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Mechanism of Silver- and Copper-Catalyzed Decarboxylation Reactions of Aryl Carboxylic Acids

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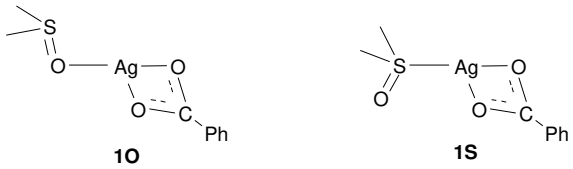
Additional Calculation Results

Scheme S1 gives the relative enegies of the two DMSO linkage isomers (**1O and 1S**) calculated with different basis sets. The results shows that inclusion of the diffuse functions for O change the relative energies only slightly.



1O **1S**

Basis set: 6-31G+* for S and 6-31G* for O	0.0	3.6
Basis set: 6-31G+* for both S and O	0.0	3.3

The calculated relative free energies in the gas phase are given in kcal/mol.

Scheme S1

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Table S1 compares the relative solvation-corrected free enerigies calculated for the species involved in silver- or copper-catalyzed decarboxylation reactions of PhCOOH → C_6H_6 + CO_2 using PCM with the UAHF radii and PCM with the UFF radii. The results show that the difference in the relative free energies obtained between the two solvation energy calculation methods is within 3 kcal/mol. More importantly, the difference in the overall free energy barriers (**TS3** or **TS5**) between the two methods is less than 1 kcal/mol.

Table S1. Comparison of the relative solvation-corrected free enerigies calculated for the species involved in silver- or copper-catalyzed decarboxylation reactions of PhCOOH → C_6H_6 + CO_2 using PCM with the UAHF radii and PCM with the UFF radii.

species	ΔG/kcalmol^{-1} (in gas phase)	ΔG_{sol}/kcalmol^{-1} (PCM with UAHF radii)	ΔG_{sol} /kcalmol^{-1} (PCM with UFF radii)
1O + PhCOOH	0.0	0.0	0.0
TS1 + PhCOOH	13.9	7.5	5.2
2 + PhCOOH	12.3	5.7	4.4
TS2 + PhCOOH	18.2	14.5	13.1
3 + PhCOOH	17.2	13.5	12.4
TS3 + PhCOOH	34.3	33.2	34.1
4 + PhCOOH + CO_2	9.5	8.2	9.5
TS4 + CO_2	18.1	20.0	23.2
1O + C_6H_6 + CO_2	-15.9	-14.0	-14.4
5 + PhCOOH	0.0	0.0	0.0
TS5 + PhCOOH	34.4	31.8	32.1
6 + PhCOOH + CO_2	16.4	16.4	15.8
7 + CO_2	17.1	24.4	21.9
TS6 + CO_2	19.0	26.2	24.2
5 + C_6H_6 + CO_2	-15.9	-11.7	-14.3

For the silver-catalyzed decarboxylation reaction of PhCOOH → C_6H_6 + CO_2, the solvent used in the calculation is DMSO. For the copper-catalyzed decarboxylation reaction of PhCOOH → C_6H_6 + CO_2, the solvent used in the calculations is NMP.

