

Electronic Supplementary Information for

The Rebound Mechanism in Catalytic C-H Oxidation by MnO(tpp)Cl from DFT Studies: Electronic Nature of the Active Species

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References for the theoretical methods

BP86 functional:

- [1] J. P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822.
- [2] J. P. Perdew, *Phys. Rev. B*, 1986, **34**, 7406.
- [3] A. Becke, *Phys. Rev. A*, 1988, **38**, 3098.

Stuttgart-Bonn ECP basis set:

- [3] D. Andrae, U. Haussermann, M. Dolg, H. Stoll and H. Preuss, *Theor. Chim. Acta*, 1990, **77**, 123.
- [4] A. W. Ehlers, M. Bohme, S. Dapprich, A. Gobbi, A. Hollwarth, V. Jonas, K. F. Kohler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 111.
- [5] A. Bergner, M. Dolg, W. Kuchle, H. Stoll and H. Preuss, *Mol. Phys.*, 1993, **30**, 1431.
- [6] A. Hollwarth, H. Bohme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Kohler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **203**, 237.

6-31g(d,p) basis set:

- [7] P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213.

Orbital diagrams

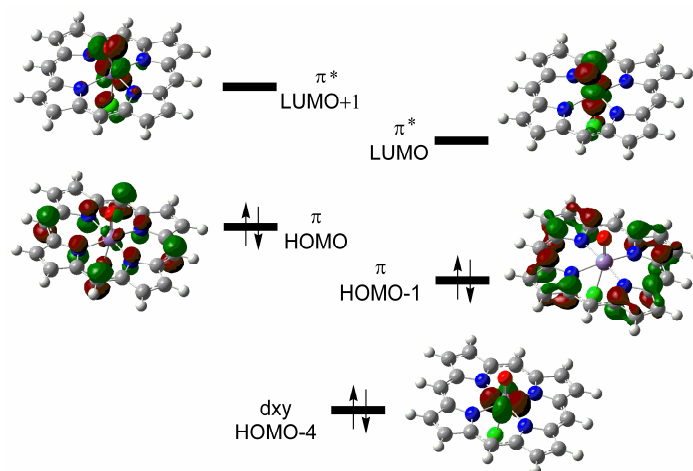


Figure 1. Frontier orbitals for the singlet (S). The π bonding orbitals associated to the Mn=O bond are even deeper in energy, well below HOMO-4.

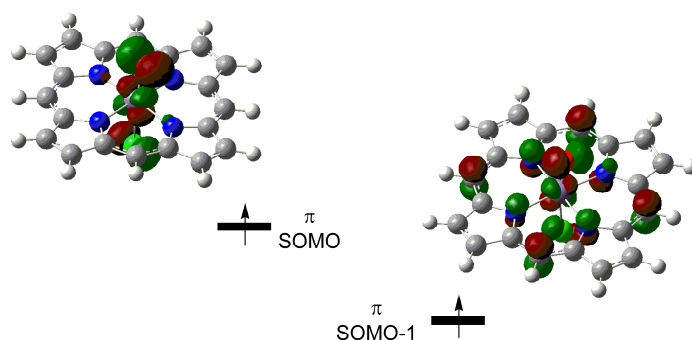


Figure 2. Highest singly occupied frontier orbitals for the triplet (T).

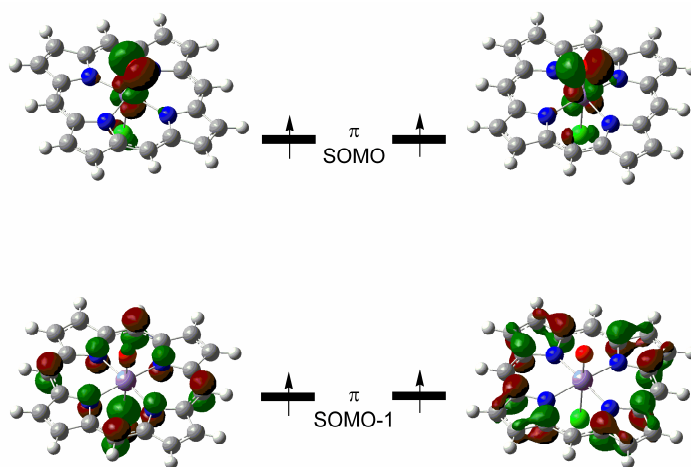


Figure 3. Highest singly occupied frontier orbitals for the quintet (**Q**).

3D geometries

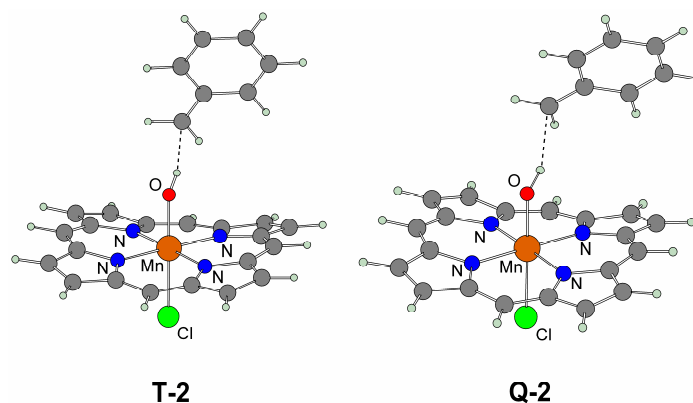


Figure 4. 3D representation of the optimized geometries of intermediates **T-2** and **Q-2**.

