Principal Components of Mn(salen) Catalysts

Supporting Information

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Equilibrium geometries at the X3LYP/DefBas-3 level of theory.

Equilibrium geometry of **1-ox-amine-S2**.

Mn	0.021349	0.235562	-0.116089
N	-1.208828	-1.119523	0.119262
N	1.235182	-1.091283	-0.014966
O	-0.114448	0.321858	-1.641671
O	1.212320	1.492630	0.122975
O	-1.200831	1.493286	0.232252
N	0.169194	0.217227	2.029556

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C	-0.663379	-2.492402	0.224238
C	0.719348	-2.422547	-0.381155
C	2.528619	1.432815	0.308052
C	-2.529157	-0.981771	0.113356
C	2.566245	-0.977361	0.200027
C	-2.505187	1.422815	0.160252
C	3.209414	0.247274	0.371184
C	-3.195189	0.245843	0.069542
H	-0.611261	-2.793220	1.274572
H	0.673224	-2.491485	-1.471167
H	-1.309105	-3.194520	-0.300382
H	1.370622	-3.209927	-0.005161
H	2.994446	2.401066	0.427046
H	-3.115118	-1.892899	0.167224
H	-3.001220	2.383741	0.233506
H	3.135078	-1.897252	0.235053
H	4.275755	0.262090	0.543530
H	-4.273977	0.261127	0.034563
H	-0.372273	-0.561063	2.401653
H	1.140250	-0.024769	2.227788
C	-0.154423	1.436856	2.843635
C	0.330994	1.306092	4.276279
H	0.302369	2.286173	2.342657
H	-1.231993	1.577403	2.807171
H	0.073782	2.206113	4.835350
H	-0.129039	0.458946	4.789104
H	1.416290	1.190456	4.327372

Equilibrium geometry of **2-ox-amine-S2**.

Mn	0.016394	0.228007	-0.094704
N	-1.267154	-1.088994	0.162259
N	1.190711	-1.131281	0.029911
O	-0.127928	0.281954	-1.622046
O	1.233206	1.459436	0.121541
O	-1.168215	1.539201	0.221800
N	0.151819	0.239739	2.042777
C	-0.733981	-2.471807	0.339716
C	0.608717	-2.437173	-0.373085
C	2.543075	1.371115	0.348327
C	-2.574700	-0.894725	0.113687
C	2.517563	-1.043740	0.285629
C	-2.468932	1.510638	0.106030
C	3.185110	0.168419	0.459737
C	-3.193833	0.357026	0.011708

H	-0.535828	-2.613187	1.410619
H	0.419019	-2.359533	-1.450665
C	-1.593604	-3.633736	-0.140804
H	3.031021	2.329607	0.455726
H	-3.207364	-1.769585	0.178637
H	-2.936038	2.488267	0.146644
H	3.070409	-1.967313	0.355661
H	4.245753	0.156963	0.665331
H	-4.269826	0.407319	-0.059288
H	-0.410591	-0.520098	2.421410
H	1.115770	-0.024861	2.248110
C	-0.144097	1.476893	2.839233
C	0.326869	1.348346	4.277139
H	0.339984	2.307326	2.332307
H	-1.216938	1.647070	2.792237
H	0.093018	2.261793	4.824570
H	-0.161960	0.520959	4.795822
H	1.407726	1.200310	4.337228
C	-0.817056	-4.944366	0.062768
H	-2.533268	-3.694101	0.411185
H	-1.843158	-3.497063	-1.196952
H	-1.399382	-5.771019	-0.346346
C	0.569219	-4.911499	-0.579493
H	-0.719966	-5.141256	1.135633
H	1.106969	-5.833187	-0.352795
H	0.468128	-4.875499	-1.668595
C	1.403204	-3.708616	-0.113805
H	2.348281	-3.695057	-0.658873
H	1.640299	-3.804845	0.950772

Equilibrium geometry of **3-ox-amine-S2**.

Mn	-0.015249	0.269301	-0.110340
N	-1.215944	-1.120313	0.153775
N	1.226254	-1.041529	-0.013991
O	-0.172618	0.326755	-1.632754
O	1.151008	1.524059	0.126513
O	-1.241288	1.470972	0.280532
N	0.152967	0.235267	2.067836
C	-0.637069	-2.476958	0.271649
C	0.730483	-2.384065	-0.360083
C	2.498006	1.533133	0.257465
C	-2.532720	-1.019797	0.151333
C	2.556962	-0.914502	0.172494
C	-2.573070	1.427252	0.149885

C	3.221433	0.319445	0.309476
C	-3.253407	0.189842	0.073312
H	-0.557824	-2.756339	1.326194
H	0.665251	-2.464834	-1.448576
H	-1.275969	-3.203589	-0.227758
H	1.403695	-3.155792	0.010376
H	-3.095525	-1.945547	0.219578
H	3.135616	-1.829439	0.199905
C	4.626359	0.389706	0.483402
C	-4.666051	0.188760	-0.016468
H	-0.417845	-0.520365	2.442442
H	1.115097	-0.040993	2.260837
C	-0.130428	1.470513	2.865881
C	0.324656	1.334171	4.308730
H	0.371845	2.294284	2.365825
H	-1.199366	1.659102	2.806191
H	0.099015	2.250513	4.855142
H	-0.181386	0.513564	4.821913
H	1.402602	1.169995	4.379519
C	-5.362572	1.372002	-0.043392
H	-5.189274	-0.758330	-0.073382
H	-6.440731	1.369102	-0.127403
C	-4.668126	2.588920	0.040766
C	-3.289301	2.621311	0.150646
H	-5.219081	3.520342	0.016787
H	-2.747990	3.555498	0.213741
C	5.262145	1.604598	0.587895
H	5.196148	-0.531204	0.520061
H	6.336193	1.644918	0.710981
C	4.519898	2.792744	0.530544
C	3.143128	2.757341	0.372245
H	5.023518	3.747571	0.604490
H	2.556691	3.664969	0.318635

Equilibrium geometry of **4-ox-amine-S2**.

Mn	-0.060536	0.262022	-0.073386
N	-1.299329	-1.108786	0.216283
N	1.156202	-1.068974	0.003511
O	-0.264060	0.306247	-1.592475
O	1.121890	1.503420	0.126731
O	-1.263784	1.496662	0.324850
N	0.133276	0.237242	2.083630
C	-0.712257	-2.469152	0.383849
C	0.600249	-2.391248	-0.378953

C	2.468686	1.495257	0.269864
C	-2.604938	-0.966321	0.171365
C	2.489584	-0.956304	0.204402
C	-2.587735	1.484028	0.146545
C	3.168833	0.270722	0.342160
C	-3.291529	0.263271	0.047709
H	-0.468107	-2.590128	1.447494
H	0.367579	-2.322233	-1.449098
C	-1.550416	-3.664017	-0.050166
H	-3.206894	-1.863357	0.241146
H	3.064633	-1.868363	0.245870
C	4.572856	0.322630	0.531310
C	-4.699033	0.290810	-0.091161
H	-0.447057	-0.505483	2.469078
H	1.092151	-0.059459	2.264123
C	-0.113466	1.479126	2.883994
C	0.350364	1.328865	4.322612
H	0.404881	2.290430	2.380254
H	-1.177686	1.693800	2.832305
H	0.151591	2.249259	4.872687
H	-0.171284	0.519802	4.838785
H	1.424482	1.138374	4.383962
C	-0.723282	-4.946123	0.131470
H	-2.464022	-3.749470	0.541135
H	-1.847268	-3.548143	-1.096691
H	-1.294754	-5.796467	-0.243017
C	0.630718	-4.871509	-0.572205
H	-0.571192	-5.127120	1.200788
H	1.209138	-5.773084	-0.364726
H	0.480244	-4.846070	-1.655957
C	1.442321	-3.638757	-0.149155
H	2.362552	-3.598586	-0.733649
H	1.727565	-3.721358	0.904803
C	-5.370137	1.488046	-0.145475
H	-5.240247	-0.645319	-0.162608
H	-6.444499	1.507719	-0.267301
C	-4.653054	2.689819	-0.038028
C	-3.279136	2.693770	0.120634
H	-5.183073	3.632701	-0.081857
H	-2.720896	3.616462	0.202715
C	5.227283	1.528571	0.628883
H	5.128197	-0.606401	0.584767
H	6.300542	1.552114	0.763840
C	4.506243	2.728295	0.548676
C	3.130709	2.711144	0.375382

H	5.024154	3.675863	0.616705
H	2.558279	3.626610	0.304551

Equilibrium geometry of **5-ox-amine-S2**.

Mn	-0.022060	0.255154	-0.109150
N	-1.216586	-1.125931	0.202411
N	1.223768	-1.050630	0.019081
O	-0.180399	0.268810	-1.632876
O	1.143912	1.517621	0.091031
O	-1.243109	1.465040	0.256148
N	0.162366	0.277870	2.075795
C	-0.636971	-2.480188	0.342535
C	0.727481	-2.399902	-0.297396
C	2.489417	1.526846	0.232507
C	-2.535618	-1.027505	0.225527
C	2.553650	-0.917740	0.202809
C	-2.578480	1.413451	0.160405
C	3.215585	0.319510	0.315367
C	-3.259617	0.177894	0.134510
H	-0.552816	-2.740839	1.401647
H	0.656386	-2.501307	-1.383764
H	-1.278280	-3.215620	-0.140923
H	1.403107	-3.164045	0.084254
H	-3.093424	-1.952984	0.328210
H	3.133120	-1.831437	0.250975
C	4.620942	0.394346	0.493123
C	-4.675317	0.173670	0.079249
H	-0.399463	-0.473356	2.471844
H	1.128277	0.015053	2.268556
C	-0.126880	1.530225	2.842389
C	0.340442	1.437798	4.284904
H	0.363007	2.345324	2.316406
H	-1.198239	1.706924	2.786537
H	0.107484	2.364993	4.809453
H	-0.151381	0.624275	4.822719
H	1.420849	1.288355	4.351246
C	-5.398995	1.344045	0.037257
H	-5.189191	-0.780892	0.060404
C	-6.900167	1.351217	-0.048867
C	-4.681718	2.559807	0.075345
C	-3.303081	2.602498	0.149472
H	-5.231745	3.493095	0.042764
H	-2.768496	3.542480	0.175496
C	5.280769	1.601606	0.577139

H	5.182455	-0.531568	0.549906
C	6.773061	1.678985	0.749474
C	4.514598	2.782884	0.490654
C	3.141154	2.749890	0.326836
H	5.014346	3.742474	0.547225
H	2.561145	3.660343	0.252145
H	-7.341906	1.902143	0.783980
H	-7.238431	1.831790	-0.969320
H	-7.306291	0.340823	-0.033718
H	7.038270	2.211762	1.665242
H	7.223021	0.688200	0.798162
H	7.237042	2.215553	-0.080816

Equilibrium geometry of **6-ox-amine-S2**.

Mn	-0.072657	0.257239	-0.074972
N	-1.295907	-1.116295	0.253771
N	1.155746	-1.064616	0.008190
O	-0.290620	0.275042	-1.592987
O	1.104338	1.509300	0.093620
O	-1.274210	1.490160	0.321029
N	0.155003	0.263363	2.084810
C	-0.698813	-2.471508	0.425203
C	0.604015	-2.393527	-0.353942
C	2.450886	1.507148	0.237787
C	-2.605000	-0.982652	0.241943
C	2.489254	-0.940855	0.198113
C	-2.603609	1.462266	0.182008
C	3.160490	0.291654	0.320987
C	-3.302600	0.239706	0.122038
H	-0.441574	-2.584389	1.486847
H	0.357687	-2.336400	-1.421706
C	-1.534446	-3.674812	0.008643
H	-3.197684	-1.883240	0.338526
H	3.070796	-1.848677	0.244638
C	4.566006	0.353174	0.503954
C	-4.714962	0.256310	0.022913
H	-0.403290	-0.486466	2.488282
H	1.122958	-0.010344	2.252673
C	-0.104896	1.510356	2.871204
C	0.386409	1.392015	4.303659
H	0.386681	2.325295	2.346871
H	-1.174493	1.701316	2.835471
H	0.175100	2.314980	4.844693
H	-0.106968	0.577939	4.839434

H	1.465633	1.227446	4.348869
C	-0.698119	-4.950872	0.190313
H	-2.441033	-3.761903	0.610258
H	-1.843546	-3.567218	-1.035208
H	-1.268640	-5.807245	-0.171882
C	0.648198	-4.874310	-0.527856
H	-0.533714	-5.123191	1.259290
H	1.233762	-5.771161	-0.319644
H	0.486203	-4.857913	-1.610152
C	1.456594	-3.633491	-0.122889
H	2.370551	-3.591987	-0.717095
H	1.753189	-3.705939	0.928715
C	-5.420664	1.437405	-0.031130
H	-5.242390	-0.690312	-0.018996
C	-6.918121	1.467693	-0.165325
C	-4.686687	2.641220	0.042555
C	-3.311151	2.662755	0.161021
H	-5.221580	3.583085	0.002794
H	-2.763865	3.594246	0.214448
C	5.238857	1.553415	0.590146
H	5.118266	-0.578366	0.562175
C	6.731571	1.612585	0.768158
C	4.487591	2.743686	0.500306
C	3.114114	2.723754	0.331992
H	4.997549	3.697795	0.557880
H	2.542985	3.639721	0.254923
H	-7.378216	2.024801	0.653332
H	-7.219755	1.953480	-1.095800
H	-7.339707	0.463407	-0.164211
H	7.000015	2.136917	1.687958
H	7.169497	0.616144	0.813021
H	7.205353	2.148180	-0.057251

Equilibrium geometry of **7-ox-amine-S2**.

Mn	-0.006385	0.255710	-0.148498
N	-1.190142	-1.136854	0.131491
N	1.248362	-1.043654	-0.018075
O	-0.141083	0.286281	-1.674797
O	1.153812	1.519159	0.075952
O	-1.239393	1.451958	0.218162
N	0.102224	0.241823	2.050493
C	-0.606875	-2.492194	0.248524
C	0.768156	-2.391684	-0.364920
C	2.499508	1.544977	0.217482

C	-2.510799	-1.046174	0.167448
C	2.568151	-0.901870	0.200320
C	-2.579053	1.399931	0.125187
C	3.225369	0.337593	0.322846
C	-3.246033	0.154638	0.099843
H	-0.542164	-2.777542	1.302473
H	0.718444	-2.474373	-1.453940
H	-1.235992	-3.217143	-0.265754
H	1.443347	-3.156676	0.015737
H	-3.061861	-1.976434	0.261001
H	3.153402	-1.811647	0.258009
C	4.625567	0.407931	0.521917
C	-4.660309	0.132040	0.055156
H	-0.702750	-0.289218	2.377916
H	0.916042	-0.314963	2.307793
C	0.149972	1.516715	2.829120
C	0.074418	1.278183	4.327810
H	1.072638	2.024574	2.561115
H	-0.675275	2.133512	2.483151
H	0.112142	2.231189	4.856579
H	-0.856775	0.783384	4.614132
H	0.909620	0.672516	4.686547
C	-5.361435	1.310698	0.020571
H	-5.175295	-0.820766	0.037565
H	-6.441958	1.303185	-0.028351
C	-4.673911	2.532859	0.046346
C	-3.288391	2.607928	0.111765
H	-5.241797	3.454760	0.010629
C	-2.556598	3.918244	0.137916
C	5.250148	1.629050	0.594155
H	5.195059	-0.510262	0.600876
H	6.321002	1.684791	0.738259
C	4.503491	2.808553	0.473067
C	3.124967	2.793511	0.285789
H	5.012269	3.763592	0.517999
C	2.325155	4.055277	0.132250
H	-3.253840	4.751530	0.073938
H	-1.975392	4.033486	1.055183
H	-1.852749	3.992036	-0.692122
H	2.961904	4.931769	0.237932
H	1.845375	4.098226	-0.847455
H	1.527521	4.119839	0.874225

Equilibrium geometry of **8-ox-amine-S2**.

Mn	-0.060776	0.244390	-0.106914
N	-1.296378	-1.123226	0.200536
N	1.157295	-1.081692	0.003154
O	-0.248964	0.263579	-1.629000
O	1.119324	1.490177	0.083504
O	-1.265856	1.483148	0.264135
N	0.126616	0.243991	2.058453
C	-0.710469	-2.484100	0.371692
C	0.609308	-2.406775	-0.377890
C	2.465383	1.490557	0.252843
C	-2.603318	-0.979721	0.183362
C	2.483766	-0.962770	0.236282
C	-2.595648	1.469182	0.112264
C	3.159710	0.266952	0.371945
C	-3.296437	0.245396	0.059416
H	-0.477346	-2.608503	1.437625
H	0.387511	-2.342173	-1.450557
C	-1.543161	-3.678505	-0.075646
H	-3.202412	-1.876602	0.275845
H	3.059425	-1.872859	0.305946
C	4.557827	0.312725	0.596911
C	-4.706616	0.259258	-0.047258
H	-0.427375	-0.517614	2.445390
H	1.095460	-0.018563	2.238938
C	-0.161627	1.477659	2.853416
C	0.297924	1.346850	4.295630
H	0.335891	2.302482	2.350486
H	-1.231842	1.660340	2.795786
H	0.068149	2.262060	4.842291
H	-0.202134	0.523507	4.810441
H	1.376840	1.188358	4.363525
C	-0.717568	-4.960886	0.112279
H	-2.463615	-3.766947	0.504335
H	-1.828041	-3.558201	-1.124910
H	-1.283403	-5.809981	-0.273514
C	0.646794	-4.884503	-0.571530
H	-0.580825	-5.145993	1.182987
H	1.222478	-5.786170	-0.356943
H	0.511965	-4.857654	-1.657329
C	1.451338	-3.651427	-0.135836
H	2.379950	-3.608664	-0.706911
H	1.721374	-3.734125	0.922078
C	-5.374361	1.455676	-0.115824
H	-5.245977	-0.679645	-0.083814
H	-6.451394	1.477810	-0.212772

C	-4.654643	2.658399	-0.058911
C	-3.272859	2.696942	0.068134
H	-5.195219	3.595435	-0.119372
C	-2.506675	3.985950	0.130802
C	5.206363	1.521216	0.677200
H	5.107959	-0.616142	0.688695
H	6.275515	1.553627	0.841056
C	4.488778	2.716662	0.539191
C	3.113633	2.726401	0.326965
H	5.015852	3.661340	0.590845
C	2.341798	4.003160	0.155113
H	-3.175699	4.839106	0.034187
H	-1.967405	4.083291	1.075387
H	-1.761310	4.038707	-0.663770
H	2.996116	4.867033	0.257994
H	1.869854	4.047467	-0.828312
H	1.540356	4.093097	0.890818

Equilibrium geometry of **9-ox-amine-S2**.

Mn	-0.018471	0.243822	-0.136917
N	-1.211111	-1.134971	0.184035
N	1.226947	-1.059056	0.009690
O	-0.169123	0.243889	-1.662451
O	1.147422	1.508243	0.055671
O	-1.241968	1.454874	0.212191
N	0.163719	0.277630	2.050680
C	-0.633098	-2.490420	0.322245
C	0.735506	-2.409172	-0.309080
C	2.493095	1.523553	0.215930
C	-2.529814	-1.034447	0.224916
C	2.551761	-0.922214	0.220534
C	-2.580766	1.405271	0.130702
C	3.212534	0.315933	0.335107
C	-3.257684	0.168297	0.134913
H	-0.555294	-2.755160	1.380958
H	0.671825	-2.510748	-1.395857
H	-1.272645	-3.223421	-0.167289
H	1.409885	-3.172066	0.077185
H	-3.086308	-1.959193	0.340587
H	3.131254	-1.834604	0.288959
C	4.613435	0.381998	0.542041
C	-4.673245	0.152489	0.099649
H	-0.376486	-0.490263	2.444508
H	1.137094	0.040857	2.240102

C	-0.157112	1.517452	2.821258
C	0.303515	1.429533	4.266454
H	0.318928	2.345221	2.302307
H	-1.231994	1.671106	2.760192
H	0.048625	2.349322	4.793926
H	-0.174762	0.603718	4.797578
H	1.386276	1.301289	4.338439
C	-5.393086	1.322847	0.046928
H	-5.184395	-0.803441	0.103708
C	-6.895559	1.333755	-0.016648
C	-4.675127	2.537593	0.049727
C	-3.291712	2.612855	0.103441
H	-5.235202	3.465458	0.003656
C	-2.559812	3.923506	0.104492
C	5.268986	1.590388	0.613869
H	5.169492	-0.544617	0.629101
C	6.756533	1.674782	0.821984
C	4.507138	2.768646	0.478869
C	3.132474	2.765217	0.282737
H	5.017409	3.724513	0.521161
C	2.348102	4.035276	0.116796
H	-7.323182	1.894946	0.816868
H	-7.246865	1.805381	-0.936828
H	-7.303636	0.324534	0.016171
H	6.997066	2.215682	1.739927
H	7.207806	0.685682	0.890402
H	7.239765	2.206083	-0.000602
H	-3.257436	4.756567	0.040891
H	-1.965101	4.047058	1.011858
H	-1.867627	3.987423	-0.736226
H	2.995765	4.905141	0.210714
H	1.864666	4.072917	-0.861235
H	1.554260	4.119499	0.861285

Equilibrium geometry of **10-ox-amine-S2**.

Mn	-0.068667	0.239737	-0.113434
N	-1.289686	-1.128041	0.231631
N	1.160491	-1.078226	0.003747
O	-0.268801	0.232413	-1.634737
O	1.108621	1.494260	0.046416
O	-1.270676	1.477476	0.252548
N	0.148748	0.271803	2.054656
C	-0.695948	-2.485193	0.405609
C	0.615059	-2.408621	-0.359051

C	2.453987	1.498567	0.216915
C	-2.599471	-0.991218	0.249095
C	2.486891	-0.950328	0.227031
C	-2.605198	1.451472	0.141946
C	3.156420	0.283885	0.348046
C	-3.301879	0.227694	0.129750
H	-0.450938	-2.602742	1.469847
H	0.380683	-2.353985	-1.429568
C	-1.527853	-3.686030	-0.026522
H	-3.189961	-1.890355	0.369288
H	3.067428	-1.857062	0.301774
C	4.556089	0.337948	0.567582
C	-4.715910	0.233800	0.064955
H	-0.390715	-0.491689	2.457704
H	1.123286	0.024562	2.225770
C	-0.146081	1.512877	2.833775
C	0.339905	1.414905	4.269843
H	0.328490	2.337387	2.308608
H	-1.220275	1.676991	2.792143
H	0.103119	2.334799	4.805558
H	-0.136248	0.591298	4.806476
H	1.422528	1.276492	4.321326
C	-0.695215	-4.963910	0.160742
H	-2.442334	-3.775319	0.562503
H	-1.823590	-3.572477	-1.073530
H	-1.261404	-5.817884	-0.213759
C	0.662054	-4.886745	-0.537028
H	-0.546688	-5.141543	1.231198
H	1.243411	-5.784841	-0.322473
H	0.516290	-4.867193	-1.621586
C	1.465443	-3.647498	-0.117148
H	2.388225	-3.603872	-0.697612
H	1.746207	-3.722462	0.938576
C	-5.416562	1.415084	-0.002371
H	-5.242456	-0.713949	0.059081
C	-6.917086	1.450138	-0.097555
C	-4.679253	2.618013	0.017946
C	-3.296998	2.671187	0.102117
H	-5.223493	3.554766	-0.038534
C	-2.543253	3.969115	0.123234
C	5.224458	1.539696	0.637053
H	5.102150	-0.593724	0.665138
C	6.710996	1.607502	0.859330
C	4.478281	2.725941	0.486470
C	3.105230	2.734119	0.278649

H	4.998561	3.676527	0.525627
C	2.334314	4.010221	0.096688
H	-7.353477	2.016582	0.727840
H	-7.241782	1.928275	-1.024182
H	-7.341936	0.447426	-0.075239
H	6.948996	2.136939	1.784733
H	7.151801	0.613244	0.922311
H	7.207299	2.141969	0.046617
H	-3.224277	4.814238	0.040325
H	-1.972048	4.082805	1.046943
H	-1.826498	4.020183	-0.697441
H	2.992231	4.874079	0.173991
H	1.845727	4.038324	-0.879050
H	1.545305	4.115113	0.843980

Equilibrium geometry of **11-ox-amine-S2**.

Mn	-0.046156	0.341414	0.081437
N	-1.236282	-1.062156	0.340263
N	1.202419	-0.963729	0.123937
O	-0.243017	0.429986	-1.435337
O	1.114489	1.596694	0.320322
O	-1.273808	1.524168	0.526298
N	0.165965	0.263105	2.255832
C	-0.644831	-2.412564	0.448798
C	0.706796	-2.307969	-0.214343
C	2.469379	1.612024	0.376119
C	-2.552686	-0.969803	0.325563
C	2.541759	-0.830740	0.256899
C	-2.604455	1.473563	0.367488
C	3.204604	0.407098	0.371169
C	-3.278244	0.237653	0.250779
H	-0.538236	-2.688932	1.501853
H	0.615767	-2.388111	-1.301287
H	-1.288707	-3.146530	-0.033326
H	1.393699	-3.076324	0.138199
H	-3.110592	-1.899717	0.377954
H	3.124799	-1.743233	0.250929
C	4.613802	0.485035	0.462812
C	-4.685277	0.227451	0.126899
H	-0.399483	-0.497598	2.628285
H	1.131585	-0.019303	2.419865
C	-0.096579	1.484252	3.080631
C	0.385327	1.321340	4.512062
H	0.399640	2.314461	2.585283

H	-1.165544	1.678321	3.043796
H	0.173459	2.228605	5.078975
H	-0.113470	0.493239	5.020417
H	1.463856	1.152359	4.559173
C	-5.430253	1.391955	0.096489
H	-5.174538	-0.735313	0.041544
C	-6.956342	1.336470	-0.077696
C	-4.718306	2.601251	0.229671
C	-3.341104	2.649439	0.377951
H	-5.253597	3.539440	0.214192
H	-2.822327	3.593774	0.474801
C	5.288801	1.691839	0.542526
H	5.166162	-0.446926	0.452838
C	6.824514	1.717548	0.616132
C	4.508738	2.863491	0.547591
C	3.122752	2.827642	0.473742
H	4.986490	3.830139	0.603492
H	2.540543	3.739887	0.470616
C	-7.591524	2.732933	-0.079226
C	-7.288928	0.653181	-1.419437
C	-7.574982	0.525767	1.078430
C	7.380605	3.146959	0.660491
C	7.286957	0.979677	1.888226
C	7.409318	1.013950	-0.624978
H	-8.370450	0.603055	-1.558155
H	-6.868171	1.206943	-2.260536
H	-6.906261	-0.367646	-1.467520
H	-8.670875	2.641038	-0.205250
H	-7.420809	3.264513	0.859037
H	-7.223914	3.351978	-0.899778
H	-8.658986	0.474289	0.962656
H	-7.202468	-0.499436	1.108621
H	-7.362004	0.988150	2.044086
H	8.500204	1.026538	-0.584776
H	7.097414	-0.029327	-0.693141
H	7.101399	1.514566	-1.544670
H	8.377062	0.979647	1.949456
H	6.901360	1.463436	2.787737
H	6.958453	-0.060890	1.901025
H	8.470131	3.112973	0.705649
H	7.112705	3.719699	-0.229385
H	7.039406	3.695035	1.540711

Equilibrium geometry of **12-ox-amine-S2**.

Mn	-0.071529	0.248002	-0.071080
N	-1.295990	-1.124380	0.256810
N	1.155916	-1.074098	0.016679
O	-0.285850	0.264702	-1.589854
O	1.105497	1.499977	0.099632
O	-1.274300	1.482108	0.320239
N	0.151410	0.257421	2.089770
C	-0.700112	-2.479384	0.431250
C	0.604336	-2.402969	-0.345179
C	2.451970	1.495265	0.243658
C	-2.605416	-0.990211	0.242836
C	2.489834	-0.950647	0.207624
C	-2.603279	1.452130	0.179297
C	3.161484	0.281867	0.328247
C	-3.302610	0.231369	0.120525
H	-0.444883	-2.591455	1.493540
H	0.360223	-2.347163	-1.413583
C	-1.535731	-3.682586	0.014390
H	-3.198240	-1.890686	0.339757
H	3.070435	-1.858979	0.256366
C	4.568843	0.338853	0.508185
C	-4.716166	0.243135	0.019442
H	-0.406954	-0.492710	2.492491
H	1.119483	-0.015090	2.258801
C	-0.110910	1.505008	2.873663
C	0.378360	1.389701	4.307127
H	0.380577	2.319640	2.348741
H	-1.180641	1.695001	2.836055
H	0.166453	2.313780	4.846038
H	-0.115727	0.576627	4.843808
H	1.457527	1.225079	4.354068
C	-0.700951	-4.959146	0.198894
H	-2.443562	-3.768124	0.614355
H	-1.842886	-3.575845	-1.030123
H	-1.271397	-5.815424	-0.163760
C	0.646939	-4.884050	-0.516528
H	-0.538834	-5.130717	1.268354
H	1.231490	-5.781179	-0.306512
H	0.486959	-4.868400	-1.599158
C	1.455353	-3.643455	-0.110926
H	2.370734	-3.603300	-0.703026
H	1.749480	-3.715059	0.941415
C	-5.433706	1.418385	-0.038521
H	-5.222891	-0.711730	-0.018957
C	-6.960613	1.470700	-0.174389

C	-4.691254	2.620702	0.033483
C	-3.316413	2.648108	0.154187
H	-5.212524	3.568024	-0.009116
H	-2.774679	3.583099	0.205495
C	5.254589	1.533614	0.591704
H	5.099619	-0.601921	0.564213
C	6.777550	1.617372	0.763177
C	4.494197	2.722114	0.503464
C	3.121030	2.707741	0.338264
H	4.990060	3.681725	0.559313
H	2.555206	3.627289	0.263081
C	-7.556147	2.230596	1.027961
C	-7.327961	2.205296	-1.479749
C	-7.585996	0.071061	-0.216424
C	7.105258	2.372019	2.067207
C	7.433495	0.232694	0.832298
C	7.383210	2.377577	-0.434359
H	-8.642626	2.281320	0.937482
H	-7.320477	1.729211	1.968716
H	-7.188298	3.255323	1.094152
H	-8.412966	2.262217	-1.585638
H	-6.945024	3.226460	-1.500915
H	-6.932262	1.682535	-2.352311
H	-8.669076	0.157362	-0.310804
H	-7.234967	-0.510587	-1.071273
H	-7.387011	-0.495555	0.695982
H	8.186744	2.451010	2.194655
H	6.702358	3.385525	2.070097
H	6.702768	1.849593	2.937369
H	8.511627	0.344765	0.954011
H	7.072449	-0.351281	1.681539
H	7.270675	-0.344654	-0.080254
H	8.466945	2.448761	-0.324026
H	7.173206	1.864033	-1.374354
H	6.996435	3.393960	-0.516732

Equilibrium geometry of **13-ox-amine-S2**.

Mn	-0.017470	0.299598	-0.077518
N	-1.191920	-1.123178	0.132456
N	1.222674	-1.011969	-0.052228
O	-0.187478	0.427640	-1.596190
O	1.173728	1.539542	0.187385
O	-1.284549	1.463097	0.358582
N	0.174592	0.140635	2.072810

C	-0.609044	-2.483709	0.122960
C	0.746169	-2.322753	-0.515578
C	2.533313	1.549441	0.321073
C	-2.503104	-1.042711	0.217230
C	2.530851	-0.908792	0.245472
C	-2.628701	1.413488	0.218334
C	3.206731	0.307672	0.450600
C	-3.260126	0.143153	0.197835
H	-0.512080	-2.855253	1.147426
H	0.668604	-2.302104	-1.606036
H	-1.254452	-3.163963	-0.430252
H	1.435123	-3.114609	-0.225984
H	-3.044733	-1.981076	0.285891
H	3.096460	-1.831235	0.287981
C	4.596213	0.291927	0.713860
C	-4.668073	0.037811	0.153693
H	-0.353535	-0.672364	2.385186
H	1.151313	-0.105619	2.233782
C	-0.152910	1.276526	2.988420
C	0.247579	0.980344	4.424261
H	0.365346	2.151375	2.607095
H	-1.219718	1.464852	2.907095
H	-0.007479	1.827682	5.061469
H	-0.271344	0.104415	4.820373
H	1.323101	0.813000	4.518188
C	-5.424177	1.175222	0.098289
H	-5.127189	-0.943146	0.147178
H	-6.503534	1.122856	0.050397
C	-4.786246	2.420564	0.088322
C	-3.404004	2.594998	0.153860
H	-5.413812	3.295352	0.020138
C	-2.799287	4.009288	0.128686
C	5.282742	1.472908	0.801318
H	5.102801	-0.659661	0.820336
H	6.346507	1.477698	0.999586
C	4.610264	2.682522	0.598816
C	3.240486	2.768899	0.342330
H	5.192227	3.589819	0.633145
C	2.586409	4.127358	0.035852
C	-3.863790	5.093875	-0.105422
C	-2.141451	4.302566	1.490072
C	-1.780666	4.122513	-1.021965
C	3.601198	5.282115	0.073651
C	1.991501	4.085570	-1.387392
C	1.495302	4.443518	1.072012

H	-3.370494	6.065727	-0.140238
H	-4.386701	4.963684	-1.054451
H	-4.602507	5.140629	0.696431
H	-1.686421	5.294645	1.483215
H	-2.884891	4.283201	2.289493
H	-1.364068	3.582495	1.726925
H	-1.367363	5.132085	-1.051758
H	-0.956406	3.425884	-0.916390
H	-2.263298	3.933739	-1.982702
H	3.085016	6.211908	-0.167055
H	4.050841	5.410190	1.060262
H	4.399374	5.159562	-0.659822
H	1.509017	5.037308	-1.619047
H	2.777136	3.924936	-2.127872
H	1.251825	3.297544	-1.504671
H	1.061659	5.424559	0.871190
H	0.692823	3.714679	1.040534
H	1.911567	4.467976	2.082224

Equilibrium geometry of **14-ox-amine-S2**.

Mn	-0.065185	0.274595	0.018459
N	-1.281274	-1.126605	0.270864
N	1.149161	-1.055238	0.072856
O	-0.257013	0.359060	-1.501656
O	1.142333	1.502047	0.240451
O	-1.311903	1.483154	0.422795
N	0.116589	0.170630	2.161246
C	-0.693391	-2.496204	0.339742
C	0.620185	-2.353405	-0.404432
C	2.500427	1.494748	0.399108
C	-2.584708	-0.998812	0.319092
C	2.451469	-0.965576	0.410506
C	-2.650122	1.462270	0.252604
C	3.143518	0.246956	0.593367
C	-3.309732	0.208193	0.241029
H	-0.457861	-2.702557	1.392131
H	0.395591	-2.209495	-1.468659
C	-1.521554	-3.654127	-0.204301
H	-3.166131	-1.907568	0.409395
H	3.006631	-1.886501	0.500888
C	4.525290	0.217597	0.893337
C	-4.717494	0.132523	0.165447
H	-0.448158	-0.607311	2.497663
H	1.081388	-0.116752	2.328925

C	-0.156404	1.346449	3.043855
C	0.233020	1.073066	4.487087
H	0.400326	2.185686	2.636907
H	-1.213422	1.580811	2.957778
H	0.020953	1.950056	5.099573
H	-0.327120	0.235499	4.909422
H	1.299299	0.856260	4.584919
C	-0.687205	-4.943159	-0.130040
H	-2.439508	-3.800486	0.368015
H	-1.811362	-3.444761	-1.237989
H	-1.248607	-5.758293	-0.588700
C	0.677860	-4.801589	-0.803958
H	-0.548769	-5.220507	0.920208
H	1.258092	-5.715160	-0.664662
H	0.544476	-4.683382	-1.883569
C	1.473684	-3.605281	-0.262011
H	2.405816	-3.504017	-0.820208
H	1.736303	-3.778860	0.786514
C	-5.447779	1.284461	0.071677
H	-5.198539	-0.838091	0.167851
H	-6.526659	1.254709	-0.000359
C	-4.781905	2.514884	0.056829
C	-3.398606	2.659943	0.151337
H	-5.388154	3.402126	-0.038643
C	-2.761407	4.059418	0.116485
C	5.233471	1.388299	0.947556
H	5.010855	-0.737718	1.052524
H	6.291902	1.380730	1.172948
C	4.592038	2.600728	0.674462
C	3.230558	2.700230	0.380356
H	5.191441	3.497178	0.682423
C	2.609842	4.055022	-0.002263
C	-3.797134	5.164955	-0.145615
C	-2.113233	4.357780	1.481729
C	-1.725972	4.131288	-1.022450
C	3.649330	5.188297	-0.011162
C	2.027959	3.956080	-1.428161
C	1.515906	4.445603	1.004969
H	-3.281645	6.125060	-0.185463
H	-4.310450	5.035006	-1.099866
H	-4.545314	5.237370	0.645628
H	-1.635261	5.338931	1.465414
H	-2.866479	4.367643	2.272096
H	-1.355860	3.623691	1.738867
H	-1.285709	5.129105	-1.060063

H	-0.922226	3.414249	-0.896582
H	-2.201441	3.941792	-1.986639
H	3.157836	6.115066	-0.308783
H	4.088546	5.358496	0.973640
H	4.454740	5.008306	-0.724976
H	1.567769	4.905079	-1.710845
H	2.817443	3.743400	-2.151376
H	1.273397	3.178445	-1.515143
H	1.101183	5.421788	0.747870
H	0.701079	3.729597	1.006158
H	1.924166	4.517236	2.016226

Equilibrium geometry of **15-ox-amine-S2**.

Mn	-0.023722	0.349353	-0.108787
N	-1.198322	-1.064945	0.134204
N	1.215045	-0.963761	-0.075977
O	-0.207985	0.458646	-1.627795
O	1.170887	1.590274	0.128559
O	-1.277514	1.521736	0.330338
N	0.196675	0.214941	2.048351
C	-0.620230	-2.426754	0.141488
C	0.730728	-2.281415	-0.510015
C	2.531391	1.595236	0.244107
C	-2.510202	-0.978998	0.230515
C	2.528184	-0.857436	0.201911
C	-2.623839	1.470967	0.209137
C	3.207424	0.361008	0.379937
C	-3.261667	0.208946	0.205452
H	-0.517253	-2.783732	1.170718
H	0.644610	-2.282533	-1.600125
H	-1.271978	-3.113456	-0.396445
H	1.419392	-3.069988	-0.210457
H	-3.053402	-1.915054	0.315858
H	3.092574	-1.780463	0.249439
C	4.602944	0.344149	0.621067
C	-4.672009	0.105625	0.174927
H	-0.325614	-0.595930	2.375419
H	1.176321	-0.026873	2.197504
C	-0.122250	1.360029	2.953417
C	0.291173	1.082220	4.389291
H	0.391679	2.230776	2.556998
H	-1.189884	1.547359	2.879823
H	0.042874	1.937788	5.018277
H	-0.224786	0.211808	4.801138

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H       1.367367      0.914597      4.475271
C      -5.459102      1.227433      0.118008
H      -5.106013     -0.884585      0.180885
C      -6.991422      1.187365      0.063574
C      -4.785403      2.466545      0.098598
C      -3.405935      2.646756      0.149598
H      -5.395232      3.353053      0.032730
C      -2.804632      4.063022      0.109043
C       5.326736      1.509580      0.689346
H       5.081862     -0.619610      0.726802
C       6.837758      1.551820      0.954134
C       4.620062      2.711684      0.478137
C       3.250656      2.806786      0.241961
H       5.187467      3.627777      0.488457
C       2.601395      4.166401     -0.072732
C      -7.565659      1.942593      1.278947
C      -7.474604      1.862280     -1.236062
C      -7.531009     -0.248192      0.089749
C       7.103543      2.342672      2.250686
C       7.435915      0.148366      1.115384
C       7.551317      2.245229     -0.224229
C      -3.871497      5.148073     -0.110884
C      -2.122238      4.363004      1.456692
C      -1.804608      4.172941     -1.058449
C       3.621693      5.316644     -0.067778
C       1.981969      4.109724     -1.485108
C       1.527922      4.503434      0.975398
H      -8.656713      1.933701      1.245093
H      -7.255236      1.476871      2.216306
H      -7.249130      2.986283      1.303929
H      -8.565194      1.849974     -1.281903
H      -7.157755      2.904053     -1.303562
H      -7.095495      1.340944     -2.116869
H      -8.621078     -0.230768      0.051318
H      -7.188976     -0.831113     -0.767910
H      -7.249948     -0.775732      1.003652
H       8.176252      2.396873      2.446659
H       6.729704      3.365706      2.191853
H       6.630248      1.862346      3.109407
H       8.506701      0.226764      1.307297
H       6.995880     -0.391085      1.956487
H       7.312708     -0.456078      0.214086
H       8.628375      2.267367     -0.048322
H       7.373893      1.713369     -1.160749
H       7.222897      3.276393     -0.358590
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H	-3.377955	6.119494	-0.154850
H	-4.408643	5.017175	-1.051890
H	-4.598195	5.196659	0.701931
H	-1.668578	5.355706	1.437538
H	-2.850588	4.345673	2.270099
H	-1.339478	3.644933	1.681188
H	-1.391777	5.182531	-1.098353
H	-0.978774	3.476416	-0.963277
H	-2.302479	3.980352	-2.010677
H	3.105789	6.245536	-0.312772
H	4.088451	5.455882	0.909400
H	4.406893	5.180485	-0.813001
H	1.499858	5.060730	-1.720925
H	2.754039	3.935169	-2.236774
H	1.236626	3.323967	-1.579090
H	1.095385	5.483606	0.767207
H	0.721670	3.777823	0.966865
H	1.959823	4.540075	1.978706

Equilibrium geometry of **16-ox-amine-S2**.

