-2.865143	0.052411	1.133826
C	-3.275636	-1.291608	1.140321
C	-4.479932	-1.699694	0.470463
O	-5.277893	-0.993353	-0.148300
O	-4.693124	-3.070600	0.585840
C	-5.876444	-3.526704	-0.048157
H	-2.091476	0.360127	1.835380
H	-3.637805	0.796215	0.946366
H	-2.660737	-2.070010	1.586269
H	-5.917306	-4.607352	0.124835
H	-5.863778	-3.320817	-1.126393
H	-6.770893	-3.047114	0.370150

inner sphere Co(II)-salen / methyl acrylate (β-carbon) transition state – triplet

Co	1.003342	0.304855	-0.069765
O	0.582308	2.093294	0.290117
O	2.852401	0.729258	0.232333
N	-0.730158	-0.124834	-0.659342
N	1.377364	-1.550860	-0.269482
C	-0.540423	2.723867	0.031270

C	-0.564363	4.138260	0.194232
C	-1.708646	4.889278	-0.052605
C	-2.893873	4.261456	-0.475438
C	-2.898158	2.877548	-0.635902
C	-1.753252	2.086635	-0.396941
C	-1.859758	0.628595	-0.533331
C	3.876283	-0.056765	0.160345
C	5.188774	0.492110	0.335572
C	6.323439	-0.296309	0.268896
C	6.237793	-1.687680	0.023265
C	4.985932	-2.252618	-0.151851
C	3.800128	-1.477331	-0.090956
C	2.537443	-2.136088	-0.282765
C	-0.879098	-1.488741	-1.141847
C	0.152610	-2.350180	-0.406707
H	0.360727	4.609936	0.519332
H	-1.681119	5.970692	0.081335
H	-3.792045	4.842402	-0.674920
H	-3.810489	2.371983	-0.954701
H	-2.726866	0.286949	-1.107339
H	5.250301	1.561129	0.524125
H	7.301295	0.163737	0.409148
H	7.136179	-2.297991	-0.026194
H	4.892029	-3.322600	-0.342680
H	2.567932	-3.221711	-0.446251
H	-1.889322	-1.879426	-0.956438
H	-0.686932	-1.540233	-2.230902
H	0.351509	-3.304592	-0.918739
H	-0.224821	-2.566090	0.603258
C	-2.857959	0.112382	1.241254
C	-3.221099	-1.246043	1.288111
C	-4.428207	-1.711308	0.668889
O	-5.277513	-1.049003	0.066805
O	-4.583089	-3.090916	0.810953
C	-5.767111	-3.601272	0.223826
H	-2.062707	0.458431	1.900196
H	-3.659600	0.830374	1.074471
H	-2.560373	-1.993841	1.721158
H	-5.758473	-4.681047	0.408472
H	-5.801489	-3.407634	-0.856474
H	-6.666545	-3.154559	0.667810

inner sphere Co(II)-salen / methyl acrylate (β-carbon) intermediate – singlet

Co	1.048323	0.229497	0.129689
O	0.573858	1.997858	0.581746
O	2.874609	0.719972	0.499507
N	-0.641509	-0.235741	-0.437658
N	1.542560	-1.558495	-0.292685
C	-0.491648	2.637220	0.165028
C	-0.488965	4.062734	0.231590
C	-1.571894	4.824068	-0.193434
C	-2.719926	4.202208	-0.711659
C	-2.747720	2.807245	-0.776146
C	-1.670856	2.011704	-0.350665
C	-1.840600	0.512088	-0.381128
C	3.946618	0.029659	0.284532
C	5.223970	0.631876	0.527786
C	6.407527	-0.050783	0.306098
C	6.408319	-1.383642	-0.167149
C	5.190790	-2.001671	-0.403960
C	3.959393	-1.334086	-0.191040
C	2.735195	-2.053380	-0.425723
C	-0.793977	-1.572188	-0.969777
C	0.372410	-2.428032	-0.459227