Geometries and energies

Optimized geometries and absolute potential energies with basis set II:

toluene	E=-271.559165557		
C	-1.412174	-0.821667	2.319366
H	-0.747148	-0.833137	1.433577
H	-1.794759	0.208543	2.427069
H	-2.268154	-1.481664	2.093282
C	-0.675267	-1.274330	3.566965
C	-0.626475	-2.641969	3.924599
C	0.081061	-3.067349	5.064401
C	0.752650	-2.128899	5.871475
C	0.708910	-0.763527	5.529734
C	0.000185	-0.342389	4.389033
H	-1.150350	-3.377590	3.303237
H	0.104251	-4.130876	5.324441
H	1.300966	-2.457798	6.760005
H	1.223175	-0.024994	6.153710
H	-0.033029	0.722567	4.131295
S	E=-1183.14402810		
Mn	0.047012	-0.040925	-0.290065
Cl	-0.089730	0.076798	2.085057
O	-0.147747	0.120844	-1.843316
C	2.771497	-1.377263	-0.179312
C	4.182089	-1.055072	-0.129129
C	4.286846	0.317086	-0.081309
C	2.942730	0.857849	-0.107715
N	2.010579	-0.196647	-0.179537
H	4.981886	-1.793992	-0.122597
H	5.190204	0.923155	-0.030312
C	2.647660	2.217086	-0.076203
C	1.051859	4.185827	-0.074276
C	-0.319281	4.295457	-0.114049
C	-0.857849	2.943725	-0.151726
N	0.191440	2.023113	-0.138465
C	1.363271	2.765126	-0.094373
H	1.793950	4.981855	-0.036563
H	-0.925624	5.200085	-0.112065
C	2.248864	-2.666933	-0.192352
N	-0.140747	-2.016706	-0.165807
C	-1.340228	-2.749405	-0.092940
C	-1.039762	-4.167311	-0.058746
C	0.330366	-4.300832	-0.106608
C	0.888165	-2.965699	-0.165631
H	-1.792489	-4.952502	-0.005132
H	0.920863	-5.215657	-0.097175
C	-2.630267	-2.225727	-0.071803
N	-2.030428	0.163917	-0.138828

C	-2.760634	1.349480	-0.161321
C	-4.185325	1.046566	-0.135329
C	-4.306891	-0.323260	-0.094511
C	-2.956763	-0.868368	-0.101763
H	-4.975703	1.795761	-0.139729
H	-5.216252	-0.921494	-0.062234
C	-2.217779	2.634659	-0.169069
H	-2.919584	3.473760	-0.173347
H	-3.456239	-2.941470	-0.028118
H	2.954209	-3.502206	-0.191289
H	3.492154	2.910619	-0.031783

T	E=-1183.13861870		
Mn	0.041729	-0.000633	-0.225106
Cl	-0.113383	0.019872	2.183251
O	-0.258927	0.010879	-1.858737
C	2.765769	-1.360759	-0.201521
C	4.180283	-1.049399	-0.142437
C	4.296785	0.318990	-0.053593
C	2.956210	0.869899	-0.070297
N	2.020899	-0.171820	-0.164816
H	4.973228	-1.795401	-0.154946
H	5.204261	0.916530	0.016098
C	2.656581	2.229977	-0.026560
C	1.056256	4.190479	-0.072781
C	-0.312538	4.297946	-0.156430
C	-0.849947	2.947277	-0.197564
N	0.199125	2.026393	-0.151367
C	1.372288	2.772394	-0.072586
H	1.795745	4.987685	-0.017952
H	-0.919604	5.201649	-0.176577
C	2.238956	-2.650163	-0.241374
N	-0.148256	-2.030855	-0.139012
C	-1.337386	-2.758530	-0.061500
C	-1.037033	-4.181740	-0.065516
C	0.329429	-4.310226	-0.155371
C	0.880624	-2.966075	-0.195353
H	-1.787664	-4.968420	-0.007948
H	0.923260	-5.222344	-0.183411
C	-2.624896	-2.222413	-0.010544
N	-2.024687	0.176836	-0.092284
C	-2.759063	1.358326	-0.172738
C	-4.180411	1.047427	-0.155778
C	-4.296201	-0.320830	-0.071535
C	-2.947362	-0.866256	-0.045982
H	-4.974527	1.791258	-0.196800
H	-5.203988	-0.920910	-0.034300
C	-2.210957	2.639613	-0.223748
H	-2.909266	3.480470	-0.263632
H	-3.456174	-2.931575	0.038126