Mn	-0.064846	0.302631	0.018997
N	-1.282958	-1.096722	0.275764
N	1.148304	-1.028704	0.079592
O	-0.254305	0.378869	-1.502511
O	1.140959	1.530143	0.239989
O	-1.307937	1.513636	0.418231
N	0.116456	0.203946	2.164551
C	-0.696648	-2.465894	0.349687
C	0.617624	-2.326935	-0.394251
C	2.500111	1.519256	0.399601
C	-2.586825	-0.967702	0.321938
C	2.453222	-0.938773	0.410295
C	-2.647602	1.489777	0.244275
C	3.146694	0.275015	0.587848
C	-3.310072	0.240006	0.237912
H	-0.461818	-2.669864	1.402824
H	0.393182	-2.185881	-1.459025
C	-1.525966	-3.624746	-0.190899
H	-3.168904	-1.875736	0.414978
H	3.008499	-1.859905	0.497623
C	4.528004	0.244247	0.874353
C	-4.714853	0.163989	0.160271
H	-0.443383	-0.577505	2.500765
H	1.083289	-0.076145	2.332524

C	-0.166369	1.380052	3.042234
C	0.224117	1.116176	4.487016
H	0.383917	2.221918	2.632430
H	-1.225121	1.606041	2.954089
H	0.005536	1.994329	5.095637
H	-0.329858	0.276239	4.912804
H	1.291945	0.907421	4.586021
C	-0.693866	-4.914634	-0.111415
H	-2.444783	-3.767281	0.380967
H	-1.814555	-3.418477	-1.225578
H	-1.256109	-5.731041	-0.566948
C	0.671548	-4.777174	-0.785426
H	-0.555945	-5.187940	0.940015
H	1.250537	-5.691154	-0.643174
H	0.538057	-4.662331	-1.865436
C	1.468850	-3.579962	-0.247884
H	2.401000	-3.482267	-0.806672
H	1.731817	-3.749855	0.801169
C	-5.485132	1.299757	0.057854
H	-5.170676	-0.818608	0.168898
C	-7.015727	1.203842	-0.041574
C	-4.790694	2.521562	0.040233
C	-3.405600	2.674533	0.136985
H	-5.375519	3.419332	-0.060181
C	-2.777380	4.079050	0.095760
C	5.277298	1.400072	0.933980
H	4.989745	-0.724716	1.021042
C	6.782539	1.338326	1.242470
C	4.605314	2.604700	0.669371
C	3.239401	2.713385	0.387867
H	5.183194	3.511843	0.671900
C	2.624836	4.076848	0.022489
C	-3.816534	5.180913	-0.167777
C	-2.126219	4.385477	1.457852
C	-1.743037	4.153208	-1.044277
C	3.667012	5.207600	0.019507
C	2.033908	3.995716	-1.400696
C	1.536097	4.462603	1.037761
H	-3.303475	6.142409	-0.209154
H	-4.329563	5.048596	-1.121907
H	-4.564997	5.253108	0.623267
H	-1.654639	5.369832	1.437836
H	-2.876714	4.391979	2.251031
H	-1.362828	3.656914	1.713379
H	-1.306524	5.152785	-1.084448

H	-0.936373	3.439420	-0.917624
H	-2.218924	3.959676	-2.007530
H	3.174844	6.139118	-0.262048
H	4.115180	5.364744	1.002578
H	4.465933	5.035799	-0.703639
H	1.578569	4.950425	-1.672370
H	2.817721	3.783644	-2.130372
H	1.273347	3.224071	-1.489438
H	1.127224	5.444925	0.794534
H	0.716110	3.752355	1.031497
H	1.947857	4.518077	2.048691
C	-7.683986	2.582044	-0.128568
C	-7.396140	0.402652	-1.302522
C	-7.562528	0.481587	1.206121
H	-8.765817	2.458497	-0.191643
H	-7.480589	3.195127	0.752020
H	-7.371730	3.135996	-1.015891
H	-8.481720	0.317663	-1.382103
H	-7.030844	0.891781	-2.207212
H	-6.990349	-0.610065	-1.283896
H	-8.649468	0.400523	1.148012
H	-7.165595	-0.530397	1.302774
H	-7.314704	1.026300	2.119189
C	7.433484	2.727418	1.277665
C	6.994960	0.675893	2.618095
C	7.492172	0.503842	0.157328
H	8.494332	2.625714	1.510204
H	7.362341	3.240542	0.316808
H	6.993644	3.368616	2.043821
H	8.060278	0.616345	2.849185
H	6.512072	1.251048	3.410670
H	6.596496	-0.339376	2.651513
H	8.562543	0.446776	0.364696
H	7.112679	-0.518042	0.111293
H	7.363710	0.951709	-0.829713

Absolute energies.

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory.

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m01	Acacen	EDA	None	None	Nothing	V	S0	TPSS	def2-SV(P)	-1796.419235
m01	Acacen	EDA	None	None	Cl	V	S0	TPSS	def2-SV(P)	-2256.727571
m01	Acacen	EDA	None	None	Amine	V	S0	TPSS	def2-SV(P)	-1931.520859
m01	Acacen	EDA	None	None	Amide	V	S0	TPSS	def2-SV(P)	-1931.101144
m01	Acacen	EDA	None	None	Nothing	III	S0	TPSS	def2-SV(P)	-1721.192884
m01	Acacen	EDA	None	None	Cl	III	S0	TPSS	def2-SV(P)	-2181.564277
m01	Acacen	EDA	None	None	Amine	III	S0	TPSS	def2-SV(P)	-1856.355592
m01	Acacen	EDA	None	None	Amide	III	S0	TPSS	def2-SV(P)	-1855.957702
m02	Acacen	CHDA	None	None	Nothing	V	S0	TPSS	def2-SV(P)	-1952.385631
m02	Acacen	CHDA	None	None	Cl	V	S0	TPSS	def2-SV(P)	-2412.688457
m02	Acacen	CHDA	None	None	Amine	V	S0	TPSS	def2-SV(P)	-2087.486040
m02	Acacen	CHDA	None	None	Amide	V	S0	TPSS	def2-SV(P)	-2087.061933
m02	Acacen	CHDA	None	None	Nothing	III	S0	TPSS	def2-SV(P)	-1877.158081
m02	Acacen	CHDA	None	None	Cl	III	S0	TPSS	def2-SV(P)	-2337.524812
m02	Acacen	CHDA	None	None	Amine	III	S0	TPSS	def2-SV(P)	-2012.319468
m02	Acacen	CHDA	None	None	Amide	III	S0	TPSS	def2-SV(P)	-2011.916757
m03	Salen	EDA	H	H	Nothing	V	S0	TPSS	def2-SV(P)	-2103.564223
m03	Salen	EDA	H	H	Cl	V	S0	TPSS	def2-SV(P)	-2563.861658
m03	Salen	EDA	H	H	Amine	V	S0	TPSS	def2-SV(P)	-2238.661944
m03	Salen	EDA	H	H	Amide	V	S0	TPSS	def2-SV(P)	-2238.229717
m03	Salen	EDA	H	H	Nothing	III	S0	TPSS	def2-SV(P)	-2028.341531
m03	Salen	EDA	H	H	Cl	III	S0	TPSS	def2-SV(P)	-2488.703677
m03	Salen	EDA	H	H	Amine	III	S0	TPSS	def2-SV(P)	-2163.500669
m03	Salen	EDA	H	H	Amide	III	S0	TPSS	def2-SV(P)	-2163.092466
m04	Salen	CHDA	H	H	Nothing	V	S0	TPSS	def2-SV(P)	-2259.529899
m04	Salen	CHDA	H	H	Cl	V	S0	TPSS	def2-SV(P)	-2719.823561
m04	Salen	CHDA	H	H	Amine	V	S0	TPSS	def2-SV(P)	-2394.627248
m04	Salen	CHDA	H	H	Amide	V	S0	TPSS	def2-SV(P)	-2394.190900
m04	Salen	CHDA	H	H	Nothing	III	S0	TPSS	def2-SV(P)	-2184.306621
m04	Salen	CHDA	H	H	Cl	III	S0	TPSS	def2-SV(P)	-2644.664569
m04	Salen	CHDA	H	H	Amine	III	S0	TPSS	def2-SV(P)	-2319.464639
m04	Salen	CHDA	H	H	Amide	III	S0	TPSS	def2-SV(P)	-2319.051985
m05	Salen	EDA	H	Me	Nothing	V	S0	TPSS	def2-SV(P)	-2182.152431
m05	Salen	EDA	H	Me	Cl	V	S0	TPSS	def2-SV(P)	-2642.445563
m05	Salen	EDA	H	Me	Amine	V	S0	TPSS	def2-SV(P)	-2317.249266
m05	Salen	EDA	H	Me	Amide	V	S0	TPSS	def2-SV(P)	-2316.813578
m05	Salen	EDA	H	Me	Nothing	III	S0	TPSS	def2-SV(P)	-2106.930006
m05	Salen	EDA	H	Me	Cl	III	S0	TPSS	def2-SV(P)	-2567.287132
m05	Salen	EDA	H	Me	Amine	III	S0	TPSS	def2-SV(P)	-2242.087352
m05	Salen	EDA	H	Me	Amide	III	S0	TPSS	def2-SV(P)	-2241.675325
m06	Salen	CHDA	H	Me	Nothing	V	S0	TPSS	def2-SV(P)	-2338.117674
m06	Salen	CHDA	H	Me	Cl	V	S0	TPSS	def2-SV(P)	-2798.407355
m06	Salen	CHDA	H	Me	Amine	V	S0	TPSS	def2-SV(P)	-2473.214212
m06	Salen	CHDA	H	Me	Amide	V	S0	TPSS	def2-SV(P)	-2472.774001
m06	Salen	CHDA	H	Me	Nothing	III	S0	TPSS	def2-SV(P)	-2262.894609
m06	Salen	CHDA	H	Me	Cl	III	S0	TPSS	def2-SV(P)	-2723.247980
m06	Salen	CHDA	H	Me	Amine	III	S0	TPSS	def2-SV(P)	-2398.051034
m06	Salen	CHDA	H	Me	Amide	III	S0	TPSS	def2-SV(P)	-2397.634699
m07	Salen	EDA	Me	H	Nothing	V	S0	TPSS	def2-SV(P)	-2182.154261
m07	Salen	EDA	Me	H	Cl	V	S0	TPSS	def2-SV(P)	-2642.449814
m07	Salen	EDA	Me	H	Amine	V	S0	TPSS	def2-SV(P)	-2317.250346
m07	Salen	EDA	Me	H	Amide	V	S0	TPSS	def2-SV(P)	-2316.818078
m07	Salen	EDA	Me	H	Nothing	III	S0	TPSS	def2-SV(P)	-2106.932181
m07	Salen	EDA	Me	H	Cl	III	S0	TPSS	def2-SV(P)	-2567.291203
m07	Salen	EDA	Me	H	Amine	III	S0	TPSS	def2-SV(P)	-2242.088414
m07	Salen	EDA	Me	H	Amide	III	S0	TPSS	def2-SV(P)	-2241.679197
m08	Salen	CHDA	Me	H	Nothing	V	S0	TPSS	def2-SV(P)	-2338.119758
m08	Salen	CHDA	Me	H	Cl	V	S0	TPSS	def2-SV(P)	-2798.411718
m08	Salen	CHDA	Me	H	Amine	V	S0	TPSS	def2-SV(P)	-2473.215435
m08	Salen	CHDA	Me	H	Amide	V	S0	TPSS	def2-SV(P)	-2472.778728
m08	Salen	CHDA	Me	H	Nothing	III	S0	TPSS	def2-SV(P)	-2262.896970
m08	Salen	CHDA	Me	H	Cl	III	S0	TPSS	def2-SV(P)	-2723.251989
m08	Salen	CHDA	Me	H	Amine	III	S0	TPSS	def2-SV(P)	-2398.052201
m08	Salen	CHDA	Me	H	Amide	III	S0	TPSS	def2-SV(P)	-2397.638727
m09	Salen	EDA	Me	Me	Nothing	V	S0	TPSS	def2-SV(P)	-2260.742220
m09	Salen	EDA	Me	Me	Cl	V	S0	TPSS	def2-SV(P)	-2721.033709

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m09	Salen	EDA	Me	Me	Amine	V	S0	TPSS	def2-SV(P)	-2395.837444
m09	Salen	EDA	Me	Me	Amide	V	S0	TPSS	def2-SV(P)	-2395.401324
m09	Salen	EDA	Me	Me	Nothing	III	S0	TPSS	def2-SV(P)	-2185.520281
m09	Salen	EDA	Me	Me	Cl	III	S0	TPSS	def2-SV(P)	-2645.874630
m09	Salen	EDA	Me	Me	Amine	III	S0	TPSS	def2-SV(P)	-2320.674890
m09	Salen	EDA	Me	Me	Amide	III	S0	TPSS	def2-SV(P)	-2320.262131
m10	Salen	CHDA	Me	Me	Nothing	V	S0	TPSS	def2-SV(P)	-2416.707314
m10	Salen	CHDA	Me	Me	Cl	V	S0	TPSS	def2-SV(P)	-2876.995496
m10	Salen	CHDA	Me	Me	Amine	V	S0	TPSS	def2-SV(P)	-2551.802782
m10	Salen	CHDA	Me	Me	Amide	V	S0	TPSS	def2-SV(P)	-2551.361894
m10	Salen	CHDA	Me	Me	Nothing	III	S0	TPSS	def2-SV(P)	-2341.484695
m10	Salen	CHDA	Me	Me	Cl	III	S0	TPSS	def2-SV(P)	-2801.835368
m10	Salen	CHDA	Me	Me	Amine	III	S0	TPSS	def2-SV(P)	-2476.638372
m10	Salen	CHDA	Me	Me	Amide	III	S0	TPSS	def2-SV(P)	-2476.221553
m11	Salen	EDA	H	t-Bu	Nothing	V	S0	TPSS	def2-SV(P)	-2417.877508
m11	Salen	EDA	H	t-Bu	Cl	V	S0	TPSS	def2-SV(P)	-2878.167509
m11	Salen	EDA	H	t-Bu	Amine	V	S0	TPSS	def2-SV(P)	-2552.972225
m11	Salen	EDA	H	t-Bu	Amide	V	S0	TPSS	def2-SV(P)	-2552.534829
m11	Salen	EDA	H	t-Bu	Nothing	III	S0	TPSS	def2-SV(P)	-2342.654014
m11	Salen	EDA	H	t-Bu	Cl	III	S0	TPSS	def2-SV(P)	-2803.008485
m11	Salen	EDA	H	t-Bu	Amine	III	S0	TPSS	def2-SV(P)	-2477.810129
m11	Salen	EDA	H	t-Bu	Amide	III	S0	TPSS	def2-SV(P)	-2477.395996
m12	Salen	CHDA	H	t-Bu	Nothing	V	S0	TPSS	def2-SV(P)	-2573.841306
m12	Salen	CHDA	H	t-Bu	Cl	V	S0	TPSS	def2-SV(P)	-3034.129335
m12	Salen	CHDA	H	t-Bu	Amine	V	S0	TPSS	def2-SV(P)	-2708.937994
m12	Salen	CHDA	H	t-Bu	Amide	V	S0	TPSS	def2-SV(P)	-2708.496004
m12	Salen	CHDA	H	t-Bu	Nothing	III	S0	TPSS	def2-SV(P)	-2498.619139
m12	Salen	CHDA	H	t-Bu	Cl	III	S0	TPSS	def2-SV(P)	-2958.970659
m12	Salen	CHDA	H	t-Bu	Amine	III	S0	TPSS	def2-SV(P)	-2633.774301
m12	Salen	CHDA	H	t-Bu	Amide	III	S0	TPSS	def2-SV(P)	-2633.355979
m13	Salen	EDA	t-Bu	H	Nothing	V	S0	TPSS	def2-SV(P)	-2417.867009
m13	Salen	EDA	t-Bu	H	Cl	V	S0	TPSS	def2-SV(P)	-2878.164254
m13	Salen	EDA	t-Bu	H	Amine	V	S0	TPSS	def2-SV(P)	-2552.963289
m13	Salen	EDA	t-Bu	H	Amide	V	S0	TPSS	def2-SV(P)	-2552.534991
m13	Salen	EDA	t-Bu	H	Nothing	III	S0	TPSS	def2-SV(P)	-2342.651109
m13	Salen	EDA	t-Bu	H	Cl	III	S0	TPSS	def2-SV(P)	-2802.999799
m13	Salen	EDA	t-Bu	H	Amine	III	S0	TPSS	def2-SV(P)	-2477.801450
m13	Salen	EDA	t-Bu	H	Amide	III	S0	TPSS	def2-SV(P)	-2477.392447
m14	Salen	CHDA	t-Bu	H	Nothing	V	S0	TPSS	def2-SV(P)	-2573.832112
m14	Salen	CHDA	t-Bu	H	Cl	V	S0	TPSS	def2-SV(P)	-3034.126078
m14	Salen	CHDA	t-Bu	H	Amine	V	S0	TPSS	def2-SV(P)	-2708.930885
m14	Salen	CHDA	t-Bu	H	Amide	V	S0	TPSS	def2-SV(P)	-2708.493710
m14	Salen	CHDA	t-Bu	H	Nothing	III	S0	TPSS	def2-SV(P)	-2498.615108
m14	Salen	CHDA	t-Bu	H	Cl	III	S0	TPSS	def2-SV(P)	-2958.959819
m14	Salen	CHDA	t-Bu	H	Amine	III	S0	TPSS	def2-SV(P)	-2633.764153
m14	Salen	CHDA	t-Bu	H	Amide	III	S0	TPSS	def2-SV(P)	-2633.352041
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S0	TPSS	def2-SV(P)	-2732.180047
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S0	TPSS	def2-SV(P)	-3192.471586
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S0	TPSS	def2-SV(P)	-2867.278040
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S0	TPSS	def2-SV(P)	-2866.840267
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S0	TPSS	def2-SV(P)	-2656.962286
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S0	TPSS	def2-SV(P)	-3117.305291
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S0	TPSS	def2-SV(P)	-2792.111651
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S0	TPSS	def2-SV(P)	-2791.696449
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S0	TPSS	def2-SV(P)	-2888.144564
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S0	TPSS	def2-SV(P)	-3348.433257
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S0	TPSS	def2-SV(P)	-3023.239484
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S0	TPSS	def2-SV(P)	-3022.801068
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S0	TPSS	def2-SV(P)	-2812.926284
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S0	TPSS	def2-SV(P)	-3273.266653
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S0	TPSS	def2-SV(P)	-2948.072632
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S0	TPSS	def2-SV(P)	-2947.656001
m01	Acacen	EDA	None	None	Nothing	V	S2	TPSS	def2-SV(P)	-1796.408789
m01	Acacen	EDA	None	None	Cl	V	S2	TPSS	def2-SV(P)	-2256.727083
m01	Acacen	EDA	None	None	Amine	V	S2	TPSS	def2-SV(P)	-1931.521588
m01	Acacen	EDA	None	None	Amide	V	S2	TPSS	def2-SV(P)	-1931.102259
m01	Acacen	EDA	None	None	Nothing	III	S2	TPSS	def2-SV(P)	-1721.248826
m01	Acacen	EDA	None	None	Cl	III	S2	TPSS	def2-SV(P)	-2181.593095
m01	Acacen	EDA	None	None	Amine	III	S2	TPSS	def2-SV(P)	-1856.387420
m01	Acacen	EDA	None	None	Amide	III	S2	TPSS	def2-SV(P)	-1855.965030
m02	Acacen	CHDA	None	None	Nothing	V	S2	TPSS	def2-SV(P)	-1952.376267

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m02	Acacen	CHDA	None	None	Cl	V	S2	TPSS	def2-SV(P)	-2412.689404
m02	Acacen	CHDA	None	None	Amine	V	S2	TPSS	def2-SV(P)	-2087.488000
m02	Acacen	CHDA	None	None	Amide	V	S2	TPSS	def2-SV(P)	-2087.063763
m02	Acacen	CHDA	None	None	Nothing	III	S2	TPSS	def2-SV(P)	-1877.213882
m02	Acacen	CHDA	None	None	Cl	III	S2	TPSS	def2-SV(P)	-2337.553262
m02	Acacen	CHDA	None	None	Amine	III	S2	TPSS	def2-SV(P)	-2012.351066
m02	Acacen	CHDA	None	None	Amide	III	S2	TPSS	def2-SV(P)	-2011.926707
m03	Salen	EDA	H	H	Nothing	V	S2	TPSS	def2-SV(P)	-2103.558235
m03	Salen	EDA	H	H	Cl	V	S2	TPSS	def2-SV(P)	-2563.863640
m03	Salen	EDA	H	H	Amine	V	S2	TPSS	def2-SV(P)	-2238.666143
m03	Salen	EDA	H	H	Amide	V	S2	TPSS	def2-SV(P)	-2238.235948
m03	Salen	EDA	H	H	Nothing	III	S2	TPSS	def2-SV(P)	-2028.395729
m03	Salen	EDA	H	H	Cl	III	S2	TPSS	def2-SV(P)	-2488.730056
m03	Salen	EDA	H	H	Amine	III	S2	TPSS	def2-SV(P)	-2163.527617
m03	Salen	EDA	H	H	Amide	III	S2	TPSS	def2-SV(P)	-2163.101386
m04	Salen	CHDA	H	H	Nothing	V	S2	TPSS	def2-SV(P)	-2259.524692
m04	Salen	CHDA	H	H	Cl	V	S2	TPSS	def2-SV(P)	-2719.826282
m04	Salen	CHDA	H	H	Amine	V	S2	TPSS	def2-SV(P)	-2394.631772
m04	Salen	CHDA	H	H	Amide	V	S2	TPSS	def2-SV(P)	-2394.198000
m04	Salen	CHDA	H	H	Nothing	III	S2	TPSS	def2-SV(P)	-2184.360075
m04	Salen	CHDA	H	H	Cl	III	S2	TPSS	def2-SV(P)	-2644.690393
m04	Salen	CHDA	H	H	Amine	III	S2	TPSS	def2-SV(P)	-2319.490916
m04	Salen	CHDA	H	H	Amide	III	S2	TPSS	def2-SV(P)	-2319.060818
m05	Salen	EDA	H	Me	Nothing	V	S2	TPSS	def2-SV(P)	-2182.146493
m05	Salen	EDA	H	Me	Cl	V	S2	TPSS	def2-SV(P)	-2642.447421
m05	Salen	EDA	H	Me	Amine	V	S2	TPSS	def2-SV(P)	-2317.253723
m05	Salen	EDA	H	Me	Amide	V	S2	TPSS	def2-SV(P)	-2316.818865
m05	Salen	EDA	H	Me	Nothing	III	S2	TPSS	def2-SV(P)	-2106.984718
m05	Salen	EDA	H	Me	Cl	III	S2	TPSS	def2-SV(P)	-2567.312765
m05	Salen	EDA	H	Me	Amine	III	S2	TPSS	def2-SV(P)	-2242.114022
m05	Salen	EDA	H	Me	Amide	III	S2	TPSS	def2-SV(P)	-2241.684242
m06	Salen	CHDA	H	Me	Nothing	V	S2	TPSS	def2-SV(P)	-2338.112485
m06	Salen	CHDA	H	Me	Cl	V	S2	TPSS	def2-SV(P)	-2798.409975
m06	Salen	CHDA	H	Me	Amine	V	S2	TPSS	def2-SV(P)	-2473.218913
m06	Salen	CHDA	H	Me	Amide	V	S2	TPSS	def2-SV(P)	-2472.780834
m06	Salen	CHDA	H	Me	Nothing	III	S2	TPSS	def2-SV(P)	-2262.948004
m06	Salen	CHDA	H	Me	Cl	III	S2	TPSS	def2-SV(P)	-2723.273666
m06	Salen	CHDA	H	Me	Amine	III	S2	TPSS	def2-SV(P)	-2398.076994
m06	Salen	CHDA	H	Me	Amide	III	S2	TPSS	def2-SV(P)	-2397.643511
m07	Salen	EDA	Me	H	Nothing	V	S2	TPSS	def2-SV(P)	-2182.148327
m07	Salen	EDA	Me	H	Cl	V	S2	TPSS	def2-SV(P)	-2642.452126
m07	Salen	EDA	Me	H	Amine	V	S2	TPSS	def2-SV(P)	-2317.255285
m07	Salen	EDA	Me	H	Amide	V	S2	TPSS	def2-SV(P)	-2316.823631
m07	Salen	EDA	Me	H	Nothing	III	S2	TPSS	def2-SV(P)	-2106.985777
m07	Salen	EDA	Me	H	Cl	III	S2	TPSS	def2-SV(P)	-2567.317684
m07	Salen	EDA	Me	H	Amine	III	S2	TPSS	def2-SV(P)	-2242.115520
m07	Salen	EDA	Me	H	Amide	III	S2	TPSS	def2-SV(P)	-2241.688231
m08	Salen	CHDA	Me	H	Nothing	V	S2	TPSS	def2-SV(P)	-2338.114543
m08	Salen	CHDA	Me	H	Cl	V	S2	TPSS	def2-SV(P)	-2798.414747
m08	Salen	CHDA	Me	H	Amine	V	S2	TPSS	def2-SV(P)	-2473.220762
m08	Salen	CHDA	Me	H	Amide	V	S2	TPSS	def2-SV(P)	-2472.785683
m08	Salen	CHDA	Me	H	Nothing	III	S2	TPSS	def2-SV(P)	-2262.949828
m08	Salen	CHDA	Me	H	Cl	III	S2	TPSS	def2-SV(P)	-2723.277941
m08	Salen	CHDA	Me	H	Amine	III	S2	TPSS	def2-SV(P)	-2398.078708
m08	Salen	CHDA	Me	H	Amide	III	S2	TPSS	def2-SV(P)	-2397.647685
m09	Salen	EDA	Me	Me	Nothing	V	S2	TPSS	def2-SV(P)	-2260.736394
m09	Salen	EDA	Me	Me	Cl	V	S2	TPSS	def2-SV(P)	-2721.035931
m09	Salen	EDA	Me	Me	Amine	V	S2	TPSS	def2-SV(P)	-2395.842707
m09	Salen	EDA	Me	Me	Amide	V	S2	TPSS	def2-SV(P)	-2395.406554
m09	Salen	EDA	Me	Me	Nothing	III	S2	TPSS	def2-SV(P)	-2185.574775
m09	Salen	EDA	Me	Me	Cl	III	S2	TPSS	def2-SV(P)	-2645.900339
m09	Salen	EDA	Me	Me	Amine	III	S2	TPSS	def2-SV(P)	-2320.701723
m09	Salen	EDA	Me	Me	Amide	III	S2	TPSS	def2-SV(P)	-2320.271090
m10	Salen	CHDA	Me	Me	Nothing	V	S2	TPSS	def2-SV(P)	-2416.702144
m10	Salen	CHDA	Me	Me	Cl	V	S2	TPSS	def2-SV(P)	-2876.998450
m10	Salen	CHDA	Me	Me	Amine	V	S2	TPSS	def2-SV(P)	-2551.807786
m10	Salen	CHDA	Me	Me	Amide	V	S2	TPSS	def2-SV(P)	-2551.368529
m10	Salen	CHDA	Me	Me	Nothing	III	S2	TPSS	def2-SV(P)	-2341.537973
m10	Salen	CHDA	Me	Me	Cl	III	S2	TPSS	def2-SV(P)	-2801.861188
m10	Salen	CHDA	Me	Me	Amine	III	S2	TPSS	def2-SV(P)	-2476.664656
m10	Salen	CHDA	Me	Me	Amide	III	S2	TPSS	def2-SV(P)	-2476.230452

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m11	Salen	EDA	H	t-Bu	Nothing	V	S2	TPSS	def2-SV(P)	-2417.871506
m11	Salen	EDA	H	t-Bu	Cl	V	S2	TPSS	def2-SV(P)	-2878.169582
m11	Salen	EDA	H	t-Bu	Amine	V	S2	TPSS	def2-SV(P)	-2552.977223
m11	Salen	EDA	H	t-Bu	Amide	V	S2	TPSS	def2-SV(P)	-2552.540857
m11	Salen	EDA	H	t-Bu	Nothing	III	S2	TPSS	def2-SV(P)	-2342.708490
m11	Salen	EDA	H	t-Bu	Cl	III	S2	TPSS	def2-SV(P)	-2803.035362
m11	Salen	EDA	H	t-Bu	Amine	III	S2	TPSS	def2-SV(P)	-2477.836926
m11	Salen	EDA	H	t-Bu	Amide	III	S2	TPSS	def2-SV(P)	-2477.405038
m12	Salen	CHDA	H	t-Bu	Nothing	V	S2	TPSS	def2-SV(P)	-2573.836076
m12	Salen	CHDA	H	t-Bu	Cl	V	S2	TPSS	def2-SV(P)	-3034.131624
m12	Salen	CHDA	H	t-Bu	Amine	V	S2	TPSS	def2-SV(P)	-2708.943229
m12	Salen	CHDA	H	t-Bu	Amide	V	S2	TPSS	def2-SV(P)	-2708.502760
m12	Salen	CHDA	H	t-Bu	Nothing	III	S2	TPSS	def2-SV(P)	-2498.672822
m12	Salen	CHDA	H	t-Bu	Cl	III	S2	TPSS	def2-SV(P)	-2958.996410
m12	Salen	CHDA	H	t-Bu	Amine	III	S2	TPSS	def2-SV(P)	-2633.799833
m12	Salen	CHDA	H	t-Bu	Amide	III	S2	TPSS	def2-SV(P)	-2633.365361
m13	Salen	EDA	t-Bu	H	Nothing	V	S2	TPSS	def2-SV(P)	-2417.865487
m13	Salen	EDA	t-Bu	H	Cl	V	S2	TPSS	def2-SV(P)	-2878.169622
m13	Salen	EDA	t-Bu	H	Amine	V	S2	TPSS	def2-SV(P)	-2552.972354
m13	Salen	EDA	t-Bu	H	Amide	V	S2	TPSS	def2-SV(P)	-2552.540665
m13	Salen	EDA	t-Bu	H	Nothing	III	S2	TPSS	def2-SV(P)	-2342.703065
m13	Salen	EDA	t-Bu	H	Cl	III	S2	TPSS	def2-SV(P)	-2803.034434
m13	Salen	EDA	t-Bu	H	Amine	III	S2	TPSS	def2-SV(P)	-2477.830526
m13	Salen	EDA	t-Bu	H	Amide	III	S2	TPSS	def2-SV(P)	-2477.402281
m14	Salen	CHDA	t-Bu	H	Nothing	V	S2	TPSS	def2-SV(P)	-2573.831534
m14	Salen	CHDA	t-Bu	H	Cl	V	S2	TPSS	def2-SV(P)	-3034.132151
m14	Salen	CHDA	t-Bu	H	Amine	V	S2	TPSS	def2-SV(P)	-2708.937522
m14	Salen	CHDA	t-Bu	H	Amide	V	S2	TPSS	def2-SV(P)	-2708.501455
m14	Salen	CHDA	t-Bu	H	Nothing	III	S2	TPSS	def2-SV(P)	-2498.667223
m14	Salen	CHDA	t-Bu	H	Cl	III	S2	TPSS	def2-SV(P)	-2958.994808
m14	Salen	CHDA	t-Bu	H	Amine	III	S2	TPSS	def2-SV(P)	-2633.793683
m14	Salen	CHDA	t-Bu	H	Amide	III	S2	TPSS	def2-SV(P)	-2633.361639
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S2	TPSS	def2-SV(P)	-2732.178079
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S2	TPSS	def2-SV(P)	-3192.476841
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S2	TPSS	def2-SV(P)	-2867.281568
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S2	TPSS	def2-SV(P)	-2866.845639
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S2	TPSS	def2-SV(P)	-2657.015353
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S2	TPSS	def2-SV(P)	-3117.339866
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S2	TPSS	def2-SV(P)	-2792.139624
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S2	TPSS	def2-SV(P)	-2791.706156
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S2	TPSS	def2-SV(P)	-2888.143607
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S2	TPSS	def2-SV(P)	-3348.439123
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S2	TPSS	def2-SV(P)	-3023.246779
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S2	TPSS	def2-SV(P)	-3022.806918
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S2	TPSS	def2-SV(P)	-2812.978554
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S2	TPSS	def2-SV(P)	-3273.301150
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S2	TPSS	def2-SV(P)	-2948.101226
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S2	TPSS	def2-SV(P)	-2947.665580
m01	Acacen	EDA	None	None	Nothing	V	S4	TPSS	def2-SV(P)	-1796.381929
m01	Acacen	EDA	None	None	Cl	V	S4	TPSS	def2-SV(P)	-2256.711597
m01	Acacen	EDA	None	None	Amine	V	S4	TPSS	def2-SV(P)	-1931.506224
m01	Acacen	EDA	None	None	Amide	V	S4	TPSS	def2-SV(P)	-1931.085044
m01	Acacen	EDA	None	None	Nothing	III	S4	TPSS	def2-SV(P)	-1721.273964
m01	Acacen	EDA	None	None	Cl	III	S4	TPSS	def2-SV(P)	-2181.607414
m01	Acacen	EDA	None	None	Amine	III	S4	TPSS	def2-SV(P)	-1856.398333
m01	Acacen	EDA	None	None	Amide	III	S4	TPSS	def2-SV(P)	-1855.965243
m02	Acacen	CHDA	None	None	Nothing	V	S4	TPSS	def2-SV(P)	-1952.348422
m02	Acacen	CHDA	None	None	Cl	V	S4	TPSS	def2-SV(P)	-2412.673220
m02	Acacen	CHDA	None	None	Amine	V	S4	TPSS	def2-SV(P)	-2087.471360
m02	Acacen	CHDA	None	None	Amide	V	S4	TPSS	def2-SV(P)	-2087.045707
m02	Acacen	CHDA	None	None	Nothing	III	S4	TPSS	def2-SV(P)	-1877.240027
m02	Acacen	CHDA	None	None	Cl	III	S4	TPSS	def2-SV(P)	-2337.568915
m02	Acacen	CHDA	None	None	Amine	III	S4	TPSS	def2-SV(P)	-2012.363031
m02	Acacen	CHDA	None	None	Amide	III	S4	TPSS	def2-SV(P)	-2011.916728
m03	Salen	EDA	H	H	Nothing	V	S4	TPSS	def2-SV(P)	-2103.533295
m03	Salen	EDA	H	H	Cl	V	S4	TPSS	def2-SV(P)	-2563.847246
m03	Salen	EDA	H	H	Amine	V	S4	TPSS	def2-SV(P)	-2238.650679
m03	Salen	EDA	H	H	Amide	V	S4	TPSS	def2-SV(P)	-2238.219868
m03	Salen	EDA	H	H	Nothing	III	S4	TPSS	def2-SV(P)	-2028.421183
m03	Salen	EDA	H	H	Cl	III	S4	TPSS	def2-SV(P)	-2488.742897
m03	Salen	EDA	H	H	Amine	III	S4	TPSS	def2-SV(P)	-2163.540037

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m03	Salen	EDA	H	H	Amide	III	S4	TPSS	def2-SV(P)	-2163.097411
m04	Salen	CHDA	H	H	Nothing	V	S4	TPSS	def2-SV(P)	-2259.498793
m04	Salen	CHDA	H	H	Cl	V	S4	TPSS	def2-SV(P)	-2719.809198
m04	Salen	CHDA	H	H	Amine	V	S4	TPSS	def2-SV(P)	-2394.615250
m04	Salen	CHDA	H	H	Amide	V	S4	TPSS	def2-SV(P)	-2394.181216
m04	Salen	CHDA	H	H	Nothing	III	S4	TPSS	def2-SV(P)	-2184.386712
m04	Salen	CHDA	H	H	Cl	III	S4	TPSS	def2-SV(P)	-2644.704751
m04	Salen	CHDA	H	H	Amine	III	S4	TPSS	def2-SV(P)	-2319.504467
m04	Salen	CHDA	H	H	Amide	III	S4	TPSS	def2-SV(P)	-2319.058418
m05	Salen	EDA	H	Me	Nothing	V	S4	TPSS	def2-SV(P)	-2182.124219
m05	Salen	EDA	H	Me	Cl	V	S4	TPSS	def2-SV(P)	-2642.431753
m05	Salen	EDA	H	Me	Amine	V	S4	TPSS	def2-SV(P)	-2317.239484
m05	Salen	EDA	H	Me	Amide	V	S4	TPSS	def2-SV(P)	-2316.802715
m05	Salen	EDA	H	Me	Nothing	III	S4	TPSS	def2-SV(P)	-2107.008213
m05	Salen	EDA	H	Me	Cl	III	S4	TPSS	def2-SV(P)	-2567.326003
m05	Salen	EDA	H	Me	Amine	III	S4	TPSS	def2-SV(P)	-2242.126061
m05	Salen	EDA	H	Me	Amide	III	S4	TPSS	def2-SV(P)	-2241.680251
m06	Salen	CHDA	H	Me	Nothing	V	S4	TPSS	def2-SV(P)	-2338.089244
m06	Salen	CHDA	H	Me	Cl	V	S4	TPSS	def2-SV(P)	-2798.393474
m06	Salen	CHDA	H	Me	Amine	V	S4	TPSS	def2-SV(P)	-2473.203645
m06	Salen	CHDA	H	Me	Amide	V	S4	TPSS	def2-SV(P)	-2472.763989
m06	Salen	CHDA	H	Me	Nothing	III	S4	TPSS	def2-SV(P)	-2262.973363
m06	Salen	CHDA	H	Me	Cl	III	S4	TPSS	def2-SV(P)	-2723.287818
m06	Salen	CHDA	H	Me	Amine	III	S4	TPSS	def2-SV(P)	-2398.090126
m06	Salen	CHDA	H	Me	Amide	III	S4	TPSS	def2-SV(P)	-2397.641182
m07	Salen	EDA	Me	H	Nothing	V	S4	TPSS	def2-SV(P)	-2182.125542
m07	Salen	EDA	Me	H	Cl	V	S4	TPSS	def2-SV(P)	-2642.436399
m07	Salen	EDA	Me	H	Amine	V	S4	TPSS	def2-SV(P)	-2317.241131
m07	Salen	EDA	Me	H	Amide	V	S4	TPSS	def2-SV(P)	-2316.807333
m07	Salen	EDA	Me	H	Nothing	III	S4	TPSS	def2-SV(P)	-2107.010474
m07	Salen	EDA	Me	H	Cl	III	S4	TPSS	def2-SV(P)	-2567.330862
m07	Salen	EDA	Me	H	Amine	III	S4	TPSS	def2-SV(P)	-2242.128303
m07	Salen	EDA	Me	H	Amide	III	S4	TPSS	def2-SV(P)	-2241.684640
m08	Salen	CHDA	Me	H	Nothing	V	S4	TPSS	def2-SV(P)	-2338.090806
m08	Salen	CHDA	Me	H	Cl	V	S4	TPSS	def2-SV(P)	-2798.398209
m08	Salen	CHDA	Me	H	Amine	V	S4	TPSS	def2-SV(P)	-2473.205552
m08	Salen	CHDA	Me	H	Amide	V	S4	TPSS	def2-SV(P)	-2472.768466
m08	Salen	CHDA	Me	H	Nothing	III	S4	TPSS	def2-SV(P)	-2262.975729
m08	Salen	CHDA	Me	H	Cl	III	S4	TPSS	def2-SV(P)	-2723.292618
m08	Salen	CHDA	Me	H	Amine	III	S4	TPSS	def2-SV(P)	-2398.092610
m08	Salen	CHDA	Me	H	Amide	III	S4	TPSS	def2-SV(P)	-2397.645566
m09	Salen	EDA	Me	Me	Nothing	V	S4	TPSS	def2-SV(P)	-2260.715901
m09	Salen	EDA	Me	Me	Cl	V	S4	TPSS	def2-SV(P)	-2721.020878
m09	Salen	EDA	Me	Me	Amine	V	S4	TPSS	def2-SV(P)	-2395.829636
m09	Salen	EDA	Me	Me	Amide	V	S4	TPSS	def2-SV(P)	-2395.390058
m09	Salen	EDA	Me	Me	Nothing	III	S4	TPSS	def2-SV(P)	-2185.597223
m09	Salen	EDA	Me	Me	Cl	III	S4	TPSS	def2-SV(P)	-2645.913976
m09	Salen	EDA	Me	Me	Amine	III	S4	TPSS	def2-SV(P)	-2320.714158
m09	Salen	EDA	Me	Me	Amide	III	S4	TPSS	def2-SV(P)	-2320.267489
m10	Salen	CHDA	Me	Me	Nothing	V	S4	TPSS	def2-SV(P)	-2416.680752
m10	Salen	CHDA	Me	Me	Cl	V	S4	TPSS	def2-SV(P)	-2876.982611
m10	Salen	CHDA	Me	Me	Amine	V	S4	TPSS	def2-SV(P)	-2551.793723
m10	Salen	CHDA	Me	Me	Amide	V	S4	TPSS	def2-SV(P)	-2551.351271
m10	Salen	CHDA	Me	Me	Nothing	III	S4	TPSS	def2-SV(P)	-2341.562133
m10	Salen	CHDA	Me	Me	Cl	III	S4	TPSS	def2-SV(P)	-2801.875421
m10	Salen	CHDA	Me	Me	Amine	III	S4	TPSS	def2-SV(P)	-2476.678135
m10	Salen	CHDA	Me	Me	Amide	III	S4	TPSS	def2-SV(P)	-2476.228236
m11	Salen	EDA	H	t-Bu	Nothing	V	S4	TPSS	def2-SV(P)	-2417.849407
m11	Salen	EDA	H	t-Bu	Cl	V	S4	TPSS	def2-SV(P)	-2878.153740
m11	Salen	EDA	H	t-Bu	Amine	V	S4	TPSS	def2-SV(P)	-2552.963171
m11	Salen	EDA	H	t-Bu	Amide	V	S4	TPSS	def2-SV(P)	-2552.524772
m11	Salen	EDA	H	t-Bu	Nothing	III	S4	TPSS	def2-SV(P)	-2342.732019
m11	Salen	EDA	H	t-Bu	Cl	III	S4	TPSS	def2-SV(P)	-2803.047744
m11	Salen	EDA	H	t-Bu	Amine	III	S4	TPSS	def2-SV(P)	-2477.849297
m11	Salen	EDA	H	t-Bu	Amide	III	S4	TPSS	def2-SV(P)	-2477.401123
m12	Salen	CHDA	H	t-Bu	Nothing	V	S4	TPSS	def2-SV(P)	-2573.813437
m12	Salen	CHDA	H	t-Bu	Cl	V	S4	TPSS	def2-SV(P)	-3034.115642
m12	Salen	CHDA	H	t-Bu	Amine	V	S4	TPSS	def2-SV(P)	-2708.928091
m12	Salen	CHDA	H	t-Bu	Amide	V	S4	TPSS	def2-SV(P)	-2708.486007
m12	Salen	CHDA	H	t-Bu	Nothing	III	S4	TPSS	def2-SV(P)	-2498.697910
m12	Salen	CHDA	H	t-Bu	Cl	III	S4	TPSS	def2-SV(P)	-2959.010518