H	0.408930	4.532028	0.628814
H	-1.522260	5.911407	-0.127852
H	-3.568609	4.789302	-1.056631
H	-3.635896	2.303084	-1.161081
H	-2.522658	0.242705	-1.204837
H	5.219514	1.657209	0.889617
H	7.355995	0.449744	0.500121
H	7.343483	-1.911425	-0.337834
H	5.162779	-3.031890	-0.762269
H	2.831703	-3.106587	-0.723211
H	-1.751956	-2.020386	-0.637174
H	-0.817537	-1.566782	-2.076987
H	0.593724	-3.279571	-1.121348
H	0.110790	-2.825987	0.532279
C	-2.758019	0.091036	0.970639
C	-3.247192	-1.283579	1.011277
C	-4.445469	-1.652572	0.320220
O	-5.175735	-0.921518	-0.353461
O	-4.743137	-3.001616	0.476808
C	-5.926024	-3.414327	-0.188522
H	-2.109510	0.341696	1.815657
H	-3.593980	0.795634	0.910297
H	-2.697548	-2.066700	1.527596
H	-6.039415	-4.481611	0.028018
H	-5.855883	-3.257863	-1.272714
H	-6.805167	-2.863843	0.170453

inner sphere Co(II)-salen / methyl acrylate (β-carbon) intermediate – triplet

Co	1.013056	0.226802	0.069372
O	0.558225	2.002470	0.511023
O	2.832503	0.667534	0.507190
N	-0.701893	-0.217802	-0.485614
N	1.475541	-1.561278	-0.377789
C	-0.506984	2.653700	0.114566
C	-0.480067	4.079903	0.172879
C	-1.559073	4.856308	-0.232908
C	-2.728113	4.249609	-0.722362
C	-2.779526	2.855121	-0.777754
C	-1.707028	2.043179	-0.372294
C	-1.897378	0.544283	-0.390836
C	3.895737	-0.042447	0.311829
C	5.177276	0.525037	0.609857
C	6.351958	-0.180412	0.413938
C	6.337978	-1.503567	-0.085820
C	5.115448	-2.088229	-0.375466
C	3.892784	-1.396133	-0.191433
C	2.660924	-2.082495	-0.477926
C	-0.841780	-1.515381	-1.107307
C	0.292853	-2.405919	-0.587201
H	0.433746	4.536366	0.548143
H	-1.490704	5.943065	-0.175346
H	-3.574267	4.848410	-1.053329
H	-3.683560	2.364554	-1.142783
H	-2.597383	0.289928	-1.205140
H	5.183724	1.542780	0.992573
H	7.304492	0.293692	0.649851
H	7.266039	-2.050064	-0.235320
H	5.076090	-3.110727	-0.754268
H	2.742905	-3.134229	-0.784506
H	-1.811458	-1.985597	-0.855462
H	-0.800428	-1.454468	-2.214577
H	0.516017	-3.249199	-1.259584
H	-0.000408	-2.814487	0.391247
C	-2.767774	0.146650	0.973900
C	-3.208795	-1.247335	1.041692
C	-4.464492	-1.657314	0.481170
O	-5.301101	-0.945415	-0.076668
O	-4.677867	-3.020224	0.633418
C	-5.912795	-3.476317	0.102832
H	-2.098932	0.414070	1.798684
H	-3.631553	0.819821	0.951150
H	-2.569886	-2.019731	1.462778
H	-5.951069	-4.551395	0.305148
H	-5.978458	-3.295652	-0.977689
H	-6.765420	-2.974167	0.577446