H	2.949818	-3.480366	-0.273775
H	3.497344	2.926111	0.036928

T-1 E=-1454.69905483

Mn	-1.037138	0.020281	0.332555
Cl	-2.821414	0.363893	1.916465
C	0.702029	-0.946298	2.671699
C	1.657310	-0.462692	3.652840
C	1.813868	0.886863	3.433658
C	0.941514	1.249480	2.328994
N	0.276253	0.110169	1.867429
H	2.140619	-1.086595	4.402967
H	2.444745	1.590446	3.974567
C	0.748828	2.553189	1.869219
C	-0.447610	4.320756	0.502003
C	-1.476768	4.281820	-0.410172
C	-1.846391	2.884705	-0.583638
N	-1.057106	2.090959	0.246654
C	-0.185997	2.949456	0.912684
H	0.087880	5.190454	0.879359
H	-1.946849	5.112644	-0.933961
C	0.304071	-2.274252	2.515979
N	-1.155749	-1.954380	0.529831
C	-1.881361	-2.838092	-0.283719
C	-1.702574	-4.194911	0.195545
C	-0.895276	-4.135054	1.308897
C	-0.547470	-2.743258	1.516923
H	-2.159418	-5.071652	-0.260720
H	-0.553363	-4.954052	1.939643
C	-2.709013	-2.475194	-1.345279
N	-2.482134	-0.028730	-1.116282
C	-3.082305	1.065866	-1.739510
C	-4.016541	0.595868	-2.751431
C	-3.963036	-0.778791	-2.748939
C	-3.009448	-1.164708	-1.721230
H	-4.622067	1.247481	-3.379461
H	-4.520248	-1.478883	-3.369332
C	-2.802700	2.408754	-1.480547
H	-3.353561	3.152493	-2.063381
H	-3.204402	-3.282908	-1.891216
H	0.713473	-3.010100	3.213482
H	1.354533	3.337644	2.331716
O	0.142502	0.165587	-0.837640
H	1.878913	-0.957387	-1.217568
C	2.745313	-1.616946	-1.454510
H	2.851937	-2.327589	-0.615672
H	2.476764	-2.187278	-2.361606
C	4.006515	-0.807335	-1.659025
C	4.330045	-0.272629	-2.930230
C	5.489446	0.501055	-3.117541

C	6.353109	0.756716	-2.034033
C	6.045520	0.231761	-0.763460
C	4.884950	-0.541860	-0.580313
H	3.661575	-0.467736	-3.776438
H	5.721215	0.902816	-4.109681
H	7.257313	1.356751	-2.179042
H	6.712547	0.422110	0.084234
H	4.650967	-0.948989	0.410016

T-TS1 E=-1454.69470369

Mn	0.048561	0.278650	-0.884812
Cl	0.181871	1.829071	-2.680106
C	-0.999868	2.598428	0.830981
C	-0.542152	3.595213	1.782268
C	0.808213	3.392983	1.968350
C	1.202456	2.287967	1.112151
N	0.078753	1.802336	0.434037
H	-1.182500	4.344883	2.244950
H	1.492912	3.953771	2.603114
C	2.516280	1.856485	0.924011
C	4.314148	0.590821	-0.330465
C	4.298081	-0.285556	-1.391105
C	2.903627	-0.519630	-1.735317
N	2.086222	0.235922	-0.896593
C	2.930258	0.924299	-0.028856
H	5.175456	0.995987	0.198555
H	5.143356	-0.750139	-1.896625
C	-2.325361	2.410133	0.435166
N	-1.960982	0.375544	-0.936265
C	-2.817862	-0.517719	-1.590844
C	-4.193076	-0.090615	-1.404488
C	-4.165523	1.073934	-0.669432
C	-2.774939	1.361534	-0.368568
H	-5.058861	-0.610632	-1.811995
H	-5.004956	1.687853	-0.346231
C	-2.418962	-1.591321	-2.387831
N	0.023115	-1.205372	-2.279170
C	1.122969	-1.762882	-2.929769
C	0.672111	-2.819321	-3.823163
C	-0.694244	-2.911224	-3.688570
C	-1.099929	-1.893293	-2.731325
H	1.330338	-3.413925	-4.454901
H	-1.379358	-3.588132	-4.196836
C	2.456819	-1.422780	-2.700790
H	3.216445	-1.950189	-3.284512
H	-3.207836	-2.201116	-2.837158
H	-3.073250	3.108006	0.821329
H	3.292049	2.338072	1.525939
O	0.101042	-0.958687	0.359734
H	-0.658035	-0.887303	1.354964

C	-1.495119	-0.849958	2.358298
H	-1.785728	0.210880	2.349464
H	-2.286182	-1.516856	1.983525
C	-0.775566	-1.311450	3.547399
C	-0.738572	-2.695274	3.891362
C	-0.035647	-3.136756	5.020717
C	0.655047	-2.211274	5.832695
C	0.638140	-0.838419	5.503446
C	-0.063236	-0.392685	4.374817
H	-1.270127	-3.413090	3.257675
H	-0.022069	-4.201700	5.273008
H	1.204612	-2.557494	6.713560
H	1.174356	-0.119773	6.131282
H	-0.073078	0.671075	4.114241