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m12	Salen	CHDA	H	t-Bu	Amine	III	S4	TPSS	def2-SV(P)	-2633.813008
m12	Salen	CHDA	H	t-Bu	Amide	III	S4	TPSS	def2-SV(P)	-2633.363148
m13	Salen	EDA	t-Bu	H	Nothing	V	S4	TPSS	def2-SV(P)	-2417.842957
m13	Salen	EDA	t-Bu	H	Cl	V	S4	TPSS	def2-SV(P)	-2878.154840
m13	Salen	EDA	t-Bu	H	Amine	V	S4	TPSS	def2-SV(P)	-2552.958489
m13	Salen	EDA	t-Bu	H	Amide	V	S4	TPSS	def2-SV(P)	-2552.524378
m13	Salen	EDA	t-Bu	H	Nothing	III	S4	TPSS	def2-SV(P)	-2342.727195
m13	Salen	EDA	t-Bu	H	Cl	III	S4	TPSS	def2-SV(P)	-2803.048246
m13	Salen	EDA	t-Bu	H	Amine	III	S4	TPSS	def2-SV(P)	-2477.844359
m13	Salen	EDA	t-Bu	H	Amide	III	S4	TPSS	def2-SV(P)	-2477.400928
m14	Salen	CHDA	t-Bu	H	Nothing	V	S4	TPSS	def2-SV(P)	-2573.808114
m14	Salen	CHDA	t-Bu	H	Cl	V	S4	TPSS	def2-SV(P)	-3034.116551
m14	Salen	CHDA	t-Bu	H	Amine	V	S4	TPSS	def2-SV(P)	-2708.922630
m14	Salen	CHDA	t-Bu	H	Amide	V	S4	TPSS	def2-SV(P)	-2708.484494
m14	Salen	CHDA	t-Bu	H	Nothing	III	S4	TPSS	def2-SV(P)	-2498.692518
m14	Salen	CHDA	t-Bu	H	Cl	III	S4	TPSS	def2-SV(P)	-2959.010165
m14	Salen	CHDA	t-Bu	H	Amine	III	S4	TPSS	def2-SV(P)	-2633.808401
m14	Salen	CHDA	t-Bu	H	Amide	III	S4	TPSS	def2-SV(P)	-2633.361731
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S4	TPSS	def2-SV(P)	-2732.157971
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S4	TPSS	def2-SV(P)	-3192.462510
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S4	TPSS	def2-SV(P)	-2867.270447
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S4	TPSS	def2-SV(P)	-2866.829559
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S4	TPSS	def2-SV(P)	-2657.037518
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S4	TPSS	def2-SV(P)	-3117.353493
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S4	TPSS	def2-SV(P)	-2792.153325
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S4	TPSS	def2-SV(P)	-2791.704798
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S4	TPSS	def2-SV(P)	-2888.122490
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S4	TPSS	def2-SV(P)	-3348.423892
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S4	TPSS	def2-SV(P)	-3023.233552
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S4	TPSS	def2-SV(P)	-3022.788891
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S4	TPSS	def2-SV(P)	-2813.002223
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S4	TPSS	def2-SV(P)	-3273.316396
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S4	TPSS	def2-SV(P)	-2948.115789
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S4	TPSS	def2-SV(P)	-2947.665501
m01	Acacen	EDA	None	None	Nothing	V	S0	TPSS	def2-TZVP	-1794.666406
m01	Acacen	EDA	None	None	Cl	V	S0	TPSS	def2-TZVP	-2255.145906
m01	Acacen	EDA	None	None	Amine	V	S0	TPSS	def2-TZVP	-1929.942425
m01	Acacen	EDA	None	None	Amide	V	S0	TPSS	def2-TZVP	-1929.536071
m01	Acacen	EDA	None	None	Nothing	III	S0	TPSS	def2-TZVP	-1719.307942
m01	Acacen	EDA	None	None	Cl	III	S0	TPSS	def2-TZVP	-2179.776957
m01	Acacen	EDA	None	None	Amine	III	S0	TPSS	def2-TZVP	-1854.565538
m01	Acacen	EDA	None	None	Amide	III	S0	TPSS	def2-TZVP	-1854.197933
m02	Acacen	CHDA	None	None	Nothing	V	S0	TPSS	def2-TZVP	-1950.803176
m02	Acacen	CHDA	None	None	Cl	V	S0	TPSS	def2-TZVP	-2411.273938
m02	Acacen	CHDA	None	None	Amine	V	S0	TPSS	def2-TZVP	-2086.074386
m02	Acacen	CHDA	None	None	Amide	V	S0	TPSS	def2-TZVP	-2085.664603
m02	Acacen	CHDA	None	None	Nothing	III	S0	TPSS	def2-TZVP	-1875.440189
m02	Acacen	CHDA	None	None	Cl	III	S0	TPSS	def2-TZVP	-2335.904752
m02	Acacen	CHDA	None	None	Amine	III	S0	TPSS	def2-TZVP	-2010.701117
m02	Acacen	CHDA	None	None	Amide	III	S0	TPSS	def2-TZVP	-2010.307960
m03	Salen	EDA	H	H	Nothing	V	S0	TPSS	def2-TZVP	-2102.143447
m03	Salen	EDA	H	H	Cl	V	S0	TPSS	def2-TZVP	-2562.612451
m03	Salen	EDA	H	H	Amine	V	S0	TPSS	def2-TZVP	-2237.418131
m03	Salen	EDA	H	H	Amide	V	S0	TPSS	def2-TZVP	-2237.006115
m03	Salen	EDA	H	H	Nothing	III	S0	TPSS	def2-TZVP	-2026.778618
m03	Salen	EDA	H	H	Cl	III	S0	TPSS	def2-TZVP	-2487.247332
m03	Salen	EDA	H	H	Amine	III	S0	TPSS	def2-TZVP	-2162.043634
m03	Salen	EDA	H	H	Amide	III	S0	TPSS	def2-TZVP	-2161.666654
m04	Salen	CHDA	H	H	Nothing	V	S0	TPSS	def2-TZVP	-2258.275887
m04	Salen	CHDA	H	H	Cl	V	S0	TPSS	def2-TZVP	-2718.743100
m04	Salen	CHDA	H	H	Amine	V	S0	TPSS	def2-TZVP	-2393.551507
m04	Salen	CHDA	H	H	Amide	V	S0	TPSS	def2-TZVP	-2393.134402
m04	Salen	CHDA	H	H	Nothing	III	S0	TPSS	def2-TZVP	-2182.909303
m04	Salen	CHDA	H	H	Cl	III	S0	TPSS	def2-TZVP	-2643.375028
m04	Salen	CHDA	H	H	Amine	III	S0	TPSS	def2-TZVP	-2318.175271
m04	Salen	CHDA	H	H	Amide	III	S0	TPSS	def2-TZVP	-2317.793826
m05	Salen	EDA	H	Me	Nothing	V	S0	TPSS	def2-TZVP	-2180.821282
m05	Salen	EDA	H	Me	Cl	V	S0	TPSS	def2-TZVP	-2641.285533
m05	Salen	EDA	H	Me	Amine	V	S0	TPSS	def2-TZVP	-2316.094638
m05	Salen	EDA	H	Me	Amide	V	S0	TPSS	def2-TZVP	-2315.678929
m05	Salen	EDA	H	Me	Nothing	III	S0	TPSS	def2-TZVP	-2105.456976

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m05	Salen	EDA	H	Me	Cl	III	S0	TPSS	def2-TZVP	-2565.921132
m05	Salen	EDA	H	Me	Amine	III	S0	TPSS	def2-TZVP	-2240.720198
m05	Salen	EDA	H	Me	Amide	III	S0	TPSS	def2-TZVP	-2240.340053
m06	Salen	CHDA	H	Me	Nothing	V	S0	TPSS	def2-TZVP	-2336.953299
m06	Salen	CHDA	H	Me	Cl	V	S0	TPSS	def2-TZVP	-2797.416182
m06	Salen	CHDA	H	Me	Amine	V	S0	TPSS	def2-TZVP	-2472.227852
m06	Salen	CHDA	H	Me	Amide	V	S0	TPSS	def2-TZVP	-2471.807209
m06	Salen	CHDA	H	Me	Nothing	III	S0	TPSS	def2-TZVP	-2261.587216
m06	Salen	CHDA	H	Me	Cl	III	S0	TPSS	def2-TZVP	-2722.048664
m06	Salen	CHDA	H	Me	Amine	III	S0	TPSS	def2-TZVP	-2396.851542
m06	Salen	CHDA	H	Me	Amide	III	S0	TPSS	def2-TZVP	-2396.467081
m07	Salen	EDA	Me	H	Nothing	V	S0	TPSS	def2-TZVP	-2180.822407
m07	Salen	EDA	Me	H	Cl	V	S0	TPSS	def2-TZVP	-2641.288214
m07	Salen	EDA	Me	H	Amine	V	S0	TPSS	def2-TZVP	-2316.095372
m07	Salen	EDA	Me	H	Amide	V	S0	TPSS	def2-TZVP	-2315.681381
m07	Salen	EDA	Me	H	Nothing	III	S0	TPSS	def2-TZVP	-2105.458282
m07	Salen	EDA	Me	H	Cl	III	S0	TPSS	def2-TZVP	-2565.922768
m07	Salen	EDA	Me	H	Amine	III	S0	TPSS	def2-TZVP	-2240.720195
m07	Salen	EDA	Me	H	Amide	III	S0	TPSS	def2-TZVP	-2240.340924
m08	Salen	CHDA	Me	H	Nothing	V	S0	TPSS	def2-TZVP	-2336.954514
m08	Salen	CHDA	Me	H	Cl	V	S0	TPSS	def2-TZVP	-2797.419314
m08	Salen	CHDA	Me	H	Amine	V	S0	TPSS	def2-TZVP	-2472.228482
m08	Salen	CHDA	Me	H	Amide	V	S0	TPSS	def2-TZVP	-2471.809628
m08	Salen	CHDA	Me	H	Nothing	III	S0	TPSS	def2-TZVP	-2261.588652
m08	Salen	CHDA	Me	H	Cl	III	S0	TPSS	def2-TZVP	-2722.050524
m08	Salen	CHDA	Me	H	Amine	III	S0	TPSS	def2-TZVP	-2396.851527
m08	Salen	CHDA	Me	H	Amide	III	S0	TPSS	def2-TZVP	-2396.468078
m09	Salen	EDA	Me	Me	Nothing	V	S0	TPSS	def2-TZVP	-2259.499935
m09	Salen	EDA	Me	Me	Cl	V	S0	TPSS	def2-TZVP	-2719.961192
m09	Salen	EDA	Me	Me	Amine	V	S0	TPSS	def2-TZVP	-2394.771764
m09	Salen	EDA	Me	Me	Amide	V	S0	TPSS	def2-TZVP	-2394.354248
m09	Salen	EDA	Me	Me	Nothing	III	S0	TPSS	def2-TZVP	-2184.136256
m09	Salen	EDA	Me	Me	Cl	III	S0	TPSS	def2-TZVP	-2644.596600
m09	Salen	EDA	Me	Me	Amine	III	S0	TPSS	def2-TZVP	-2319.396545
m09	Salen	EDA	Me	Me	Amide	III	S0	TPSS	def2-TZVP	-2319.014271
m10	Salen	CHDA	Me	Me	Nothing	V	S0	TPSS	def2-TZVP	-2415.631649
m10	Salen	CHDA	Me	Me	Cl	V	S0	TPSS	def2-TZVP	-2876.092465
m10	Salen	CHDA	Me	Me	Amine	V	S0	TPSS	def2-TZVP	-2550.904596
m10	Salen	CHDA	Me	Me	Amide	V	S0	TPSS	def2-TZVP	-2550.482449
m10	Salen	CHDA	Me	Me	Nothing	III	S0	TPSS	def2-TZVP	-2340.266235
m10	Salen	CHDA	Me	Me	Cl	III	S0	TPSS	def2-TZVP	-2800.724209
m10	Salen	CHDA	Me	Me	Amine	III	S0	TPSS	def2-TZVP	-2475.527589
m10	Salen	CHDA	Me	Me	Amide	III	S0	TPSS	def2-TZVP	-2475.141349
m11	Salen	EDA	H	t-Bu	Nothing	V	S0	TPSS	def2-TZVP	-2416.815832
m11	Salen	EDA	H	t-Bu	Cl	V	S0	TPSS	def2-TZVP	-2877.277458
m11	Salen	EDA	H	t-Bu	Amine	V	S0	TPSS	def2-TZVP	-2552.087913
m11	Salen	EDA	H	t-Bu	Amide	V	S0	TPSS	def2-TZVP	-2551.671148
m11	Salen	EDA	H	t-Bu	Nothing	III	S0	TPSS	def2-TZVP	-2341.450177
m11	Salen	EDA	H	t-Bu	Cl	III	S0	TPSS	def2-TZVP	-2801.912263
m11	Salen	EDA	H	t-Bu	Amine	III	S0	TPSS	def2-TZVP	-2476.712680
m11	Salen	EDA	H	t-Bu	Amide	III	S0	TPSS	def2-TZVP	-2476.330445
m12	Salen	CHDA	H	t-Bu	Nothing	V	S0	TPSS	def2-TZVP	-2572.947025
m12	Salen	CHDA	H	t-Bu	Cl	V	S0	TPSS	def2-TZVP	-3033.407839
m12	Salen	CHDA	H	t-Bu	Amine	V	S0	TPSS	def2-TZVP	-2708.221770
m12	Salen	CHDA	H	t-Bu	Amide	V	S0	TPSS	def2-TZVP	-2707.799085
m12	Salen	CHDA	H	t-Bu	Nothing	III	S0	TPSS	def2-TZVP	-2497.581296
m12	Salen	CHDA	H	t-Bu	Cl	III	S0	TPSS	def2-TZVP	-2958.040758
m12	Salen	CHDA	H	t-Bu	Amine	III	S0	TPSS	def2-TZVP	-2632.843963
m12	Salen	CHDA	H	t-Bu	Amide	III	S0	TPSS	def2-TZVP	-2632.457694
m13	Salen	EDA	t-Bu	H	Nothing	V	S0	TPSS	def2-TZVP	-2416.801769
m13	Salen	EDA	t-Bu	H	Cl	V	S0	TPSS	def2-TZVP	-2877.269937
m13	Salen	EDA	t-Bu	H	Amine	V	S0	TPSS	def2-TZVP	-2552.073906
m13	Salen	EDA	t-Bu	H	Amide	V	S0	TPSS	def2-TZVP	-2551.659446
m13	Salen	EDA	t-Bu	H	Nothing	III	S0	TPSS	def2-TZVP	-2341.438719
m13	Salen	EDA	t-Bu	H	Cl	III	S0	TPSS	def2-TZVP	-2801.901456
m13	Salen	EDA	t-Bu	H	Amine	III	S0	TPSS	def2-TZVP	-2476.699240
m13	Salen	EDA	t-Bu	H	Amide	III	S0	TPSS	def2-TZVP	-2476.313703
m14	Salen	CHDA	t-Bu	H	Nothing	V	S0	TPSS	def2-TZVP	-2572.928931
m14	Salen	CHDA	t-Bu	H	Cl	V	S0	TPSS	def2-TZVP	-3033.396996
m14	Salen	CHDA	t-Bu	H	Amine	V	S0	TPSS	def2-TZVP	-2708.206064
m14	Salen	CHDA	t-Bu	H	Amide	V	S0	TPSS	def2-TZVP	-2707.785106

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m14	Salen	CHDA	t-Bu	H	Nothing	III	S0	TPSS	def2-TZVP	-2497.571896
m14	Salen	CHDA	t-Bu	H	Cl	III	S0	TPSS	def2-TZVP	-2958.013306
m14	Salen	CHDA	t-Bu	H	Amine	III	S0	TPSS	def2-TZVP	-2632.830599
m14	Salen	CHDA	t-Bu	H	Amide	III	S0	TPSS	def2-TZVP	-2632.440467
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S0	TPSS	def2-TZVP	-2731.473861
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S0	TPSS	def2-TZVP	-3191.935231
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S0	TPSS	def2-TZVP	-2866.744189
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S0	TPSS	def2-TZVP	-2866.323879
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S0	TPSS	def2-TZVP	-2656.109724
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S0	TPSS	def2-TZVP	-3116.566858
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S0	TPSS	def2-TZVP	-2791.367971
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S0	TPSS	def2-TZVP	-2790.977514
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S0	TPSS	def2-TZVP	-2887.604491
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S0	TPSS	def2-TZVP	-3348.063084
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S0	TPSS	def2-TZVP	-3022.876467
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S0	TPSS	def2-TZVP	-3022.452040
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S0	TPSS	def2-TZVP	-2812.241946
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S0	TPSS	def2-TZVP	-3272.695261
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S0	TPSS	def2-TZVP	-2947.498153
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S0	TPSS	def2-TZVP	-2947.104249
m01	Acacen	EDA	None	None	Nothing	V	S2	TPSS	def2-TZVP	-1794.672240
m01	Acacen	EDA	None	None	Cl	V	S2	TPSS	def2-TZVP	-2255.149513
m01	Acacen	EDA	None	None	Amine	V	S2	TPSS	def2-TZVP	-1929.948810
m01	Acacen	EDA	None	None	Amide	V	S2	TPSS	def2-TZVP	-1929.539021
m01	Acacen	EDA	None	None	Nothing	III	S2	TPSS	def2-TZVP	-1719.281195
m01	Acacen	EDA	None	None	Cl	III	S2	TPSS	def2-TZVP	-2179.777808
m01	Acacen	EDA	None	None	Amine	III	S2	TPSS	def2-TZVP	-1854.574006
m01	Acacen	EDA	None	None	Amide	III	S2	TPSS	def2-TZVP	-1854.193057
m02	Acacen	CHDA	None	None	Nothing	V	S2	TPSS	def2-TZVP	-1950.806756
m02	Acacen	CHDA	None	None	Cl	V	S2	TPSS	def2-TZVP	-2411.278927
m02	Acacen	CHDA	None	None	Amine	V	S2	TPSS	def2-TZVP	-2086.082820
m02	Acacen	CHDA	None	None	Amide	V	S2	TPSS	def2-TZVP	-2085.668669
m02	Acacen	CHDA	None	None	Nothing	III	S2	TPSS	def2-TZVP	-1875.415581
m02	Acacen	CHDA	None	None	Cl	III	S2	TPSS	def2-TZVP	-2335.905080
m02	Acacen	CHDA	None	None	Amine	III	S2	TPSS	def2-TZVP	-2010.705721
m02	Acacen	CHDA	None	None	Amide	III	S2	TPSS	def2-TZVP	-2010.313676
m03	Salen	EDA	H	H	Nothing	V	S2	TPSS	def2-TZVP	-2102.151759
m03	Salen	EDA	H	H	Cl	V	S2	TPSS	def2-TZVP	-2562.614221
m03	Salen	EDA	H	H	Amine	V	S2	TPSS	def2-TZVP	-2237.419568
m03	Salen	EDA	H	H	Amide	V	S2	TPSS	def2-TZVP	-2237.003505
m03	Salen	EDA	H	H	Nothing	III	S2	TPSS	def2-TZVP	-2026.758304
m03	Salen	EDA	H	H	Cl	III	S2	TPSS	def2-TZVP	-2487.248785
m03	Salen	EDA	H	H	Amine	III	S2	TPSS	def2-TZVP	-2162.044893
m03	Salen	EDA	H	H	Amide	III	S2	TPSS	def2-TZVP	-2161.666202
m04	Salen	CHDA	H	H	Nothing	V	S2	TPSS	def2-TZVP	-2258.285219
m04	Salen	CHDA	H	H	Cl	V	S2	TPSS	def2-TZVP	-2718.743855
m04	Salen	CHDA	H	H	Amine	V	S2	TPSS	def2-TZVP	-2393.552748
m04	Salen	CHDA	H	H	Amide	V	S2	TPSS	def2-TZVP	-2393.133677
m04	Salen	CHDA	H	H	Nothing	III	S2	TPSS	def2-TZVP	-2182.890986
m04	Salen	CHDA	H	H	Cl	III	S2	TPSS	def2-TZVP	-2643.376065
m04	Salen	CHDA	H	H	Amine	III	S2	TPSS	def2-TZVP	-2318.176729
m04	Salen	CHDA	H	H	Amide	III	S2	TPSS	def2-TZVP	-2317.792991
m05	Salen	EDA	H	Me	Nothing	V	S2	TPSS	def2-TZVP	-2180.829621
m05	Salen	EDA	H	Me	Cl	V	S2	TPSS	def2-TZVP	-2641.287438
m05	Salen	EDA	H	Me	Amine	V	S2	TPSS	def2-TZVP	-2316.096246
m05	Salen	EDA	H	Me	Amide	V	S2	TPSS	def2-TZVP	-2315.676676
m05	Salen	EDA	H	Me	Nothing	III	S2	TPSS	def2-TZVP	-2105.436422
m05	Salen	EDA	H	Me	Cl	III	S2	TPSS	def2-TZVP	-2565.921973
m05	Salen	EDA	H	Me	Amine	III	S2	TPSS	def2-TZVP	-2240.721436
m05	Salen	EDA	H	Me	Amide	III	S2	TPSS	def2-TZVP	-2240.339151
m06	Salen	CHDA	H	Me	Nothing	V	S2	TPSS	def2-TZVP	-2336.962631
m06	Salen	CHDA	H	Me	Cl	V	S2	TPSS	def2-TZVP	-2797.417027
m06	Salen	CHDA	H	Me	Amine	V	S2	TPSS	def2-TZVP	-2472.229089
m06	Salen	CHDA	H	Me	Amide	V	S2	TPSS	def2-TZVP	-2471.806233
m06	Salen	CHDA	H	Me	Nothing	III	S2	TPSS	def2-TZVP	-2261.568652
m06	Salen	CHDA	H	Me	Cl	III	S2	TPSS	def2-TZVP	-2722.049393
m06	Salen	CHDA	H	Me	Amine	III	S2	TPSS	def2-TZVP	-2396.852943
m06	Salen	CHDA	H	Me	Amide	III	S2	TPSS	def2-TZVP	-2396.465850
m07	Salen	EDA	Me	H	Nothing	V	S2	TPSS	def2-TZVP	-2180.830563
m07	Salen	EDA	Me	H	Cl	V	S2	TPSS	def2-TZVP	-2641.291113
m07	Salen	EDA	Me	H	Amine	V	S2	TPSS	def2-TZVP	-2316.096870

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m07	Salen	EDA	Me	H	Amide	V	S2	TPSS	def2-TZVP	-2315.679443
m07	Salen	EDA	Me	H	Nothing	III	S2	TPSS	def2-TZVP	-2105.437608
m07	Salen	EDA	Me	H	Cl	III	S2	TPSS	def2-TZVP	-2565.924462
m07	Salen	EDA	Me	H	Amine	III	S2	TPSS	def2-TZVP	-2240.721706
m07	Salen	EDA	Me	H	Amide	III	S2	TPSS	def2-TZVP	-2240.340368
m08	Salen	CHDA	Me	H	Nothing	V	S2	TPSS	def2-TZVP	-2336.963771
m08	Salen	CHDA	Me	H	Cl	V	S2	TPSS	def2-TZVP	-2797.420601
m08	Salen	CHDA	Me	H	Amine	V	S2	TPSS	def2-TZVP	-2472.229897
m08	Salen	CHDA	Me	H	Amide	V	S2	TPSS	def2-TZVP	-2471.809219
m08	Salen	CHDA	Me	H	Nothing	III	S2	TPSS	def2-TZVP	-2261.569930
m08	Salen	CHDA	Me	H	Cl	III	S2	TPSS	def2-TZVP	-2722.051718
m08	Salen	CHDA	Me	H	Amine	III	S2	TPSS	def2-TZVP	-2396.853488
m08	Salen	CHDA	Me	H	Amide	III	S2	TPSS	def2-TZVP	-2396.467062
m09	Salen	EDA	Me	Me	Nothing	V	S2	TPSS	def2-TZVP	-2259.508156
m09	Salen	EDA	Me	Me	Cl	V	S2	TPSS	def2-TZVP	-2719.964340
m09	Salen	EDA	Me	Me	Amine	V	S2	TPSS	def2-TZVP	-2394.773309
m09	Salen	EDA	Me	Me	Amide	V	S2	TPSS	def2-TZVP	-2394.352359
m09	Salen	EDA	Me	Me	Nothing	III	S2	TPSS	def2-TZVP	-2184.115366
m09	Salen	EDA	Me	Me	Cl	III	S2	TPSS	def2-TZVP	-2644.597601
m09	Salen	EDA	Me	Me	Amine	III	S2	TPSS	def2-TZVP	-2319.397982
m09	Salen	EDA	Me	Me	Amide	III	S2	TPSS	def2-TZVP	-2319.013343
m10	Salen	CHDA	Me	Me	Nothing	V	S2	TPSS	def2-TZVP	-2415.640959
m10	Salen	CHDA	Me	Me	Cl	V	S2	TPSS	def2-TZVP	-2876.093788
m10	Salen	CHDA	Me	Me	Amine	V	S2	TPSS	def2-TZVP	-2550.906034
m10	Salen	CHDA	Me	Me	Amide	V	S2	TPSS	def2-TZVP	-2550.482043
m10	Salen	CHDA	Me	Me	Nothing	III	S2	TPSS	def2-TZVP	-2340.247243
m10	Salen	CHDA	Me	Me	Cl	III	S2	TPSS	def2-TZVP	-2800.725096
m10	Salen	CHDA	Me	Me	Amine	III	S2	TPSS	def2-TZVP	-2475.529408
m10	Salen	CHDA	Me	Me	Amide	III	S2	TPSS	def2-TZVP	-2475.139987
m11	Salen	EDA	H	t-Bu	Nothing	V	S2	TPSS	def2-TZVP	-2416.824189
m11	Salen	EDA	H	t-Bu	Cl	V	S2	TPSS	def2-TZVP	-2877.278367
m11	Salen	EDA	H	t-Bu	Amine	V	S2	TPSS	def2-TZVP	-2552.088420
m11	Salen	EDA	H	t-Bu	Amide	V	S2	TPSS	def2-TZVP	-2551.668460
m11	Salen	EDA	H	t-Bu	Nothing	III	S2	TPSS	def2-TZVP	-2341.430100
m11	Salen	EDA	H	t-Bu	Cl	III	S2	TPSS	def2-TZVP	-2801.913819
m11	Salen	EDA	H	t-Bu	Amine	III	S2	TPSS	def2-TZVP	-2476.714202
m11	Salen	EDA	H	t-Bu	Amide	III	S2	TPSS	def2-TZVP	-2476.330044
m12	Salen	CHDA	H	t-Bu	Nothing	V	S2	TPSS	def2-TZVP	-2572.955874
m12	Salen	CHDA	H	t-Bu	Cl	V	S2	TPSS	def2-TZVP	-3033.407791
m12	Salen	CHDA	H	t-Bu	Amine	V	S2	TPSS	def2-TZVP	-2708.223018
m12	Salen	CHDA	H	t-Bu	Amide	V	S2	TPSS	def2-TZVP	-2707.798277
m12	Salen	CHDA	H	t-Bu	Nothing	III	S2	TPSS	def2-TZVP	-2497.563014
m12	Salen	CHDA	H	t-Bu	Cl	III	S2	TPSS	def2-TZVP	-2958.041529
m12	Salen	CHDA	H	t-Bu	Amine	III	S2	TPSS	def2-TZVP	-2632.845510
m12	Salen	CHDA	H	t-Bu	Amide	III	S2	TPSS	def2-TZVP	-2632.457066
m13	Salen	EDA	t-Bu	H	Nothing	V	S2	TPSS	def2-TZVP	-2416.807015
m13	Salen	EDA	t-Bu	H	Cl	V	S2	TPSS	def2-TZVP	-2877.271271
m13	Salen	EDA	t-Bu	H	Amine	V	S2	TPSS	def2-TZVP	-2552.074994
m13	Salen	EDA	t-Bu	H	Amide	V	S2	TPSS	def2-TZVP	-2551.659505
m13	Salen	EDA	t-Bu	H	Nothing	III	S2	TPSS	def2-TZVP	-2341.420571
m13	Salen	EDA	t-Bu	H	Cl	III	S2	TPSS	def2-TZVP	-2801.904314
m13	Salen	EDA	t-Bu	H	Amine	III	S2	TPSS	def2-TZVP	-2476.703912
m13	Salen	EDA	t-Bu	H	Amide	III	S2	TPSS	def2-TZVP	-2476.315657
m14	Salen	CHDA	t-Bu	H	Nothing	V	S2	TPSS	def2-TZVP	-2572.942163
m14	Salen	CHDA	t-Bu	H	Cl	V	S2	TPSS	def2-TZVP	-3033.400533
m14	Salen	CHDA	t-Bu	H	Amine	V	S2	TPSS	def2-TZVP	-2708.208254
m14	Salen	CHDA	t-Bu	H	Amide	V	S2	TPSS	def2-TZVP	-2707.789062
m14	Salen	CHDA	t-Bu	H	Nothing	III	S2	TPSS	def2-TZVP	-2497.552847
m14	Salen	CHDA	t-Bu	H	Cl	III	S2	TPSS	def2-TZVP	-2958.031668
m14	Salen	CHDA	t-Bu	H	Amine	III	S2	TPSS	def2-TZVP	-2632.835633
m14	Salen	CHDA	t-Bu	H	Amide	III	S2	TPSS	def2-TZVP	-2632.442147
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S2	TPSS	def2-TZVP	-2731.479048
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S2	TPSS	def2-TZVP	-3191.937267
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S2	TPSS	def2-TZVP	-2866.746208
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S2	TPSS	def2-TZVP	-2866.324248
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S2	TPSS	def2-TZVP	-2656.091547
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S2	TPSS	def2-TZVP	-3116.569302
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S2	TPSS	def2-TZVP	-2791.372882
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S2	TPSS	def2-TZVP	-2790.979618
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S2	TPSS	def2-TZVP	-2887.610741
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S2	TPSS	def2-TZVP	-3348.066814

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S2	TPSS	def2-TZVP	-3022.878745
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S2	TPSS	def2-TZVP	-3022.453802
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S2	TPSS	def2-TZVP	-2812.223264
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S2	TPSS	def2-TZVP	-3272.697471
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S2	TPSS	def2-TZVP	-2947.503519
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S2	TPSS	def2-TZVP	-2947.105959
m01	Acacen	EDA	None	None	Nothing	V	S4	TPSS	def2-TZVP	-1794.578751
m01	Acacen	EDA	None	None	Cl	V	S4	TPSS	def2-TZVP	-2255.059263
m01	Acacen	EDA	None	None	Amine	V	S4	TPSS	def2-TZVP	-1929.855184
m01	Acacen	EDA	None	None	Amide	V	S4	TPSS	def2-TZVP	-1929.468691
m01	Acacen	EDA	None	None	Nothing	III	S4	TPSS	def2-TZVP	-1719.245949
m01	Acacen	EDA	None	None	Cl	III	S4	TPSS	def2-TZVP	-2179.748816
m01	Acacen	EDA	None	None	Amine	III	S4	TPSS	def2-TZVP	-1854.548449
m01	Acacen	EDA	None	None	Amide	III	S4	TPSS	def2-TZVP	-1854.157658
m02	Acacen	CHDA	None	None	Nothing	V	S4	TPSS	def2-TZVP	-1950.712892
m02	Acacen	CHDA	None	None	Cl	V	S4	TPSS	def2-TZVP	-2411.187409
m02	Acacen	CHDA	None	None	Amine	V	S4	TPSS	def2-TZVP	-2085.987733
m02	Acacen	CHDA	None	None	Amide	V	S4	TPSS	def2-TZVP	-2085.596140
m02	Acacen	CHDA	None	None	Nothing	III	S4	TPSS	def2-TZVP	-1875.380224
m02	Acacen	CHDA	None	None	Cl	III	S4	TPSS	def2-TZVP	-2335.878906
m02	Acacen	CHDA	None	None	Amine	III	S4	TPSS	def2-TZVP	-2010.669318
m02	Acacen	CHDA	None	None	Amide	III	S4	TPSS	def2-TZVP	-2010.280837
m03	Salen	EDA	H	H	Nothing	V	S4	TPSS	def2-TZVP	-2102.066648
m03	Salen	EDA	H	H	Cl	V	S4	TPSS	def2-TZVP	-2562.531067
m03	Salen	EDA	H	H	Amine	V	S4	TPSS	def2-TZVP	-2237.335289
m03	Salen	EDA	H	H	Amide	V	S4	TPSS	def2-TZVP	-2236.938598
m03	Salen	EDA	H	H	Nothing	III	S4	TPSS	def2-TZVP	-2026.729683
m03	Salen	EDA	H	H	Cl	III	S4	TPSS	def2-TZVP	-2487.223140
m03	Salen	EDA	H	H	Amine	III	S4	TPSS	def2-TZVP	-2162.021028
m03	Salen	EDA	H	H	Amide	III	S4	TPSS	def2-TZVP	-2161.630742
m04	Salen	CHDA	H	H	Nothing	V	S4	TPSS	def2-TZVP	-2258.198442
m04	Salen	CHDA	H	H	Cl	V	S4	TPSS	def2-TZVP	-2718.659001
m04	Salen	CHDA	H	H	Amine	V	S4	TPSS	def2-TZVP	-2393.466944
m04	Salen	CHDA	H	H	Amide	V	S4	TPSS	def2-TZVP	-2393.066399
m04	Salen	CHDA	H	H	Nothing	III	S4	TPSS	def2-TZVP	-2182.862470
m04	Salen	CHDA	H	H	Cl	III	S4	TPSS	def2-TZVP	-2643.350924
m04	Salen	CHDA	H	H	Amine	III	S4	TPSS	def2-TZVP	-2318.150305
m04	Salen	CHDA	H	H	Amide	III	S4	TPSS	def2-TZVP	-2317.757954
m05	Salen	EDA	H	Me	Nothing	V	S4	TPSS	def2-TZVP	-2180.751618
m05	Salen	EDA	H	Me	Cl	V	S4	TPSS	def2-TZVP	-2641.207765
m05	Salen	EDA	H	Me	Amine	V	S4	TPSS	def2-TZVP	-2316.017957
m05	Salen	EDA	H	Me	Amide	V	S4	TPSS	def2-TZVP	-2315.612535
m05	Salen	EDA	H	Me	Nothing	III	S4	TPSS	def2-TZVP	-2105.407029
m05	Salen	EDA	H	Me	Cl	III	S4	TPSS	def2-TZVP	-2565.896848
m05	Salen	EDA	H	Me	Amine	III	S4	TPSS	def2-TZVP	-2240.699943
m05	Salen	EDA	H	Me	Amide	III	S4	TPSS	def2-TZVP	-2240.303578
m06	Salen	CHDA	H	Me	Nothing	V	S4	TPSS	def2-TZVP	-2336.882708
m06	Salen	CHDA	H	Me	Cl	V	S4	TPSS	def2-TZVP	-2797.335455
m06	Salen	CHDA	H	Me	Amine	V	S4	TPSS	def2-TZVP	-2472.149172
m06	Salen	CHDA	H	Me	Amide	V	S4	TPSS	def2-TZVP	-2471.740338
m06	Salen	CHDA	H	Me	Nothing	III	S4	TPSS	def2-TZVP	-2261.539387
m06	Salen	CHDA	H	Me	Cl	III	S4	TPSS	def2-TZVP	-2722.023834
m06	Salen	CHDA	H	Me	Amine	III	S4	TPSS	def2-TZVP	-2396.826200
m06	Salen	CHDA	H	Me	Amide	III	S4	TPSS	def2-TZVP	-2396.430538
m07	Salen	EDA	Me	H	Nothing	V	S4	TPSS	def2-TZVP	-2180.749470
m07	Salen	EDA	Me	H	Cl	V	S4	TPSS	def2-TZVP	-2641.207093
m07	Salen	EDA	Me	H	Amine	V	S4	TPSS	def2-TZVP	-2316.015697
m07	Salen	EDA	Me	H	Amide	V	S4	TPSS	def2-TZVP	-2315.613477
m07	Salen	EDA	Me	H	Nothing	III	S4	TPSS	def2-TZVP	-2105.408058
m07	Salen	EDA	Me	H	Cl	III	S4	TPSS	def2-TZVP	-2565.899550
m07	Salen	EDA	Me	H	Amine	III	S4	TPSS	def2-TZVP	-2240.683646
m07	Salen	EDA	Me	H	Amide	III	S4	TPSS	def2-TZVP	-2240.305030
m08	Salen	CHDA	Me	H	Nothing	V	S4	TPSS	def2-TZVP	-2336.880899
m08	Salen	CHDA	Me	H	Cl	V	S4	TPSS	def2-TZVP	-2797.335393
m08	Salen	CHDA	Me	H	Amine	V	S4	TPSS	def2-TZVP	-2472.144988
m08	Salen	CHDA	Me	H	Amide	V	S4	TPSS	def2-TZVP	-2471.741248
m08	Salen	CHDA	Me	H	Nothing	III	S4	TPSS	def2-TZVP	-2261.540539
m08	Salen	CHDA	Me	H	Cl	III	S4	TPSS	def2-TZVP	-2722.027252
m08	Salen	CHDA	Me	H	Amine	III	S4	TPSS	def2-TZVP	-2396.815918
m08	Salen	CHDA	Me	H	Amide	III	S4	TPSS	def2-TZVP	-2396.432279
m09	Salen	EDA	Me	Me	Nothing	V	S4	TPSS	def2-TZVP	-2259.433052