Cu(II)-salen

Cu	0.000002	0.086871	-0.000014
O	-1.389265	-1.243185	-0.039347
O	1.389270	-1.243188	0.039286
N	-1.298026	1.564431	0.221843
N	1.298033	1.564438	-0.221799
C	-2.671406	-1.057620	-0.039591
C	-3.524001	-2.202209	-0.150355
C	-4.900271	-2.083282	-0.162052
C	-5.533701	-0.819346	-0.061689
C	-4.745780	0.307559	0.050983
C	-3.323967	0.229361	0.066432
C	-2.594335	1.452220	0.200375
C	2.671411	-1.057623	0.039554
C	3.524005	-2.202215	0.150283
C	4.900275	-2.083288	0.162005
C	5.533705	-0.819348	0.061701
C	4.745785	0.307561	-0.050938
C	3.323972	0.229362	-0.066409
C	2.594342	1.452226	-0.200314
C	-0.649648	2.860045	0.412595
C	0.649657	2.860059	-0.412502
H	-3.037048	-3.170578	-0.227386
H	-5.510262	-2.980762	-0.249817
H	-6.617170	-0.742697	-0.071591
H	-5.207786	1.291375	0.133128
H	-3.194484	2.368014	0.297012
H	3.037052	-3.170588	0.227267
H	5.510265	-2.980771	0.249740
H	6.617175	-0.742698	0.071623
H	5.207792	1.291381	-0.133036
H	3.194492	2.368025	-0.296904
H	-1.302265	3.695040	0.119060
H	-0.398323	2.979169	1.477079
H	1.302275	3.695042	-0.118937
H	0.398332	2.979222	-1.476982

reduced Cu(II)-salen

Cu	0.000003	-0.338233	0.000000
O	-1.705566	-1.500713	-0.031269
O	1.705571	-1.500714	0.031229
N	-1.266984	1.313704	0.525752
N	1.266990	1.313722	-0.525694
C	-2.932516	-1.146933	-0.045801
C	-3.955004	-2.139087	-0.290723
C	-5.303326	-1.837951	-0.301791
C	-5.760043	-0.513462	-0.096277
C	-4.814281	0.476536	0.119662
C	-3.422121	0.212508	0.164505
C	-2.549235	1.348923	0.348805
C	2.932521	-1.146935	0.045773
C	3.955009	-2.139098	0.290661
C	5.303332	-1.837963	0.301739
C	5.760049	-0.513467	0.096271
C	4.814287	0.476539	-0.119633
C	3.422127	0.212513	-0.164486
C	2.549241	1.348935	-0.348745
C	-0.537062	2.567622	0.558129
C	0.537068	2.567642	-0.558027
H	-3.603778	-3.156052	-0.454728
H	-6.027974	-2.634623	-0.476538
H	-6.822178	-0.279348	-0.114302
H	-5.139360	1.508811	0.268805
H	-3.053862	2.334825	0.305989

H	3.603783	-3.156069	0.454630
H	6.027979	-2.634642	0.476458
H	6.822184	-0.279354	0.114304
H	5.139366	1.508819	-0.268740
H	3.053868	2.334835	-0.305895
H	-1.195435	3.450207	0.436863
H	-0.022229	2.655114	1.527400
H	1.195441	3.450222	-0.436731
H	0.022235	2.655167	-1.527295

inner sphere Cu(II)-salen / acrylonitrile (α-carbon) transition state

Cu	0.446490	0.167859	-0.263649
O	-0.670582	1.668716	0.097830
O	2.112933	1.185175	0.139058
N	-0.955265	-0.902131	-1.079450
N	1.518976	-1.534831	-0.315962
C	-1.947252	1.754445	-0.206395
C	-2.559852	3.038174	-0.123745
C	-3.907424	3.237109	-0.407049
C	-4.717934	2.159485	-0.793729
C	-4.140606	0.891141	-0.884880
C	-2.782113	0.656318	-0.605002
C	-2.272462	-0.744043	-0.704409
C	3.329180	0.771179	0.170991
C	4.384205	1.720857	0.405118
C	5.713581	1.347049	0.450906
C	6.106853	-0.001329	0.267902
C	5.122591	-0.947226	0.041742
C	3.746136	-0.606810	-0.011455
C	2.804087	-1.669050	-0.243575
C	-0.506643	-2.229279	-1.460544
C	0.646610	-2.684485	-0.536011
H	-1.919750	3.865458	0.176536
H	-4.329561	4.239531	-0.329230
H	-5.772626	2.302500	-1.018926
H	-4.759370	0.041632	-1.171944
H	-2.973939	-1.389659	-1.255674
H	4.081303	2.755739	0.545398
H	6.474284	2.106374	0.632196
H	7.155791	-0.284403	0.306032
H	5.396487	-1.994003	-0.100286
H	3.233408	-2.677071	-0.363456
H	-1.315987	-2.978263	-1.423160
H	-0.124904	-2.222214	-2.497746
H	1.200757	-3.542584	-0.954139
H	0.228933	-2.985821	0.436893
C	-2.070547	-0.826026	2.132209
C	-2.593843	-1.578923	1.015178
C	-4.018219	-1.844044	1.033807
N	-5.165741	-2.058325	0.970237
H	-0.998844	-0.828536	2.314977
H	-2.645861	-0.003460	2.547129
H	-2.054479	-2.512130	0.816577