T-2 E=-1454.70569496

Mn	0.050299	0.257676	-0.965727
Cl	0.091873	1.787698	-2.756111
C	-0.657102	2.678651	0.792061
C	-0.038884	3.639968	1.686938
C	1.296652	3.311549	1.782464
C	1.522494	2.164794	0.921481
N	0.312092	1.779426	0.335527
H	-0.570168	4.453552	2.178902
H	2.074391	3.812463	2.357203
C	2.772648	1.613234	0.635227
C	4.342511	0.219167	-0.773925
C	4.165484	-0.633743	-1.839593
C	2.733114	-0.757272	-2.059281
N	2.052907	0.044839	-1.144115
C	3.022073	0.654874	-0.347944
H	5.276048	0.547010	-0.319118
H	4.924880	-1.153509	-2.421828
C	-2.022308	2.602304	0.507967
N	-1.949081	0.508334	-0.816899
C	-2.926878	-0.343529	-1.339412
C	-4.243189	0.190872	-1.036768
C	-4.058451	1.378544	-0.363260
C	-2.626815	1.571842	-0.214201
H	-5.180720	-0.278953	-1.330624
H	-4.815187	2.064382	0.014971
C	-2.682494	-1.469656	-2.127425
N	-0.218767	-1.243647	-2.288942
C	0.762364	-1.877332	-3.050819
C	0.148110	-2.915337	-3.862718
C	-1.196587	-2.922208	-3.567468
C	-1.428764	-1.866746	-2.594946
H	0.691142	-3.559873	-4.552328
H	-1.974610	-3.564271	-3.977713
C	2.132594	-1.624327	-2.972992

H	2.790455	-2.202058	-3.627875
H	-3.550442	-2.038891	-2.471801
H	-2.672099	3.371444	0.934258
H	3.635208	2.022093	1.168747
O	0.042844	-0.964797	0.391638
H	-0.426783	-0.665137	1.232441
C	-1.609791	-0.407812	2.934137
H	-1.570143	0.675824	2.787041
H	-2.396683	-0.958731	2.410026
C	-0.793256	-1.045805	3.904704
C	-0.905804	-2.456730	4.163405
C	-0.102735	-3.078044	5.123202
C	0.841620	-2.326858	5.861206
C	0.974800	-0.938771	5.623431
C	0.178203	-0.305298	4.665990
H	-1.632708	-3.040245	3.588690
H	-0.203662	-4.152964	5.303531
H	1.469134	-2.818176	6.610918
H	1.707453	-0.357479	6.192441
H	0.284735	0.768479	4.478329

T-TS2 E=-1454.70170213

Mn	0.015206	0.379166	-0.829194
Cl	0.045818	2.034375	-2.490617
C	-2.889002	-0.366460	-1.534054
C	-4.262195	0.020999	-1.261478
C	-4.219155	1.080879	-0.384023
C	-2.819631	1.347187	-0.099142
N	-2.017330	0.450657	-0.811067
H	-5.135966	-0.457117	-1.702057
H	-5.051077	1.640556	0.041252
C	-2.358854	2.326824	0.780764
C	-0.547606	3.527647	2.070518
C	0.822919	3.408499	2.134751
C	1.209666	2.363571	1.203676
N	0.065747	1.833333	0.594318
C	-1.021333	2.548366	1.109198
H	-1.192368	4.211000	2.621329
H	1.522350	3.979921	2.743281
C	-2.504850	-1.370622	-2.423092
N	-0.046956	-1.078852	-2.220736
C	1.045085	-1.640946	-2.891308
C	0.574158	-2.622070	-3.853354
C	-0.798749	-2.656994	-3.763259
C	-1.188275	-1.685994	-2.755875
H	1.223277	-3.201627	-4.508294
H	-1.498164	-3.267579	-4.332601
C	2.385894	-1.335972	-2.660494
N	2.047388	0.345419	-0.873715
C	2.911776	1.060720	-0.043241

C	4.288471	0.725337	-0.369605
C	4.251435	-0.185167	-1.401076
C	2.851486	-0.428825	-1.708477
H	5.159960	1.149079	0.127449
H	5.086432	-0.661717	-1.912734
C	2.524138	1.986064	0.926396
H	3.317699	2.483748	1.490869
H	3.132046	-1.868975	-3.256390
H	-3.299108	-1.922991	-2.933024
H	-3.107583	2.958507	1.266801
O	0.069310	-0.852885	0.568194
H	-0.046855	-0.410007	1.448028
C	-0.358853	-2.943706	1.681982
H	-1.352653	-3.093620	1.254468
H	0.496087	-3.275488	1.092348
C	-0.195438	-2.452534	3.005641
C	1.114468	-2.245221	3.562028
C	1.274063	-1.715927	4.846927
C	0.144261	-1.376332	5.626439
C	-1.154588	-1.571532	5.102025
C	-1.327517	-2.096382	3.817199
H	1.989353	-2.498005	2.954209
H	2.280047	-1.559420	5.249382
H	0.274351	-0.959603	6.629816
H	-2.029849	-1.307397	5.704124
H	-2.334090	-2.242074	3.410539

T-3 E=-1454.75117563

Mn	0.029775	0.362957	0.896626
Cl	0.091608	1.610457	2.791026
C	2.170184	2.164701	-0.409667
C	2.313809	3.398265	-1.163520
C	1.043587	3.861171	-1.429043
C	0.110780	2.915406	-0.840013
N	0.812516	1.870255	-0.225018
H	3.266972	3.847125	-1.440998
H	0.753688	4.763796	-1.965918
C	-1.280250	3.042956	-0.876978
C	-3.631961	2.330107	-0.289377
C	-4.165754	1.275525	0.420429
C	-3.057632	0.449180	0.861793
N	-1.845867	0.989678	0.403337
C	-2.190709	2.161833	-0.289540
H	-4.158647	3.157782	-0.763089
H	-5.213654	1.073927	0.639848
C	3.230508	1.386647	0.061075
N	1.887088	-0.378582	1.180610
C	2.231940	-1.508518	1.934391
C	3.677035	-1.638030	2.002340
C	4.213441	-0.578135	1.304532