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m09	Salen	EDA	Me	Me	Cl	V	S4	TPSS	def2-TZVP	-2719.885757
m09	Salen	EDA	Me	Me	Amine	V	S4	TPSS	def2-TZVP	-2394.697294
m09	Salen	EDA	Me	Me	Amide	V	S4	TPSS	def2-TZVP	-2394.287538
m09	Salen	EDA	Me	Me	Nothing	III	S4	TPSS	def2-TZVP	-2184.085102
m09	Salen	EDA	Me	Me	Cl	III	S4	TPSS	def2-TZVP	-2644.572937
m09	Salen	EDA	Me	Me	Amine	III	S4	TPSS	def2-TZVP	-2319.373014
m09	Salen	EDA	Me	Me	Amide	III	S4	TPSS	def2-TZVP	-2318.977643
m10	Salen	CHDA	Me	Me	Nothing	V	S4	TPSS	def2-TZVP	-2415.563929
m10	Salen	CHDA	Me	Me	Cl	V	S4	TPSS	def2-TZVP	-2876.013948
m10	Salen	CHDA	Me	Me	Amine	V	S4	TPSS	def2-TZVP	-2550.828210
m10	Salen	CHDA	Me	Me	Amide	V	S4	TPSS	def2-TZVP	-2550.415267
m10	Salen	CHDA	Me	Me	Nothing	III	S4	TPSS	def2-TZVP	-2340.217183
m10	Salen	CHDA	Me	Me	Cl	III	S4	TPSS	def2-TZVP	-2800.700145
m10	Salen	CHDA	Me	Me	Amine	III	S4	TPSS	def2-TZVP	-2475.491961
m10	Salen	CHDA	Me	Me	Amide	III	S4	TPSS	def2-TZVP	-2475.104874
m11	Salen	EDA	H	t-Bu	Nothing	V	S4	TPSS	def2-TZVP	-2416.746432
m11	Salen	EDA	H	t-Bu	Cl	V	S4	TPSS	def2-TZVP	-2877.198995
m11	Salen	EDA	H	t-Bu	Amine	V	S4	TPSS	def2-TZVP	-2552.011022
m11	Salen	EDA	H	t-Bu	Amide	V	S4	TPSS	def2-TZVP	-2551.603612
m11	Salen	EDA	H	t-Bu	Nothing	III	S4	TPSS	def2-TZVP	-2341.400811
m11	Salen	EDA	H	t-Bu	Cl	III	S4	TPSS	def2-TZVP	-2801.888909
m11	Salen	EDA	H	t-Bu	Amine	III	S4	TPSS	def2-TZVP	-2476.692946
m11	Salen	EDA	H	t-Bu	Amide	III	S4	TPSS	def2-TZVP	-2476.294196
m12	Salen	CHDA	H	t-Bu	Nothing	V	S4	TPSS	def2-TZVP	-2572.876975
m12	Salen	CHDA	H	t-Bu	Cl	V	S4	TPSS	def2-TZVP	-3033.327009
m12	Salen	CHDA	H	t-Bu	Amine	V	S4	TPSS	def2-TZVP	-2708.142777
m12	Salen	CHDA	H	t-Bu	Amide	V	S4	TPSS	def2-TZVP	-2707.731505
m12	Salen	CHDA	H	t-Bu	Nothing	III	S4	TPSS	def2-TZVP	-2497.533567
m12	Salen	CHDA	H	t-Bu	Cl	III	S4	TPSS	def2-TZVP	-2958.016127
m12	Salen	CHDA	H	t-Bu	Amine	III	S4	TPSS	def2-TZVP	-2632.818960
m12	Salen	CHDA	H	t-Bu	Amide	III	S4	TPSS	def2-TZVP	-2632.421845
m13	Salen	EDA	t-Bu	H	Nothing	V	S4	TPSS	def2-TZVP	-2416.730240
m13	Salen	EDA	t-Bu	H	Cl	V	S4	TPSS	def2-TZVP	-2877.188555
m13	Salen	EDA	t-Bu	H	Amine	V	S4	TPSS	def2-TZVP	-2551.994172
m13	Salen	EDA	t-Bu	H	Amide	V	S4	TPSS	def2-TZVP	-2551.590404
m13	Salen	EDA	t-Bu	H	Nothing	III	S4	TPSS	def2-TZVP	-2341.387128
m13	Salen	EDA	t-Bu	H	Cl	III	S4	TPSS	def2-TZVP	-2801.878852
m13	Salen	EDA	t-Bu	H	Amine	III	S4	TPSS	def2-TZVP	-2476.672732
m13	Salen	EDA	t-Bu	H	Amide	III	S4	TPSS	def2-TZVP	-2476.282769
m14	Salen	CHDA	t-Bu	H	Nothing	V	S4	TPSS	def2-TZVP	-2572.853650
m14	Salen	CHDA	t-Bu	H	Cl	V	S4	TPSS	def2-TZVP	-3033.316040
m14	Salen	CHDA	t-Bu	H	Amine	V	S4	TPSS	def2-TZVP	-2708.126678
m14	Salen	CHDA	t-Bu	H	Amide	V	S4	TPSS	def2-TZVP	-2707.717970
m14	Salen	CHDA	t-Bu	H	Nothing	III	S4	TPSS	def2-TZVP	-2497.518524
m14	Salen	CHDA	t-Bu	H	Cl	III	S4	TPSS	def2-TZVP	-2958.006301
m14	Salen	CHDA	t-Bu	H	Amine	III	S4	TPSS	def2-TZVP	-2632.803848
m14	Salen	CHDA	t-Bu	H	Amide	III	S4	TPSS	def2-TZVP	-2632.409825
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S4	TPSS	def2-TZVP	-2731.407458
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S4	TPSS	def2-TZVP	-3191.856657
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S4	TPSS	def2-TZVP	-2866.667174
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S4	TPSS	def2-TZVP	-2866.255624
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S4	TPSS	def2-TZVP	-2656.057844
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S4	TPSS	def2-TZVP	-3116.543704
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S4	TPSS	def2-TZVP	-2791.341563
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S4	TPSS	def2-TZVP	-2790.946267
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S4	TPSS	def2-TZVP	-2887.538537
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S4	TPSS	def2-TZVP	-3347.984763
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S4	TPSS	def2-TZVP	-3022.800095
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S4	TPSS	def2-TZVP	-3022.383291
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S4	TPSS	def2-TZVP	-2812.188734
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S4	TPSS	def2-TZVP	-3272.672103
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S4	TPSS	def2-TZVP	-2947.471880
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S4	TPSS	def2-TZVP	-2947.073296
m01	Acacen	EDA	None	None	Nothing	V	S0	TPSS	DefBas-3	-1794.599650
m01	Acacen	EDA	None	None	Cl	V	S0	TPSS	DefBas-3	-2255.074336
m01	Acacen	EDA	None	None	Amine	V	S0	TPSS	DefBas-3	-1929.862511
m01	Acacen	EDA	None	None	Amide	V	S0	TPSS	DefBas-3	-1929.455282
m01	Acacen	EDA	None	None	Nothing	III	S0	TPSS	DefBas-3	-1719.243725
m01	Acacen	EDA	None	None	Cl	III	S0	TPSS	DefBas-3	-2179.709017
m01	Acacen	EDA	None	None	Amine	III	S0	TPSS	DefBas-3	-1854.490615
m01	Acacen	EDA	None	None	Amide	III	S0	TPSS	DefBas-3	-1854.123569

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m02	Acacen	CHDA	None	None	Nothing	V	S0	TPSS	DefBas-3	-1950.725188
m02	Acacen	CHDA	None	None	Cl	V	S0	TPSS	DefBas-3	-2411.190671
m02	Acacen	CHDA	None	None	Amine	V	S0	TPSS	DefBas-3	-2085.982871
m02	Acacen	CHDA	None	None	Amide	V	S0	TPSS	DefBas-3	-2085.572007
m02	Acacen	CHDA	None	None	Nothing	III	S0	TPSS	DefBas-3	-1875.365148
m02	Acacen	CHDA	None	None	Cl	III	S0	TPSS	DefBas-3	-2335.825376
m02	Acacen	CHDA	None	None	Amine	III	S0	TPSS	DefBas-3	-2010.615219
m02	Acacen	CHDA	None	None	Amide	III	S0	TPSS	DefBas-3	-2010.222376
m03	Salen	EDA	H	H	Nothing	V	S0	TPSS	DefBas-3	-2102.055485
m03	Salen	EDA	H	H	Cl	V	S0	TPSS	DefBas-3	-2562.519410
m03	Salen	EDA	H	H	Amine	V	S0	TPSS	DefBas-3	-2237.316941
m03	Salen	EDA	H	H	Amide	V	S0	TPSS	DefBas-3	-2236.904250
m03	Salen	EDA	H	H	Nothing	III	S0	TPSS	DefBas-3	-2026.694250
m03	Salen	EDA	H	H	Cl	III	S0	TPSS	DefBas-3	-2487.159078
m03	Salen	EDA	H	H	Amine	III	S0	TPSS	DefBas-3	-2161.948605
m03	Salen	EDA	H	H	Amide	III	S0	TPSS	DefBas-3	-2161.571924
m04	Salen	CHDA	H	H	Nothing	V	S0	TPSS	DefBas-3	-2258.176472
m04	Salen	CHDA	H	H	Cl	V	S0	TPSS	DefBas-3	-2718.638510
m04	Salen	CHDA	H	H	Amine	V	S0	TPSS	DefBas-3	-2393.438473
m04	Salen	CHDA	H	H	Amide	V	S0	TPSS	DefBas-3	-2393.020811
m04	Salen	CHDA	H	H	Nothing	III	S0	TPSS	DefBas-3	-2182.814079
m04	Salen	CHDA	H	H	Cl	III	S0	TPSS	DefBas-3	-2643.275348
m04	Salen	CHDA	H	H	Amine	III	S0	TPSS	DefBas-3	-2318.068969
m04	Salen	CHDA	H	H	Amide	III	S0	TPSS	DefBas-3	-2317.687629
m05	Salen	EDA	H	Me	Nothing	V	S0	TPSS	DefBas-3	-2180.726735
m05	Salen	EDA	H	Me	Cl	V	S0	TPSS	DefBas-3	-2641.186068
m05	Salen	EDA	H	Me	Amine	V	S0	TPSS	DefBas-3	-2315.986867
m05	Salen	EDA	H	Me	Amide	V	S0	TPSS	DefBas-3	-2315.570507
m05	Salen	EDA	H	Me	Nothing	III	S0	TPSS	DefBas-3	-2105.365905
m05	Salen	EDA	H	Me	Cl	III	S0	TPSS	DefBas-3	-2565.826221
m05	Salen	EDA	H	Me	Amine	III	S0	TPSS	DefBas-3	-2240.618546
m05	Salen	EDA	H	Me	Amide	III	S0	TPSS	DefBas-3	-2240.238695
m06	Salen	CHDA	H	Me	Nothing	V	S0	TPSS	DefBas-3	-2336.847274
m06	Salen	CHDA	H	Me	Cl	V	S0	TPSS	DefBas-3	-2797.305128
m06	Salen	CHDA	H	Me	Amine	V	S0	TPSS	DefBas-3	-2472.108216
m06	Salen	CHDA	H	Me	Amide	V	S0	TPSS	DefBas-3	-2471.687072
m06	Salen	CHDA	H	Me	Nothing	III	S0	TPSS	DefBas-3	-2261.485310
m06	Salen	CHDA	H	Me	Cl	III	S0	TPSS	DefBas-3	-2721.931399
m06	Salen	CHDA	H	Me	Amine	III	S0	TPSS	DefBas-3	-2396.738608
m06	Salen	CHDA	H	Me	Amide	III	S0	TPSS	DefBas-3	-2396.354254
m07	Salen	EDA	Me	H	Nothing	V	S0	TPSS	DefBas-3	-2180.728118
m07	Salen	EDA	Me	H	Cl	V	S0	TPSS	DefBas-3	-2641.189976
m07	Salen	EDA	Me	H	Amine	V	S0	TPSS	DefBas-3	-2315.987725
m07	Salen	EDA	Me	H	Amide	V	S0	TPSS	DefBas-3	-2315.573120
m07	Salen	EDA	Me	H	Nothing	III	S0	TPSS	DefBas-3	-2105.367224
m07	Salen	EDA	Me	H	Cl	III	S0	TPSS	DefBas-3	-2565.828095
m07	Salen	EDA	Me	H	Amine	III	S0	TPSS	DefBas-3	-2240.618495
m07	Salen	EDA	Me	H	Amide	III	S0	TPSS	DefBas-3	-2240.239645
m08	Salen	CHDA	Me	H	Nothing	V	S0	TPSS	DefBas-3	-2336.848840
m08	Salen	CHDA	Me	H	Cl	V	S0	TPSS	DefBas-3	-2797.308459
m08	Salen	CHDA	Me	H	Amine	V	S0	TPSS	DefBas-3	-2472.109017
m08	Salen	CHDA	Me	H	Amide	V	S0	TPSS	DefBas-3	-2471.689640
m08	Salen	CHDA	Me	H	Nothing	III	S0	TPSS	DefBas-3	-2261.486750
m08	Salen	CHDA	Me	H	Cl	III	S0	TPSS	DefBas-3	-2721.944449
m08	Salen	CHDA	Me	H	Amine	III	S0	TPSS	DefBas-3	-2396.738635
m08	Salen	CHDA	Me	H	Amide	III	S0	TPSS	DefBas-3	-2396.355323
m09	Salen	EDA	Me	Me	Nothing	V	S0	TPSS	DefBas-3	-2259.399144
m09	Salen	EDA	Me	Me	Cl	V	S0	TPSS	DefBas-3	-2719.856535
m09	Salen	EDA	Me	Me	Amine	V	S0	TPSS	DefBas-3	-2394.657544
m09	Salen	EDA	Me	Me	Amide	V	S0	TPSS	DefBas-3	-2394.239447
m09	Salen	EDA	Me	Me	Nothing	III	S0	TPSS	DefBas-3	-2184.038548
m09	Salen	EDA	Me	Me	Cl	III	S0	TPSS	DefBas-3	-2644.495350
m09	Salen	EDA	Me	Me	Amine	III	S0	TPSS	DefBas-3	-2319.288250
m09	Salen	EDA	Me	Me	Amide	III	S0	TPSS	DefBas-3	-2318.906390
m10	Salen	CHDA	Me	Me	Nothing	V	S0	TPSS	DefBas-3	-2415.519460
m10	Salen	CHDA	Me	Me	Cl	V	S0	TPSS	DefBas-3	-2875.975127
m10	Salen	CHDA	Me	Me	Amine	V	S0	TPSS	DefBas-3	-2550.778558
m10	Salen	CHDA	Me	Me	Amide	V	S0	TPSS	DefBas-3	-2550.355941
m10	Salen	CHDA	Me	Me	Nothing	III	S0	TPSS	DefBas-3	-2340.157686
m10	Salen	CHDA	Me	Me	Cl	III	S0	TPSS	DefBas-3	-2800.611566
m10	Salen	CHDA	Me	Me	Amine	III	S0	TPSS	DefBas-3	-2475.408106

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m10	Salen	CHDA	Me	Me	Amide	III	S0	TPSS	DefBas-3	-2475.021997
m11	Salen	EDA	H	t-Bu	Nothing	V	S0	TPSS	DefBas-3	-2416.701427
m11	Salen	EDA	H	t-Bu	Cl	V	S0	TPSS	DefBas-3	-2877.157986
m11	Salen	EDA	H	t-Bu	Amine	V	S0	TPSS	DefBas-3	-2551.960224
m11	Salen	EDA	H	t-Bu	Amide	V	S0	TPSS	DefBas-3	-2551.542788
m11	Salen	EDA	H	t-Bu	Nothing	III	S0	TPSS	DefBas-3	-2341.339176
m11	Salen	EDA	H	t-Bu	Cl	III	S0	TPSS	DefBas-3	-2801.797436
m11	Salen	EDA	H	t-Bu	Amine	III	S0	TPSS	DefBas-3	-2476.591021
m11	Salen	EDA	H	t-Bu	Amide	III	S0	TPSS	DefBas-3	-2476.209194
m12	Salen	CHDA	H	t-Bu	Nothing	V	S0	TPSS	DefBas-3	-2572.821001
m12	Salen	CHDA	H	t-Bu	Cl	V	S0	TPSS	DefBas-3	-3033.276814
m12	Salen	CHDA	H	t-Bu	Amine	V	S0	TPSS	DefBas-3	-2708.082217
m12	Salen	CHDA	H	t-Bu	Amide	V	S0	TPSS	DefBas-3	-2707.659072
m12	Salen	CHDA	H	t-Bu	Nothing	III	S0	TPSS	DefBas-3	-2497.459465
m12	Salen	CHDA	H	t-Bu	Cl	III	S0	TPSS	DefBas-3	-2957.914590
m12	Salen	CHDA	H	t-Bu	Amine	III	S0	TPSS	DefBas-3	-2632.711182
m12	Salen	CHDA	H	t-Bu	Amide	III	S0	TPSS	DefBas-3	-2632.324923
m13	Salen	EDA	t-Bu	H	Nothing	V	S0	TPSS	DefBas-3	-2416.687795
m13	Salen	EDA	t-Bu	H	Cl	V	S0	TPSS	DefBas-3	-2877.152290
m13	Salen	EDA	t-Bu	H	Amine	V	S0	TPSS	DefBas-3	-2551.946810
m13	Salen	EDA	t-Bu	H	Amide	V	S0	TPSS	DefBas-3	-2551.532304
m13	Salen	EDA	t-Bu	H	Nothing	III	S0	TPSS	DefBas-3	-2341.328359
m13	Salen	EDA	t-Bu	H	Cl	III	S0	TPSS	DefBas-3	-2801.786971
m13	Salen	EDA	t-Bu	H	Amine	III	S0	TPSS	DefBas-3	-2476.577321
m13	Salen	EDA	t-Bu	H	Amide	III	S0	TPSS	DefBas-3	-2476.192756
m14	Salen	CHDA	t-Bu	H	Nothing	V	S0	TPSS	DefBas-3	-2572.807821
m14	Salen	CHDA	t-Bu	H	Cl	V	S0	TPSS	DefBas-3	-3033.266736
m14	Salen	CHDA	t-Bu	H	Amine	V	S0	TPSS	DefBas-3	-2708.066823
m14	Salen	CHDA	t-Bu	H	Amide	V	S0	TPSS	DefBas-3	-2707.646476
m14	Salen	CHDA	t-Bu	H	Nothing	III	S0	TPSS	DefBas-3	-2497.450272
m14	Salen	CHDA	t-Bu	H	Cl	III	S0	TPSS	DefBas-3	-2957.889561
m14	Salen	CHDA	t-Bu	H	Amine	III	S0	TPSS	DefBas-3	-2632.697564
m14	Salen	CHDA	t-Bu	H	Amide	III	S0	TPSS	DefBas-3	-2632.308041
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S0	TPSS	DefBas-3	-2731.333546
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S0	TPSS	DefBas-3	-3191.791501
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S0	TPSS	DefBas-3	-2866.590553
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S0	TPSS	DefBas-3	-2866.169835
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S0	TPSS	DefBas-3	-2655.972867
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S0	TPSS	DefBas-3	-3116.425525
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S0	TPSS	DefBas-3	-2791.219550
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S0	TPSS	DefBas-3	-2790.830075
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S0	TPSS	DefBas-3	-2887.452972
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S0	TPSS	DefBas-3	-3347.906471
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S0	TPSS	DefBas-3	-3022.711042
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S0	TPSS	DefBas-3	-3022.286242
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S0	TPSS	DefBas-3	-2812.093897
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S0	TPSS	DefBas-3	-3272.543086
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S0	TPSS	DefBas-3	-2947.338779
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S0	TPSS	DefBas-3	-2946.945559
m01	Acacen	EDA	None	None	Nothing	V	S2	TPSS	DefBas-3	-1794.604464
m01	Acacen	EDA	None	None	Cl	V	S2	TPSS	DefBas-3	-2255.077898
m01	Acacen	EDA	None	None	Amine	V	S2	TPSS	DefBas-3	-1929.868364
m01	Acacen	EDA	None	None	Amide	V	S2	TPSS	DefBas-3	-1929.457983
m01	Acacen	EDA	None	None	Nothing	III	S2	TPSS	DefBas-3	-1719.220548
m01	Acacen	EDA	None	None	Cl	III	S2	TPSS	DefBas-3	-2179.710759
m01	Acacen	EDA	None	None	Amine	III	S2	TPSS	DefBas-3	-1854.500294
m01	Acacen	EDA	None	None	Amide	III	S2	TPSS	DefBas-3	-1854.118008
m02	Acacen	CHDA	None	None	Nothing	V	S2	TPSS	DefBas-3	-1950.727223
m02	Acacen	CHDA	None	None	Cl	V	S2	TPSS	DefBas-3	-2411.195703
m02	Acacen	CHDA	None	None	Amine	V	S2	TPSS	DefBas-3	-2085.990609
m02	Acacen	CHDA	None	None	Amide	V	S2	TPSS	DefBas-3	-2085.576002
m02	Acacen	CHDA	None	None	Nothing	III	S2	TPSS	DefBas-3	-1875.343617
m02	Acacen	CHDA	None	None	Cl	III	S2	TPSS	DefBas-3	-2335.826820
m02	Acacen	CHDA	None	None	Amine	III	S2	TPSS	DefBas-3	-2010.620201
m02	Acacen	CHDA	None	None	Amide	III	S2	TPSS	DefBas-3	-2010.227247
m03	Salen	EDA	H	H	Nothing	V	S2	TPSS	DefBas-3	-2102.063409
m03	Salen	EDA	H	H	Cl	V	S2	TPSS	DefBas-3	-2562.522257
m03	Salen	EDA	H	H	Amine	V	S2	TPSS	DefBas-3	-2237.318914
m03	Salen	EDA	H	H	Amide	V	S2	TPSS	DefBas-3	-2236.902087
m03	Salen	EDA	H	H	Nothing	III	S2	TPSS	DefBas-3	-2026.677539
m03	Salen	EDA	H	H	Cl	III	S2	TPSS	DefBas-3	-2487.160977

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m03	Salen	EDA	H	H	Amine	III	S2	TPSS	DefBas-3	-2161.950385
m03	Salen	EDA	H	H	Amide	III	S2	TPSS	DefBas-3	-2161.571061
m04	Salen	CHDA	H	H	Nothing	V	S2	TPSS	DefBas-3	-2258.185118
m04	Salen	CHDA	H	H	Cl	V	S2	TPSS	DefBas-3	-2718.640212
m04	Salen	CHDA	H	H	Amine	V	S2	TPSS	DefBas-3	-2393.440364
m04	Salen	CHDA	H	H	Amide	V	S2	TPSS	DefBas-3	-2393.020391
m04	Salen	CHDA	H	H	Nothing	III	S2	TPSS	DefBas-3	-2182.798916
m04	Salen	CHDA	H	H	Cl	III	S2	TPSS	DefBas-3	-2643.277084
m04	Salen	CHDA	H	H	Amine	III	S2	TPSS	DefBas-3	-2318.070750
m04	Salen	CHDA	H	H	Amide	III	S2	TPSS	DefBas-3	-2317.686558
m05	Salen	EDA	H	Me	Nothing	V	S2	TPSS	DefBas-3	-2180.734643
m05	Salen	EDA	H	Me	Cl	V	S2	TPSS	DefBas-3	-2641.189067
m05	Salen	EDA	H	Me	Amine	V	S2	TPSS	DefBas-3	-2315.989020
m05	Salen	EDA	H	Me	Amide	V	S2	TPSS	DefBas-3	-2315.568515
m05	Salen	EDA	H	Me	Nothing	III	S2	TPSS	DefBas-3	-2105.349076
m05	Salen	EDA	H	Me	Cl	III	S2	TPSS	DefBas-3	-2565.827566
m05	Salen	EDA	H	Me	Amine	III	S2	TPSS	DefBas-3	-2240.620262
m05	Salen	EDA	H	Me	Amide	III	S2	TPSS	DefBas-3	-2240.237342
m06	Salen	CHDA	H	Me	Nothing	V	S2	TPSS	DefBas-3	-2336.855934
m06	Salen	CHDA	H	Me	Cl	V	S2	TPSS	DefBas-3	-2797.306986
m06	Salen	CHDA	H	Me	Amine	V	S2	TPSS	DefBas-3	-2472.110121
m06	Salen	CHDA	H	Me	Amide	V	S2	TPSS	DefBas-3	-2471.686680
m06	Salen	CHDA	H	Me	Nothing	III	S2	TPSS	DefBas-3	-2261.469996
m06	Salen	CHDA	H	Me	Cl	III	S2	TPSS	DefBas-3	-2721.943805
m06	Salen	CHDA	H	Me	Amine	III	S2	TPSS	DefBas-3	-2396.740274
m06	Salen	CHDA	H	Me	Amide	III	S2	TPSS	DefBas-3	-2396.352724
m07	Salen	EDA	Me	H	Nothing	V	S2	TPSS	DefBas-3	-2180.735709
m07	Salen	EDA	Me	H	Cl	V	S2	TPSS	DefBas-3	-2641.192819
m07	Salen	EDA	Me	H	Amine	V	S2	TPSS	DefBas-3	-2315.989728
m07	Salen	EDA	Me	H	Amide	V	S2	TPSS	DefBas-3	-2315.571245
m07	Salen	EDA	Me	H	Nothing	III	S2	TPSS	DefBas-3	-2105.350349
m07	Salen	EDA	Me	H	Cl	III	S2	TPSS	DefBas-3	-2565.830312
m07	Salen	EDA	Me	H	Amine	III	S2	TPSS	DefBas-3	-2240.620597
m07	Salen	EDA	Me	H	Amide	III	S2	TPSS	DefBas-3	-2240.238686
m08	Salen	CHDA	Me	H	Nothing	V	S2	TPSS	DefBas-3	-2336.857191
m08	Salen	CHDA	Me	H	Cl	V	S2	TPSS	DefBas-3	-2797.310637
m08	Salen	CHDA	Me	H	Amine	V	S2	TPSS	DefBas-3	-2472.111011
m08	Salen	CHDA	Me	H	Amide	V	S2	TPSS	DefBas-3	-2471.689394
m08	Salen	CHDA	Me	H	Nothing	III	S2	TPSS	DefBas-3	-2261.471375
m08	Salen	CHDA	Me	H	Cl	III	S2	TPSS	DefBas-3	-2721.946384
m08	Salen	CHDA	Me	H	Amine	III	S2	TPSS	DefBas-3	-2396.740990
m08	Salen	CHDA	Me	H	Amide	III	S2	TPSS	DefBas-3	-2396.354100
m09	Salen	EDA	Me	Me	Nothing	V	S2	TPSS	DefBas-3	-2259.406697
m09	Salen	EDA	Me	Me	Cl	V	S2	TPSS	DefBas-3	-2719.859707
m09	Salen	EDA	Me	Me	Amine	V	S2	TPSS	DefBas-3	-2394.659582
m09	Salen	EDA	Me	Me	Amide	V	S2	TPSS	DefBas-3	-2394.237871
m09	Salen	EDA	Me	Me	Nothing	III	S2	TPSS	DefBas-3	-2184.021565
m09	Salen	EDA	Me	Me	Cl	III	S2	TPSS	DefBas-3	-2644.497215
m09	Salen	EDA	Me	Me	Amine	III	S2	TPSS	DefBas-3	-2319.290289
m09	Salen	EDA	Me	Me	Amide	III	S2	TPSS	DefBas-3	-2318.905005
m10	Salen	CHDA	Me	Me	Nothing	V	S2	TPSS	DefBas-3	-2415.527816
m10	Salen	CHDA	Me	Me	Cl	V	S2	TPSS	DefBas-3	-2875.977410
m10	Salen	CHDA	Me	Me	Amine	V	S2	TPSS	DefBas-3	-2550.780580
m10	Salen	CHDA	Me	Me	Amide	V	S2	TPSS	DefBas-3	-2550.355904
m10	Salen	CHDA	Me	Me	Nothing	III	S2	TPSS	DefBas-3	-2340.142138
m10	Salen	CHDA	Me	Me	Cl	III	S2	TPSS	DefBas-3	-2800.613192
m10	Salen	CHDA	Me	Me	Amine	III	S2	TPSS	DefBas-3	-2475.410310
m10	Salen	CHDA	Me	Me	Amide	III	S2	TPSS	DefBas-3	-2475.020365
m11	Salen	EDA	H	t-Bu	Nothing	V	S2	TPSS	DefBas-3	-2416.709310
m11	Salen	EDA	H	t-Bu	Cl	V	S2	TPSS	DefBas-3	-2877.160392
m11	Salen	EDA	H	t-Bu	Amine	V	S2	TPSS	DefBas-3	-2551.961481
m11	Salen	EDA	H	t-Bu	Amide	V	S2	TPSS	DefBas-3	-2551.540303
m11	Salen	EDA	H	t-Bu	Nothing	III	S2	TPSS	DefBas-3	-2341.322798
m11	Salen	EDA	H	t-Bu	Cl	III	S2	TPSS	DefBas-3	-2801.799507
m11	Salen	EDA	H	t-Bu	Amine	III	S2	TPSS	DefBas-3	-2476.593054
m11	Salen	EDA	H	t-Bu	Amide	III	S2	TPSS	DefBas-3	-2476.208294
m12	Salen	CHDA	H	t-Bu	Nothing	V	S2	TPSS	DefBas-3	-2572.829326
m12	Salen	CHDA	H	t-Bu	Cl	V	S2	TPSS	DefBas-3	-3033.278157
m12	Salen	CHDA	H	t-Bu	Amine	V	S2	TPSS	DefBas-3	-2708.084136
m12	Salen	CHDA	H	t-Bu	Amide	V	S2	TPSS	DefBas-3	-2707.658448
m12	Salen	CHDA	H	t-Bu	Nothing	III	S2	TPSS	DefBas-3	-2497.444465

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m12	Salen	CHDA	H	t-Bu	Cl	III	S2	TPSS	DefBas-3	-2957.916085
m12	Salen	CHDA	H	t-Bu	Amine	III	S2	TPSS	DefBas-3	-2632.712927
m12	Salen	CHDA	H	t-Bu	Amide	III	S2	TPSS	DefBas-3	-2632.324102
m13	Salen	EDA	t-Bu	H	Nothing	V	S2	TPSS	DefBas-3	-2416.692693
m13	Salen	EDA	t-Bu	H	Cl	V	S2	TPSS	DefBas-3	-2877.153318
m13	Salen	EDA	t-Bu	H	Amine	V	S2	TPSS	DefBas-3	-2551.948509
m13	Salen	EDA	t-Bu	H	Amide	V	S2	TPSS	DefBas-3	-2551.531428
m13	Salen	EDA	t-Bu	H	Nothing	III	S2	TPSS	DefBas-3	-2341.313538
m13	Salen	EDA	t-Bu	H	Cl	III	S2	TPSS	DefBas-3	-2801.790430
m13	Salen	EDA	t-Bu	H	Amine	III	S2	TPSS	DefBas-3	-2476.583241
m13	Salen	EDA	t-Bu	H	Amide	III	S2	TPSS	DefBas-3	-2476.194397
m14	Salen	CHDA	t-Bu	H	Nothing	V	S2	TPSS	DefBas-3	-2572.813456
m14	Salen	CHDA	t-Bu	H	Cl	V	S2	TPSS	DefBas-3	-3033.270930
m14	Salen	CHDA	t-Bu	H	Amine	V	S2	TPSS	DefBas-3	-2708.070133
m14	Salen	CHDA	t-Bu	H	Amide	V	S2	TPSS	DefBas-3	-2707.649432
m14	Salen	CHDA	t-Bu	H	Nothing	III	S2	TPSS	DefBas-3	-2497.434569
m14	Salen	CHDA	t-Bu	H	Cl	III	S2	TPSS	DefBas-3	-2957.906680
m14	Salen	CHDA	t-Bu	H	Amine	III	S2	TPSS	DefBas-3	-2632.703667
m14	Salen	CHDA	t-Bu	H	Amide	III	S2	TPSS	DefBas-3	-2632.309511
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S2	TPSS	DefBas-3	-2731.338279
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S2	TPSS	DefBas-3	-3191.793202
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S2	TPSS	DefBas-3	-2866.593013
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S2	TPSS	DefBas-3	-2866.169885
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S2	TPSS	DefBas-3	-2655.958138
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S2	TPSS	DefBas-3	-3116.429137
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S2	TPSS	DefBas-3	-2791.225725
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S2	TPSS	DefBas-3	-2790.831978
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S2	TPSS	DefBas-3	-2887.458423
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S2	TPSS	DefBas-3	-3347.910927
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S2	TPSS	DefBas-3	-3022.713783
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S2	TPSS	DefBas-3	-3022.287829
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S2	TPSS	DefBas-3	-2812.078572
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S2	TPSS	DefBas-3	-3272.546145
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S2	TPSS	DefBas-3	-2947.345063
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S2	TPSS	DefBas-3	-2946.946869
m01	Acacen	EDA	None	None	Nothing	V	S4	TPSS	DefBas-3	-1794.509873
m01	Acacen	EDA	None	None	Cl	V	S4	TPSS	DefBas-3	-2254.986731
m01	Acacen	EDA	None	None	Amine	V	S4	TPSS	DefBas-3	-1929.774083
m01	Acacen	EDA	None	None	Amide	V	S4	TPSS	DefBas-3	-1929.387158
m01	Acacen	EDA	None	None	Nothing	III	S4	TPSS	DefBas-3	-1719.185839
m01	Acacen	EDA	None	None	Cl	III	S4	TPSS	DefBas-3	-2179.682338
m01	Acacen	EDA	None	None	Amine	III	S4	TPSS	DefBas-3	-1854.474590
m01	Acacen	EDA	None	None	Amide	III	S4	TPSS	DefBas-3	-1854.083291
m02	Acacen	CHDA	None	None	Nothing	V	S4	TPSS	DefBas-3	-1950.632480
m02	Acacen	CHDA	None	None	Cl	V	S4	TPSS	DefBas-3	-2411.103209
m02	Acacen	CHDA	None	None	Amine	V	S4	TPSS	DefBas-3	-2085.894932
m02	Acacen	CHDA	None	None	Amide	V	S4	TPSS	DefBas-3	-2085.503000
m02	Acacen	CHDA	None	None	Nothing	III	S4	TPSS	DefBas-3	-1875.309331
m02	Acacen	CHDA	None	None	Cl	III	S4	TPSS	DefBas-3	-2335.800925
m02	Acacen	CHDA	None	None	Amine	III	S4	TPSS	DefBas-3	-2010.584781
m02	Acacen	CHDA	None	None	Amide	III	S4	TPSS	DefBas-3	-2010.195428
m03	Salen	EDA	H	H	Nothing	V	S4	TPSS	DefBas-3	-2101.977760
m03	Salen	EDA	H	H	Cl	V	S4	TPSS	DefBas-3	-2562.438490
m03	Salen	EDA	H	H	Amine	V	S4	TPSS	DefBas-3	-2237.234402
m03	Salen	EDA	H	H	Amide	V	S4	TPSS	DefBas-3	-2236.837093
m03	Salen	EDA	H	H	Nothing	III	S4	TPSS	DefBas-3	-2026.649372
m03	Salen	EDA	H	H	Cl	III	S4	TPSS	DefBas-3	-2487.136838
m03	Salen	EDA	H	H	Amine	III	S4	TPSS	DefBas-3	-2161.926583
m03	Salen	EDA	H	H	Amide	III	S4	TPSS	DefBas-3	-2161.536351
m04	Salen	CHDA	H	H	Nothing	V	S4	TPSS	DefBas-3	-2258.097988
m04	Salen	CHDA	H	H	Cl	V	S4	TPSS	DefBas-3	-2718.554634
m04	Salen	CHDA	H	H	Amine	V	S4	TPSS	DefBas-3	-2393.354123
m04	Salen	CHDA	H	H	Amide	V	S4	TPSS	DefBas-3	-2392.953219
m04	Salen	CHDA	H	H	Nothing	III	S4	TPSS	DefBas-3	-2182.771296
m04	Salen	CHDA	H	H	Cl	III	S4	TPSS	DefBas-3	-2643.253340
m04	Salen	CHDA	H	H	Amine	III	S4	TPSS	DefBas-3	-2318.050173
m04	Salen	CHDA	H	H	Amide	III	S4	TPSS	DefBas-3	-2317.652584
m05	Salen	EDA	H	Me	Nothing	V	S4	TPSS	DefBas-3	-2180.655885
m05	Salen	EDA	H	Me	Cl	V	S4	TPSS	DefBas-3	-2641.107157
m05	Salen	EDA	H	Me	Amine	V	S4	TPSS	DefBas-3	-2315.910255
m05	Salen	EDA	H	Me	Amide	V	S4	TPSS	DefBas-3	-2315.504395

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m05	Salen	EDA	H	Me	Nothing	III	S4	TPSS	DefBas-3	-2105.320063
m05	Salen	EDA	H	Me	Cl	III	S4	TPSS	DefBas-3	-2565.803557
m05	Salen	EDA	H	Me	Amine	III	S4	TPSS	DefBas-3	-2240.596142
m05	Salen	EDA	H	Me	Amide	III	S4	TPSS	DefBas-3	-2240.202533
m06	Salen	CHDA	H	Me	Nothing	V	S4	TPSS	DefBas-3	-2336.775405
m06	Salen	CHDA	H	Me	Cl	V	S4	TPSS	DefBas-3	-2797.224441
m06	Salen	CHDA	H	Me	Amine	V	S4	TPSS	DefBas-3	-2472.029535
m06	Salen	CHDA	H	Me	Amide	V	S4	TPSS	DefBas-3	-2471.620477
m06	Salen	CHDA	H	Me	Nothing	III	S4	TPSS	DefBas-3	-2261.441576
m06	Salen	CHDA	H	Me	Cl	III	S4	TPSS	DefBas-3	-2721.919685
m06	Salen	CHDA	H	Me	Amine	III	S4	TPSS	DefBas-3	-2396.713811
m06	Salen	CHDA	H	Me	Amide	III	S4	TPSS	DefBas-3	-2396.318474
m07	Salen	EDA	Me	H	Nothing	V	S4	TPSS	DefBas-3	-2180.654108
m07	Salen	EDA	Me	H	Cl	V	S4	TPSS	DefBas-3	-2641.108877
m07	Salen	EDA	Me	H	Amine	V	S4	TPSS	DefBas-3	-2315.908295
m07	Salen	EDA	Me	H	Amide	V	S4	TPSS	DefBas-3	-2315.505489
m07	Salen	EDA	Me	H	Nothing	III	S4	TPSS	DefBas-3	-2105.321246
m07	Salen	EDA	Me	H	Cl	III	S4	TPSS	DefBas-3	-2565.806889
m07	Salen	EDA	Me	H	Amine	III	S4	TPSS	DefBas-3	-2240.583489
m07	Salen	EDA	Me	H	Amide	III	S4	TPSS	DefBas-3	-2240.204130
m08	Salen	CHDA	Me	H	Nothing	V	S4	TPSS	DefBas-3	-2336.773991
m08	Salen	CHDA	Me	H	Cl	V	S4	TPSS	DefBas-3	-2797.225505
m08	Salen	CHDA	Me	H	Amine	V	S4	TPSS	DefBas-3	-2472.025748
m08	Salen	CHDA	Me	H	Amide	V	S4	TPSS	DefBas-3	-2471.621585
m08	Salen	CHDA	Me	H	Nothing	III	S4	TPSS	DefBas-3	-2261.442910
m08	Salen	CHDA	Me	H	Cl	III	S4	TPSS	DefBas-3	-2721.923300
m08	Salen	CHDA	Me	H	Amine	III	S4	TPSS	DefBas-3	-2396.704410
m08	Salen	CHDA	Me	H	Amide	III	S4	TPSS	DefBas-3	-2396.320198
m09	Salen	EDA	Me	Me	Nothing	V	S4	TPSS	DefBas-3	-2259.330890
m09	Salen	EDA	Me	Me	Cl	V	S4	TPSS	DefBas-3	-2719.779000
m09	Salen	EDA	Me	Me	Amine	V	S4	TPSS	DefBas-3	-2394.583143
m09	Salen	EDA	Me	Me	Amide	V	S4	TPSS	DefBas-3	-2394.172914
m09	Salen	EDA	Me	Me	Nothing	III	S4	TPSS	DefBas-3	-2183.991647
m09	Salen	EDA	Me	Me	Cl	III	S4	TPSS	DefBas-3	-2644.473587
m09	Salen	EDA	Me	Me	Amine	III	S4	TPSS	DefBas-3	-2319.253103
m09	Salen	EDA	Me	Me	Amide	III	S4	TPSS	DefBas-3	-2318.870387
m10	Salen	CHDA	Me	Me	Nothing	V	S4	TPSS	DefBas-3	-2415.450228
m10	Salen	CHDA	Me	Me	Cl	V	S4	TPSS	DefBas-3	-2875.895561
m10	Salen	CHDA	Me	Me	Amine	V	S4	TPSS	DefBas-3	-2550.702207
m10	Salen	CHDA	Me	Me	Amide	V	S4	TPSS	DefBas-3	-2550.288912
m10	Salen	CHDA	Me	Me	Nothing	III	S4	TPSS	DefBas-3	-2340.112924
m10	Salen	CHDA	Me	Me	Cl	III	S4	TPSS	DefBas-3	-2800.589679
m10	Salen	CHDA	Me	Me	Amine	III	S4	TPSS	DefBas-3	-2475.373750
m10	Salen	CHDA	Me	Me	Amide	III	S4	TPSS	DefBas-3	-2474.986009
m11	Salen	EDA	H	t-Bu	Nothing	V	S4	TPSS	DefBas-3	-2416.630854
m11	Salen	EDA	H	t-Bu	Cl	V	S4	TPSS	DefBas-3	-2877.079978
m11	Salen	EDA	H	t-Bu	Amine	V	S4	TPSS	DefBas-3	-2551.883636
m11	Salen	EDA	H	t-Bu	Amide	V	S4	TPSS	DefBas-3	-2551.475647
m11	Salen	EDA	H	t-Bu	Nothing	III	S4	TPSS	DefBas-3	-2341.293909
m11	Salen	EDA	H	t-Bu	Cl	III	S4	TPSS	DefBas-3	-2801.775719
m11	Salen	EDA	H	t-Bu	Amine	III	S4	TPSS	DefBas-3	-2476.572304
m11	Salen	EDA	H	t-Bu	Amide	III	S4	TPSS	DefBas-3	-2476.173129
m12	Salen	CHDA	H	t-Bu	Nothing	V	S4	TPSS	DefBas-3	-2572.749724
m12	Salen	CHDA	H	t-Bu	Cl	V	S4	TPSS	DefBas-3	-3033.196228
m12	Salen	CHDA	H	t-Bu	Amine	V	S4	TPSS	DefBas-3	-2708.003341
m12	Salen	CHDA	H	t-Bu	Amide	V	S4	TPSS	DefBas-3	-2707.591868
m12	Salen	CHDA	H	t-Bu	Nothing	III	S4	TPSS	DefBas-3	-2497.415814
m12	Salen	CHDA	H	t-Bu	Cl	III	S4	TPSS	DefBas-3	-2957.892031
m12	Salen	CHDA	H	t-Bu	Amine	III	S4	TPSS	DefBas-3	-2632.686586
m12	Salen	CHDA	H	t-Bu	Amide	III	S4	TPSS	DefBas-3	-2632.289392
m13	Salen	EDA	t-Bu	H	Nothing	V	S4	TPSS	DefBas-3	-2416.615316
m13	Salen	EDA	t-Bu	H	Cl	V	S4	TPSS	DefBas-3	-2877.069979
m13	Salen	EDA	t-Bu	H	Amine	V	S4	TPSS	DefBas-3	-2551.867405
m13	Salen	EDA	t-Bu	H	Amide	V	S4	TPSS	DefBas-3	-2551.462994
m13	Salen	EDA	t-Bu	H	Nothing	III	S4	TPSS	DefBas-3	-2341.280646
m13	Salen	EDA	t-Bu	H	Cl	III	S4	TPSS	DefBas-3	-2801.766707
m13	Salen	EDA	t-Bu	H	Amine	III	S4	TPSS	DefBas-3	-2476.552521
m13	Salen	EDA	t-Bu	H	Amide	III	S4	TPSS	DefBas-3	-2476.161972
m14	Salen	CHDA	t-Bu	H	Nothing	V	S4	TPSS	DefBas-3	-2572.727251
m14	Salen	CHDA	t-Bu	H	Cl	V	S4	TPSS	DefBas-3	-3033.184682
m14	Salen	CHDA	t-Bu	H	Amine	V	S4	TPSS	DefBas-3	-2707.986505