inner sphere Cu(II)-salen / acrylonitrile (α-carbon) intermediate

Cu	0.510863	-0.007842	0.223224
O	-0.643860	1.436569	0.723421
O	2.150310	1.055583	0.607046
N	-0.912975	-1.188663	-0.275839
N	1.685361	-1.586389	-0.241551
C	-1.796943	1.644806	0.122651
C	-2.270869	2.986571	0.041746
C	-3.475026	3.315502	-0.573753
C	-4.268553	2.315926	-1.153343

C	-3.825942	0.991441	-1.082326
C	-2.625266	0.624498	-0.451532
C	-2.288528	-0.856332	-0.374580
C	3.375855	0.783145	0.330069
C	4.381958	1.787097	0.551452
C	5.717155	1.565274	0.271605
C	6.165353	0.326138	-0.246661
C	5.229571	-0.669987	-0.466921
C	3.850378	-0.483487	-0.194843
C	2.964597	-1.594638	-0.428260
C	-0.496324	-2.377348	-0.977588
C	0.883848	-2.790867	-0.435596
H	-1.637627	3.753000	0.484510
H	-3.791906	4.358268	-0.611675
H	-5.206473	2.558342	-1.648633
H	-4.439369	0.203157	-1.518993
H	-2.760009	-1.348641	-1.246574
H	4.036894	2.739115	0.947884
H	6.438825	2.361619	0.454092
H	7.218077	0.162032	-0.463098
H	5.547061	-1.637429	-0.859851
H	3.439460	-2.524814	-0.781746
H	-1.188401	-3.230940	-0.825631
H	-0.423812	-2.240787	-2.080562
H	1.390894	-3.515322	-1.094828
H	0.741965	-3.259226	0.550483
C	-2.881561	-0.847475	2.198734
C	-3.097417	-1.563779	0.917850
C	-4.520386	-1.753525	0.610484
N	-5.636031	-1.921877	0.314775
H	-1.866905	-0.807168	2.583982
H	-3.573168	-0.066417	2.500759
H	-2.642463	-2.565157	0.950622

inner sphere Cu(II)-salen / acrylonitrile (β-carbon) transition state

Cu	0.664654	0.128371	0.180505
O	-0.323733	1.717768	0.555446
O	2.409299	1.044326	0.431786
N	-0.917745	-0.937403	-0.195149
N	1.634405	-1.614314	-0.092512
C	-1.534620	1.972431	0.115099
C	-1.961678	3.333161	0.107257
C	-3.223351	3.715084	-0.333505
C	-4.127455	2.751359	-0.812291
C	-3.733601	1.414971	-0.824053
C	-2.468465	0.988751	-0.364106
C	-2.179097	-0.460557	-0.412310
C	3.594836	0.595816	0.213912
C	4.711593	1.495304	0.323714
C	6.011111	1.084162	0.097197
C	6.310367	-0.255952	-0.250443
C	5.265056	-1.155866	-0.357488
C	3.915997	-0.774747	-0.136405
C	2.907448	-1.794739	-0.241935
C	-0.613019	-2.236882	-0.766068
C	0.700529	-2.736019	-0.144151
H	-1.244993	4.067925	0.468578
H	-3.504367	4.768130	-0.313873
H	-5.112459	3.039011	-1.174112
H	-4.422259	0.654398	-1.191553
H	-2.766212	-0.985397	-1.178680
H	4.480697	2.523924	0.590097
H	6.821950	1.806694	0.188852
H	7.336751	-0.568518	-0.425189