C	3.101646	0.209920	0.802085
H	4.202835	-2.434314	2.528025
H	5.264142	-0.337534	1.146244
C	1.326141	-2.375973	2.548084
N	-0.762652	-1.220676	1.878747
C	-2.116303	-1.478017	2.111912
C	-2.262741	-2.680325	2.918491
C	-0.995364	-3.152481	3.173304
C	-0.063166	-2.242163	2.526069
H	-3.216157	-3.095955	3.242623
H	-0.705052	-4.031391	3.747791
C	-3.178490	-0.702991	1.641389
H	-4.189803	-1.018100	1.916095
H	1.740782	-3.222396	3.104108
H	4.244969	1.735676	-0.154631
H	-1.689741	3.919284	-1.388637
O	-0.180194	-0.767895	-0.849806
H	-0.985341	-0.366116	-1.271478
C	0.911937	-0.988152	-1.866331
H	1.476386	-0.047336	-1.969208
H	1.546010	-1.750438	-1.393024
C	0.318129	-1.438424	-3.176394
C	-0.204759	-2.746283	-3.318992
C	-0.788977	-3.149667	-4.531995
C	-0.855982	-2.252327	-5.617522
C	-0.339356	-0.949395	-5.484988
C	0.242056	-0.543712	-4.269226
H	-0.153411	-3.440842	-2.473726
H	-1.188794	-4.163325	-4.634034
H	-1.308247	-2.569038	-6.562531
H	-0.388806	-0.250517	-6.325743
H	0.645616	0.469733	-4.163953

T-4 E=-1107.96287224

Mn	-0.023998	0.004633	0.011214
Cl	-2.026664	0.341054	0.947381
C	1.477992	-0.276877	2.687767
C	2.109132	0.519387	3.721851
C	2.119694	1.822856	3.278945
C	1.495556	1.833426	1.970468
N	1.106093	0.533781	1.600576
H	2.491927	0.121971	4.660957
H	2.512753	2.704681	3.783190
C	1.317790	2.972553	1.189521
C	0.569855	4.177869	-0.888937
C	-0.041534	3.785591	-2.058408
C	-0.254775	2.354449	-1.968564
N	0.233297	1.860044	-0.745916
C	0.735239	2.989540	-0.075171
H	0.885439	5.177834	-0.594196

H	-0.325874	4.400349	-2.911400
C	1.276980	-1.652773	2.761876
N	0.198247	-1.932606	0.543840
C	-0.305489	-3.061912	-0.125828
C	-0.116451	-4.254207	0.676945
C	0.495803	-3.861986	1.845930
C	0.685872	-2.426923	1.766738
H	-0.416015	-5.256868	0.374743
H	0.797212	-4.479478	2.691051
C	-0.896414	-3.043854	-1.386577
N	-0.674829	-0.606863	-1.801846
C	-1.046482	0.203937	-2.889100
C	-1.654675	-0.596036	-3.934037
C	-1.667092	-1.899244	-3.490475
C	-1.066702	-1.905994	-2.170918
H	-2.020183	-0.201344	-4.881147
H	-2.044509	-2.783623	-4.002140
C	-0.852247	1.581001	-2.960424
H	-1.190342	2.093086	-3.866191
H	-1.249022	-3.996213	-1.793548
H	1.612975	-2.164888	3.668405
H	1.666908	3.925447	1.598259

Q	E=-1183.12626107		
Mn	-0.000415	-0.000276	-0.237085
Cl	-0.005333	0.006889	2.263075
O	0.001011	-0.002560	-1.937965
C	2.767375	-1.354066	-0.136576
C	4.189221	-1.049377	-0.113450
C	4.306450	0.320797	-0.098586
C	2.957204	0.863128	-0.114463
N	2.024992	-0.173693	-0.135347
H	4.981351	-1.796297	-0.104582
H	5.214195	0.921491	-0.075591
C	2.639837	2.223402	-0.108260
C	1.048697	4.189307	-0.103392
C	-0.321423	4.306964	-0.119939
C	-0.863720	2.957766	-0.141555
N	0.172983	2.025288	-0.138659
C	1.353486	2.767343	-0.117041
H	1.795505	4.981274	-0.080940
H	-0.922174	5.214933	-0.112794
C	2.223490	-2.640539	-0.146460
N	-0.173672	-2.025163	-0.136036
C	-1.354028	-2.767452	-0.114035
C	-1.049133	-4.189352	-0.100758
C	0.320970	-4.306915	-0.118286
C	0.863256	-2.957747	-0.139902
H	-1.795877	-4.981369	-0.077939
H	0.921775	-5.214854	-0.111602