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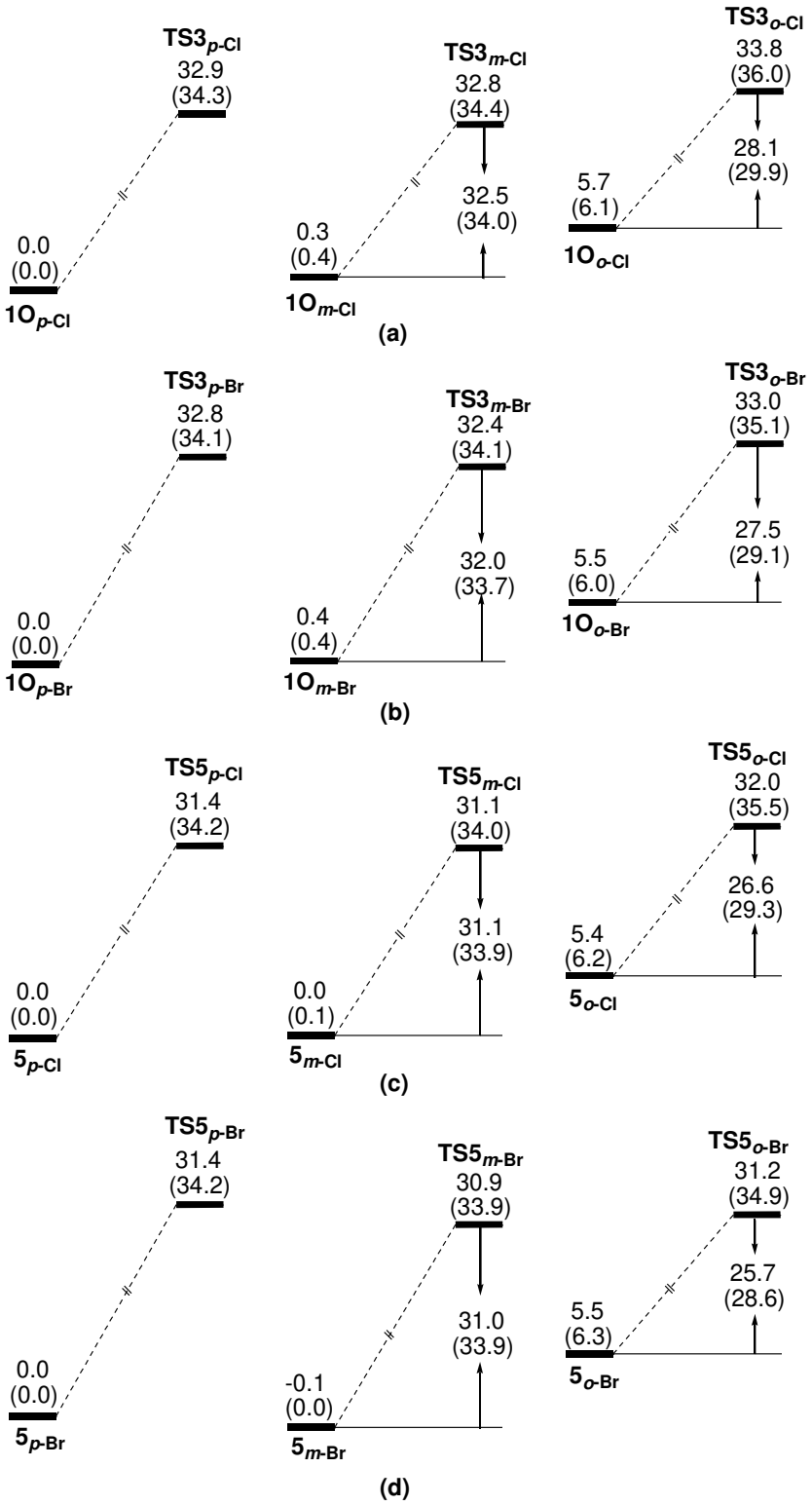

Figure S1. The relative energies calculated for $\mathbf{1O_R}$ and $\mathbf{TS3_R}$, and $\mathbf{5_R}$ and $\mathbf{TS5_R}$ (R = Cl, and Br at an *ortho*, *meta*, or *para* position). The solvation-corrected relative free energies and the gas-phase relative free energies (in parentheses) are given in kcal/mol.