H	5.466933	-2.196264	-0.617411
H	3.271396	-2.812706	-0.455613
H	-1.413174	-2.969624	-0.563382
H	-0.498074	-2.190539	-1.867407
H	1.118942	-3.591291	-0.698570
H	0.499233	-3.059665	0.888175
C	-3.282062	-1.232865	1.154283
C	-4.678459	-1.236242	0.957449
C	-5.360958	-2.297556	0.330735
H	-2.777089	-2.198329	1.151491
H	-2.877661	-0.520903	1.871201
H	-5.260592	-0.340403	1.162511
N	-5.943111	-3.189441	-0.171399

inner sphere Cu(II)-salen / acrylonitrile (β-carbon) intermediate

Cu	0.514644	0.194326	-0.069825
O	-0.544861	1.666613	0.570688
O	2.239420	1.077680	0.378809
N	-0.951502	-0.694990	-0.962442
N	1.488777	-1.551254	-0.318701
C	-1.739087	1.960962	0.099001
C	-2.186614	3.309857	0.174572
C	-3.448259	3.696455	-0.273442
C	-4.325327	2.753760	-0.826808
C	-3.903664	1.420926	-0.911906
C	-2.643227	1.002083	-0.465421
C	-2.285034	-0.470623	-0.520466
C	3.433340	0.604107	0.308676
C	4.544557	1.473611	0.587339
C	5.854297	1.036055	0.529962
C	6.169351	-0.302349	0.192257
C	5.128250	-1.173028	-0.079918
C	3.770491	-0.765588	-0.031835
C	2.765337	-1.756170	-0.318991
C	-0.619267	-2.026284	-1.432539
C	0.538599	-2.624184	-0.594838
H	-1.496612	4.033601	0.604197
H	-3.747992	4.741887	-0.194895
H	-5.309892	3.046163	-1.186277
H	-4.575339	0.672623	-1.335600
H	-3.007948	-0.987339	-1.175271
H	4.301560	2.501394	0.846412
H	6.659961	1.736544	0.749840
H	7.202970	-0.636592	0.149965
H	5.341399	-2.211194	-0.340189
H	3.135805	-2.768491	-0.549159
H	-1.478256	-2.718022	-1.393574
H	-0.285839	-1.994208	-2.487551
H	1.023339	-3.478391	-1.098996
H	0.136643	-2.975235	0.367940
C	-2.551375	-1.130852	0.972429
C	-3.967704	-1.119492	1.385339
C	-4.814628	-2.216107	1.218405
H	-2.159737	-2.154308	0.936453
H	-1.930593	-0.524075	1.642526
H	-4.429538	-0.179631	1.680246
N	-5.522443	-3.153636	1.101588

inner sphere Cu(II)-salen / methyl acrylate (α-carbon) transition state

Cu	0.872027	0.253825	-0.232142
O	-0.186909	1.774751	0.232731
O	2.584822	1.161665	0.265739
N	-0.550790	-0.674648	-1.189550
N	1.866913	-1.490824	-0.382724