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m14	Salen	CHDA	t-Bu	H	Amide	V	S4	TPSS	DefBas-3	-2707.578984
m14	Salen	CHDA	t-Bu	H	Nothing	III	S4	TPSS	DefBas-3	-2497.401056
m14	Salen	CHDA	t-Bu	H	Cl	III	S4	TPSS	DefBas-3	-2957.882843
m14	Salen	CHDA	t-Bu	H	Amine	III	S4	TPSS	DefBas-3	-2632.672199
m14	Salen	CHDA	t-Bu	H	Amide	III	S4	TPSS	DefBas-3	-2632.277685
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S4	TPSS	DefBas-3	-2731.261325
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S4	TPSS	DefBas-3	-3191.710842
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S4	TPSS	DefBas-3	-2866.513571
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S4	TPSS	DefBas-3	-2866.101805
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S4	TPSS	DefBas-3	-2655.924867
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S4	TPSS	DefBas-3	-3116.405204
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S4	TPSS	DefBas-3	-2791.194911
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S4	TPSS	DefBas-3	-2790.799084
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S4	TPSS	DefBas-3	-2887.385457
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S4	TPSS	DefBas-3	-3347.828053
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S4	TPSS	DefBas-3	-3022.634821
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S4	TPSS	DefBas-3	-3022.217815
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S4	TPSS	DefBas-3	-2812.049063
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S4	TPSS	DefBas-3	-3272.522218
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S4	TPSS	DefBas-3	-2947.313776
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S4	TPSS	DefBas-3	-2946.914683
m01	Acacen	EDA	None	None	Nothing	V	S0	X3LYP	def2-SV(P)	-1795.551608
m01	Acacen	EDA	None	None	Cl	V	S0	X3LYP	def2-SV(P)	-2255.749929
m01	Acacen	EDA	None	None	Amine	V	S0	X3LYP	def2-SV(P)	-1930.490865
m01	Acacen	EDA	None	None	Amide	V	S0	X3LYP	def2-SV(P)	-1930.070009
m01	Acacen	EDA	None	None	Nothing	III	S0	X3LYP	def2-SV(P)	-1720.415444
m01	Acacen	EDA	None	None	Cl	III	S0	X3LYP	def2-SV(P)	-2180.682110
m01	Acacen	EDA	None	None	Amine	III	S0	X3LYP	def2-SV(P)	-1855.415505
m01	Acacen	EDA	None	None	Amide	III	S0	X3LYP	def2-SV(P)	-1855.015629
m02	Acacen	CHDA	None	None	Nothing	V	S0	X3LYP	def2-SV(P)	-1951.329185
m02	Acacen	CHDA	None	None	Cl	V	S0	X3LYP	def2-SV(P)	-2411.522093
m02	Acacen	CHDA	None	None	Amine	V	S0	X3LYP	def2-SV(P)	-2086.267022
m02	Acacen	CHDA	None	None	Amide	V	S0	X3LYP	def2-SV(P)	-2085.841505
m02	Acacen	CHDA	None	None	Nothing	III	S0	X3LYP	def2-SV(P)	-1876.217570
m02	Acacen	CHDA	None	None	Cl	III	S0	X3LYP	def2-SV(P)	-2336.454144
m02	Acacen	CHDA	None	None	Amine	III	S0	X3LYP	def2-SV(P)	-2011.190940
m02	Acacen	CHDA	None	None	Amide	III	S0	X3LYP	def2-SV(P)	-2010.786250
m03	Salen	EDA	H	H	Nothing	V	S0	X3LYP	def2-SV(P)	-2102.353700
m03	Salen	EDA	H	H	Cl	V	S0	X3LYP	def2-SV(P)	-2562.541843
m03	Salen	EDA	H	H	Amine	V	S0	X3LYP	def2-SV(P)	-2237.288058
m03	Salen	EDA	H	H	Amide	V	S0	X3LYP	def2-SV(P)	-2236.854176
m03	Salen	EDA	H	H	Nothing	III	S0	X3LYP	def2-SV(P)	-2027.222232
m03	Salen	EDA	H	H	Cl	III	S0	X3LYP	def2-SV(P)	-2487.476988
m03	Salen	EDA	H	H	Amine	III	S0	X3LYP	def2-SV(P)	-2162.220060
m03	Salen	EDA	H	H	Amide	III	S0	X3LYP	def2-SV(P)	-2161.805839
m04	Salen	CHDA	H	H	Nothing	V	S0	X3LYP	def2-SV(P)	-2258.130171
m04	Salen	CHDA	H	H	Cl	V	S0	X3LYP	def2-SV(P)	-2718.314675
m04	Salen	CHDA	H	H	Amine	V	S0	X3LYP	def2-SV(P)	-2393.064042
m04	Salen	CHDA	H	H	Amide	V	S0	X3LYP	def2-SV(P)	-2392.626751
m04	Salen	CHDA	H	H	Nothing	III	S0	X3LYP	def2-SV(P)	-2183.020102
m04	Salen	CHDA	H	H	Cl	III	S0	X3LYP	def2-SV(P)	-2643.250135
m04	Salen	CHDA	H	H	Amine	III	S0	X3LYP	def2-SV(P)	-2317.996048
m04	Salen	CHDA	H	H	Amide	III	S0	X3LYP	def2-SV(P)	-2317.577543
m05	Salen	EDA	H	Me	Nothing	V	S0	X3LYP	def2-SV(P)	-2180.842115
m05	Salen	EDA	H	Me	Cl	V	S0	X3LYP	def2-SV(P)	-2641.024715
m05	Salen	EDA	H	Me	Amine	V	S0	X3LYP	def2-SV(P)	-2315.775472
m05	Salen	EDA	H	Me	Amide	V	S0	X3LYP	def2-SV(P)	-2315.335665
m05	Salen	EDA	H	Me	Nothing	III	S0	X3LYP	def2-SV(P)	-2105.728667
m05	Salen	EDA	H	Me	Cl	III	S0	X3LYP	def2-SV(P)	-2565.957810
m05	Salen	EDA	H	Me	Amine	III	S0	X3LYP	def2-SV(P)	-2240.705607
m05	Salen	EDA	H	Me	Amide	III	S0	X3LYP	def2-SV(P)	-2240.289221
m06	Salen	CHDA	H	Me	Nothing	V	S0	X3LYP	def2-SV(P)	-2336.618356
m06	Salen	CHDA	H	Me	Cl	V	S0	X3LYP	def2-SV(P)	-2796.796905
m06	Salen	CHDA	H	Me	Amine	V	S0	X3LYP	def2-SV(P)	-2471.550306
m06	Salen	CHDA	H	Me	Amide	V	S0	X3LYP	def2-SV(P)	-2471.110035
m06	Salen	CHDA	H	Me	Nothing	III	S0	X3LYP	def2-SV(P)	-2261.508300
m06	Salen	CHDA	H	Me	Cl	III	S0	X3LYP	def2-SV(P)	-2721.734035
m06	Salen	CHDA	H	Me	Amine	III	S0	X3LYP	def2-SV(P)	-2396.482232
m06	Salen	CHDA	H	Me	Amide	III	S0	X3LYP	def2-SV(P)	-2396.058494
m07	Salen	EDA	Me	H	Nothing	V	S0	X3LYP	def2-SV(P)	-2180.843801
m07	Salen	EDA	Me	H	Cl	V	S0	X3LYP	def2-SV(P)	-2641.030079

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m07	Salen	EDA	Me	H	Amine	V	S0	X3LYP	def2-SV(P)	-2315.777478
m07	Salen	EDA	Me	H	Amide	V	S0	X3LYP	def2-SV(P)	-2315.342153
m07	Salen	EDA	Me	H	Nothing	III	S0	X3LYP	def2-SV(P)	-2105.712517
m07	Salen	EDA	Me	H	Cl	III	S0	X3LYP	def2-SV(P)	-2565.965140
m07	Salen	EDA	Me	H	Amine	III	S0	X3LYP	def2-SV(P)	-2240.707949
m07	Salen	EDA	Me	H	Amide	III	S0	X3LYP	def2-SV(P)	-2240.294177
m08	Salen	CHDA	Me	H	Nothing	V	S0	X3LYP	def2-SV(P)	-2336.620313
m08	Salen	CHDA	Me	H	Cl	V	S0	X3LYP	def2-SV(P)	-2796.803223
m08	Salen	CHDA	Me	H	Amine	V	S0	X3LYP	def2-SV(P)	-2471.553527
m08	Salen	CHDA	Me	H	Amide	V	S0	X3LYP	def2-SV(P)	-2471.114728
m08	Salen	CHDA	Me	H	Nothing	III	S0	X3LYP	def2-SV(P)	-2261.508494
m08	Salen	CHDA	Me	H	Cl	III	S0	X3LYP	def2-SV(P)	-2721.737012
m08	Salen	CHDA	Me	H	Amine	III	S0	X3LYP	def2-SV(P)	-2396.482945
m08	Salen	CHDA	Me	H	Amide	III	S0	X3LYP	def2-SV(P)	-2396.065188
m09	Salen	EDA	Me	Me	Nothing	V	S0	X3LYP	def2-SV(P)	-2259.331571
m09	Salen	EDA	Me	Me	Cl	V	S0	X3LYP	def2-SV(P)	-2719.513309
m09	Salen	EDA	Me	Me	Amine	V	S0	X3LYP	def2-SV(P)	-2394.264860
m09	Salen	EDA	Me	Me	Amide	V	S0	X3LYP	def2-SV(P)	-2393.824301
m09	Salen	EDA	Me	Me	Nothing	III	S0	X3LYP	def2-SV(P)	-2184.200525
m09	Salen	EDA	Me	Me	Cl	III	S0	X3LYP	def2-SV(P)	-2644.448971
m09	Salen	EDA	Me	Me	Amine	III	S0	X3LYP	def2-SV(P)	-2319.193463
m09	Salen	EDA	Me	Me	Amide	III	S0	X3LYP	def2-SV(P)	-2318.777871
m10	Salen	CHDA	Me	Me	Nothing	V	S0	X3LYP	def2-SV(P)	-2415.108169
m10	Salen	CHDA	Me	Me	Cl	V	S0	X3LYP	def2-SV(P)	-2875.286125
m10	Salen	CHDA	Me	Me	Amine	V	S0	X3LYP	def2-SV(P)	-2550.040383
m10	Salen	CHDA	Me	Me	Amide	V	S0	X3LYP	def2-SV(P)	-2549.597925
m10	Salen	CHDA	Me	Me	Nothing	III	S0	X3LYP	def2-SV(P)	-2339.995398
m10	Salen	CHDA	Me	Me	Cl	III	S0	X3LYP	def2-SV(P)	-2800.220909
m10	Salen	CHDA	Me	Me	Amine	III	S0	X3LYP	def2-SV(P)	-2474.968405
m10	Salen	CHDA	Me	Me	Amide	III	S0	X3LYP	def2-SV(P)	-2474.548093
m11	Salen	EDA	H	t-Bu	Nothing	V	S0	X3LYP	def2-SV(P)	-2416.269640
m11	Salen	EDA	H	t-Bu	Cl	V	S0	X3LYP	def2-SV(P)	-2876.448237
m11	Salen	EDA	H	t-Bu	Amine	V	S0	X3LYP	def2-SV(P)	-2551.195048
m11	Salen	EDA	H	t-Bu	Amide	V	S0	X3LYP	def2-SV(P)	-2550.761730
m11	Salen	EDA	H	t-Bu	Nothing	III	S0	X3LYP	def2-SV(P)	-2341.153077
m11	Salen	EDA	H	t-Bu	Cl	III	S0	X3LYP	def2-SV(P)	-2801.387200
m11	Salen	EDA	H	t-Bu	Amine	III	S0	X3LYP	def2-SV(P)	-2476.129430
m11	Salen	EDA	H	t-Bu	Amide	III	S0	X3LYP	def2-SV(P)	-2475.713512
m12	Salen	CHDA	H	t-Bu	Nothing	V	S0	X3LYP	def2-SV(P)	-2572.041089
m12	Salen	CHDA	H	t-Bu	Cl	V	S0	X3LYP	def2-SV(P)	-3032.221819
m12	Salen	CHDA	H	t-Bu	Amine	V	S0	X3LYP	def2-SV(P)	-2706.973766
m12	Salen	CHDA	H	t-Bu	Amide	V	S0	X3LYP	def2-SV(P)	-2706.530366
m12	Salen	CHDA	H	t-Bu	Nothing	III	S0	X3LYP	def2-SV(P)	-2496.908787
m12	Salen	CHDA	H	t-Bu	Cl	III	S0	X3LYP	def2-SV(P)	-2957.156278
m12	Salen	CHDA	H	t-Bu	Amine	III	S0	X3LYP	def2-SV(P)	-2631.905975
m12	Salen	CHDA	H	t-Bu	Amide	III	S0	X3LYP	def2-SV(P)	-2631.485491
m13	Salen	EDA	t-Bu	H	Nothing	V	S0	X3LYP	def2-SV(P)	-2416.258461
m13	Salen	EDA	t-Bu	H	Cl	V	S0	X3LYP	def2-SV(P)	-2876.446698
m13	Salen	EDA	t-Bu	H	Amine	V	S0	X3LYP	def2-SV(P)	-2551.192683
m13	Salen	EDA	t-Bu	H	Amide	V	S0	X3LYP	def2-SV(P)	-2550.758491
m13	Salen	EDA	t-Bu	H	Nothing	III	S0	X3LYP	def2-SV(P)	-2341.129216
m13	Salen	EDA	t-Bu	H	Cl	III	S0	X3LYP	def2-SV(P)	-2801.377076
m13	Salen	EDA	t-Bu	H	Amine	III	S0	X3LYP	def2-SV(P)	-2476.119991
m13	Salen	EDA	t-Bu	H	Amide	III	S0	X3LYP	def2-SV(P)	-2475.712586
m14	Salen	CHDA	t-Bu	H	Nothing	V	S0	X3LYP	def2-SV(P)	-2572.034718
m14	Salen	CHDA	t-Bu	H	Cl	V	S0	X3LYP	def2-SV(P)	-3032.219431
m14	Salen	CHDA	t-Bu	H	Amine	V	S0	X3LYP	def2-SV(P)	-2706.969419
m14	Salen	CHDA	t-Bu	H	Amide	V	S0	X3LYP	def2-SV(P)	-2706.532487
m14	Salen	CHDA	t-Bu	H	Nothing	III	S0	X3LYP	def2-SV(P)	-2496.905251
m14	Salen	CHDA	t-Bu	H	Cl	III	S0	X3LYP	def2-SV(P)	-2957.149311
m14	Salen	CHDA	t-Bu	H	Amine	III	S0	X3LYP	def2-SV(P)	-2631.894194
m14	Salen	CHDA	t-Bu	H	Amide	III	S0	X3LYP	def2-SV(P)	-2631.479604
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S0	X3LYP	def2-SV(P)	-2730.171202
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S0	X3LYP	def2-SV(P)	-3190.353988
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S0	X3LYP	def2-SV(P)	-2865.104802
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S0	X3LYP	def2-SV(P)	-2864.664579
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S0	X3LYP	def2-SV(P)	-2655.039007
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S0	X3LYP	def2-SV(P)	-3115.285364
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S0	X3LYP	def2-SV(P)	-2790.030920
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S0	X3LYP	def2-SV(P)	-2789.613511
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S0	X3LYP	def2-SV(P)	-2885.947408

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S0	X3LYP	def2-SV(P)	-3346.127219
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S0	X3LYP	def2-SV(P)	-3020.878283
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S0	X3LYP	def2-SV(P)	-3020.437403
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S0	X3LYP	def2-SV(P)	-2810.814368
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S0	X3LYP	def2-SV(P)	-3271.057962
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S0	X3LYP	def2-SV(P)	-2945.807055
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S0	X3LYP	def2-SV(P)	-2945.384889
m01	Acacen	EDA	None	None	Nothing	V	S2	X3LYP	def2-SV(P)	-1795.546254
m01	Acacen	EDA	None	None	Cl	V	S2	X3LYP	def2-SV(P)	-2255.767533
m01	Acacen	EDA	None	None	Amine	V	S2	X3LYP	def2-SV(P)	-1930.503713
m01	Acacen	EDA	None	None	Amide	V	S2	X3LYP	def2-SV(P)	-1930.089664
m01	Acacen	EDA	None	None	Nothing	III	S2	X3LYP	def2-SV(P)	-1720.478565
m01	Acacen	EDA	None	None	Cl	III	S2	X3LYP	def2-SV(P)	-2180.719718
m01	Acacen	EDA	None	None	Amine	III	S2	X3LYP	def2-SV(P)	-1855.456438
m01	Acacen	EDA	None	None	Amide	III	S2	X3LYP	def2-SV(P)	-1855.029727
m02	Acacen	CHDA	None	None	Nothing	V	S2	X3LYP	def2-SV(P)	-1951.324018
m02	Acacen	CHDA	None	None	Cl	V	S2	X3LYP	def2-SV(P)	-2411.540737
m02	Acacen	CHDA	None	None	Amine	V	S2	X3LYP	def2-SV(P)	-2086.280662
m02	Acacen	CHDA	None	None	Amide	V	S2	X3LYP	def2-SV(P)	-2085.861062
m02	Acacen	CHDA	None	None	Nothing	III	S2	X3LYP	def2-SV(P)	-1876.254804
m02	Acacen	CHDA	None	None	Cl	III	S2	X3LYP	def2-SV(P)	-2336.491549
m02	Acacen	CHDA	None	None	Amine	III	S2	X3LYP	def2-SV(P)	-2011.231345
m02	Acacen	CHDA	None	None	Amide	III	S2	X3LYP	def2-SV(P)	-2010.805649
m03	Salen	EDA	H	H	Nothing	V	S2	X3LYP	def2-SV(P)	-2102.352949
m03	Salen	EDA	H	H	Cl	V	S2	X3LYP	def2-SV(P)	-2562.561670
m03	Salen	EDA	H	H	Amine	V	S2	X3LYP	def2-SV(P)	-2237.304267
m03	Salen	EDA	H	H	Amide	V	S2	X3LYP	def2-SV(P)	-2236.880697
m03	Salen	EDA	H	H	Nothing	III	S2	X3LYP	def2-SV(P)	-2027.282547
m03	Salen	EDA	H	H	Cl	III	S2	X3LYP	def2-SV(P)	-2487.513790
m03	Salen	EDA	H	H	Amine	III	S2	X3LYP	def2-SV(P)	-2162.253446
m03	Salen	EDA	H	H	Amide	III	S2	X3LYP	def2-SV(P)	-2161.817131
m04	Salen	CHDA	H	H	Nothing	V	S2	X3LYP	def2-SV(P)	-2258.129654
m04	Salen	CHDA	H	H	Cl	V	S2	X3LYP	def2-SV(P)	-2718.334917
m04	Salen	CHDA	H	H	Amine	V	S2	X3LYP	def2-SV(P)	-2393.081488
m04	Salen	CHDA	H	H	Amide	V	S2	X3LYP	def2-SV(P)	-2392.653067
m04	Salen	CHDA	H	H	Nothing	III	S2	X3LYP	def2-SV(P)	-2183.058118
m04	Salen	CHDA	H	H	Cl	III	S2	X3LYP	def2-SV(P)	-2643.285573
m04	Salen	CHDA	H	H	Amine	III	S2	X3LYP	def2-SV(P)	-2318.028105
m04	Salen	CHDA	H	H	Amide	III	S2	X3LYP	def2-SV(P)	-2317.591747
m05	Salen	EDA	H	Me	Nothing	V	S2	X3LYP	def2-SV(P)	-2180.839438
m05	Salen	EDA	H	Me	Cl	V	S2	X3LYP	def2-SV(P)	-2641.045376
m05	Salen	EDA	H	Me	Amine	V	S2	X3LYP	def2-SV(P)	-2315.791982
m05	Salen	EDA	H	Me	Amide	V	S2	X3LYP	def2-SV(P)	-2315.362188
m05	Salen	EDA	H	Me	Nothing	III	S2	X3LYP	def2-SV(P)	-2105.770688
m05	Salen	EDA	H	Me	Cl	III	S2	X3LYP	def2-SV(P)	-2565.997418
m05	Salen	EDA	H	Me	Amine	III	S2	X3LYP	def2-SV(P)	-2240.739218
m05	Salen	EDA	H	Me	Amide	III	S2	X3LYP	def2-SV(P)	-2240.309050
m06	Salen	CHDA	H	Me	Nothing	V	S2	X3LYP	def2-SV(P)	-2336.617543
m06	Salen	CHDA	H	Me	Cl	V	S2	X3LYP	def2-SV(P)	-2796.818897
m06	Salen	CHDA	H	Me	Amine	V	S2	X3LYP	def2-SV(P)	-2471.567390
m06	Salen	CHDA	H	Me	Amide	V	S2	X3LYP	def2-SV(P)	-2471.135448
m06	Salen	CHDA	H	Me	Nothing	III	S2	X3LYP	def2-SV(P)	-2261.545767
m06	Salen	CHDA	H	Me	Cl	III	S2	X3LYP	def2-SV(P)	-2721.768983
m06	Salen	CHDA	H	Me	Amine	III	S2	X3LYP	def2-SV(P)	-2396.513729
m06	Salen	CHDA	H	Me	Amide	III	S2	X3LYP	def2-SV(P)	-2396.074459
m07	Salen	EDA	Me	H	Nothing	V	S2	X3LYP	def2-SV(P)	-2180.843353
m07	Salen	EDA	Me	H	Cl	V	S2	X3LYP	def2-SV(P)	-2641.049862
m07	Salen	EDA	Me	H	Amine	V	S2	X3LYP	def2-SV(P)	-2315.793625
m07	Salen	EDA	Me	H	Amide	V	S2	X3LYP	def2-SV(P)	-2315.368106
m07	Salen	EDA	Me	H	Nothing	III	S2	X3LYP	def2-SV(P)	-2105.772656
m07	Salen	EDA	Me	H	Cl	III	S2	X3LYP	def2-SV(P)	-2566.002070
m07	Salen	EDA	Me	H	Amine	III	S2	X3LYP	def2-SV(P)	-2240.741928
m07	Salen	EDA	Me	H	Amide	III	S2	X3LYP	def2-SV(P)	-2240.307060
m08	Salen	CHDA	Me	H	Nothing	V	S2	X3LYP	def2-SV(P)	-2336.620831
m08	Salen	CHDA	Me	H	Cl	V	S2	X3LYP	def2-SV(P)	-2796.823898
m08	Salen	CHDA	Me	H	Amine	V	S2	X3LYP	def2-SV(P)	-2471.570001
m08	Salen	CHDA	Me	H	Amide	V	S2	X3LYP	def2-SV(P)	-2471.140840
m08	Salen	CHDA	Me	H	Nothing	III	S2	X3LYP	def2-SV(P)	-2261.548102
m08	Salen	CHDA	Me	H	Cl	III	S2	X3LYP	def2-SV(P)	-2721.774009
m08	Salen	CHDA	Me	H	Amine	III	S2	X3LYP	def2-SV(P)	-2396.516012
m08	Salen	CHDA	Me	H	Amide	III	S2	X3LYP	def2-SV(P)	-2396.078605

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m09	Salen	EDA	Me	Me	Nothing	V	S2	X3LYP	def2-SV(P)	-2259.330956
m09	Salen	EDA	Me	Me	Cl	V	S2	X3LYP	def2-SV(P)	-2719.533259
m09	Salen	EDA	Me	Me	Amine	V	S2	X3LYP	def2-SV(P)	-2394.278162
m09	Salen	EDA	Me	Me	Amide	V	S2	X3LYP	def2-SV(P)	-2393.850825
m09	Salen	EDA	Me	Me	Nothing	III	S2	X3LYP	def2-SV(P)	-2184.260596
m09	Salen	EDA	Me	Me	Cl	III	S2	X3LYP	def2-SV(P)	-2644.485755
m09	Salen	EDA	Me	Me	Amine	III	S2	X3LYP	def2-SV(P)	-2319.227546
m09	Salen	EDA	Me	Me	Amide	III	S2	X3LYP	def2-SV(P)	-2318.792129
m10	Salen	CHDA	Me	Me	Nothing	V	S2	X3LYP	def2-SV(P)	-2415.107600
m10	Salen	CHDA	Me	Me	Cl	V	S2	X3LYP	def2-SV(P)	-2875.307054
m10	Salen	CHDA	Me	Me	Amine	V	S2	X3LYP	def2-SV(P)	-2550.053188
m10	Salen	CHDA	Me	Me	Amide	V	S2	X3LYP	def2-SV(P)	-2549.623162
m10	Salen	CHDA	Me	Me	Nothing	III	S2	X3LYP	def2-SV(P)	-2340.035717
m10	Salen	CHDA	Me	Me	Cl	III	S2	X3LYP	def2-SV(P)	-2800.257573
m10	Salen	CHDA	Me	Me	Amine	III	S2	X3LYP	def2-SV(P)	-2475.001718
m10	Salen	CHDA	Me	Me	Amide	III	S2	X3LYP	def2-SV(P)	-2474.568163
m11	Salen	EDA	H	t-Bu	Nothing	V	S2	X3LYP	def2-SV(P)	-2416.262683
m11	Salen	EDA	H	t-Bu	Cl	V	S2	X3LYP	def2-SV(P)	-2876.465377
m11	Salen	EDA	H	t-Bu	Amine	V	S2	X3LYP	def2-SV(P)	-2551.219448
m11	Salen	EDA	H	t-Bu	Amide	V	S2	X3LYP	def2-SV(P)	-2550.787477
m11	Salen	EDA	H	t-Bu	Nothing	III	S2	X3LYP	def2-SV(P)	-2341.196551
m11	Salen	EDA	H	t-Bu	Cl	III	S2	X3LYP	def2-SV(P)	-2801.419863
m11	Salen	EDA	H	t-Bu	Amine	III	S2	X3LYP	def2-SV(P)	-2476.162536
m11	Salen	EDA	H	t-Bu	Amide	III	S2	X3LYP	def2-SV(P)	-2475.725030
m12	Salen	CHDA	H	t-Bu	Nothing	V	S2	X3LYP	def2-SV(P)	-2572.040092
m12	Salen	CHDA	H	t-Bu	Cl	V	S2	X3LYP	def2-SV(P)	-3032.240138
m12	Salen	CHDA	H	t-Bu	Amine	V	S2	X3LYP	def2-SV(P)	-2706.988589
m12	Salen	CHDA	H	t-Bu	Amide	V	S2	X3LYP	def2-SV(P)	-2706.554451
m12	Salen	CHDA	H	t-Bu	Nothing	III	S2	X3LYP	def2-SV(P)	-2496.971815
m12	Salen	CHDA	H	t-Bu	Cl	III	S2	X3LYP	def2-SV(P)	-2957.194059
m12	Salen	CHDA	H	t-Bu	Amine	III	S2	X3LYP	def2-SV(P)	-2631.936131
m12	Salen	CHDA	H	t-Bu	Amide	III	S2	X3LYP	def2-SV(P)	-2631.498240
m13	Salen	EDA	t-Bu	H	Nothing	V	S2	X3LYP	def2-SV(P)	-2416.258417
m13	Salen	EDA	t-Bu	H	Cl	V	S2	X3LYP	def2-SV(P)	-2876.468190
m13	Salen	EDA	t-Bu	H	Amine	V	S2	X3LYP	def2-SV(P)	-2551.209870
m13	Salen	EDA	t-Bu	H	Amide	V	S2	X3LYP	def2-SV(P)	-2550.786507
m13	Salen	EDA	t-Bu	H	Nothing	III	S2	X3LYP	def2-SV(P)	-2341.189538
m13	Salen	EDA	t-Bu	H	Cl	III	S2	X3LYP	def2-SV(P)	-2801.419958
m13	Salen	EDA	t-Bu	H	Amine	III	S2	X3LYP	def2-SV(P)	-2476.157933
m13	Salen	EDA	t-Bu	H	Amide	III	S2	X3LYP	def2-SV(P)	-2475.727185
m14	Salen	CHDA	t-Bu	H	Nothing	V	S2	X3LYP	def2-SV(P)	-2572.035405
m14	Salen	CHDA	t-Bu	H	Cl	V	S2	X3LYP	def2-SV(P)	-3032.241581
m14	Salen	CHDA	t-Bu	H	Amine	V	S2	X3LYP	def2-SV(P)	-2706.986596
m14	Salen	CHDA	t-Bu	H	Amide	V	S2	X3LYP	def2-SV(P)	-2706.559214
m14	Salen	CHDA	t-Bu	H	Nothing	III	S2	X3LYP	def2-SV(P)	-2496.964977
m14	Salen	CHDA	t-Bu	H	Cl	III	S2	X3LYP	def2-SV(P)	-2957.191395
m14	Salen	CHDA	t-Bu	H	Amine	III	S2	X3LYP	def2-SV(P)	-2631.932723
m14	Salen	CHDA	t-Bu	H	Amide	III	S2	X3LYP	def2-SV(P)	-2631.501303
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S2	X3LYP	def2-SV(P)	-2730.173384
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S2	X3LYP	def2-SV(P)	-3190.375993
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S2	X3LYP	def2-SV(P)	-2865.122277
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S2	X3LYP	def2-SV(P)	-2864.694192
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S2	X3LYP	def2-SV(P)	-2655.100168
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S2	X3LYP	def2-SV(P)	-3115.327230
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S2	X3LYP	def2-SV(P)	-2790.065246
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S2	X3LYP	def2-SV(P)	-2789.635958
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S2	X3LYP	def2-SV(P)	-2885.950033
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S2	X3LYP	def2-SV(P)	-3346.149049
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S2	X3LYP	def2-SV(P)	-3020.897100
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S2	X3LYP	def2-SV(P)	-3020.465207
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S2	X3LYP	def2-SV(P)	-2810.876753
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S2	X3LYP	def2-SV(P)	-3271.100162
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S2	X3LYP	def2-SV(P)	-2945.840459
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S2	X3LYP	def2-SV(P)	-2945.407057
m01	Acacen	EDA	None	None	Nothing	V	S4	X3LYP	def2-SV(P)	-1795.537560
m01	Acacen	EDA	None	None	Cl	V	S4	X3LYP	def2-SV(P)	-2255.763497
m01	Acacen	EDA	None	None	Amine	V	S4	X3LYP	def2-SV(P)	-1930.502105
m01	Acacen	EDA	None	None	Amide	V	S4	X3LYP	def2-SV(P)	-1930.087191
m01	Acacen	EDA	None	None	Nothing	III	S4	X3LYP	def2-SV(P)	-1720.521779
m01	Acacen	EDA	None	None	Cl	III	S4	X3LYP	def2-SV(P)	-2180.751577
m01	Acacen	EDA	None	None	Amine	III	S4	X3LYP	def2-SV(P)	-1855.488256

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m01	Acacen	EDA	None	None	Amide	III	S4	X3LYP	def2-SV(P)	-1855.055404
m02	Acacen	CHDA	None	None	Nothing	V	S4	X3LYP	def2-SV(P)	-1951.314927
m02	Acacen	CHDA	None	None	Cl	V	S4	X3LYP	def2-SV(P)	-2411.536192
m02	Acacen	CHDA	None	None	Amine	V	S4	X3LYP	def2-SV(P)	-2086.278106
m02	Acacen	CHDA	None	None	Amide	V	S4	X3LYP	def2-SV(P)	-2085.858384
m02	Acacen	CHDA	None	None	Nothing	III	S4	X3LYP	def2-SV(P)	-1876.298830
m02	Acacen	CHDA	None	None	Cl	III	S4	X3LYP	def2-SV(P)	-2336.523783
m02	Acacen	CHDA	None	None	Amine	III	S4	X3LYP	def2-SV(P)	-2011.263851
m02	Acacen	CHDA	None	None	Amide	III	S4	X3LYP	def2-SV(P)	-2010.820294
m03	Salen	EDA	H	H	Nothing	V	S4	X3LYP	def2-SV(P)	-2102.346456
m03	Salen	EDA	H	H	Cl	V	S4	X3LYP	def2-SV(P)	-2562.556812
m03	Salen	EDA	H	H	Amine	V	S4	X3LYP	def2-SV(P)	-2237.302948
m03	Salen	EDA	H	H	Amide	V	S4	X3LYP	def2-SV(P)	-2236.879186
m03	Salen	EDA	H	H	Nothing	III	S4	X3LYP	def2-SV(P)	-2027.325527
m03	Salen	EDA	H	H	Cl	III	S4	X3LYP	def2-SV(P)	-2487.544888
m03	Salen	EDA	H	H	Amine	III	S4	X3LYP	def2-SV(P)	-2162.285822
m03	Salen	EDA	H	H	Amide	III	S4	X3LYP	def2-SV(P)	-2161.839868
m04	Salen	CHDA	H	H	Nothing	V	S4	X3LYP	def2-SV(P)	-2258.122715
m04	Salen	CHDA	H	H	Cl	V	S4	X3LYP	def2-SV(P)	-2718.329129
m04	Salen	CHDA	H	H	Amine	V	S4	X3LYP	def2-SV(P)	-2393.078108
m04	Salen	CHDA	H	H	Amide	V	S4	X3LYP	def2-SV(P)	-2392.651340
m04	Salen	CHDA	H	H	Nothing	III	S4	X3LYP	def2-SV(P)	-2183.101882
m04	Salen	CHDA	H	H	Cl	III	S4	X3LYP	def2-SV(P)	-2643.317317
m04	Salen	CHDA	H	H	Amine	III	S4	X3LYP	def2-SV(P)	-2318.061400
m04	Salen	CHDA	H	H	Amide	III	S4	X3LYP	def2-SV(P)	-2317.616017
m05	Salen	EDA	H	Me	Nothing	V	S4	X3LYP	def2-SV(P)	-2180.836764
m05	Salen	EDA	H	Me	Cl	V	S4	X3LYP	def2-SV(P)	-2641.038337
m05	Salen	EDA	H	Me	Amine	V	S4	X3LYP	def2-SV(P)	-2315.791972
m05	Salen	EDA	H	Me	Amide	V	S4	X3LYP	def2-SV(P)	-2315.362139
m05	Salen	EDA	H	Me	Nothing	III	S4	X3LYP	def2-SV(P)	-2105.812398
m05	Salen	EDA	H	Me	Cl	III	S4	X3LYP	def2-SV(P)	-2566.027969
m05	Salen	EDA	H	Me	Amine	III	S4	X3LYP	def2-SV(P)	-2240.771695
m05	Salen	EDA	H	Me	Amide	III	S4	X3LYP	def2-SV(P)	-2240.325202
m06	Salen	CHDA	H	Me	Nothing	V	S4	X3LYP	def2-SV(P)	-2336.613537
m06	Salen	CHDA	H	Me	Cl	V	S4	X3LYP	def2-SV(P)	-2796.811437
m06	Salen	CHDA	H	Me	Amine	V	S4	X3LYP	def2-SV(P)	-2471.565725
m06	Salen	CHDA	H	Me	Amide	V	S4	X3LYP	def2-SV(P)	-2471.132749
m06	Salen	CHDA	H	Me	Nothing	III	S4	X3LYP	def2-SV(P)	-2261.587971
m06	Salen	CHDA	H	Me	Cl	III	S4	X3LYP	def2-SV(P)	-2721.800522
m06	Salen	CHDA	H	Me	Amine	III	S4	X3LYP	def2-SV(P)	-2396.545583
m06	Salen	CHDA	H	Me	Amide	III	S4	X3LYP	def2-SV(P)	-2396.098953
m07	Salen	EDA	Me	H	Nothing	V	S4	X3LYP	def2-SV(P)	-2180.839431
m07	Salen	EDA	Me	H	Cl	V	S4	X3LYP	def2-SV(P)	-2641.045757
m07	Salen	EDA	Me	H	Amine	V	S4	X3LYP	def2-SV(P)	-2315.793407
m07	Salen	EDA	Me	H	Amide	V	S4	X3LYP	def2-SV(P)	-2315.366629
m07	Salen	EDA	Me	H	Nothing	III	S4	X3LYP	def2-SV(P)	-2105.814999
m07	Salen	EDA	Me	H	Cl	III	S4	X3LYP	def2-SV(P)	-2566.033287
m07	Salen	EDA	Me	H	Amine	III	S4	X3LYP	def2-SV(P)	-2240.774517
m07	Salen	EDA	Me	H	Amide	III	S4	X3LYP	def2-SV(P)	-2240.332782
m08	Salen	CHDA	Me	H	Nothing	V	S4	X3LYP	def2-SV(P)	-2336.615615
m08	Salen	CHDA	Me	H	Cl	V	S4	X3LYP	def2-SV(P)	-2796.818401
m08	Salen	CHDA	Me	H	Amine	V	S4	X3LYP	def2-SV(P)	-2471.568779
m08	Salen	CHDA	Me	H	Amide	V	S4	X3LYP	def2-SV(P)	-2471.139299
m08	Salen	CHDA	Me	H	Nothing	III	S4	X3LYP	def2-SV(P)	-2261.591171
m08	Salen	CHDA	Me	H	Cl	III	S4	X3LYP	def2-SV(P)	-2721.806082
m08	Salen	CHDA	Me	H	Amine	III	S4	X3LYP	def2-SV(P)	-2396.549714
m08	Salen	CHDA	Me	H	Amide	III	S4	X3LYP	def2-SV(P)	-2396.101934
m09	Salen	EDA	Me	Me	Nothing	V	S4	X3LYP	def2-SV(P)	-2259.329394
m09	Salen	EDA	Me	Me	Cl	V	S4	X3LYP	def2-SV(P)	-2719.527740
m09	Salen	EDA	Me	Me	Amine	V	S4	X3LYP	def2-SV(P)	-2394.282279
m09	Salen	EDA	Me	Me	Amide	V	S4	X3LYP	def2-SV(P)	-2393.849078
m09	Salen	EDA	Me	Me	Nothing	III	S4	X3LYP	def2-SV(P)	-2184.301695
m09	Salen	EDA	Me	Me	Cl	III	S4	X3LYP	def2-SV(P)	-2644.517004
m09	Salen	EDA	Me	Me	Amine	III	S4	X3LYP	def2-SV(P)	-2319.260315
m09	Salen	EDA	Me	Me	Amide	III	S4	X3LYP	def2-SV(P)	-2318.814153
m10	Salen	CHDA	Me	Me	Nothing	V	S4	X3LYP	def2-SV(P)	-2415.105196
m10	Salen	CHDA	Me	Me	Cl	V	S4	X3LYP	def2-SV(P)	-2875.302290
m10	Salen	CHDA	Me	Me	Amine	V	S4	X3LYP	def2-SV(P)	-2550.056994
m10	Salen	CHDA	Me	Me	Amide	V	S4	X3LYP	def2-SV(P)	-2549.621361
m10	Salen	CHDA	Me	Me	Nothing	III	S4	X3LYP	def2-SV(P)	-2340.077544
m10	Salen	CHDA	Me	Me	Cl	III	S4	X3LYP	def2-SV(P)	-2800.289490