C	-2.640537	-2.223691	-0.105540
N	-2.025427	0.173120	-0.137745
C	-2.767696	1.353810	-0.137771
C	-4.189526	1.049220	-0.112133
C	-4.306999	-0.320892	-0.096041
C	-2.957931	-0.863542	-0.113704
H	-4.981512	1.796284	-0.102397
H	-5.214829	-0.921376	-0.071113
C	-2.223984	2.640253	-0.148080
H	-2.928981	3.477159	-0.149408
H	-3.477348	-2.928558	-0.087344
H	2.928307	-3.477593	-0.148424
H	3.476760	2.928180	-0.091599

Q-1 E=-1454.68765690

Mn	-1.076220	0.017248	0.354086
Cl	-2.781752	0.291181	2.142326
C	0.719475	-1.312233	2.485429
C	1.756345	-1.004663	3.457574
C	1.965972	0.353503	3.405732
C	1.057133	0.885964	2.402871
N	0.299867	-0.144399	1.848741
H	2.247836	-1.741106	4.091155
H	2.664133	0.952926	3.987523
C	0.949332	2.234967	2.055479
C	-0.052606	4.188143	0.799641
C	-1.041348	4.305722	-0.148788
C	-1.536286	2.964538	-0.416077
N	-0.853174	2.037740	0.370581
C	0.062551	2.774646	1.121656
H	0.548153	4.975700	1.251398
H	-1.412620	5.208910	-0.630202
C	0.216602	-2.588882	2.225997
N	-1.427705	-1.986960	0.476442
C	-2.339676	-2.724775	-0.277202
C	-2.260021	-4.131728	0.081304
C	-1.297210	-4.244045	1.057143
C	-0.780578	-2.906728	1.300634
H	-2.870703	-4.917872	-0.359605
H	-0.960927	-5.140564	1.575377
C	-3.213499	-2.187581	-1.225726
N	-2.582145	0.195255	-0.998651
C	-3.034196	1.368736	-1.601791
C	-4.089983	1.064647	-2.554238
C	-4.274702	-0.297978	-2.529028
C	-3.334913	-0.837038	-1.559251
H	-4.614023	1.807048	-3.153896
H	-4.980792	-0.895425	-3.103347
C	-2.545798	2.648427	-1.327881
H	-2.996447	3.480044	-1.878068

H	-3.873573	-2.888444	-1.745804
H	0.638882	-3.416182	2.804524
H	1.614624	2.934607	2.570318
O	0.100615	-0.169633	-0.864817
H	1.987057	-1.115934	-1.622758
C	2.865705	-1.591023	-2.109427
H	3.034427	-2.567256	-1.620923
H	2.586147	-1.778888	-3.162201
C	4.094346	-0.709074	-2.015227
C	4.285732	0.365705	-2.917781
C	5.410905	1.203935	-2.820163
C	6.374536	0.983441	-1.815814
C	6.199783	-0.081939	-0.911782
C	5.071639	-0.917853	-1.013040
H	3.539850	0.542850	-3.700915
H	5.538605	2.027906	-3.530563
H	7.253212	1.632552	-1.741486
H	6.944940	-0.265923	-0.130087
H	4.943830	-1.748145	-0.308735
Q-TS1	E=-1454.68201038		
Mn	0.073005	0.278432	-0.932678
Cl	0.020043	2.075364	-2.493934
C	-1.337824	2.284841	0.958522
C	-1.048571	3.236996	2.017724
C	0.308589	3.183239	2.252444
C	0.864516	2.212085	1.325135
N	-0.154474	1.668127	0.548567
H	-1.795138	3.859118	2.509392
H	0.893960	3.758938	2.967910
C	2.227790	1.931179	1.183289
C	4.213199	0.938994	-0.016643
C	4.359268	0.144454	-1.130170
C	3.025038	-0.191783	-1.598734
N	2.073235	0.418404	-0.780484
C	2.788197	1.122126	0.199218
H	4.991083	1.380574	0.604355
H	5.280337	-0.201011	-1.597092
C	-2.612595	1.986901	0.472708
N	-1.961502	0.181602	-1.097790
C	-2.678293	-0.699359	-1.902839
C	-4.101881	-0.439829	-1.767333
C	-4.239857	0.614875	-0.892464
C	-2.903431	0.997653	-0.468693
H	-4.882213	-0.988356	-2.292718
H	-5.156186	1.095411	-0.552765
C	-2.115510	-1.638370	-2.773275
N	0.274382	-1.062837	-2.415912
C	1.462273	-1.477960	-3.021125
C	1.169999	-2.477836	-4.034513
C	-0.190664	-2.681605	-4.027167

C	-0.755324	-1.792041	-3.026964
H	1.921827	-2.961086	-4.656580
H	-0.775263	-3.358645	-4.648157
C	2.739329	-1.047907	-2.662160
H	3.584991	-1.456782	-3.221849
H	-2.804890	-2.266954	-3.344121
H	-3.453520	2.550508	0.886689
H	2.915517	2.433020	1.869855
O	0.106632	-1.070232	0.252917
H	-0.736212	-1.124006	1.350820
C	-1.521342	-1.254750	2.297134
H	-2.075582	-0.302292	2.285297
H	-2.150306	-2.097982	1.968271
C	-0.756537	-1.506536	3.532636
C	-0.418084	-2.833490	3.928416
C	0.326211	-3.071009	5.092418
C	0.758402	-1.989817	5.890908
C	0.440533	-0.667750	5.511177
C	-0.302364	-0.427303	4.346486
H	-0.749679	-3.671735	3.306422
H	0.572256	-4.097378	5.382765
H	1.340041	-2.175859	6.799254
H	0.775262	0.172657	6.127870
H	-0.543102	0.598661	4.047397