C	-1.449454	1.933299	-0.092572
C	-2.014330	3.234499	0.040975
C	-3.341679	3.504782	-0.277942
C	-4.179371	2.485318	-0.753455
C	-3.648544	1.199774	-0.887175
C	-2.315180	0.891274	-0.568143
C	-1.850892	-0.521769	-0.733892
C	3.777908	0.687081	0.286256
C	4.875309	1.565871	0.594862
C	6.183907	1.124247	0.633652
C	6.513682	-0.227510	0.368805
C	5.487567	-1.106542	0.068593
C	4.130635	-0.695814	0.019752
C	3.142162	-1.692290	-0.299551
C	-0.147181	-1.995198	-1.638528
C	0.945132	-2.575626	-0.707163
H	-1.353301	4.018763	0.404824
H	-3.725672	4.518651	-0.160757
H	-5.216739	2.686012	-1.013858
H	-4.284058	0.395158	-1.260552
H	-2.587158	-1.114095	-1.298259
H	4.621061	2.603478	0.798108
H	6.978005	1.831525	0.873468
H	7.546801	-0.564551	0.401885
H	5.712109	-2.154264	-0.138967
H	3.525052	-2.709463	-0.484131
H	-0.992455	-2.703125	-1.688162
H	0.280503	-1.934164	-2.655520
H	1.470530	-3.433161	-1.163142
H	0.476287	-2.916737	0.227903
C	-1.249937	-0.971383	1.973846
C	-2.108835	-1.440489	0.913538
C	-3.565247	-1.329270	1.189170
O	-4.116785	-0.636725	2.024429
O	-4.294158	-2.100427	0.307712
C	-5.705415	-1.959301	0.440734
H	-0.193871	-1.228890	1.984495
H	-1.582375	-0.161584	2.615525
H	-1.865834	-2.434429	0.524371
H	-6.146706	-2.610090	-0.320105
H	-6.013423	-0.919839	0.278108
H	-6.042414	-2.262065	1.439508

inner sphere Cu(II)-salen / methyl acrylate (α-carbon) intermediate

Cu	0.903839	0.261188	-0.247979
O	-0.138471	1.794112	0.249816
O	2.636865	1.127138	0.262455
N	-0.519630	-0.628283	-1.216912
N	1.857414	-1.515525	-0.352916
C	-1.354201	2.028464	-0.190532
C	-1.839948	3.366973	-0.144165
C	-3.116407	3.709689	-0.582262
C	-3.975384	2.730235	-1.099354
C	-3.518692	1.408655	-1.151565
C	-2.243800	1.028147	-0.705928
C	-1.854748	-0.433553	-0.776993
C	3.817080	0.622191	0.299329
C	4.934673	1.476535	0.604705
C	6.231420	1.002368	0.661147
C	6.528389	-0.360888	0.418908
C	5.481846	-1.217461	0.122564
C	4.136745	-0.773222	0.055817
C	3.125281	-1.749933	-0.256984
C	-0.154264	-1.970921	-1.628281

C	0.905577	-2.575001	-0.671807
H	-1.161101	4.120269	0.251263
H	-3.441324	4.749311	-0.527596
H	-4.971202	2.986851	-1.455746
H	-4.172269	0.634609	-1.558218
H	-2.566533	-0.946154	-1.447425
H	4.705737	2.523325	0.790514
H	7.041400	1.692758	0.897338
H	7.552131	-0.724087	0.465567
H	5.680952	-2.273606	-0.067988
H	3.483656	-2.779529	-0.422713
H	-1.020692	-2.654521	-1.675801
H	0.290198	-1.956483	-2.641430
H	1.409490	-3.458592	-1.102970
H	0.412854	-2.882556	0.263350
C	-1.404604	-0.767075	1.847275
C	-2.203477	-1.221712	0.697375
C	-3.684401	-1.103861	0.954709
O	-4.237497	-0.443490	1.810986
O	-4.398901	-1.834206	0.039187
C	-5.813207	-1.676588	0.138449
H	-0.353071	-1.030436	1.918931
H	-1.773018	0.043385	2.467318
H	-1.989968	-2.267104	0.431874
H	-6.241356	-2.304281	-0.648109
H	-6.098953	-0.629134	-0.011181
H	-6.178629	-1.995802	1.121478