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m10	Salen	CHDA	Me	Me	Amine	III	S4	X3LYP	def2-SV(P)	-2475.034639
m10	Salen	CHDA	Me	Me	Amide	III	S4	X3LYP	def2-SV(P)	-2474.586289
m11	Salen	EDA	H	t-Bu	Nothing	V	S4	X3LYP	def2-SV(P)	-2416.266108
m11	Salen	EDA	H	t-Bu	Cl	V	S4	X3LYP	def2-SV(P)	-2876.462089
m11	Salen	EDA	H	t-Bu	Amine	V	S4	X3LYP	def2-SV(P)	-2551.219777
m11	Salen	EDA	H	t-Bu	Amide	V	S4	X3LYP	def2-SV(P)	-2550.785049
m11	Salen	EDA	H	t-Bu	Nothing	III	S4	X3LYP	def2-SV(P)	-2341.238298
m11	Salen	EDA	H	t-Bu	Cl	III	S4	X3LYP	def2-SV(P)	-2801.451478
m11	Salen	EDA	H	t-Bu	Amine	III	S4	X3LYP	def2-SV(P)	-2476.199261
m11	Salen	EDA	H	t-Bu	Amide	III	S4	X3LYP	def2-SV(P)	-2475.750165
m12	Salen	CHDA	H	t-Bu	Nothing	V	S4	X3LYP	def2-SV(P)	-2572.038573
m12	Salen	CHDA	H	t-Bu	Cl	V	S4	X3LYP	def2-SV(P)	-3032.236031
m12	Salen	CHDA	H	t-Bu	Amine	V	S4	X3LYP	def2-SV(P)	-2706.989821
m12	Salen	CHDA	H	t-Bu	Amide	V	S4	X3LYP	def2-SV(P)	-2706.553670
m12	Salen	CHDA	H	t-Bu	Nothing	III	S4	X3LYP	def2-SV(P)	-2497.014395
m12	Salen	CHDA	H	t-Bu	Cl	III	S4	X3LYP	def2-SV(P)	-2957.225609
m12	Salen	CHDA	H	t-Bu	Amine	III	S4	X3LYP	def2-SV(P)	-2631.968464
m12	Salen	CHDA	H	t-Bu	Amide	III	S4	X3LYP	def2-SV(P)	-2631.523601
m13	Salen	EDA	t-Bu	H	Nothing	V	S4	X3LYP	def2-SV(P)	-2416.257534
m13	Salen	EDA	t-Bu	H	Cl	V	S4	X3LYP	def2-SV(P)	-2876.465126
m13	Salen	EDA	t-Bu	H	Amine	V	S4	X3LYP	def2-SV(P)	-2551.211254
m13	Salen	EDA	t-Bu	H	Amide	V	S4	X3LYP	def2-SV(P)	-2550.784813
m13	Salen	EDA	t-Bu	H	Nothing	III	S4	X3LYP	def2-SV(P)	-2341.231589
m13	Salen	EDA	t-Bu	H	Cl	III	S4	X3LYP	def2-SV(P)	-2801.450945
m13	Salen	EDA	t-Bu	H	Amine	III	S4	X3LYP	def2-SV(P)	-2476.191982
m13	Salen	EDA	t-Bu	H	Amide	III	S4	X3LYP	def2-SV(P)	-2475.751399
m14	Salen	CHDA	t-Bu	H	Nothing	V	S4	X3LYP	def2-SV(P)	-2572.033816
m14	Salen	CHDA	t-Bu	H	Cl	V	S4	X3LYP	def2-SV(P)	-3032.238195
m14	Salen	CHDA	t-Bu	H	Amine	V	S4	X3LYP	def2-SV(P)	-2706.986776
m14	Salen	CHDA	t-Bu	H	Amide	V	S4	X3LYP	def2-SV(P)	-2706.557173
m14	Salen	CHDA	t-Bu	H	Nothing	III	S4	X3LYP	def2-SV(P)	-2497.007985
m14	Salen	CHDA	t-Bu	H	Cl	III	S4	X3LYP	def2-SV(P)	-2957.223626
m14	Salen	CHDA	t-Bu	H	Amine	III	S4	X3LYP	def2-SV(P)	-2631.967610
m14	Salen	CHDA	t-Bu	H	Amide	III	S4	X3LYP	def2-SV(P)	-2631.515000
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S4	X3LYP	def2-SV(P)	-2730.173061
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S4	X3LYP	def2-SV(P)	-3190.373674
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S4	X3LYP	def2-SV(P)	-2865.126013
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S4	X3LYP	def2-SV(P)	-2864.689964
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S4	X3LYP	def2-SV(P)	-2655.141092
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S4	X3LYP	def2-SV(P)	-3115.357943
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S4	X3LYP	def2-SV(P)	-2790.097450
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S4	X3LYP	def2-SV(P)	-2789.655593
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S4	X3LYP	def2-SV(P)	-2885.949443
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S4	X3LYP	def2-SV(P)	-3346.146317
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S4	X3LYP	def2-SV(P)	-3020.899451
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S4	X3LYP	def2-SV(P)	-3020.463278
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S4	X3LYP	def2-SV(P)	-2810.917815
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S4	X3LYP	def2-SV(P)	-3271.132621
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S4	X3LYP	def2-SV(P)	-2945.874558
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S4	X3LYP	def2-SV(P)	-2945.422138
m01	Acacen	EDA	None	None	Nothing	V	S0	X3LYP	def2-TZVP	-1793.875538
m01	Acacen	EDA	None	None	Cl	V	S0	X3LYP	def2-TZVP	-2254.249886
m01	Acacen	EDA	None	None	Amine	V	S0	X3LYP	def2-TZVP	-1928.993190
m01	Acacen	EDA	None	None	Amide	V	S0	X3LYP	def2-TZVP	-1928.588849
m01	Acacen	EDA	None	None	Nothing	III	S0	X3LYP	def2-TZVP	-1718.568647
m01	Acacen	EDA	None	None	Cl	III	S0	X3LYP	def2-TZVP	-2178.927175
m01	Acacen	EDA	None	None	Amine	III	S0	X3LYP	def2-TZVP	-1853.669757
m01	Acacen	EDA	None	None	Amide	III	S0	X3LYP	def2-TZVP	-1853.298025
m02	Acacen	CHDA	None	None	Nothing	V	S0	X3LYP	def2-TZVP	-1949.830125
m02	Acacen	CHDA	None	None	Cl	V	S0	X3LYP	def2-TZVP	-2410.197438
m02	Acacen	CHDA	None	None	Amine	V	S0	X3LYP	def2-TZVP	-2084.947260
m02	Acacen	CHDA	None	None	Amide	V	S0	X3LYP	def2-TZVP	-2084.534633
m02	Acacen	CHDA	None	None	Nothing	III	S0	X3LYP	def2-TZVP	-1874.518704
m02	Acacen	CHDA	None	None	Cl	III	S0	X3LYP	def2-TZVP	-2334.872922
m02	Acacen	CHDA	None	None	Amine	III	S0	X3LYP	def2-TZVP	-2009.619851
m02	Acacen	CHDA	None	None	Amide	III	S0	X3LYP	def2-TZVP	-2009.242525
m03	Salen	EDA	H	H	Nothing	V	S0	X3LYP	def2-TZVP	-2101.016197
m03	Salen	EDA	H	H	Cl	V	S0	X3LYP	def2-TZVP	-2561.380874
m03	Salen	EDA	H	H	Amine	V	S0	X3LYP	def2-TZVP	-2236.132365
m03	Salen	EDA	H	H	Amide	V	S0	X3LYP	def2-TZVP	-2235.719880
m03	Salen	EDA	H	H	Nothing	III	S0	X3LYP	def2-TZVP	-2025.707459

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m03	Salen	EDA	H	H	Cl	III	S0	X3LYP	def2-TZVP	-2486.065479
m03	Salen	EDA	H	H	Amine	III	S0	X3LYP	def2-TZVP	-2160.812659
m03	Salen	EDA	H	H	Amide	III	S0	X3LYP	def2-TZVP	-2160.434148
m04	Salen	CHDA	H	H	Nothing	V	S0	X3LYP	def2-TZVP	-2256.969462
m04	Salen	CHDA	H	H	Cl	V	S0	X3LYP	def2-TZVP	-2717.330226
m04	Salen	CHDA	H	H	Amine	V	S0	X3LYP	def2-TZVP	-2392.084851
m04	Salen	CHDA	H	H	Amide	V	S0	X3LYP	def2-TZVP	-2391.668001
m04	Salen	CHDA	H	H	Nothing	III	S0	X3LYP	def2-TZVP	-2181.655897
m04	Salen	CHDA	H	H	Cl	III	S0	X3LYP	def2-TZVP	-2642.011284
m04	Salen	CHDA	H	H	Amine	III	S0	X3LYP	def2-TZVP	-2316.762078
m04	Salen	CHDA	H	H	Amide	III	S0	X3LYP	def2-TZVP	-2316.378242
m05	Salen	EDA	H	Me	Nothing	V	S0	X3LYP	def2-TZVP	-2179.597561
m05	Salen	EDA	H	Me	Cl	V	S0	X3LYP	def2-TZVP	-2639.958425
m05	Salen	EDA	H	Me	Amine	V	S0	X3LYP	def2-TZVP	-2314.712066
m05	Salen	EDA	H	Me	Amide	V	S0	X3LYP	def2-TZVP	-2314.297151
m05	Salen	EDA	H	Me	Nothing	III	S0	X3LYP	def2-TZVP	-2104.291051
m05	Salen	EDA	H	Me	Cl	III	S0	X3LYP	def2-TZVP	-2564.644130
m05	Salen	EDA	H	Me	Amine	III	S0	X3LYP	def2-TZVP	-2239.392668
m05	Salen	EDA	H	Me	Amide	III	S0	X3LYP	def2-TZVP	-2239.010592
m06	Salen	CHDA	H	Me	Nothing	V	S0	X3LYP	def2-TZVP	-2335.552067
m06	Salen	CHDA	H	Me	Cl	V	S0	X3LYP	def2-TZVP	-2795.907329
m06	Salen	CHDA	H	Me	Amine	V	S0	X3LYP	def2-TZVP	-2470.664924
m06	Salen	CHDA	H	Me	Amide	V	S0	X3LYP	def2-TZVP	-2470.246314
m06	Salen	CHDA	H	Me	Nothing	III	S0	X3LYP	def2-TZVP	-2260.239242
m06	Salen	CHDA	H	Me	Cl	III	S0	X3LYP	def2-TZVP	-2720.589470
m06	Salen	CHDA	H	Me	Amine	III	S0	X3LYP	def2-TZVP	-2395.342883
m06	Salen	CHDA	H	Me	Amide	III	S0	X3LYP	def2-TZVP	-2394.957432
m07	Salen	EDA	Me	H	Nothing	V	S0	X3LYP	def2-TZVP	-2179.600454
m07	Salen	EDA	Me	H	Cl	V	S0	X3LYP	def2-TZVP	-2639.961216
m07	Salen	EDA	Me	H	Amine	V	S0	X3LYP	def2-TZVP	-2314.714155
m07	Salen	EDA	Me	H	Amide	V	S0	X3LYP	def2-TZVP	-2314.299465
m07	Salen	EDA	Me	H	Nothing	III	S0	X3LYP	def2-TZVP	-2104.292519
m07	Salen	EDA	Me	H	Cl	III	S0	X3LYP	def2-TZVP	-2564.644999
m07	Salen	EDA	Me	H	Amine	III	S0	X3LYP	def2-TZVP	-2239.393400
m07	Salen	EDA	Me	H	Amide	III	S0	X3LYP	def2-TZVP	-2239.012490
m08	Salen	CHDA	Me	H	Nothing	V	S0	X3LYP	def2-TZVP	-2335.552221
m08	Salen	CHDA	Me	H	Cl	V	S0	X3LYP	def2-TZVP	-2795.911294
m08	Salen	CHDA	Me	H	Amine	V	S0	X3LYP	def2-TZVP	-2470.666311
m08	Salen	CHDA	Me	H	Amide	V	S0	X3LYP	def2-TZVP	-2470.247966
m08	Salen	CHDA	Me	H	Nothing	III	S0	X3LYP	def2-TZVP	-2260.240952
m08	Salen	CHDA	Me	H	Cl	III	S0	X3LYP	def2-TZVP	-2720.590919
m08	Salen	CHDA	Me	H	Amine	III	S0	X3LYP	def2-TZVP	-2395.341864
m08	Salen	CHDA	Me	H	Amide	III	S0	X3LYP	def2-TZVP	-2394.958046
m09	Salen	EDA	Me	Me	Nothing	V	S0	X3LYP	def2-TZVP	-2258.181837
m09	Salen	EDA	Me	Me	Cl	V	S0	X3LYP	def2-TZVP	-2718.540723
m09	Salen	EDA	Me	Me	Amine	V	S0	X3LYP	def2-TZVP	-2393.295316
m09	Salen	EDA	Me	Me	Amide	V	S0	X3LYP	def2-TZVP	-2392.877929
m09	Salen	EDA	Me	Me	Nothing	III	S0	X3LYP	def2-TZVP	-2182.875390
m09	Salen	EDA	Me	Me	Cl	III	S0	X3LYP	def2-TZVP	-2643.222466
m09	Salen	EDA	Me	Me	Amine	III	S0	X3LYP	def2-TZVP	-2317.972419
m09	Salen	EDA	Me	Me	Amide	III	S0	X3LYP	def2-TZVP	-2317.590784
m10	Salen	CHDA	Me	Me	Nothing	V	S0	X3LYP	def2-TZVP	-2414.135149
m10	Salen	CHDA	Me	Me	Cl	V	S0	X3LYP	def2-TZVP	-2874.489041
m10	Salen	CHDA	Me	Me	Amine	V	S0	X3LYP	def2-TZVP	-2549.247415
m10	Salen	CHDA	Me	Me	Amide	V	S0	X3LYP	def2-TZVP	-2548.825029
m10	Salen	CHDA	Me	Me	Nothing	III	S0	X3LYP	def2-TZVP	-2338.823152
m10	Salen	CHDA	Me	Me	Cl	III	S0	X3LYP	def2-TZVP	-2799.170185
m10	Salen	CHDA	Me	Me	Amine	III	S0	X3LYP	def2-TZVP	-2473.924303
m10	Salen	CHDA	Me	Me	Amide	III	S0	X3LYP	def2-TZVP	-2473.534351
m11	Salen	EDA	H	t-Bu	Nothing	V	S0	X3LYP	def2-TZVP	-2415.311223
m11	Salen	EDA	H	t-Bu	Cl	V	S0	X3LYP	def2-TZVP	-2875.668220
m11	Salen	EDA	H	t-Bu	Amine	V	S0	X3LYP	def2-TZVP	-2550.423764
m11	Salen	EDA	H	t-Bu	Amide	V	S0	X3LYP	def2-TZVP	-2550.007394
m11	Salen	EDA	H	t-Bu	Nothing	III	S0	X3LYP	def2-TZVP	-2340.001925
m11	Salen	EDA	H	t-Bu	Cl	III	S0	X3LYP	def2-TZVP	-2800.351765
m11	Salen	EDA	H	t-Bu	Amine	III	S0	X3LYP	def2-TZVP	-2475.102336
m11	Salen	EDA	H	t-Bu	Amide	III	S0	X3LYP	def2-TZVP	-2474.718981
m12	Salen	CHDA	H	t-Bu	Nothing	V	S0	X3LYP	def2-TZVP	-2571.263426
m12	Salen	CHDA	H	t-Bu	Cl	V	S0	X3LYP	def2-TZVP	-3031.617661
m12	Salen	CHDA	H	t-Bu	Amine	V	S0	X3LYP	def2-TZVP	-2706.375976
m12	Salen	CHDA	H	t-Bu	Amide	V	S0	X3LYP	def2-TZVP	-2705.955817

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m12	Salen	CHDA	H	t-Bu	Nothing	III	S0	X3LYP	def2-TZVP	-2495.949254
m12	Salen	CHDA	H	t-Bu	Cl	III	S0	X3LYP	def2-TZVP	-2956.296982
m12	Salen	CHDA	H	t-Bu	Amine	III	S0	X3LYP	def2-TZVP	-2631.051478
m12	Salen	CHDA	H	t-Bu	Amide	III	S0	X3LYP	def2-TZVP	-2630.665075
m13	Salen	EDA	t-Bu	H	Nothing	V	S0	X3LYP	def2-TZVP	-2415.294746
m13	Salen	EDA	t-Bu	H	Cl	V	S0	X3LYP	def2-TZVP	-2875.658738
m13	Salen	EDA	t-Bu	H	Amine	V	S0	X3LYP	def2-TZVP	-2550.410095
m13	Salen	EDA	t-Bu	H	Amide	V	S0	X3LYP	def2-TZVP	-2549.994366
m13	Salen	EDA	t-Bu	H	Nothing	III	S0	X3LYP	def2-TZVP	-2339.989708
m13	Salen	EDA	t-Bu	H	Cl	III	S0	X3LYP	def2-TZVP	-2800.328100
m13	Salen	EDA	t-Bu	H	Amine	III	S0	X3LYP	def2-TZVP	-2475.090701
m13	Salen	EDA	t-Bu	H	Amide	III	S0	X3LYP	def2-TZVP	-2474.704188
m14	Salen	CHDA	t-Bu	H	Nothing	V	S0	X3LYP	def2-TZVP	-2571.246604
m14	Salen	CHDA	t-Bu	H	Cl	V	S0	X3LYP	def2-TZVP	-3031.608186
m14	Salen	CHDA	t-Bu	H	Amine	V	S0	X3LYP	def2-TZVP	-2706.364182
m14	Salen	CHDA	t-Bu	H	Amide	V	S0	X3LYP	def2-TZVP	-2705.945822
m14	Salen	CHDA	t-Bu	H	Nothing	III	S0	X3LYP	def2-TZVP	-2495.937810
m14	Salen	CHDA	t-Bu	H	Cl	III	S0	X3LYP	def2-TZVP	-2956.270868
m14	Salen	CHDA	t-Bu	H	Amine	III	S0	X3LYP	def2-TZVP	-2631.029893
m14	Salen	CHDA	t-Bu	H	Amide	III	S0	X3LYP	def2-TZVP	-2630.641070
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S0	X3LYP	def2-TZVP	-2729.588070
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S0	X3LYP	def2-TZVP	-3189.947867
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S0	X3LYP	def2-TZVP	-2864.702907
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S0	X3LYP	def2-TZVP	-2864.281510
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S0	X3LYP	def2-TZVP	-2654.280149
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S0	X3LYP	def2-TZVP	-3114.629482
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S0	X3LYP	def2-TZVP	-2789.364501
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S0	X3LYP	def2-TZVP	-2788.983059
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S0	X3LYP	def2-TZVP	-2885.539932
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S0	X3LYP	def2-TZVP	-3345.893492
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S0	X3LYP	def2-TZVP	-3020.651207
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S0	X3LYP	def2-TZVP	-3020.229985
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S0	X3LYP	def2-TZVP	-2810.228483
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S0	X3LYP	def2-TZVP	-3270.572768
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S0	X3LYP	def2-TZVP	-2945.314868
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S0	X3LYP	def2-TZVP	-2944.926050
m01	Acacen	EDA	None	None	Nothing	V	S2	X3LYP	def2-TZVP	-1793.877264
m01	Acacen	EDA	None	None	Cl	V	S2	X3LYP	def2-TZVP	-2254.251233
m01	Acacen	EDA	None	None	Amine	V	S2	X3LYP	def2-TZVP	-1928.997973
m01	Acacen	EDA	None	None	Amide	V	S2	X3LYP	def2-TZVP	-1928.591071
m01	Acacen	EDA	None	None	Nothing	III	S2	X3LYP	def2-TZVP	-1718.550365
m01	Acacen	EDA	None	None	Cl	III	S2	X3LYP	def2-TZVP	-2178.937272
m01	Acacen	EDA	None	None	Amine	III	S2	X3LYP	def2-TZVP	-1853.681419
m01	Acacen	EDA	None	None	Amide	III	S2	X3LYP	def2-TZVP	-1853.302356
m02	Acacen	CHDA	None	None	Nothing	V	S2	X3LYP	def2-TZVP	-1949.830368
m02	Acacen	CHDA	None	None	Cl	V	S2	X3LYP	def2-TZVP	-2410.199304
m02	Acacen	CHDA	None	None	Amine	V	S2	X3LYP	def2-TZVP	-2084.950656
m02	Acacen	CHDA	None	None	Amide	V	S2	X3LYP	def2-TZVP	-2084.539337
m02	Acacen	CHDA	None	None	Nothing	III	S2	X3LYP	def2-TZVP	-1874.501830
m02	Acacen	CHDA	None	None	Cl	III	S2	X3LYP	def2-TZVP	-2334.882825
m02	Acacen	CHDA	None	None	Amine	III	S2	X3LYP	def2-TZVP	-2009.631446
m02	Acacen	CHDA	None	None	Amide	III	S2	X3LYP	def2-TZVP	-2009.240692
m03	Salen	EDA	H	H	Nothing	V	S2	X3LYP	def2-TZVP	-2101.025597
m03	Salen	EDA	H	H	Cl	V	S2	X3LYP	def2-TZVP	-2561.384188
m03	Salen	EDA	H	H	Amine	V	S2	X3LYP	def2-TZVP	-2236.136580
m03	Salen	EDA	H	H	Amide	V	S2	X3LYP	def2-TZVP	-2235.723613
m03	Salen	EDA	H	H	Nothing	III	S2	X3LYP	def2-TZVP	-2025.695165
m03	Salen	EDA	H	H	Cl	III	S2	X3LYP	def2-TZVP	-2486.073886
m03	Salen	EDA	H	H	Amine	III	S2	X3LYP	def2-TZVP	-2160.820294
m03	Salen	EDA	H	H	Amide	III	S2	X3LYP	def2-TZVP	-2160.443839
m04	Salen	CHDA	H	H	Nothing	V	S2	X3LYP	def2-TZVP	-2256.977630
m04	Salen	CHDA	H	H	Cl	V	S2	X3LYP	def2-TZVP	-2717.332194
m04	Salen	CHDA	H	H	Amine	V	S2	X3LYP	def2-TZVP	-2392.087650
m04	Salen	CHDA	H	H	Amide	V	S2	X3LYP	def2-TZVP	-2391.671849
m04	Salen	CHDA	H	H	Nothing	III	S2	X3LYP	def2-TZVP	-2181.644675
m04	Salen	CHDA	H	H	Cl	III	S2	X3LYP	def2-TZVP	-2642.019470
m04	Salen	CHDA	H	H	Amine	III	S2	X3LYP	def2-TZVP	-2316.770134
m04	Salen	CHDA	H	H	Amide	III	S2	X3LYP	def2-TZVP	-2316.389164
m05	Salen	EDA	H	Me	Nothing	V	S2	X3LYP	def2-TZVP	-2179.608778
m05	Salen	EDA	H	Me	Cl	V	S2	X3LYP	def2-TZVP	-2639.962023
m05	Salen	EDA	H	Me	Amine	V	S2	X3LYP	def2-TZVP	-2314.716161

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m05	Salen	EDA	H	Me	Amide	V	S2	X3LYP	def2-TZVP	-2314.299033
m05	Salen	EDA	H	Me	Nothing	III	S2	X3LYP	def2-TZVP	-2104.278682
m05	Salen	EDA	H	Me	Cl	III	S2	X3LYP	def2-TZVP	-2564.652266
m05	Salen	EDA	H	Me	Amine	III	S2	X3LYP	def2-TZVP	-2239.401374
m05	Salen	EDA	H	Me	Amide	III	S2	X3LYP	def2-TZVP	-2239.021937
m06	Salen	CHDA	H	Me	Nothing	V	S2	X3LYP	def2-TZVP	-2335.560108
m06	Salen	CHDA	H	Me	Cl	V	S2	X3LYP	def2-TZVP	-2795.909630
m06	Salen	CHDA	H	Me	Amine	V	S2	X3LYP	def2-TZVP	-2470.667994
m06	Salen	CHDA	H	Me	Amide	V	S2	X3LYP	def2-TZVP	-2470.250455
m06	Salen	CHDA	H	Me	Nothing	III	S2	X3LYP	def2-TZVP	-2260.227755
m06	Salen	CHDA	H	Me	Cl	III	S2	X3LYP	def2-TZVP	-2720.598225
m06	Salen	CHDA	H	Me	Amine	III	S2	X3LYP	def2-TZVP	-2395.350239
m06	Salen	CHDA	H	Me	Amide	III	S2	X3LYP	def2-TZVP	-2394.967401
m07	Salen	EDA	Me	H	Nothing	V	S2	X3LYP	def2-TZVP	-2179.609650
m07	Salen	EDA	Me	H	Cl	V	S2	X3LYP	def2-TZVP	-2639.966430
m07	Salen	EDA	Me	H	Amine	V	S2	X3LYP	def2-TZVP	-2314.719296
m07	Salen	EDA	Me	H	Amide	V	S2	X3LYP	def2-TZVP	-2314.304872
m07	Salen	EDA	Me	H	Nothing	III	S2	X3LYP	def2-TZVP	-2104.279794
m07	Salen	EDA	Me	H	Cl	III	S2	X3LYP	def2-TZVP	-2564.655377
m07	Salen	EDA	Me	H	Amine	III	S2	X3LYP	def2-TZVP	-2239.402486
m07	Salen	EDA	Me	H	Amide	III	S2	X3LYP	def2-TZVP	-2239.023153
m08	Salen	CHDA	Me	H	Nothing	V	S2	X3LYP	def2-TZVP	-2335.561122
m08	Salen	CHDA	Me	H	Cl	V	S2	X3LYP	def2-TZVP	-2795.914022
m08	Salen	CHDA	Me	H	Amine	V	S2	X3LYP	def2-TZVP	-2470.670395
m08	Salen	CHDA	Me	H	Amide	V	S2	X3LYP	def2-TZVP	-2470.252704
m08	Salen	CHDA	Me	H	Nothing	III	S2	X3LYP	def2-TZVP	-2260.229403
m08	Salen	CHDA	Me	H	Cl	III	S2	X3LYP	def2-TZVP	-2720.600894
m08	Salen	CHDA	Me	H	Amine	III	S2	X3LYP	def2-TZVP	-2395.352694
m08	Salen	CHDA	Me	H	Amide	III	S2	X3LYP	def2-TZVP	-2394.968498
m09	Salen	EDA	Me	Me	Nothing	V	S2	X3LYP	def2-TZVP	-2258.192556
m09	Salen	EDA	Me	Me	Cl	V	S2	X3LYP	def2-TZVP	-2718.544371
m09	Salen	EDA	Me	Me	Amine	V	S2	X3LYP	def2-TZVP	-2393.299323
m09	Salen	EDA	Me	Me	Amide	V	S2	X3LYP	def2-TZVP	-2392.882345
m09	Salen	EDA	Me	Me	Nothing	III	S2	X3LYP	def2-TZVP	-2182.862493
m09	Salen	EDA	Me	Me	Cl	III	S2	X3LYP	def2-TZVP	-2643.233484
m09	Salen	EDA	Me	Me	Amine	III	S2	X3LYP	def2-TZVP	-2317.983128
m09	Salen	EDA	Me	Me	Amide	III	S2	X3LYP	def2-TZVP	-2317.600476
m10	Salen	CHDA	Me	Me	Nothing	V	S2	X3LYP	def2-TZVP	-2414.143471
m10	Salen	CHDA	Me	Me	Cl	V	S2	X3LYP	def2-TZVP	-2874.491932
m10	Salen	CHDA	Me	Me	Amine	V	S2	X3LYP	def2-TZVP	-2549.250628
m10	Salen	CHDA	Me	Me	Amide	V	S2	X3LYP	def2-TZVP	-2548.829182
m10	Salen	CHDA	Me	Me	Nothing	III	S2	X3LYP	def2-TZVP	-2338.811293
m10	Salen	CHDA	Me	Me	Cl	III	S2	X3LYP	def2-TZVP	-2799.178756
m10	Salen	CHDA	Me	Me	Amine	III	S2	X3LYP	def2-TZVP	-2473.932591
m10	Salen	CHDA	Me	Me	Amide	III	S2	X3LYP	def2-TZVP	-2473.545124
m11	Salen	EDA	H	t-Bu	Nothing	V	S2	X3LYP	def2-TZVP	-2415.319372
m11	Salen	EDA	H	t-Bu	Cl	V	S2	X3LYP	def2-TZVP	-2875.671963
m11	Salen	EDA	H	t-Bu	Amine	V	S2	X3LYP	def2-TZVP	-2550.429333
m11	Salen	EDA	H	t-Bu	Amide	V	S2	X3LYP	def2-TZVP	-2550.010537
m11	Salen	EDA	H	t-Bu	Nothing	III	S2	X3LYP	def2-TZVP	-2339.990150
m11	Salen	EDA	H	t-Bu	Cl	III	S2	X3LYP	def2-TZVP	-2800.358719
m11	Salen	EDA	H	t-Bu	Amine	III	S2	X3LYP	def2-TZVP	-2475.109171
m11	Salen	EDA	H	t-Bu	Amide	III	S2	X3LYP	def2-TZVP	-2474.728162
m12	Salen	CHDA	H	t-Bu	Nothing	V	S2	X3LYP	def2-TZVP	-2571.269990
m12	Salen	CHDA	H	t-Bu	Cl	V	S2	X3LYP	def2-TZVP	-3031.620402
m12	Salen	CHDA	H	t-Bu	Amine	V	S2	X3LYP	def2-TZVP	-2706.383473
m12	Salen	CHDA	H	t-Bu	Amide	V	S2	X3LYP	def2-TZVP	-2705.958616
m12	Salen	CHDA	H	t-Bu	Nothing	III	S2	X3LYP	def2-TZVP	-2495.938571
m12	Salen	CHDA	H	t-Bu	Cl	III	S2	X3LYP	def2-TZVP	-2956.301104
m12	Salen	CHDA	H	t-Bu	Amine	III	S2	X3LYP	def2-TZVP	-2631.057156
m12	Salen	CHDA	H	t-Bu	Amide	III	S2	X3LYP	def2-TZVP	-2630.674357
m13	Salen	EDA	t-Bu	H	Nothing	V	S2	X3LYP	def2-TZVP	-2415.303319
m13	Salen	EDA	t-Bu	H	Cl	V	S2	X3LYP	def2-TZVP	-2875.662816
m13	Salen	EDA	t-Bu	H	Amine	V	S2	X3LYP	def2-TZVP	-2550.414778
m13	Salen	EDA	t-Bu	H	Amide	V	S2	X3LYP	def2-TZVP	-2550.000559
m13	Salen	EDA	t-Bu	H	Nothing	III	S2	X3LYP	def2-TZVP	-2339.974609
m13	Salen	EDA	t-Bu	H	Cl	III	S2	X3LYP	def2-TZVP	-2800.347488
m13	Salen	EDA	t-Bu	H	Amine	III	S2	X3LYP	def2-TZVP	-2475.093201
m13	Salen	EDA	t-Bu	H	Amide	III	S2	X3LYP	def2-TZVP	-2474.716418
m14	Salen	CHDA	t-Bu	H	Nothing	V	S2	X3LYP	def2-TZVP	-2571.254153
m14	Salen	CHDA	t-Bu	H	Cl	V	S2	X3LYP	def2-TZVP	-3031.610997

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m14	Salen	CHDA	t-Bu	H	Amine	V	S2	X3LYP	def2-TZVP	-2706.366812
m14	Salen	CHDA	t-Bu	H	Amide	V	S2	X3LYP	def2-TZVP	-2705.944610
m14	Salen	CHDA	t-Bu	H	Nothing	III	S2	X3LYP	def2-TZVP	-2495.924230
m14	Salen	CHDA	t-Bu	H	Cl	III	S2	X3LYP	def2-TZVP	-2956.291506
m14	Salen	CHDA	t-Bu	H	Amine	III	S2	X3LYP	def2-TZVP	-2631.042014
m14	Salen	CHDA	t-Bu	H	Amide	III	S2	X3LYP	def2-TZVP	-2630.661126
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S2	X3LYP	def2-TZVP	-2729.597008
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S2	X3LYP	def2-TZVP	-3189.951087
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S2	X3LYP	def2-TZVP	-2864.706301
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S2	X3LYP	def2-TZVP	-2864.286215
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S2	X3LYP	def2-TZVP	-2654.268123
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S2	X3LYP	def2-TZVP	-3114.633567
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S2	X3LYP	def2-TZVP	-2789.383219
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S2	X3LYP	def2-TZVP	-2789.000385
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S2	X3LYP	def2-TZVP	-2885.547541
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S2	X3LYP	def2-TZVP	-3345.896924
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S2	X3LYP	def2-TZVP	-3020.656235
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S2	X3LYP	def2-TZVP	-3020.233769
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S2	X3LYP	def2-TZVP	-2810.215480
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S2	X3LYP	def2-TZVP	-3270.576405
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S2	X3LYP	def2-TZVP	-2945.328962
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S2	X3LYP	def2-TZVP	-2944.935750
m01	Acacen	EDA	None	None	Nothing	V	S4	X3LYP	def2-TZVP	-1793.780829
m01	Acacen	EDA	None	None	Cl	V	S4	X3LYP	def2-TZVP	-2254.158223
m01	Acacen	EDA	None	None	Amine	V	S4	X3LYP	def2-TZVP	-1928.901113
m01	Acacen	EDA	None	None	Amide	V	S4	X3LYP	def2-TZVP	-1928.518502
m01	Acacen	EDA	None	None	Nothing	III	S4	X3LYP	def2-TZVP	-1718.513366
m01	Acacen	EDA	None	None	Cl	III	S4	X3LYP	def2-TZVP	-2178.912801
m01	Acacen	EDA	None	None	Amine	III	S4	X3LYP	def2-TZVP	-1853.652458
m01	Acacen	EDA	None	None	Amide	III	S4	X3LYP	def2-TZVP	-1853.276973
m02	Acacen	CHDA	None	None	Nothing	V	S4	X3LYP	def2-TZVP	-1949.733465
m02	Acacen	CHDA	None	None	Cl	V	S4	X3LYP	def2-TZVP	-2410.105215
m02	Acacen	CHDA	None	None	Amine	V	S4	X3LYP	def2-TZVP	-2084.852784
m02	Acacen	CHDA	None	None	Amide	V	S4	X3LYP	def2-TZVP	-2084.464946
m02	Acacen	CHDA	None	None	Nothing	III	S4	X3LYP	def2-TZVP	-1874.465834
m02	Acacen	CHDA	None	None	Cl	III	S4	X3LYP	def2-TZVP	-2334.858069
m02	Acacen	CHDA	None	None	Amine	III	S4	X3LYP	def2-TZVP	-2009.596452
m02	Acacen	CHDA	None	None	Amide	III	S4	X3LYP	def2-TZVP	-2009.219299
m03	Salen	EDA	H	H	Nothing	V	S4	X3LYP	def2-TZVP	-2100.934974
m03	Salen	EDA	H	H	Cl	V	S4	X3LYP	def2-TZVP	-2561.296146
m03	Salen	EDA	H	H	Amine	V	S4	X3LYP	def2-TZVP	-2236.047550
m03	Salen	EDA	H	H	Amide	V	S4	X3LYP	def2-TZVP	-2235.654217
m03	Salen	EDA	H	H	Nothing	III	S4	X3LYP	def2-TZVP	-2025.663925
m03	Salen	EDA	H	H	Cl	III	S4	X3LYP	def2-TZVP	-2486.054486
m03	Salen	EDA	H	H	Amine	III	S4	X3LYP	def2-TZVP	-2160.799637
m03	Salen	EDA	H	H	Amide	III	S4	X3LYP	def2-TZVP	-2160.417795
m04	Salen	CHDA	H	H	Nothing	V	S4	X3LYP	def2-TZVP	-2256.884779
m04	Salen	CHDA	H	H	Cl	V	S4	X3LYP	def2-TZVP	-2717.243063
m04	Salen	CHDA	H	H	Amine	V	S4	X3LYP	def2-TZVP	-2391.996970
m04	Salen	CHDA	H	H	Amide	V	S4	X3LYP	def2-TZVP	-2391.600202
m04	Salen	CHDA	H	H	Nothing	III	S4	X3LYP	def2-TZVP	-2181.614509
m04	Salen	CHDA	H	H	Cl	III	S4	X3LYP	def2-TZVP	-2641.999975
m04	Salen	CHDA	H	H	Amine	III	S4	X3LYP	def2-TZVP	-2316.746686
m04	Salen	CHDA	H	H	Amide	III	S4	X3LYP	def2-TZVP	-2316.362724
m05	Salen	EDA	H	Me	Nothing	V	S4	X3LYP	def2-TZVP	-2179.525743
m05	Salen	EDA	H	Me	Cl	V	S4	X3LYP	def2-TZVP	-2639.878228
m05	Salen	EDA	H	Me	Amine	V	S4	X3LYP	def2-TZVP	-2314.637917
m05	Salen	EDA	H	Me	Amide	V	S4	X3LYP	def2-TZVP	-2314.231855
m05	Salen	EDA	H	Me	Nothing	III	S4	X3LYP	def2-TZVP	-2104.246476
m05	Salen	EDA	H	Me	Cl	III	S4	X3LYP	def2-TZVP	-2564.632395
m05	Salen	EDA	H	Me	Amine	III	S4	X3LYP	def2-TZVP	-2239.377801
m05	Salen	EDA	H	Me	Amide	III	S4	X3LYP	def2-TZVP	-2238.995640
m06	Salen	CHDA	H	Me	Nothing	V	S4	X3LYP	def2-TZVP	-2335.474312
m06	Salen	CHDA	H	Me	Cl	V	S4	X3LYP	def2-TZVP	-2795.823886
m06	Salen	CHDA	H	Me	Amine	V	S4	X3LYP	def2-TZVP	-2470.584758
m06	Salen	CHDA	H	Me	Amide	V	S4	X3LYP	def2-TZVP	-2470.180193
m06	Salen	CHDA	H	Me	Nothing	III	S4	X3LYP	def2-TZVP	-2260.196717
m06	Salen	CHDA	H	Me	Cl	III	S4	X3LYP	def2-TZVP	-2720.577853
m06	Salen	CHDA	H	Me	Amine	III	S4	X3LYP	def2-TZVP	-2395.325899
m06	Salen	CHDA	H	Me	Amide	III	S4	X3LYP	def2-TZVP	-2394.941110
m07	Salen	EDA	Me	H	Nothing	V	S4	X3LYP	def2-TZVP	-2179.524129