Q-2 E=-1454.70517976

Mn	-1.015660	0.079151	0.275773
Cl	-2.517130	0.077685	2.085698
C	1.003899	-1.133585	2.254398
C	2.096973	-0.747774	3.127697
C	2.297102	0.606332	2.961059
C	1.308638	1.075051	2.007619
N	0.535710	-0.006090	1.570688
H	2.637249	-1.434526	3.777858
H	3.026537	1.246024	3.455678
C	1.091336	2.413214	1.674015
C	-0.312411	4.293295	0.734223
C	-1.506026	4.344089	0.050917
C	-1.911984	2.972353	-0.210161
N	-0.976837	2.098501	0.343288
C	0.012098	2.889548	0.929574
H	0.295115	5.121840	1.095019
H	-2.063329	5.222650	-0.270562
C	0.551447	-2.440200	2.059404
N	-1.075690	-1.945119	0.256968
C	-1.836081	-2.737004	-0.606954
C	-1.611062	-4.139175	-0.300029
C	-0.738852	-4.190241	0.764713
C	-0.393058	-2.820746	1.104666
H	-2.083710	-4.967838	-0.825257

H	-0.346560	-5.069186	1.274194
C	-2.750605	-2.259526	-1.547176
N	-2.566356	0.155409	-1.007400
C	-3.290230	1.286973	-1.384215
C	-4.318487	0.906843	-2.338044
C	-4.195599	-0.447734	-2.553176
C	-3.111630	-0.921370	-1.709318
H	-5.025832	1.600592	-2.789923
H	-4.791306	-1.084223	-3.205735
C	-3.009757	2.593966	-0.983792
H	-3.658428	3.388299	-1.362719
H	-3.281693	-2.999768	-2.151970
H	1.013366	-3.229972	2.658077
H	1.778347	3.152934	2.093985
O	0.128726	0.088744	-1.159452
H	0.985033	-0.406697	-1.000331
C	2.705493	-1.799183	-1.306137
H	2.467558	-2.186071	-0.310327
H	2.128773	-2.188289	-2.150509
C	3.804750	-0.926442	-1.510871
C	4.167442	-0.477894	-2.829948
C	5.259389	0.371368	-3.026659
C	6.033240	0.810449	-1.926842
C	5.694531	0.389358	-0.619516
C	4.604599	-0.459428	-0.408359
H	3.567705	-0.814022	-3.682433
H	5.516945	0.699727	-4.038739
H	6.887749	1.475020	-2.086467
H	6.290312	0.731315	0.233098
H	4.338621	-0.777331	0.605458

Q-TS2 E=-1454.70333434

Mn	0.000874	0.327236	-0.944216
Cl	-0.005614	1.730898	-2.854897
C	-2.815677	-0.606646	-1.768506
C	-4.222582	-0.320884	-1.537984
C	-4.285492	0.712342	-0.631234
C	-2.917492	1.083839	-0.307524
N	-2.032884	0.267544	-1.013594
H	-5.044704	-0.856498	-2.010454
H	-5.169121	1.196667	-0.218189
C	-2.552375	2.126085	0.544684
C	-0.880166	3.708832	1.575090
C	0.490444	3.835997	1.509323
C	0.988908	2.737974	0.704183
N	-0.085157	1.940730	0.285956
C	-1.243972	2.540342	0.797108
H	-1.593543	4.353309	2.086599
H	1.119148	4.601454	1.961789
C	-2.330923	-1.634108	-2.577481

N	0.088630	-1.312118	-2.127049
C	1.242871	-1.996657	-2.514269
C	0.879096	-3.116370	-3.364647
C	-0.490855	-3.094669	-3.504633
C	-0.985516	-1.971716	-2.727885
H	1.591841	-3.812664	-3.804120
H	-1.122105	-3.773659	-4.076010
C	2.550649	-1.630825	-2.193739
N	2.033919	0.424933	-0.902831
C	2.819457	1.415623	-0.311502
C	4.225128	1.109676	-0.519626
C	4.284718	-0.073245	-1.220830
C	2.916463	-0.498532	-1.466047
H	5.048798	1.725864	-0.162091
H	5.167248	-0.614806	-1.558247
C	2.333958	2.500044	0.419482
H	3.065712	3.204902	0.823337
H	3.356501	-2.260488	-2.581054
H	-3.065014	-2.243432	-3.111781
H	-3.357777	2.694408	1.017966
O	0.015030	-0.821941	0.553149
H	0.147062	-0.294543	1.385815
C	-0.031776	-2.718647	2.252149
H	-0.969786	-2.944596	1.742948
H	0.890831	-3.023077	1.754843
C	-0.015571	-2.141721	3.549486
C	1.220878	-1.890348	4.241179
C	1.228726	-1.324207	5.519555
C	0.014266	-0.986380	6.160915
C	-1.214952	-1.222207	5.502105
C	-1.236210	-1.787248	4.223511
H	2.162635	-2.152245	3.746582
H	2.181282	-1.142927	6.028066
H	0.025646	-0.544868	7.162069
H	-2.156115	-0.961356	5.997023
H	-2.188763	-1.967782	3.713831