inner sphere Cu(II)-salen / methyl acrylate (β-carbon) transition state

Cu	1.102032	0.329633	0.226995
O	0.566439	2.130700	0.567257
O	3.038260	0.778547	0.335329
N	-0.719520	-0.315063	-0.017355
N	1.581223	-1.615214	0.019428
C	-0.566698	2.665187	0.176279
C	-0.645517	4.089593	0.139960
C	-1.791972	4.762576	-0.264023
C	-2.927282	4.042878	-0.676546
C	-2.877480	2.651597	-0.655664
C	-1.737005	1.933949	-0.230014
C	-1.820656	0.456205	-0.253637
C	4.054254	0.030891	0.085095
C	5.367403	0.617672	0.076092
C	6.502543	-0.124300	-0.189350
C	6.428668	-1.512142	-0.461962
C	5.184188	-2.117172	-0.455423
C	3.993740	-1.392073	-0.190815
C	2.754139	-2.122977	-0.181598
C	-0.785420	-1.673676	-0.518570
C	0.389824	-2.459685	0.079370
H	0.246448	4.631487	0.447937
H	-1.803311	5.852662	-0.267098
H	-3.826350	4.557646	-1.008922
H	-3.748303	2.076762	-0.974208
H	-2.519458	0.084147	-1.015996
H	5.422993	1.683368	0.284999
H	7.474098	0.369778	-0.187967
H	7.328245	-2.086662	-0.668086
H	5.097997	-3.186252	-0.656575
H	2.833815	-3.209137	-0.350620
H	-1.738976	-2.147825	-0.227660
H	-0.727686	-1.712790	-1.625085
H	0.545894	-3.422952	-0.431997
H	0.171238	-2.663072	1.138585

C	-3.152441	0.044683	1.258418
C	-3.632457	-1.277740	1.224529
C	-4.733883	-1.636270	0.373912
O	-5.377999	-0.901308	-0.377471
O	-5.044077	-2.989323	0.473954
C	-6.128040	-3.395935	-0.344583
H	-2.475037	0.326313	2.062687
H	-3.855206	0.819842	0.958805
H	-3.142865	-2.075878	1.777252
H	-6.253851	-4.470049	-0.171640
H	-5.925440	-3.209185	-1.407173
H	-7.053411	-2.865137	-0.085445

inner sphere Cu(II)-salen / methyl acrylate (β-carbon) intermediate

Cu	1.098749	0.304062	0.305246
O	0.584870	2.093701	0.705147
O	3.029441	0.736863	0.495329
N	-0.696902	-0.313516	-0.019938
N	1.588748	-1.619647	-0.035593
C	-0.514646	2.658640	0.253854
C	-0.538307	4.084653	0.196481
C	-1.639421	4.795189	-0.266554
C	-2.782106	4.112659	-0.712313
C	-2.782982	2.717876	-0.662541
C	-1.691556	1.968950	-0.184501
C	-1.867389	0.460135	-0.154188
C	4.052393	0.017210	0.194880
C	5.362587	0.606941	0.253332
C	6.504335	-0.106076	-0.060263
C	6.439783	-1.465185	-0.452387
C	5.197497	-2.072422	-0.514328
C	4.001591	-1.376425	-0.203189
C	2.763278	-2.107371	-0.270507
C	-0.783271	-1.633907	-0.581371
C	0.398228	-2.466885	-0.058916
H	0.360058	4.596805	0.535485
H	-1.606397	5.884785	-0.289383
H	-3.647141	4.652577	-1.092044
H	-3.664055	2.170494	-1.002031
H	-2.458943	0.167500	-1.040707
H	5.411016	1.650989	0.553452
H	7.473686	0.389192	-0.004027
H	7.344274	-2.016939	-0.696041
H	5.118203	-3.120389	-0.808128
H	2.845801	-3.174371	-0.533890
H	-1.736084	-2.121788	-0.282203
H	-0.778662	-1.631777	-1.692823
H	0.559969	-3.379543	-0.655009
H	0.180591	-2.766890	0.977342
C	-2.943804	0.107844	1.098654
C	-3.487891	-1.246603	1.090064
C	-4.598169	-1.576263	0.248568
O	-5.204452	-0.823206	-0.518072
O	-4.968704	-2.910691	0.370330
C	-6.066001	-3.283309	-0.447679
H	-2.379226	0.339834	2.006499
H	-3.740921	0.843006	0.947613
H	-3.042289	-2.044297	1.678705
H	-6.248754	-4.343894	-0.245905
H	-5.844059	-3.137896	-1.512782
H	-6.963862	-2.697315	-0.212371