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m07	Salen	EDA	Me	H	Cl	V	S4	X3LYP	def2-TZVP	-2639.880197
m07	Salen	EDA	Me	H	Amine	V	S4	X3LYP	def2-TZVP	-2314.634151
m07	Salen	EDA	Me	H	Amide	V	S4	X3LYP	def2-TZVP	-2314.234846
m07	Salen	EDA	Me	H	Nothing	III	S4	X3LYP	def2-TZVP	-2104.247503
m07	Salen	EDA	Me	H	Cl	III	S4	X3LYP	def2-TZVP	-2564.637412
m07	Salen	EDA	Me	H	Amine	III	S4	X3LYP	def2-TZVP	-2239.379287
m07	Salen	EDA	Me	H	Amide	III	S4	X3LYP	def2-TZVP	-2238.996264
m08	Salen	CHDA	Me	H	Nothing	V	S4	X3LYP	def2-TZVP	-2335.473551
m08	Salen	CHDA	Me	H	Cl	V	S4	X3LYP	def2-TZVP	-2795.826908
m08	Salen	CHDA	Me	H	Amine	V	S4	X3LYP	def2-TZVP	-2470.583204
m08	Salen	CHDA	Me	H	Amide	V	S4	X3LYP	def2-TZVP	-2470.181309
m08	Salen	CHDA	Me	H	Nothing	III	S4	X3LYP	def2-TZVP	-2260.198328
m08	Salen	CHDA	Me	H	Cl	III	S4	X3LYP	def2-TZVP	-2720.583630
m08	Salen	CHDA	Me	H	Amine	III	S4	X3LYP	def2-TZVP	-2395.328558
m08	Salen	CHDA	Me	H	Amide	III	S4	X3LYP	def2-TZVP	-2394.941458
m09	Salen	EDA	Me	Me	Nothing	V	S4	X3LYP	def2-TZVP	-2258.113280
m09	Salen	EDA	Me	Me	Cl	V	S4	X3LYP	def2-TZVP	-2718.462188
m09	Salen	EDA	Me	Me	Amine	V	S4	X3LYP	def2-TZVP	-2393.220913
m09	Salen	EDA	Me	Me	Amide	V	S4	X3LYP	def2-TZVP	-2392.814038
m09	Salen	EDA	Me	Me	Nothing	III	S4	X3LYP	def2-TZVP	-2182.829566
m09	Salen	EDA	Me	Me	Cl	III	S4	X3LYP	def2-TZVP	-2643.215785
m09	Salen	EDA	Me	Me	Amine	III	S4	X3LYP	def2-TZVP	-2317.959369
m09	Salen	EDA	Me	Me	Amide	III	S4	X3LYP	def2-TZVP	-2317.574462
m10	Salen	CHDA	Me	Me	Nothing	V	S4	X3LYP	def2-TZVP	-2414.061619
m10	Salen	CHDA	Me	Me	Cl	V	S4	X3LYP	def2-TZVP	-2874.408688
m10	Salen	CHDA	Me	Me	Amine	V	S4	X3LYP	def2-TZVP	-2549.169919
m10	Salen	CHDA	Me	Me	Amide	V	S4	X3LYP	def2-TZVP	-2548.759355
m10	Salen	CHDA	Me	Me	Nothing	III	S4	X3LYP	def2-TZVP	-2338.779412
m10	Salen	CHDA	Me	Me	Cl	III	S4	X3LYP	def2-TZVP	-2799.161031
m10	Salen	CHDA	Me	Me	Amine	III	S4	X3LYP	def2-TZVP	-2473.909227
m10	Salen	CHDA	Me	Me	Amide	III	S4	X3LYP	def2-TZVP	-2473.518909
m11	Salen	EDA	H	t-Bu	Nothing	V	S4	X3LYP	def2-TZVP	-2415.236529
m11	Salen	EDA	H	t-Bu	Cl	V	S4	X3LYP	def2-TZVP	-2875.585498
m11	Salen	EDA	H	t-Bu	Amine	V	S4	X3LYP	def2-TZVP	-2550.345785
m11	Salen	EDA	H	t-Bu	Amide	V	S4	X3LYP	def2-TZVP	-2549.942625
m11	Salen	EDA	H	t-Bu	Nothing	III	S4	X3LYP	def2-TZVP	-2339.957509
m11	Salen	EDA	H	t-Bu	Cl	III	S4	X3LYP	def2-TZVP	-2800.336125
m11	Salen	EDA	H	t-Bu	Amine	III	S4	X3LYP	def2-TZVP	-2475.088051
m11	Salen	EDA	H	t-Bu	Amide	III	S4	X3LYP	def2-TZVP	-2474.704656
m12	Salen	CHDA	H	t-Bu	Nothing	V	S4	X3LYP	def2-TZVP	-2571.183793
m12	Salen	CHDA	H	t-Bu	Cl	V	S4	X3LYP	def2-TZVP	-3031.532987
m12	Salen	CHDA	H	t-Bu	Amine	V	S4	X3LYP	def2-TZVP	-2706.293604
m12	Salen	CHDA	H	t-Bu	Amide	V	S4	X3LYP	def2-TZVP	-2705.885803
m12	Salen	CHDA	H	t-Bu	Nothing	III	S4	X3LYP	def2-TZVP	-2495.906492
m12	Salen	CHDA	H	t-Bu	Cl	III	S4	X3LYP	def2-TZVP	-2956.283525
m12	Salen	CHDA	H	t-Bu	Amine	III	S4	X3LYP	def2-TZVP	-2631.038195
m12	Salen	CHDA	H	t-Bu	Amide	III	S4	X3LYP	def2-TZVP	-2630.642886
m13	Salen	EDA	t-Bu	H	Nothing	V	S4	X3LYP	def2-TZVP	-2415.222431
m13	Salen	EDA	t-Bu	H	Cl	V	S4	X3LYP	def2-TZVP	-2875.575499
m13	Salen	EDA	t-Bu	H	Amine	V	S4	X3LYP	def2-TZVP	-2550.328892
m13	Salen	EDA	t-Bu	H	Amide	V	S4	X3LYP	def2-TZVP	-2549.927326
m13	Salen	EDA	t-Bu	H	Nothing	III	S4	X3LYP	def2-TZVP	-2339.942938
m13	Salen	EDA	t-Bu	H	Cl	III	S4	X3LYP	def2-TZVP	-2800.332422
m13	Salen	EDA	t-Bu	H	Amine	III	S4	X3LYP	def2-TZVP	-2475.074138
m13	Salen	EDA	t-Bu	H	Amide	III	S4	X3LYP	def2-TZVP	-2474.691835
m14	Salen	CHDA	t-Bu	H	Nothing	V	S4	X3LYP	def2-TZVP	-2571.163418
m14	Salen	CHDA	t-Bu	H	Cl	V	S4	X3LYP	def2-TZVP	-3031.522308
m14	Salen	CHDA	t-Bu	H	Amine	V	S4	X3LYP	def2-TZVP	-2706.278463
m14	Salen	CHDA	t-Bu	H	Amide	V	S4	X3LYP	def2-TZVP	-2705.874866
m14	Salen	CHDA	t-Bu	H	Nothing	III	S4	X3LYP	def2-TZVP	-2495.893929
m14	Salen	CHDA	t-Bu	H	Cl	III	S4	X3LYP	def2-TZVP	-2956.277193
m14	Salen	CHDA	t-Bu	H	Amine	III	S4	X3LYP	def2-TZVP	-2631.023046
m14	Salen	CHDA	t-Bu	H	Amide	III	S4	X3LYP	def2-TZVP	-2630.623926
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S4	X3LYP	def2-TZVP	-2729.518855
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S4	X3LYP	def2-TZVP	-3189.866778
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S4	X3LYP	def2-TZVP	-2864.625458
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S4	X3LYP	def2-TZVP	-2864.215156
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S4	X3LYP	def2-TZVP	-2654.232674
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S4	X3LYP	def2-TZVP	-3114.619577
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S4	X3LYP	def2-TZVP	-2789.362062
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S4	X3LYP	def2-TZVP	-2788.975665

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S4	X3LYP	def2-TZVP	-2885.460768
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S4	X3LYP	def2-TZVP	-3345.810461
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S4	X3LYP	def2-TZVP	-3020.572428
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S4	X3LYP	def2-TZVP	-3020.161700
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S4	X3LYP	def2-TZVP	-2810.184258
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S4	X3LYP	def2-TZVP	-3270.561863
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S4	X3LYP	def2-TZVP	-2945.310567
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S4	X3LYP	def2-TZVP	-2944.914141
m01	Acacen	EDA	None	None	Nothing	V	S0	X3LYP	DefBas-3	-1793.805778
m01	Acacen	EDA	None	None	Cl	V	S0	X3LYP	DefBas-3	-2254.174288
m01	Acacen	EDA	None	None	Amine	V	S0	X3LYP	DefBas-3	-1928.908568
m01	Acacen	EDA	None	None	Amide	V	S0	X3LYP	DefBas-3	-1928.504156
m01	Acacen	EDA	None	None	Nothing	III	S0	X3LYP	DefBas-3	-1718.500021
m01	Acacen	EDA	None	None	Cl	III	S0	X3LYP	DefBas-3	-2178.855703
m01	Acacen	EDA	None	None	Amine	III	S0	X3LYP	DefBas-3	-1853.589814
m01	Acacen	EDA	None	None	Amide	III	S0	X3LYP	DefBas-3	-1853.219534
m02	Acacen	CHDA	None	None	Nothing	V	S0	X3LYP	DefBas-3	-1949.747194
m02	Acacen	CHDA	None	None	Cl	V	S0	X3LYP	DefBas-3	-2410.108861
m02	Acacen	CHDA	None	None	Amine	V	S0	X3LYP	DefBas-3	-2084.848645
m02	Acacen	CHDA	None	None	Amide	V	S0	X3LYP	DefBas-3	-2084.438020
m02	Acacen	CHDA	None	None	Nothing	III	S0	X3LYP	DefBas-3	-1874.438509
m02	Acacen	CHDA	None	None	Cl	III	S0	X3LYP	DefBas-3	-2334.789261
m02	Acacen	CHDA	None	None	Amine	III	S0	X3LYP	DefBas-3	-2009.525428
m02	Acacen	CHDA	None	None	Amide	III	S0	X3LYP	DefBas-3	-2009.152577
m03	Salen	EDA	H	H	Nothing	V	S0	X3LYP	DefBas-3	-2100.924478
m03	Salen	EDA	H	H	Cl	V	S0	X3LYP	DefBas-3	-2561.283102
m03	Salen	EDA	H	H	Amine	V	S0	X3LYP	DefBas-3	-2236.025173
m03	Salen	EDA	H	H	Amide	V	S0	X3LYP	DefBas-3	-2235.610431
m03	Salen	EDA	H	H	Nothing	III	S0	X3LYP	DefBas-3	-2025.617702
m03	Salen	EDA	H	H	Cl	III	S0	X3LYP	DefBas-3	-2485.972615
m03	Salen	EDA	H	H	Amine	III	S0	X3LYP	DefBas-3	-2160.710941
m03	Salen	EDA	H	H	Amide	III	S0	X3LYP	DefBas-3	-2160.334121
m04	Salen	CHDA	H	H	Nothing	V	S0	X3LYP	DefBas-3	-2256.865035
m04	Salen	CHDA	H	H	Cl	V	S0	X3LYP	DefBas-3	-2717.219891
m04	Salen	CHDA	H	H	Amine	V	S0	X3LYP	DefBas-3	-2391.965301
m04	Salen	CHDA	H	H	Amide	V	S0	X3LYP	DefBas-3	-2391.546681
m04	Salen	CHDA	H	H	Nothing	III	S0	X3LYP	DefBas-3	-2181.554488
m04	Salen	CHDA	H	H	Cl	III	S0	X3LYP	DefBas-3	-2641.906296
m04	Salen	CHDA	H	H	Amine	III	S0	X3LYP	DefBas-3	-2316.648578
m04	Salen	CHDA	H	H	Amide	III	S0	X3LYP	DefBas-3	-2316.265880
m05	Salen	EDA	H	Me	Nothing	V	S0	X3LYP	DefBas-3	-2179.500023
m05	Salen	EDA	H	Me	Cl	V	S0	X3LYP	DefBas-3	-2639.853672
m05	Salen	EDA	H	Me	Amine	V	S0	X3LYP	DefBas-3	-2314.598119
m05	Salen	EDA	H	Me	Amide	V	S0	X3LYP	DefBas-3	-2314.180985
m05	Salen	EDA	H	Me	Nothing	III	S0	X3LYP	DefBas-3	-2104.193525
m05	Salen	EDA	H	Me	Cl	III	S0	X3LYP	DefBas-3	-2564.544757
m05	Salen	EDA	H	Me	Amine	III	S0	X3LYP	DefBas-3	-2239.281363
m05	Salen	EDA	H	Me	Amide	III	S0	X3LYP	DefBas-3	-2238.905150
m06	Salen	CHDA	H	Me	Nothing	V	S0	X3LYP	DefBas-3	-2335.440267
m06	Salen	CHDA	H	Me	Cl	V	S0	X3LYP	DefBas-3	-2795.790210
m06	Salen	CHDA	H	Me	Amine	V	S0	X3LYP	DefBas-3	-2470.537912
m06	Salen	CHDA	H	Me	Amide	V	S0	X3LYP	DefBas-3	-2470.116808
m06	Salen	CHDA	H	Me	Nothing	III	S0	X3LYP	DefBas-3	-2260.130405
m06	Salen	CHDA	H	Me	Cl	III	S0	X3LYP	DefBas-3	-2720.478226
m06	Salen	CHDA	H	Me	Amine	III	S0	X3LYP	DefBas-3	-2395.204747
m06	Salen	CHDA	H	Me	Amide	III	S0	X3LYP	DefBas-3	-2394.837794
m07	Salen	EDA	Me	H	Nothing	V	S0	X3LYP	DefBas-3	-2179.501476
m07	Salen	EDA	Me	H	Cl	V	S0	X3LYP	DefBas-3	-2639.858099
m07	Salen	EDA	Me	H	Amine	V	S0	X3LYP	DefBas-3	-2314.600942
m07	Salen	EDA	Me	H	Amide	V	S0	X3LYP	DefBas-3	-2314.183704
m07	Salen	EDA	Me	H	Nothing	III	S0	X3LYP	DefBas-3	-2104.195527
m07	Salen	EDA	Me	H	Cl	III	S0	X3LYP	DefBas-3	-2564.546213
m07	Salen	EDA	Me	H	Amine	III	S0	X3LYP	DefBas-3	-2239.285179
m07	Salen	EDA	Me	H	Amide	III	S0	X3LYP	DefBas-3	-2238.905677
m08	Salen	CHDA	Me	H	Nothing	V	S0	X3LYP	DefBas-3	-2335.441454
m08	Salen	CHDA	Me	H	Cl	V	S0	X3LYP	DefBas-3	-2795.794153
m08	Salen	CHDA	Me	H	Amine	V	S0	X3LYP	DefBas-3	-2470.539491
m08	Salen	CHDA	Me	H	Amide	V	S0	X3LYP	DefBas-3	-2470.119935
m08	Salen	CHDA	Me	H	Nothing	III	S0	X3LYP	DefBas-3	-2260.132330
m08	Salen	CHDA	Me	H	Cl	III	S0	X3LYP	DefBas-3	-2720.479870
m08	Salen	CHDA	Me	H	Amine	III	S0	X3LYP	DefBas-3	-2395.222075

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m08	Salen	CHDA	Me	H	Amide	III	S0	X3LYP	DefBas-3	-2394.837201
m09	Salen	EDA	Me	Me	Nothing	V	S0	X3LYP	DefBas-3	-2258.077471
m09	Salen	EDA	Me	Me	Cl	V	S0	X3LYP	DefBas-3	-2718.429145
m09	Salen	EDA	Me	Me	Amine	V	S0	X3LYP	DefBas-3	-2393.174792
m09	Salen	EDA	Me	Me	Amide	V	S0	X3LYP	DefBas-3	-2392.753785
m09	Salen	EDA	Me	Me	Nothing	III	S0	X3LYP	DefBas-3	-2182.771510
m09	Salen	EDA	Me	Me	Cl	III	S0	X3LYP	DefBas-3	-2643.118101
m09	Salen	EDA	Me	Me	Amine	III	S0	X3LYP	DefBas-3	-2317.843966
m09	Salen	EDA	Me	Me	Amide	III	S0	X3LYP	DefBas-3	-2317.477684
m10	Salen	CHDA	Me	Me	Nothing	V	S0	X3LYP	DefBas-3	-2414.017135
m10	Salen	CHDA	Me	Me	Cl	V	S0	X3LYP	DefBas-3	-2874.365450
m10	Salen	CHDA	Me	Me	Amine	V	S0	X3LYP	DefBas-3	-2549.114128
m10	Salen	CHDA	Me	Me	Amide	V	S0	X3LYP	DefBas-3	-2548.689959
m10	Salen	CHDA	Me	Me	Nothing	III	S0	X3LYP	DefBas-3	-2338.707465
m10	Salen	CHDA	Me	Me	Cl	III	S0	X3LYP	DefBas-3	-2799.052460
m10	Salen	CHDA	Me	Me	Amine	III	S0	X3LYP	DefBas-3	-2473.796416
m10	Salen	CHDA	Me	Me	Amide	III	S0	X3LYP	DefBas-3	-2473.409700
m11	Salen	EDA	H	t-Bu	Nothing	V	S0	X3LYP	DefBas-3	-2415.188507
m11	Salen	EDA	H	t-Bu	Cl	V	S0	X3LYP	DefBas-3	-2875.542407
m11	Salen	EDA	H	t-Bu	Amine	V	S0	X3LYP	DefBas-3	-2550.287569
m11	Salen	EDA	H	t-Bu	Amide	V	S0	X3LYP	DefBas-3	-2549.865834
m11	Salen	EDA	H	t-Bu	Nothing	III	S0	X3LYP	DefBas-3	-2339.883344
m11	Salen	EDA	H	t-Bu	Cl	III	S0	X3LYP	DefBas-3	-2800.228994
m11	Salen	EDA	H	t-Bu	Amine	III	S0	X3LYP	DefBas-3	-2474.972818
m11	Salen	EDA	H	t-Bu	Amide	III	S0	X3LYP	DefBas-3	-2474.589977
m12	Salen	CHDA	H	t-Bu	Nothing	V	S0	X3LYP	DefBas-3	-2571.128458
m12	Salen	CHDA	H	t-Bu	Cl	V	S0	X3LYP	DefBas-3	-3031.476878
m12	Salen	CHDA	H	t-Bu	Amine	V	S0	X3LYP	DefBas-3	-2706.225523
m12	Salen	CHDA	H	t-Bu	Amide	V	S0	X3LYP	DefBas-3	-2705.801984
m12	Salen	CHDA	H	t-Bu	Nothing	III	S0	X3LYP	DefBas-3	-2495.816939
m12	Salen	CHDA	H	t-Bu	Cl	III	S0	X3LYP	DefBas-3	-2956.155712
m12	Salen	CHDA	H	t-Bu	Amine	III	S0	X3LYP	DefBas-3	-2630.894236
m12	Salen	CHDA	H	t-Bu	Amide	III	S0	X3LYP	DefBas-3	-2630.524168
m13	Salen	EDA	t-Bu	H	Nothing	V	S0	X3LYP	DefBas-3	-2415.174559
m13	Salen	EDA	t-Bu	H	Cl	V	S0	X3LYP	DefBas-3	-2875.533950
m13	Salen	EDA	t-Bu	H	Amine	V	S0	X3LYP	DefBas-3	-2550.275478
m13	Salen	EDA	t-Bu	H	Amide	V	S0	X3LYP	DefBas-3	-2549.861229
m13	Salen	EDA	t-Bu	H	Nothing	III	S0	X3LYP	DefBas-3	-2339.871665
m13	Salen	EDA	t-Bu	H	Cl	III	S0	X3LYP	DefBas-3	-2800.208737
m13	Salen	EDA	t-Bu	H	Amine	III	S0	X3LYP	DefBas-3	-2474.953780
m13	Salen	EDA	t-Bu	H	Amide	III	S0	X3LYP	DefBas-3	-2474.570611
m14	Salen	CHDA	t-Bu	H	Nothing	V	S0	X3LYP	DefBas-3	-2571.113729
m14	Salen	CHDA	t-Bu	H	Cl	V	S0	X3LYP	DefBas-3	-3031.470299
m14	Salen	CHDA	t-Bu	H	Amine	V	S0	X3LYP	DefBas-3	-2706.214676
m14	Salen	CHDA	t-Bu	H	Amide	V	S0	X3LYP	DefBas-3	-2705.797123
m14	Salen	CHDA	t-Bu	H	Nothing	III	S0	X3LYP	DefBas-3	-2495.807682
m14	Salen	CHDA	t-Bu	H	Cl	III	S0	X3LYP	DefBas-3	-2956.139096
m14	Salen	CHDA	t-Bu	H	Amine	III	S0	X3LYP	DefBas-3	-2630.888917
m14	Salen	CHDA	t-Bu	H	Amide	III	S0	X3LYP	DefBas-3	-2630.501129
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S0	X3LYP	DefBas-3	-2729.439557
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S0	X3LYP	DefBas-3	-3189.791298
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S0	X3LYP	DefBas-3	-2864.535790
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S0	X3LYP	DefBas-3	-2864.118609
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S0	X3LYP	DefBas-3	-2654.136372
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S0	X3LYP	DefBas-3	-3114.477424
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S0	X3LYP	DefBas-3	-2789.204959
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S0	X3LYP	DefBas-3	-2788.825248
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S0	X3LYP	DefBas-3	-2885.378187
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S0	X3LYP	DefBas-3	-3345.724526
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S0	X3LYP	DefBas-3	-3020.477788
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S0	X3LYP	DefBas-3	-3020.053469
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S0	X3LYP	DefBas-3	-2810.066931
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S0	X3LYP	DefBas-3	-3270.408969
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S0	X3LYP	DefBas-3	-2945.141379
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S0	X3LYP	DefBas-3	-2944.756362
m01	Acacen	EDA	None	None	Nothing	V	S2	X3LYP	DefBas-3	-1793.804513
m01	Acacen	EDA	None	None	Cl	V	S2	X3LYP	DefBas-3	-2254.174539
m01	Acacen	EDA	None	None	Amine	V	S2	X3LYP	DefBas-3	-1928.911510
m01	Acacen	EDA	None	None	Amide	V	S2	X3LYP	DefBas-3	-1928.503169
m01	Acacen	EDA	None	None	Nothing	III	S2	X3LYP	DefBas-3	-1718.486839
m01	Acacen	EDA	None	None	Cl	III	S2	X3LYP	DefBas-3	-2178.866528

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m01	Acacen	EDA	None	None	Amine	III	S2	X3LYP	DefBas-3	-1853.602562
m01	Acacen	EDA	None	None	Amide	III	S2	X3LYP	DefBas-3	-1853.222686
m02	Acacen	CHDA	None	None	Nothing	V	S2	X3LYP	DefBas-3	-1949.744806
m02	Acacen	CHDA	None	None	Cl	V	S2	X3LYP	DefBas-3	-2410.110190
m02	Acacen	CHDA	None	None	Amine	V	S2	X3LYP	DefBas-3	-2084.851383
m02	Acacen	CHDA	None	None	Amide	V	S2	X3LYP	DefBas-3	-2084.439022
m02	Acacen	CHDA	None	None	Nothing	III	S2	X3LYP	DefBas-3	-1874.426035
m02	Acacen	CHDA	None	None	Cl	III	S2	X3LYP	DefBas-3	-2334.800112
m02	Acacen	CHDA	None	None	Amine	III	S2	X3LYP	DefBas-3	-2009.540161
m02	Acacen	CHDA	None	None	Amide	III	S2	X3LYP	DefBas-3	-2009.148235
m03	Salen	EDA	H	H	Nothing	V	S2	X3LYP	DefBas-3	-2100.931206
m03	Salen	EDA	H	H	Cl	V	S2	X3LYP	DefBas-3	-2561.286122
m03	Salen	EDA	H	H	Amine	V	S2	X3LYP	DefBas-3	-2236.029015
m03	Salen	EDA	H	H	Amide	V	S2	X3LYP	DefBas-3	-2235.614368
m03	Salen	EDA	H	H	Nothing	III	S2	X3LYP	DefBas-3	-2025.610528
m03	Salen	EDA	H	H	Cl	III	S2	X3LYP	DefBas-3	-2485.981814
m03	Salen	EDA	H	H	Amine	III	S2	X3LYP	DefBas-3	-2160.720117
m03	Salen	EDA	H	H	Amide	III	S2	X3LYP	DefBas-3	-2160.343521
m04	Salen	CHDA	H	H	Nothing	V	S2	X3LYP	DefBas-3	-2256.870537
m04	Salen	CHDA	H	H	Cl	V	S2	X3LYP	DefBas-3	-2717.221710
m04	Salen	CHDA	H	H	Amine	V	S2	X3LYP	DefBas-3	-2391.967219
m04	Salen	CHDA	H	H	Amide	V	S2	X3LYP	DefBas-3	-2391.550154
m04	Salen	CHDA	H	H	Nothing	III	S2	X3LYP	DefBas-3	-2181.548043
m04	Salen	CHDA	H	H	Cl	III	S2	X3LYP	DefBas-3	-2641.915315
m04	Salen	CHDA	H	H	Amine	III	S2	X3LYP	DefBas-3	-2316.657444
m04	Salen	CHDA	H	H	Amide	III	S2	X3LYP	DefBas-3	-2316.276315
m05	Salen	EDA	H	Me	Nothing	V	S2	X3LYP	DefBas-3	-2179.506900
m05	Salen	EDA	H	Me	Cl	V	S2	X3LYP	DefBas-3	-2639.857138
m05	Salen	EDA	H	Me	Amine	V	S2	X3LYP	DefBas-3	-2314.602116
m05	Salen	EDA	H	Me	Amide	V	S2	X3LYP	DefBas-3	-2314.182598
m05	Salen	EDA	H	Me	Nothing	III	S2	X3LYP	DefBas-3	-2104.186612
m05	Salen	EDA	H	Me	Cl	III	S2	X3LYP	DefBas-3	-2564.552719
m05	Salen	EDA	H	Me	Amine	III	S2	X3LYP	DefBas-3	-2239.294016
m05	Salen	EDA	H	Me	Amide	III	S2	X3LYP	DefBas-3	-2238.914416
m06	Salen	CHDA	H	Me	Nothing	V	S2	X3LYP	DefBas-3	-2335.445623
m06	Salen	CHDA	H	Me	Cl	V	S2	X3LYP	DefBas-3	-2795.792396
m06	Salen	CHDA	H	Me	Amine	V	S2	X3LYP	DefBas-3	-2470.540451
m06	Salen	CHDA	H	Me	Amide	V	S2	X3LYP	DefBas-3	-2470.121900
m06	Salen	CHDA	H	Me	Nothing	III	S2	X3LYP	DefBas-3	-2260.123631
m06	Salen	CHDA	H	Me	Cl	III	S2	X3LYP	DefBas-3	-2720.486533
m06	Salen	CHDA	H	Me	Amine	III	S2	X3LYP	DefBas-3	-2395.230872
m06	Salen	CHDA	H	Me	Amide	III	S2	X3LYP	DefBas-3	-2394.847435
m07	Salen	EDA	Me	H	Nothing	V	S2	X3LYP	DefBas-3	-2179.508260
m07	Salen	EDA	Me	H	Cl	V	S2	X3LYP	DefBas-3	-2639.861483
m07	Salen	EDA	Me	H	Amine	V	S2	X3LYP	DefBas-3	-2314.604991
m07	Salen	EDA	Me	H	Amide	V	S2	X3LYP	DefBas-3	-2314.188430
m07	Salen	EDA	Me	H	Nothing	III	S2	X3LYP	DefBas-3	-2104.188154
m07	Salen	EDA	Me	H	Cl	III	S2	X3LYP	DefBas-3	-2564.556520
m07	Salen	EDA	Me	H	Amine	III	S2	X3LYP	DefBas-3	-2239.296148
m07	Salen	EDA	Me	H	Amide	III	S2	X3LYP	DefBas-3	-2238.915736
m08	Salen	CHDA	Me	H	Nothing	V	S2	X3LYP	DefBas-3	-2335.446648
m08	Salen	CHDA	Me	H	Cl	V	S2	X3LYP	DefBas-3	-2795.796657
m08	Salen	CHDA	Me	H	Amine	V	S2	X3LYP	DefBas-3	-2470.543182
m08	Salen	CHDA	Me	H	Amide	V	S2	X3LYP	DefBas-3	-2470.124166
m08	Salen	CHDA	Me	H	Nothing	III	S2	X3LYP	DefBas-3	-2260.125763
m08	Salen	CHDA	Me	H	Cl	III	S2	X3LYP	DefBas-3	-2720.490072
m08	Salen	CHDA	Me	H	Amine	III	S2	X3LYP	DefBas-3	-2395.232756
m08	Salen	CHDA	Me	H	Amide	III	S2	X3LYP	DefBas-3	-2394.848396
m09	Salen	EDA	Me	Me	Nothing	V	S2	X3LYP	DefBas-3	-2258.083965
m09	Salen	EDA	Me	Me	Cl	V	S2	X3LYP	DefBas-3	-2718.432927
m09	Salen	EDA	Me	Me	Amine	V	S2	X3LYP	DefBas-3	-2393.178343
m09	Salen	EDA	Me	Me	Amide	V	S2	X3LYP	DefBas-3	-2392.759824
m09	Salen	EDA	Me	Me	Nothing	III	S2	X3LYP	DefBas-3	-2182.763592
m09	Salen	EDA	Me	Me	Cl	III	S2	X3LYP	DefBas-3	-2643.127425
m09	Salen	EDA	Me	Me	Amine	III	S2	X3LYP	DefBas-3	-2317.869108
m09	Salen	EDA	Me	Me	Amide	III	S2	X3LYP	DefBas-3	-2317.485889
m10	Salen	CHDA	Me	Me	Nothing	V	S2	X3LYP	DefBas-3	-2414.022346
m10	Salen	CHDA	Me	Me	Cl	V	S2	X3LYP	DefBas-3	-2874.368092
m10	Salen	CHDA	Me	Me	Amine	V	S2	X3LYP	DefBas-3	-2549.116983
m10	Salen	CHDA	Me	Me	Amide	V	S2	X3LYP	DefBas-3	-2548.694279
m10	Salen	CHDA	Me	Me	Nothing	III	S2	X3LYP	DefBas-3	-2338.700737

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m10	Salen	CHDA	Me	Me	Cl	III	S2	X3LYP	DefBas-3	-2799.060392
m10	Salen	CHDA	Me	Me	Amine	III	S2	X3LYP	DefBas-3	-2473.805092
m10	Salen	CHDA	Me	Me	Amide	III	S2	X3LYP	DefBas-3	-2473.418171
m11	Salen	EDA	H	t-Bu	Nothing	V	S2	X3LYP	DefBas-3	-2415.196182
m11	Salen	EDA	H	t-Bu	Cl	V	S2	X3LYP	DefBas-3	-2875.543743
m11	Salen	EDA	H	t-Bu	Amine	V	S2	X3LYP	DefBas-3	-2550.290286
m11	Salen	EDA	H	t-Bu	Amide	V	S2	X3LYP	DefBas-3	-2549.871185
m11	Salen	EDA	H	t-Bu	Nothing	III	S2	X3LYP	DefBas-3	-2339.875777
m11	Salen	EDA	H	t-Bu	Cl	III	S2	X3LYP	DefBas-3	-2800.237910
m11	Salen	EDA	H	t-Bu	Amine	III	S2	X3LYP	DefBas-3	-2474.978538
m11	Salen	EDA	H	t-Bu	Amide	III	S2	X3LYP	DefBas-3	-2474.598419
m12	Salen	CHDA	H	t-Bu	Nothing	V	S2	X3LYP	DefBas-3	-2571.134260
m12	Salen	CHDA	H	t-Bu	Cl	V	S2	X3LYP	DefBas-3	-3031.479875
m12	Salen	CHDA	H	t-Bu	Amine	V	S2	X3LYP	DefBas-3	-2706.231336
m12	Salen	CHDA	H	t-Bu	Amide	V	S2	X3LYP	DefBas-3	-2705.806572
m12	Salen	CHDA	H	t-Bu	Nothing	III	S2	X3LYP	DefBas-3	-2495.812721
m12	Salen	CHDA	H	t-Bu	Cl	III	S2	X3LYP	DefBas-3	-2956.166209
m12	Salen	CHDA	H	t-Bu	Amine	III	S2	X3LYP	DefBas-3	-2630.915000
m12	Salen	CHDA	H	t-Bu	Amide	III	S2	X3LYP	DefBas-3	-2630.533747
m13	Salen	EDA	t-Bu	H	Nothing	V	S2	X3LYP	DefBas-3	-2415.181000
m13	Salen	EDA	t-Bu	H	Cl	V	S2	X3LYP	DefBas-3	-2875.537020
m13	Salen	EDA	t-Bu	H	Amine	V	S2	X3LYP	DefBas-3	-2550.278922
m13	Salen	EDA	t-Bu	H	Amide	V	S2	X3LYP	DefBas-3	-2549.862927
m13	Salen	EDA	t-Bu	H	Nothing	III	S2	X3LYP	DefBas-3	-2339.862374
m13	Salen	EDA	t-Bu	H	Cl	III	S2	X3LYP	DefBas-3	-2800.227072
m13	Salen	EDA	t-Bu	H	Amine	III	S2	X3LYP	DefBas-3	-2474.964366
m13	Salen	EDA	t-Bu	H	Amide	III	S2	X3LYP	DefBas-3	-2474.587317
m14	Salen	CHDA	t-Bu	H	Nothing	V	S2	X3LYP	DefBas-3	-2571.119215
m14	Salen	CHDA	t-Bu	H	Cl	V	S2	X3LYP	DefBas-3	-3031.472189
m14	Salen	CHDA	t-Bu	H	Amine	V	S2	X3LYP	DefBas-3	-2706.215697
m14	Salen	CHDA	t-Bu	H	Amide	V	S2	X3LYP	DefBas-3	-2705.793491
m14	Salen	CHDA	t-Bu	H	Nothing	III	S2	X3LYP	DefBas-3	-2495.799346
m14	Salen	CHDA	t-Bu	H	Cl	III	S2	X3LYP	DefBas-3	-2956.159080
m14	Salen	CHDA	t-Bu	H	Amine	III	S2	X3LYP	DefBas-3	-2630.901530
m14	Salen	CHDA	t-Bu	H	Amide	III	S2	X3LYP	DefBas-3	-2630.509644
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S2	X3LYP	DefBas-3	-2729.445849
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S2	X3LYP	DefBas-3	-3189.796370
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S2	X3LYP	DefBas-3	-2864.540871
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S2	X3LYP	DefBas-3	-2864.120515
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S2	X3LYP	DefBas-3	-2654.125001
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S2	X3LYP	DefBas-3	-3114.483565
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S2	X3LYP	DefBas-3	-2789.225830
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S2	X3LYP	DefBas-3	-2788.836508
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S2	X3LYP	DefBas-3	-2885.383585
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S2	X3LYP	DefBas-3	-3345.730790
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S2	X3LYP	DefBas-3	-3020.479125
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S2	X3LYP	DefBas-3	-3020.056201
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S2	X3LYP	DefBas-3	-2810.061163
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S2	X3LYP	DefBas-3	-3270.416587
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S2	X3LYP	DefBas-3	-2945.159211
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S2	X3LYP	DefBas-3	-2944.765255
m01	Acacen	EDA	None	None	Nothing	V	S4	X3LYP	DefBas-3	-1793.706725
m01	Acacen	EDA	None	None	Cl	V	S4	X3LYP	DefBas-3	-2254.080756
m01	Acacen	EDA	None	None	Amine	V	S4	X3LYP	DefBas-3	-1928.813695
m01	Acacen	EDA	None	None	Amide	V	S4	X3LYP	DefBas-3	-1928.429259
m01	Acacen	EDA	None	None	Nothing	III	S4	X3LYP	DefBas-3	-1718.449929
m01	Acacen	EDA	None	None	Cl	III	S4	X3LYP	DefBas-3	-2178.842412
m01	Acacen	EDA	None	None	Amine	III	S4	X3LYP	DefBas-3	-1853.580644
m01	Acacen	EDA	None	None	Amide	III	S4	X3LYP	DefBas-3	-1853.197908
m02	Acacen	CHDA	None	None	Nothing	V	S4	X3LYP	DefBas-3	-1949.646863
m02	Acacen	CHDA	None	None	Cl	V	S4	X3LYP	DefBas-3	-2410.014476
m02	Acacen	CHDA	None	None	Amine	V	S4	X3LYP	DefBas-3	-2084.752466
m02	Acacen	CHDA	None	None	Amide	V	S4	X3LYP	DefBas-3	-2084.361565
m02	Acacen	CHDA	None	None	Nothing	III	S4	X3LYP	DefBas-3	-1874.390793
m02	Acacen	CHDA	None	None	Cl	III	S4	X3LYP	DefBas-3	-2334.778774
m02	Acacen	CHDA	None	None	Amine	III	S4	X3LYP	DefBas-3	-2009.506129
m02	Acacen	CHDA	None	None	Amide	III	S4	X3LYP	DefBas-3	-2009.128385
m03	Salen	EDA	H	H	Nothing	V	S4	X3LYP	DefBas-3	-2100.839811
m03	Salen	EDA	H	H	Cl	V	S4	X3LYP	DefBas-3	-2561.197617
m03	Salen	EDA	H	H	Amine	V	S4	X3LYP	DefBas-3	-2235.938784
m03	Salen	EDA	H	H	Amide	V	S4	X3LYP	DefBas-3	-2235.546709

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m03	Salen	EDA	H	H	Nothing	III	S4	X3LYP	DefBas-3	-2025.579136
m03	Salen	EDA	H	H	Cl	III	S4	X3LYP	DefBas-3	-2485.964160
m03	Salen	EDA	H	H	Amine	III	S4	X3LYP	DefBas-3	-2160.702752
m03	Salen	EDA	H	H	Amide	III	S4	X3LYP	DefBas-3	-2160.317000
m04	Salen	CHDA	H	H	Nothing	V	S4	X3LYP	DefBas-3	-2256.776908
m04	Salen	CHDA	H	H	Cl	V	S4	X3LYP	DefBas-3	-2717.131844
m04	Salen	CHDA	H	H	Amine	V	S4	X3LYP	DefBas-3	-2391.875452
m04	Salen	CHDA	H	H	Amide	V	S4	X3LYP	DefBas-3	-2391.478890
m04	Salen	CHDA	H	H	Nothing	III	S4	X3LYP	DefBas-3	-2181.518057
m04	Salen	CHDA	H	H	Cl	III	S4	X3LYP	DefBas-3	-2641.897062
m04	Salen	CHDA	H	H	Amine	III	S4	X3LYP	DefBas-3	-2316.640779
m04	Salen	CHDA	H	H	Amide	III	S4	X3LYP	DefBas-3	-2316.251257
m05	Salen	EDA	H	Me	Nothing	V	S4	X3LYP	DefBas-3	-2179.423191
m05	Salen	EDA	H	Me	Cl	V	S4	X3LYP	DefBas-3	-2639.772678
m05	Salen	EDA	H	Me	Amine	V	S4	X3LYP	DefBas-3	-2314.518536
m05	Salen	EDA	H	Me	Amide	V	S4	X3LYP	DefBas-3	-2314.117942
m05	Salen	EDA	H	Me	Nothing	III	S4	X3LYP	DefBas-3	-2104.153921
m05	Salen	EDA	H	Me	Cl	III	S4	X3LYP	DefBas-3	-2564.535311
m05	Salen	EDA	H	Me	Amine	III	S4	X3LYP	DefBas-3	-2239.276497
m05	Salen	EDA	H	Me	Amide	III	S4	X3LYP	DefBas-3	-2238.885200
m06	Salen	CHDA	H	Me	Nothing	V	S4	X3LYP	DefBas-3	-2335.359257
m06	Salen	CHDA	H	Me	Cl	V	S4	X3LYP	DefBas-3	-2795.705452
m06	Salen	CHDA	H	Me	Amine	V	S4	X3LYP	DefBas-3	-2470.455726
m06	Salen	CHDA	H	Me	Amide	V	S4	X3LYP	DefBas-3	-2470.052101
m06	Salen	CHDA	H	Me	Nothing	III	S4	X3LYP	DefBas-3	-2260.091828
m06	Salen	CHDA	H	Me	Cl	III	S4	X3LYP	DefBas-3	-2720.467911
m06	Salen	CHDA	H	Me	Amine	III	S4	X3LYP	DefBas-3	-2395.214462
m06	Salen	CHDA	H	Me	Amide	III	S4	X3LYP	DefBas-3	-2394.821890
m07	Salen	EDA	Me	H	Nothing	V	S4	X3LYP	DefBas-3	-2179.421663
m07	Salen	EDA	Me	H	Cl	V	S4	X3LYP	DefBas-3	-2639.774666
m07	Salen	EDA	Me	H	Amine	V	S4	X3LYP	DefBas-3	-2314.518153
m07	Salen	EDA	Me	H	Amide	V	S4	X3LYP	DefBas-3	-2314.119030
m07	Salen	EDA	Me	H	Nothing	III	S4	X3LYP	DefBas-3	-2104.155702
m07	Salen	EDA	Me	H	Cl	III	S4	X3LYP	DefBas-3	-2564.539219
m07	Salen	EDA	Me	H	Amine	III	S4	X3LYP	DefBas-3	-2239.276218
m07	Salen	EDA	Me	H	Amide	III	S4	X3LYP	DefBas-3	-2238.889811
m08	Salen	CHDA	Me	H	Nothing	V	S4	X3LYP	DefBas-3	-2335.358310
m08	Salen	CHDA	Me	H	Cl	V	S4	X3LYP	DefBas-3	-2795.708831
m08	Salen	CHDA	Me	H	Amine	V	S4	X3LYP	DefBas-3	-2470.455166
m08	Salen	CHDA	Me	H	Amide	V	S4	X3LYP	DefBas-3	-2470.053017
m08	Salen	CHDA	Me	H	Nothing	III	S4	X3LYP	DefBas-3	-2260.094997
m08	Salen	CHDA	Me	H	Cl	III	S4	X3LYP	DefBas-3	-2720.473047
m08	Salen	CHDA	Me	H	Amine	III	S4	X3LYP	DefBas-3	-2395.208485
m08	Salen	CHDA	Me	H	Amide	III	S4	X3LYP	DefBas-3	-2394.821773
m09	Salen	EDA	Me	Me	Nothing	V	S4	X3LYP	DefBas-3	-2258.003972
m09	Salen	EDA	Me	Me	Cl	V	S4	X3LYP	DefBas-3	-2718.349963
m09	Salen	EDA	Me	Me	Amine	V	S4	X3LYP	DefBas-3	-2393.097867
m09	Salen	EDA	Me	Me	Amide	V	S4	X3LYP	DefBas-3	-2392.690482
m09	Salen	EDA	Me	Me	Nothing	III	S4	X3LYP	DefBas-3	-2182.729873
m09	Salen	EDA	Me	Me	Cl	III	S4	X3LYP	DefBas-3	-2643.110234
m09	Salen	EDA	Me	Me	Amine	III	S4	X3LYP	DefBas-3	-2317.848122
m09	Salen	EDA	Me	Me	Amide	III	S4	X3LYP	DefBas-3	-2317.459025
m10	Salen	CHDA	Me	Me	Nothing	V	S4	X3LYP	DefBas-3	-2413.939780
m10	Salen	CHDA	Me	Me	Cl	V	S4	X3LYP	DefBas-3	-2874.284009
m10	Salen	CHDA	Me	Me	Amine	V	S4	X3LYP	DefBas-3	-2549.034246
m10	Salen	CHDA	Me	Me	Amide	V	S4	X3LYP	DefBas-3	-2548.623722
m10	Salen	CHDA	Me	Me	Nothing	III	S4	X3LYP	DefBas-3	-2338.668914
m10	Salen	CHDA	Me	Me	Cl	III	S4	X3LYP	DefBas-3	-2799.043707
m10	Salen	CHDA	Me	Me	Amine	III	S4	X3LYP	DefBas-3	-2473.781536
m10	Salen	CHDA	Me	Me	Amide	III	S4	X3LYP	DefBas-3	-2473.392937
m11	Salen	EDA	H	t-Bu	Nothing	V	S4	X3LYP	DefBas-3	-2415.112583
m11	Salen	EDA	H	t-Bu	Cl	V	S4	X3LYP	DefBas-3	-2875.456157
m11	Salen	EDA	H	t-Bu	Amine	V	S4	X3LYP	DefBas-3	-2550.204883
m11	Salen	EDA	H	t-Bu	Amide	V	S4	X3LYP	DefBas-3	-2549.802177
m11	Salen	EDA	H	t-Bu	Nothing	III	S4	X3LYP	DefBas-3	-2339.843377
m11	Salen	EDA	H	t-Bu	Cl	III	S4	X3LYP	DefBas-3	-2800.220393
m11	Salen	EDA	H	t-Bu	Amine	III	S4	X3LYP	DefBas-3	-2474.951338
m11	Salen	EDA	H	t-Bu	Amide	III	S4	X3LYP	DefBas-3	-2474.575720
m12	Salen	CHDA	H	t-Bu	Nothing	V	S4	X3LYP	DefBas-3	-2571.048393
m12	Salen	CHDA	H	t-Bu	Cl	V	S4	X3LYP	DefBas-3	-3031.391373
m12	Salen	CHDA	H	t-Bu	Amine	V	S4	X3LYP	DefBas-3	-2706.145113