Q-3 E=-1454.75430634

Mn	-0.931848	0.118298	0.502327
Cl	-3.044702	-0.442387	1.591504
C	-0.765353	-2.649611	-0.852336
C	-0.298996	-4.005043	-0.612672
C	0.333374	-4.007849	0.611115
C	0.260234	-2.655271	1.136714
N	-0.413179	-1.834071	0.227483
H	-0.447736	-4.839009	-1.297268
H	0.804737	-4.844514	1.124961
C	0.788086	-2.246292	2.363415
C	1.249357	-0.545067	4.174227
C	0.965087	0.794801	4.327931

C	0.266339	1.226892	3.131053
N	0.141899	0.149597	2.244705
C	0.727412	-0.951311	2.882416
H	1.756651	-1.209845	4.871923
H	1.194415	1.439692	5.175143
C	-1.451233	-2.228761	-1.994004
N	-1.712086	0.164708	-1.381702
C	-2.331160	1.255823	-2.001918
C	-2.886859	0.841163	-3.277658
C	-2.616918	-0.501983	-3.423932
C	-1.892797	-0.926951	-2.239186
H	-3.421193	1.499490	-3.961241
H	-2.886946	-1.157829	-4.250500
C	-2.416826	2.544864	-1.472036
N	-1.233950	2.127310	0.671012
C	-0.907294	2.935067	1.764095
C	-1.389487	4.286631	1.534086
C	-2.007258	4.294831	0.303645
C	-1.910808	2.948487	-0.234821
H	-1.267654	5.112627	2.233442
H	-2.490834	5.128758	-0.203219
C	-0.214756	2.517895	2.902903
H	-0.042203	3.262575	3.685112
H	-2.933913	3.299269	-2.071852
H	-1.666678	-2.982887	-2.756317
H	1.279882	-3.007908	2.975257
O	1.233233	0.689183	-0.423409
H	1.901231	0.801781	0.297838
C	1.858663	0.858183	-1.761949
H	1.055297	0.548597	-2.448432
H	2.080160	1.928444	-1.934303
C	3.108513	0.021536	-1.924475
C	4.360124	0.640339	-2.141834
C	5.528148	-0.132930	-2.284842
C	5.455424	-1.536025	-2.202538
C	4.211821	-2.162180	-1.978946
C	3.045192	-1.390381	-1.842276
H	4.416318	1.733543	-2.204464
H	6.490824	0.358740	-2.457197
H	6.361820	-2.139965	-2.311548
H	4.152166	-3.253333	-1.915142
H	2.079567	-1.876142	-1.667999

Q-4 E=-1107.98070646

Mn	-1.347569	0.120520	0.301176
Cl	-3.495353	0.501716	1.303321
C	0.147251	-0.159920	2.988814
C	0.781359	0.639098	4.019365
C	0.786910	1.943775	3.578853
C	0.160884	1.958527	2.271023

N	-0.226031	0.659119	1.913725
H	1.165977	0.241382	4.957238
H	1.177449	2.825660	4.084312
C	-0.014371	3.096994	1.486478
C	-0.756282	4.300313	-0.599634
C	-1.366289	3.907624	-1.769983
C	-1.582947	2.476619	-1.682376
N	-1.092772	1.994261	-0.460388
C	-0.591829	3.114370	0.218150
H	-0.443168	5.300458	-0.304012
H	-1.651654	4.522583	-2.622110
C	-0.050023	-1.537895	3.059593
N	-1.145560	-1.830554	0.849082
C	-1.643640	-2.950786	0.168579
C	-1.441940	-4.142709	0.969239
C	-0.827430	-3.750737	2.137650
C	-0.643523	-2.314238	2.065760
H	-1.737625	-5.145685	0.665356
H	-0.520078	-4.369256	2.979498
C	-2.235680	-2.930476	-1.093037
N	-2.029119	-0.491280	-1.517940
C	-2.385140	0.324887	-2.600867
C	-2.986748	-0.479544	-3.646593
C	-3.003497	-1.782411	-3.200935
C	-2.409413	-1.791940	-1.878182
H	-3.347700	-0.085675	-4.595435
H	-3.380223	-2.666565	-3.712880
C	-2.183540	1.701958	-2.673218
H	-2.518673	2.213608	-3.579451
H	-2.584036	-3.882746	-1.501861
H	0.292166	-2.050466	3.962646
H	0.332902	4.049557	1.895602

benzyl alcohol E=-346.765127856

O	0.903035	0.204217	-0.906662
H	0.084412	0.753749	-0.847985
C	1.931330	0.959008	-1.624719
H	1.547903	1.294406	-2.614089
H	2.221864	1.871119	-1.059745
C	3.147640	0.074038	-1.823400
C	4.357157	0.641167	-2.283985
C	5.486948	-0.167285	-2.501991
C	5.421305	-1.553131	-2.255308
C	4.219880	-2.120400	-1.790546
C	3.086179	-1.312672	-1.576718
H	4.415939	1.720547	-2.470468
H	6.418574	0.284139	-2.858620
H	6.301220	-2.183036	-2.421186
H	4.163381	-3.195910	-1.592318
H	2.149143	-1.737817	-1.210614