Table 1: Absolute energies (in Hartrees) for the Mn(salen) complexes at the different levels of theory. *(continued)*

Model	Eq. Lig.	Bridge	R_1	R_2	Ax. Lig.	Ox. St.	Spin St.	Funct.	Basis Set	Energy
m12	Salen	CHDA	H	t-Bu	Amide	V	S4	X3LYP	DefBas-3	-2705.736228
m12	Salen	CHDA	H	t-Bu	Nothing	III	S4	X3LYP	DefBas-3	-2495.779681
m12	Salen	CHDA	H	t-Bu	Cl	III	S4	X3LYP	DefBas-3	-2956.150792
m12	Salen	CHDA	H	t-Bu	Amine	III	S4	X3LYP	DefBas-3	-2630.895763
m12	Salen	CHDA	H	t-Bu	Amide	III	S4	X3LYP	DefBas-3	-2630.508899
m13	Salen	EDA	t-Bu	H	Nothing	V	S4	X3LYP	DefBas-3	-2415.091684
m13	Salen	EDA	t-Bu	H	Cl	V	S4	X3LYP	DefBas-3	-2875.449242
m13	Salen	EDA	t-Bu	H	Amine	V	S4	X3LYP	DefBas-3	-2550.192422
m13	Salen	EDA	t-Bu	H	Amide	V	S4	X3LYP	DefBas-3	-2549.792743
m13	Salen	EDA	t-Bu	H	Nothing	III	S4	X3LYP	DefBas-3	-2339.830325
m13	Salen	EDA	t-Bu	H	Cl	III	S4	X3LYP	DefBas-3	-2800.213521
m13	Salen	EDA	t-Bu	H	Amine	III	S4	X3LYP	DefBas-3	-2474.945794
m13	Salen	EDA	t-Bu	H	Amide	III	S4	X3LYP	DefBas-3	-2474.563163
m14	Salen	CHDA	t-Bu	H	Nothing	V	S4	X3LYP	DefBas-3	-2571.028022
m14	Salen	CHDA	t-Bu	H	Cl	V	S4	X3LYP	DefBas-3	-3031.383045
m14	Salen	CHDA	t-Bu	H	Amine	V	S4	X3LYP	DefBas-3	-2706.128598
m14	Salen	CHDA	t-Bu	H	Amide	V	S4	X3LYP	DefBas-3	-2705.725897
m14	Salen	CHDA	t-Bu	H	Nothing	III	S4	X3LYP	DefBas-3	-2495.768459
m14	Salen	CHDA	t-Bu	H	Cl	III	S4	X3LYP	DefBas-3	-2956.146235
m14	Salen	CHDA	t-Bu	H	Amine	III	S4	X3LYP	DefBas-3	-2630.882263
m14	Salen	CHDA	t-Bu	H	Amide	III	S4	X3LYP	DefBas-3	-2630.483696
m15	Salen	EDA	t-Bu	t-Bu	Nothing	V	S4	X3LYP	DefBas-3	-2729.360728
m15	Salen	EDA	t-Bu	t-Bu	Cl	V	S4	X3LYP	DefBas-3	-3189.712052
m15	Salen	EDA	t-Bu	t-Bu	Amine	V	S4	X3LYP	DefBas-3	-2864.460445
m15	Salen	EDA	t-Bu	t-Bu	Amide	V	S4	X3LYP	DefBas-3	-2864.047438
m15	Salen	EDA	t-Bu	t-Bu	Nothing	III	S4	X3LYP	DefBas-3	-2654.091388
m15	Salen	EDA	t-Bu	t-Bu	Cl	III	S4	X3LYP	DefBas-3	-3114.474648
m15	Salen	EDA	t-Bu	t-Bu	Amine	III	S4	X3LYP	DefBas-3	-2789.203754
m15	Salen	EDA	t-Bu	t-Bu	Amide	III	S4	X3LYP	DefBas-3	-2788.821823
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	V	S4	X3LYP	DefBas-3	-2885.296318
m16	Salen	CHDA	t-Bu	t-Bu	Cl	V	S4	X3LYP	DefBas-3	-3345.643244
m16	Salen	CHDA	t-Bu	t-Bu	Amine	V	S4	X3LYP	DefBas-3	-3020.395207
m16	Salen	CHDA	t-Bu	t-Bu	Amide	V	S4	X3LYP	DefBas-3	-3019.980555
m16	Salen	CHDA	t-Bu	t-Bu	Nothing	III	S4	X3LYP	DefBas-3	-2810.027850
m16	Salen	CHDA	t-Bu	t-Bu	Cl	III	S4	X3LYP	DefBas-3	-3270.403357
m16	Salen	CHDA	t-Bu	t-Bu	Amine	III	S4	X3LYP	DefBas-3	-2945.140918
m16	Salen	CHDA	t-Bu	t-Bu	Amide	III	S4	X3LYP	DefBas-3	-2944.745190

Description of DB0

Table 2: Continuous variables in the DB0 dataset, organized by group.

	Group	Variables
1	Bond Distances	D·Mn−O_{ax}, D·Mn−N_2, D·Mn−N_3, D·Mn−O_4, D·Mn−O_5, D·N_2−C_{20}, D·N_2−C_6, D·N_3−C_{21}, D·N_3−C_7, D·O_4−C_{10}, D·O_5−C_{11}, D·C_6−C_8, D·C_7−C_9, D·C_8−C_{10}, D·C_9−C_{11}, D·C_{20}−C_{21}, D·C_{10}−C_{12}, D·C_{11}−C_{13}, D·C_{12}−C_{14}, D·C_{13}−C_{15}, D·C_{14}−C_{16}, D·C_{15}−C_{17}, D·C_{16}−C_{18}, D·C_{17}−C_{19}, D·C_{18}−C_8, D·C_{19}−C_9
2	Bond Angles	A·C_{10}−O_4−Mn, A·C_{11}−O_5−Mn, A·L_{ax}−Mn−N_2, A·L_{ax}−Mn−N_3, A·L_{ax}−Mn−O_4, A·L_{ax}−Mn−O_5, A·Mn−N_2−C_{20}, A·Mn−N_2−C_6, A·Mn−N_3−C_7, A·N_2−C_{20}−C_{21}, A·N_2−C_6−C_8, A·N_2−Mn−N_3, A·C_9−C_{11}−O_5, A·N_3−C_7−C_9, A·O_4−Mn−N_2, A·O_4−Mn−O_5, A·O_5−Mn−N_3, A·O_{ax}−Mn−L_{ax}, A·O_{ax}−Mn−N_2, A·O_{ax}−Mn−N_3, A·O_{ax}−Mn−O_4, A·O_{ax}−Mn−O_5, A·C_{20}−C_{21}−N_3, A·C_{21}−N_3−Mn, A·C_6−C_8−C_{10}, A·C_7−C_9−C_{11}, A·C_{10}−C_{12}−C_{14}, A·C_{11}−C_{13}−C_{15}, A·C_{12}−C_{14}−C_{16}, A·C_{13}−C_{15}−C_{17}, A·C_{14}−C_{16}−C_{18}, A·C_{15}−C_{17}−C_{19}, A·C_{16}−C_{18}−C_8, A·C_{17}−C_{19}−C_9, A·C_8−C_{10}−C_{12}, A·C_8−C_{10}−O_4, A·C_9−C_{11}−C_{13}
3	Natural Charges	Q·O_{ax}, S·O_{ax}, Q·EqLig, S·EqLig, Q·AxLig, S·AxLig, Q·Mn, Q·N_2, Q·N_3, Q·O_4, Q·O_5, Q·C_6, Q·C_7, Q·C_8, Q·C_9, Q·C_{10}, Q·C_{11}, Q·C_{12}, Q·C_{13}, Q·C_{14}, Q·C_{15}, Q·C_{16}, Q·C_{17}, Q·C_{18}, Q·C_{19}, Q·C_{20}, Q·C_{21}
4	Natural Spin Densities	S·Mn, S·N_2, S·N_3, S·O_4, S·O_5, S·C_6, S·C_7, S·C_8, S·C_9, S·C_{10}, S·C_{11}, S·C_{12}, S·C_{13}, S·C_{14}, S·C_{15}, S·C_{16}, S·C_{17}, S·C_{18}, S·C_{19}, S·C_{20}, S·C_{21}
5	General Geometric Measurements	d_P, ϕ_e, ϕ_u, *CCM.acacen*, *CCM.ssalen*
6	Energies	ΔE_{ox}, ΔE_{epox}, $\Delta E_{0,2}$, $\Delta E_{0,4}$, $\Delta E_{2,4}$

Factor Analysis

```
======================================================================
DB1
======================================================================
Summary for PCA of db1
      Comp.      %Var.   %C. Var. Association
 ---------------------------------------------
        PC1       30.6       30.6      EqLig
        PC2       23.3       53.9   BasisSet
        PC3        8.2       62.1     SpinSt
        PC4        5.0       67.1       OxSt
        PC5        4.6       71.6      AxLig
        PC6        3.5       75.1       OxSt
        PC7        3.0       78.1     Bridge
        PC8        2.8       80.9     Bridge
        PC9        2.3       83.2
       PC10        2.0       85.3         R2
       PC11        1.9       87.2
       PC12        1.5       88.7         R1
       PC13        1.4       90.1
       PC14        1.3       91.4 Functional
 ---------------------------------------------
Associated Overlaps:

PC1:
            Acacen        Salen
Acacen 1.000745e+00 6.392762e-17
Salen  6.392762e-17 1.001063e+00

PC2:
          def2-SV(P)  def2-TZVP   DefBas-3
def2-SV(P) 1.00097761 0.02296503 0.02154844
def2-TZVP  0.02296503 1.00097878 0.95782400
DefBas-3   0.02154844 0.95782400 1.00097788

PC3:
           S0        S2         S4
S0 1.00096726 0.4831312 0.08824091
S2 0.48313124 1.0009783 0.26165915
S4 0.08824091 0.2616592 1.00097843

PC4:
            V       III
V   1.0009781 0.4305428
III 0.4305428 1.0009744

PC5:
          Nothing        Cl     Amine     Amide
Nothing 1.0009748 0.4446921 0.6049953 0.3681638
Cl      0.4446921 1.0009786 0.8236873 0.7963754
Amine   0.6049953 0.8236873 1.0009789 0.6941031
Amide   0.3681638 0.7963754 0.6941031 1.0009318

PC6:
            V       III
V   1.0009780 0.5747908
III 0.5747908 1.0009735

PC7:
           EDA      CHDA
EDA  1.0009759 0.6417746
CHDA 0.6417746 1.0009753

PC8:
            EDA       CHDA
EDA  1.00097799 0.07200161
CHDA 0.07200161 1.00097881

PC10:
           None         H        Me      t-Bu
None 1.0009785 0.4114676 0.5348415 0.5514032
H    0.4114676 1.0009786 0.3116187 0.3481594
Me   0.5348415 0.3116187 1.0009780 0.8823070
t-Bu 0.5514032 0.3481594 0.8823070 1.0009744

PC12:
           None         H        Me      t-Bu
None 1.0009790 0.6783955 0.6914035 0.6750193
H    0.6783955 1.0009749 0.5697448 0.4971778
Me   0.6914035 0.5697448 1.0009707 0.8144356
t-Bu 0.6750193 0.4971778 0.8144356 1.0009786

PC14:
             TPSS     X3LYP
TPSS  1.0009783 0.6816425
X3LYP 0.6816425 1.0009743


Most Prominent Loadings:
PC01(+):   D.C11.C13( 1.0)   D.C10.C12( 1.0) A.C10.C12.C14( 1.0)   D.C15.C17( 1.0)   D.C14.C16( 1.0) A.C11.C13.C15( 1.0)
PC01(-):       Q.C19(-1.0)       Q.C18(-1.0)       Q.C15(-0.9) CCM.acacen1(-0.9)       Q.C14(-0.9)       Q.C13(-0.4)
PC02(+):     D.N2.C6( 0.9)     D.N3.C7( 0.9)    D.O5.C11( 0.8)    D.O4.C10( 0.8)  A.Mn.N3.C7( 0.8)        Q.Mn( 0.7)
PC02(-):     D.Mn.N3(-0.9)     D.Mn.N2(-0.9)        Q.C7(-0.8)        Q.C6(-0.8)     D.Mn.O5(-0.8)     D.Mn.O4(-0.8)
PC03(+):     S.EqLig( 0.7)        S.O4( 0.7)        S.C7( 0.7)        S.O5( 0.6)        S.C6( 0.6)       S.C19( 0.6)
PC03(-):        Q.N2(-0.5)        Q.N3(-0.5)    D.O4.C10(-0.4)        Q.O5(-0.4)    D.N3.C21(-0.4) A.C10.O4.Mn(-0.4)
PC04(+):        S.N3( 0.7)        S.N2( 0.6)        S.C16( 0.6)        Q.O4( 0.6)        Q.O5( 0.6)       S.C12( 0.6)
PC04(-):        S.Mn(-0.5)       S.C21(-0.4)       S.C20(-0.3)       PhiE(-0.3) A.C21.N3.Mn(-0.2)    D.N3.C21(-0.2)
PC05(+): A.C11.O5.Mn( 0.7) A.C10.O4.Mn( 0.6)  A.O4.Mn.O5( 0.5)  A.N3.C7.C9( 0.4)       S.Mn( 0.3)  A.N2.C6.C8( 0.3)
PC05(-):  A.O5.Mn.N3(-0.8)  A.O4.Mn.N2(-0.8)        Q.N2(-0.5) A.C8.C10.O4(-0.5) A.C9.C11.O5(-0.5)        Q.N3(-0.4)
PC06(+):     Q.EqLig( 0.6) A.Mn.N2.C20( 0.6)        Q.C6( 0.4)  A.N2.C6.C8( 0.4)        Q.C7( 0.4)    D.N2.C20( 0.4)
PC06(-):  A.Mn.N2.C6(-0.4) A.C21.N3.Mn(-0.4)       S.C8(-0.3)      S.C13(-0.3)         Dp(-0.3)     D.Mn.O5(-0.3)
PC07(+):       S.C17( 0.7)       S.C13( 0.6)       S.C9( 0.5)        S.O5( 0.4)    D.N2.C20( 0.4)       Q.C20( 0.3)
PC07(-):       S.N2(-0.4) A.C21.N3.Mn(-0.4)       S.C15(-0.2)       S.C8(-0.2)       S.C19(-0.2)     D.N3.C7(-0.2)
PC08(+):       Q.C21( 0.9)       Q.C20( 0.9)    D.N3.C21( 0.3) CCM.acacen1( 0.3)       S.C12( 0.2)    D.N2.C20( 0.2)
PC08(-): A.N2.C20.C21(-0.4) A.C20.C21.N3(-0.4) A.Mn.N2.C20(-0.3)       S.C17(-0.2)       Q.C17(-0.2)        S.C9(-0.2)
PC09(+):       S.C12( 0.5)       S.C16( 0.5)  A.N2.Mn.N3( 0.4)       PhiE( 0.3)       S.C8( 0.3)       S.O4( 0.3)
PC09(-):          Dp(-0.5)        S.N3(-0.4)       Q.C20(-0.2)       S.C14(-0.2)       Q.C21(-0.2)    D.O4.C10(-0.1)
PC10(+):       Q.C13( 0.5)       Q.C12( 0.5) CCM.acacen1( 0.3)  CCM.salen1( 0.3)       S.C13( 0.2)       Q.N3( 0.2)
PC10(-):       Q.C16(-0.7)       Q.C17(-0.6)       S.C16(-0.2)         Dp(-0.2)       S.C12(-0.2) A.C8.C10.O4(-0.1)
PC11(+):  A.O4.Mn.O5( 0.5)        PhiU( 0.4)        Q.O5( 0.3)        Q.O4( 0.2)  A.O5.Mn.N3( 0.2)  A.N3.C7.C9( 0.2)
PC11(-):          Dp(-0.6)       S.C12(-0.3)       Q.Mn(-0.3)      S.C16(-0.3)       Q.C12(-0.3)    D.N2.C20(-0.2)
PC12(+):       Q.C13( 0.5)       Q.C12( 0.5)       Q.C17( 0.5)       Q.C16( 0.5) A.C21.N3.Mn( 0.2)  A.O5.Mn.N3( 0.2)
PC12(-):          Dp(-0.2)        PhiE(-0.2)  A.Mn.N3.C7(-0.2) A.C11.O5.Mn(-0.2)  CCM.salen1(-0.1)  A.Mn.N2.C6(-0.1)
PC13(+):        PhiU( 0.7)  A.Mn.N3.C7( 0.3)          Dp( 0.3)  A.N3.C7.C9( 0.2)     D.Mn.O5( 0.2)    D.N3.C21( 0.2)
PC13(-):  A.O4.Mn.O5(-0.3)    D.O5.C11(-0.2)  A.O4.Mn.N2(-0.2)       PhiE(-0.2)       S.C10(-0.2) A.N2.C20.C21(-0.2)
PC14(+):       PhiE( 0.6)        PhiU( 0.3) A.C10.O4.Mn( 0.2)  A.Mn.N2.C6( 0.2)       S.N2( 0.2)       S.N3( 0.2)
PC14(-):       S.C21(-0.2)  A.O4.Mn.O5(-0.2) A.C21.N3.Mn(-0.2)       S.O5(-0.2)       S.C20(-0.2)       Q.O5(-0.2)
```

Summary for rPCA of db1

rComp.	%Var.	%C. Var.	Association
RC1	30.0	30.0	EqLig
RC2	18.5	48.5	BasisSet
RC3	12.0	60.5	SpinSt
RC4	4.5	65.0	AxLig
RC5	3.9	68.9	OxSt
RC6	3.5	72.4	
RC7	3.4	75.8	AxLig
RC8	3.3	79.1	
RC9	2.8	81.9	Bridge
RC10	2.1	84.0	R2
RC11	2.0	86.0	R1
RC12	2.0	88.0	
RC13	1.8	89.8	Functional
RC14	1.6	91.4	

Associated Overlaps:

RC1:

	Acacen	Salen
Acacen	1.000958e+00	1.247091e-16
Salen	1.247091e-16	1.000895e+00

RC2:

	def2-SV(P)	def2-TZVP	DefBas-3
def2-SV(P)	1.0009792	0.1246290	0.1133072
def2-TZVP	0.1246290	1.0009774	0.9647615
DefBas-3	0.1133072	0.9647615	1.0009780

RC3:

	S0	S2	S4
S0	1.00097840	0.1636736	0.06893227
S2	0.16367356	1.0009781	0.36154069
S4	0.06893227	0.3615407	1.00093074

RC4:

	Nothing	Cl	Amine	Amide
Nothing	1.0009770	0.3807532	0.5001306	0.4518430
Cl	0.3807532	1.0009781	0.8424024	0.7499814
Amine	0.5001306	0.8424024	1.0009784	0.7752959
Amide	0.4518430	0.7499814	0.7752959	1.0005875

RC5:

	V	III
V	1.0009784	0.4417481
III	0.4417481	1.0009760

RC7:

	Nothing	Cl	Amine	Amide
Nothing	1.0009276	0.6270186	0.7070013	0.5010798
Cl	0.6270186	1.0009786	0.7679933	0.7705187
Amine	0.7070013	0.7679933	1.0009784	0.6606454
Amide	0.5010798	0.7705187	0.6606454	1.0009784

RC9:

	EDA	CHDA
EDA	1.000984e+00	1.851465e-16
CHDA	1.851465e-16	1.000959e+00

RC10:

	None	H	Me	t-Bu
None	1.0009782	1.514083e-01	0.3491111552	2.219561e-01
H	0.1514083	1.000978e+00	0.0003104907	3.207283e-05
Me	0.3491112	3.104907e-04	1.0009787136	7.978097e-01
t-Bu	0.2219561	3.207283e-05	0.7978096638	1.000979e+00

RC11:

	None	H	Me	t-Bu
None	1.000978623	8.744934e-03	3.160476e-01	1.130664e-01
H	0.008744934	1.001005e+00	7.128333e-10	2.293527e-16
Me	0.316047648	7.128333e-10	1.000978e+00	5.437855e-01
t-Bu	0.113066431	2.293527e-16	5.437855e-01	1.000979e+00

RC13:

	TPSS	X3LYP
TPSS	1.0009771	0.6784403
X3LYP	0.6784403	1.0009759

Most Prominent Loadings:

RC01(+):	D.C16.C18(1.0)	A.C17.C19.C9(1.0)	A.C16.C18.C8(1.0)	D.C12.C14(1.0)	D.C17.C19(1.0)	D.C13.C15(1.0)
RC01(-):	Q.C19(-1.0)	Q.C18(-1.0)	Q.C15(-0.9)	Q.C14(-0.9)	CCM.acacen1(-0.9)	Q.C13(-0.4)
RC02(+):	D.Mn.O4(0.9)	D.Mn.N2(0.9)	D.Mn.N3(0.8)	Q.C6(0.8)	Q.C7(0.8)	Q.C10(0.8)
RC02(-):	D.O4.C10(-0.9)	A.Mn.N2.C6(-0.8)	D.O5.C11(-0.8)	D.N3.C21(-0.8)	D.N3.C7(-0.8)	D.N2.C6(-0.7)
RC03(+):	S.EqLig(0.9)	S.C6(0.9)	S.C7(0.9)	S.C18(0.8)	S.C10(0.8)	S.C19(0.8)
RC03(-):	S.C9(-0.5)	D.C6.C8(-0.4)	S.C8(-0.4)	D.C7.C9(-0.4)	Q.N2(-0.3)	A.O4.Mn.O5(-0.3)
RC04(+):	A.O4.Mn.N2(0.8)	A.O5.Mn.N3(0.8)	Q.N2(0.6)	Q.N3(0.6)	A.N2.Mn.N3(0.4)	A.C8.C10.O4(0.4)
RC04(-):	A.C11.O5.Mn(-0.7)	A.C10.O4.Mn(-0.6)	A.O4.Mn.O5(-0.4)	A.N3.C7.C9(-0.4)	S.Mn(-0.3)	A.N2.C6.C8(-0.3)
RC05(+):	A.Mn.N2.C20(0.7)	Q.EqLig(0.7)	Q.O4(0.6)	Q.O5(0.5)	Q.N3(0.5)	D.N2.C20(0.4)
RC05(-):	D.Mn.O5(-0.4)	A.C21.N3.Mn(-0.4)	S.Mn(-0.3)	D.C6.C8(-0.3)	A.Mn.N2.C6(-0.3)	A.C20.C21.N3(-0.3)
RC06(+):	S.C17(0.9)	S.C13(0.9)	S.C9(0.7)	S.O5(0.5)	S.N3(0.4)	D.C9.C11(0.3)
RC06(-):	S.C15(-0.4)	S.C19(-0.3)	S.C7(-0.3)	D.O5.C11(-0.2)	A.C21.N3.Mn(-0.2)	S.C21(-0.2)
RC07(+):	S.N3(0.8)	S.N2(0.8)	Q.O5(0.4)	Q.O4(0.3)	Q.N2(0.3)	Q.N3(0.3)
RC07(-):	S.Mn(-0.5)	S.C20(-0.5)	D.N2.C20(-0.4)	S.C21(-0.4)	A.N2.Mn.N3(-0.4)	D.N3.C21(-0.4)
RC08(+):	S.C12(0.9)	S.C16(0.9)	S.C8(0.6)	S.O4(0.5)	S.N2(0.3)	D.C8.C10(0.3)
RC08(-):	S.C14(-0.3)	D.O4.C10(-0.3)	S.C20(-0.2)	S.C6(-0.2)	A.O4.Mn.N2(-0.2)	Q.C14(-0.2)
RC09(+):	Q.C20(1.0)	Q.C21(1.0)	D.N2.C20(0.3)	D.N3.C21(0.3)	CCM.acacen1(0.2)	A.N2.C6.C8(0.2)
RC09(-):	A.C20.C21.N3(-0.4)	A.N2.C20.C21(-0.4)	A.C21.N3.Mn(-0.3)	A.Mn.N2.C20(-0.3)	A.Mn.N3.C7(-0.2)	A.Mn.N2.C6(-0.1)
RC10(+):	Q.C16(0.9)	Q.C17(0.9)	Q.EqLig(0.1)	S.C18(0.1)	S.C17(0.1)	S.C16(0.1)
RC10(-):	CCM.salen1(-0.4)	CCM.acacen1(-0.3)	S.Mn(-0.1)	D.C8.C10(-0.1)	D.C9.C11(-0.1)	S.C8(-0.1)
RC11(+):	Q.C12(0.9)	Q.C13(0.9)	CCM.acacen1(0.2)	A.Mn.N2.C20(0.2)	A.N2.C6.C8(0.1)	A.N3.C7.C9(0.1)
RC11(-):	A.C9.C11.O5(-0.2)	A.C8.C10.O4(-0.2)	Q.O5(-0.1)	Q.O4(-0.1)	D.C6.C8(-0.1)	S.Mn(-0.1)
RC12(+):	A.O4.Mn.O5(0.7)	A.N2.Mn.N3(0.2)	Q.O5(0.2)	S.Mn(0.2)	D.C6.C8(0.2)	A.N3.C7.C9(0.2)
RC12(-):	Dp(-0.9)	Q.Mn(-0.3)	A.Mn.N3.C7(-0.2)	D.N2.C20(-0.2)	A.C9.C11.O5(-0.2)	A.C8.C10.O4(-0.2)
RC13(+):	PhiE(0.8)	A.Mn.N2.C6(0.3)	A.C10.O4.Mn(0.3)	A.N2.C20.C21(0.3)	A.N2.Mn.N3(0.3)	A.O4.Mn.N2(0.2)
RC13(-):	Q.O5(-0.3)	Q.O4(-0.2)	A.N3.C7.C9(-0.2)	D.Mn.O5(-0.2)	Dp(-0.2)	A.C21.N3.Mn(-0.2)
RC14(+):	PhiU(0.9)	A.Mn.N3.C7(0.4)	Q.O5(0.2)	A.C11.O5.Mn(0.2)	A.N3.C7.C9(0.2)	A.N2.Mn.N3(0.2)
RC14(-):	Q.Mn(-0.2)	D.C7.C9(-0.2)	D.O5.C11(-0.2)	A.O4.Mn.O5(-0.1)	S.Mn(-0.1)	A.C21.N3.Mn(-0.1)

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======================================================================
DB2
======================================================================
Summary for PCA of db2
      Comp.      %Var.   %C. Var. Association
 ---------------------------------------------
        PC1       34.8       34.8   BasisSet
        PC2       10.8       45.5     SpinSt
        PC3        9.2       54.7      EqLig
        PC4        6.9       61.7       OxSt
        PC5        6.1       67.7      EqLig
        PC6        4.9       72.7      AxLig
        PC7        4.4       77.1     Bridge
        PC8        3.2       80.3
        PC9        2.9       83.2
       PC10        2.2       85.4
       PC11        2.0       87.4 Functional
 ---------------------------------------------

Associated Overlaps:

PC1:
           def2-SV(P)  def2-TZVP   DefBas-3
def2-SV(P) 1.00097964 0.01811272 0.01687923
def2-TZVP  0.01811272 1.00097846 0.95264966
DefBas-3   0.01687923 0.95264966 1.00097843

PC2:
          S0        S2        S4
S0 1.0009663 0.4316030 0.1004411
S2 0.4316030 1.0009782 0.3042606
S4 0.1004411 0.3042606 1.0009784

PC3:
          Acacen     Salen
Acacen 1.0009669 0.1033964
Salen  0.1033964 1.0009786

PC4:
          V      III
V   1.000979 0.265570
III 0.265570 1.000979

PC5:
          Acacen     Salen
Acacen 1.0009517 0.3296115
Salen  0.3296115 1.0009766

PC6:
          Nothing        Cl     Amine     Amide
Nothing 1.0009712 0.5691285 0.6601578 0.3237887
Cl      0.5691285 1.0009777 0.8559007 0.7117459
Amine   0.6601578 0.8559007 1.0009751 0.5702389
Amide   0.3237887 0.7117459 0.5702389 1.0009785

PC7:
             EDA        CHDA
EDA  1.000978551 0.009794608
CHDA 0.009794608 1.000978441

PC11:
           TPSS     X3LYP
TPSS  1.0009784 0.6181949
X3LYP 0.6181949 1.0009742
 ---------------------------------------------

Most Prominent Loadings:
PC01(+):     D.N2.C6( 0.9)     D.N3.C7( 0.9)    D.O5.C11( 0.8)    D.O4.C10( 0.8)  A.Mn.N3.C7( 0.8)  A.Mn.N2.C6( 0.7)
PC01(-):     D.Mn.N2(-0.9)     D.Mn.N3(-0.9)        Q.C7(-0.9)        Q.C6(-0.8)       Q.C11(-0.8)       Q.C10(-0.8)
PC02(+):     S.EqLig( 0.7)        S.O4( 0.7)       S.C11( 0.7)       S.C10( 0.7)        S.C7( 0.6)        S.O5( 0.6)
PC02(-):        Q.N2(-0.5)        Q.N3(-0.5) A.C10.O4.Mn(-0.4)        Q.O5(-0.4)    D.O4.C10(-0.4)    D.N3.C21(-0.3)
PC03(+):        Q.C9( 0.8)        Q.C8( 0.7)    D.C8.C10( 0.6)    D.C9.C11( 0.6) A.C11.O5.Mn( 0.5) A.C10.O4.Mn( 0.4)
PC03(-): CCM.acacen1(-0.7) A.C9.C11.O5(-0.5) A.C8.C10.O4(-0.5)  A.O5.Mn.N3(-0.5)  A.O4.Mn.N2(-0.5)        Q.N2(-0.3)
PC04(+):        S.N2( 0.7)        S.N3( 0.6)        Q.N3( 0.6)        Q.O4( 0.6)        Q.O5( 0.6)        Q.N2( 0.5)
PC04(-):        S.Mn(-0.5)        PhiE(-0.4)  A.Mn.N2.C6(-0.3) A.C21.N3.Mn(-0.3)    D.N3.C21(-0.3)       S.C20(-0.3)
PC05(+):  A.O5.Mn.N3( 0.6)  A.O4.Mn.N2( 0.6)     D.C6.C8( 0.4)  A.N2.Mn.N3( 0.4)        Q.N2( 0.4)    D.C9.C11( 0.4)
PC05(-): A.C11.O5.Mn(-0.5) CCM.acacen1(-0.5) A.C10.O4.Mn(-0.4)     Q.EqLig(-0.3) A.Mn.N2.C20(-0.3)  A.O4.Mn.O5(-0.3)
PC06(+):     Q.EqLig( 0.6)    D.N2.C20( 0.5) A.Mn.N2.C20( 0.4)        Q.C6( 0.4)  A.N2.C6.C8( 0.4)        Q.C7( 0.4)
PC06(-): A.C21.N3.Mn(-0.5)        S.N2(-0.4)        S.C8(-0.4)          Dp(-0.3)        S.N3(-0.3)  A.Mn.N2.C6(-0.3)
PC07(+):       Q.C21( 0.9)       Q.C20( 0.9)    D.N3.C21( 0.3) CCM.acacen1( 0.3)    D.N2.C20( 0.2)        S.N2( 0.2)
PC07(-): A.Mn.N2.C20(-0.4) A.N2.C20.C21(-0.4) A.C20.C21.N3(-0.4)  A.Mn.N3.C7(-0.2) A.C21.N3.Mn(-0.2)        Q.C7(-0.1)
PC08(+):        PhiU( 0.5)        PhiE( 0.4)  A.O4.Mn.O5( 0.4)  A.N2.Mn.N3( 0.4)        S.C8( 0.3)        S.O4( 0.2)
PC08(-):          Dp(-0.7)        Q.Mn(-0.3) A.Mn.N2.C20(-0.2)    D.O5.C11(-0.1)    D.N2.C20(-0.1)    D.O4.C10(-0.1)
PC09(+):        S.C9( 0.7)        S.N3( 0.4)        PhiE( 0.3)        S.O5( 0.3)  A.Mn.N2.C6( 0.3)          Dp( 0.2)
PC09(-): A.C21.N3.Mn(-0.3)        S.C7(-0.3)  A.O5.Mn.N3(-0.2)  A.N3.C7.C9(-0.2)        S.N2(-0.2)  A.O4.Mn.O5(-0.2)
PC10(+):        PhiU( 0.6)          Dp( 0.4)  A.Mn.N3.C7( 0.4)  A.Mn.N2.C6( 0.2)        S.C8( 0.2) A.C11.O5.Mn( 0.2)
PC10(-):  A.O4.Mn.O5(-0.4) A.C21.N3.Mn(-0.2)  A.O4.Mn.N2(-0.2) A.Mn.N2.C20(-0.1)        S.N3(-0.1)        S.C9(-0.1)
PC11(+):        Q.O5( 0.3)        S.O5( 0.3)       S.C20( 0.3)     D.Mn.O5( 0.2)        PhiU( 0.2)       S.C21( 0.2)
PC11(-):        PhiE(-0.5)        S.N2(-0.3)        Q.Mn(-0.3) A.N2.C20.C21(-0.2)    D.O5.C11(-0.2) A.C10.O4.Mn(-0.2)
```

Summary for rPCA of db2

rComp.	%Var.	%C. Var.	Association
RC1	24.3	24.3	BasisSet
RC2	10.8	35.1	SpinSt
RC3	9.3	44.4	OxSt
RC4	8.1	52.5	EqLig
RC5	7.7	60.2	AxLig
RC6	6.2	66.4	OxSt
RC7	4.5	70.9	Bridge
RC8	3.6	74.5	
RC9	3.2	77.7	
RC10	3.1	80.8	
RC11	2.6	83.4	

Associated Overlaps:

RC1:

	def2-SV(P)	def2-TZVP	DefBas-3
def2-SV(P)	1.0009782	0.2846262	0.2904804
def2-TZVP	0.2846262	1.0009748	0.9678334
DefBas-3	0.2904804	0.9678334	1.0009779

RC2:

	S0	S2	S4
S0	1.00098092	0.1749892	0.06631784
S2	0.17498917	1.0009763	0.42435946
S4	0.06631784	0.4243595	1.00094648

RC3:

	V	III
V	1.0009782	0.4295907
III	0.4295907	1.0009734

RC4:

	Acacen	Salen
Acacen	1.000684e+00	2.045025e-14
Salen	2.045025e-14	1.000979e+00

RC5:

	Nothing	Cl	Amine	Amide
Nothing	1.0009765	0.2841053	0.4209321	0.2458286
Cl	0.2841053	1.0009782	0.8027189	0.7805731
Amine	0.4209321	0.8027189	1.0009788	0.6746245
Amide	0.2458286	0.7805731	0.6746245	1.0009656

RC6:

	V	III
V	1.0009790	0.5654614
III	0.5654614	1.0006880

RC7:

	EDA	CHDA
EDA	1.000982e+00	2.166658e-16
CHDA	2.166658e-16	1.000980e+00

Most Prominent Loadings:

RC01(+):	A.N2.C6.C8(0.9)	Q.C6(0.9)	Q.C7(0.9)	Q.C10(0.8)	D.Mn.O4(0.8)	D.Mn.N3(0.8)
RC01(-):	D.O4.C10(-0.8)	A.Mn.N2.C6(-0.8)	D.N3.C7(-0.8)	A.C21.N3.Mn(-0.8)	D.N3.C21(-0.7)	D.N2.C6(-0.7)
RC02(+):	S.EqLig(1.0)	S.C10(0.9)	S.C6(0.9)	S.C11(0.8)	S.O4(0.8)	S.C7(0.8)
RC02(-):	D.C6.C8(-0.5)	D.C7.C9(-0.4)	S.C9(-0.4)	Q.C7(-0.3)	A.O4.Mn.O5(-0.3)	D.Mn.N2(-0.3)
RC03(+):	Q.N3(0.8)	Q.O4(0.8)	Q.O5(0.8)	Q.N2(0.6)	A.Mn.N2.C20(0.6)	Q.EqLig(0.4)
RC03(-):	S.Mn(-0.7)	D.Mn.O5(-0.4)	A.C20.C21.N3(-0.4)	A.N3.C7.C9(-0.4)	D.Mn.N2(-0.3)	Q.C11(-0.3)
RC04(+):	Q.C9(0.9)	Q.C8(0.9)	D.C9.C11(0.8)	D.C8.C10(0.7)	D.C6.C8(0.5)	D.C7.C9(0.5)
RC04(-):	CCM.acacen1(-0.9)	A.C9.C11.O5(-0.3)	A.C8.C10.O4(-0.3)	S.C11(-0.2)	S.C10(-0.2)	A.Mn.N2.C20(-0.1)
RC05(+):	A.O5.Mn.N3(0.7)	A.O4.Mn.N2(0.7)	A.C8.C10.O4(0.6)	A.C9.C11.O5(0.6)	Q.N2(0.4)	D.Mn.O5(0.4)
RC05(-):	A.C11.O5.Mn(-0.9)	A.C10.O4.Mn(-0.7)	A.O4.Mn.O5(-0.3)	A.Mn.N2.C20(-0.3)	Q.EqLig(-0.3)	D.N2.C6(-0.3)
RC06(+):	S.N2(0.8)	S.C8(0.7)	S.N3(0.5)	D.Mn.N2(0.4)	D.Mn.O4(0.3)	A.O4.Mn.O5(0.3)
RC06(-):	S.C20(-0.6)	D.N2.C20(-0.6)	S.C21(-0.4)	A.N2.Mn.N3(-0.4)	D.N3.C21(-0.4)	A.Mn.N2.C20(-0.3)
RC07(+):	Q.C20(1.0)	Q.C21(1.0)	D.N3.C21(0.3)	D.N2.C20(0.3)	CCM.acacen1(0.2)	A.N2.C6.C8(0.1)
RC07(-):	A.C20.C21.N3(-0.4)	A.N2.C20.C21(-0.4)	A.Mn.N2.C20(-0.3)	A.C21.N3.Mn(-0.3)	A.Mn.N3.C7(-0.1)	A.Mn.N2.C6(-0.1)
RC08(+):	S.C9(0.8)	S.N3(0.4)	S.O5(0.4)	D.Mn.O5(0.3)	D.Mn.N3(0.3)	D.C9.C11(0.3)
RC08(-):	S.C7(-0.3)	D.O5.C11(-0.3)	Q.Mn(-0.3)	S.C21(-0.2)	A.C21.N3.Mn(-0.2)	A.O5.Mn.N3(-0.2)
RC09(+):	PhiE(0.8)	A.N2.Mn.N3(0.4)	A.Mn.N2.C6(0.4)	A.O4.Mn.N2(0.3)	A.C10.O4.Mn(0.3)	D.N2.C20(0.3)
RC09(-):	A.N3.C7.C9(-0.4)	D.Mn.O5(-0.3)	D.C9.C11(-0.2)	A.O4.Mn.O5(-0.2)	Dp(-0.2)	A.C21.N3.Mn(-0.2)
RC10(+):	A.O4.Mn.O5(0.6)	A.N2.Mn.N3(0.2)	D.C6.C8(0.2)	A.O5.Mn.N3(0.2)	S.Mn(0.2)	A.N3.C7.C9(0.2)
RC10(-):	Dp(-0.9)	Q.Mn(-0.3)	A.Mn.N3.C7(-0.2)	S.N3(-0.2)	D.N2.C20(-0.1)	A.Mn.N2.C6(-0.1)
RC11(+):	PhiU(0.8)	A.Mn.N3.C7(0.4)	A.N2.Mn.N3(0.3)	A.C11.O5.Mn(0.2)	A.Mn.N2.C6(0.2)	D.N3.C21(0.2)
RC11(-):	S.N3(-0.3)	A.O4.Mn.O5(-0.2)	Q.Mn(-0.1)	A.C21.N3.Mn(-0.1)	A.Mn.N2.C20(-0.1)	S.C9(-0.1)