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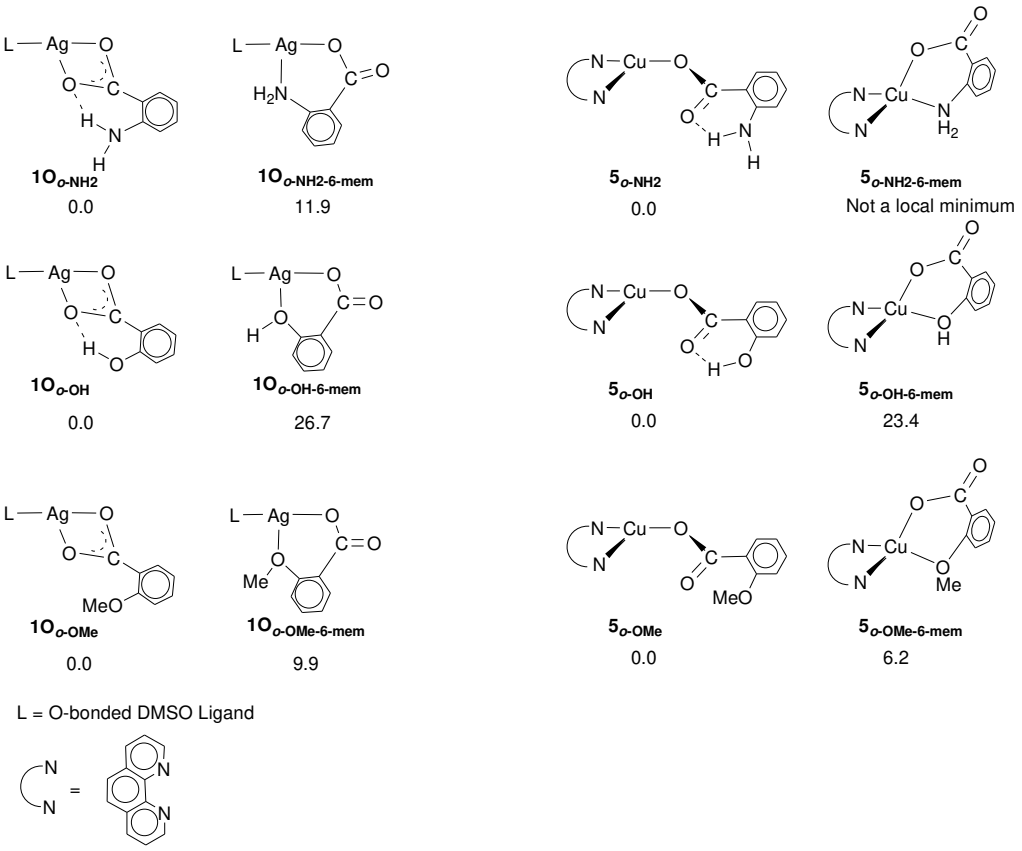
For a carboxylate complex having an *ortho* substituent that is capable of coordinating with the metal center, an alternative structure, which considers the possible metal coordination of one carboxylate oxygen atom and the coordinating atom from the *ortho* substituent, is also possible. However, Such alternative structures were found to be much less stable than the structures which consider the possible metal coordination of the two carboxylate oxygen atoms. The detailed calculation results are given below in Scheme S2.



The calculated relative free energies in the gas phase are given in kcal/mol.

Scheme S2

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Cartesian coordinates for all the species calculated at the B3PW91 level in this study

1O
E = -1120.226171 a.u.

Ag	0.419367	-1.595705	0.320622
O	1.703737	0.702129	-0.182395
O	2.523206	-1.339787	0.264452
C	2.656339	-0.087219	-0.009369
O	-1.746481	-1.427058	0.309800
S	-2.246580	-0.225140	-0.535833
C	-3.964659	-0.040462	-0.002411
C	-1.560468	1.269559	0.216732
H	-4.505142	-0.930412	-0.333241
H	-4.393878	0.850454	-0.470789
H	-3.997855	0.032701	1.088162
H	-1.806982	1.292897	1.282665
H	-1.976727	2.139887	-0.301664
H	-0.472276	1.232228	0.077005
C	4.067341	0.415191	-0.120351
C	5.155976	-0.443160	0.068184
C	4.296186	1.762707	-0.417184
C	6.457004	0.042380	-0.039216
H	4.964232	-1.486494	0.297602
C	5.596738	2.247622	-0.524373
H	3.437931	2.411918	-0.560282
C	6.679654	1.387714	-0.335462
H	7.299691	-0.628989	0.108041
H	5.768059	3.296381	-0.755454
H	7.696077	1.765551	-0.419167

1S
E = -1120.220486 a.u.

Ag	0.271245	-0.390786	0.001307
O	2.364875	-0.952755	0.000806
O	2.072533	1.256404	0.003282
C	2.822036	0.246622	0.001908
S	-2.092348	-0.030309	0.000108
O	-3.096930	-1.140940	-0.002555
C	-2.457577	1.090994	-1.373994
C	-2.459928	1.086552	1.377216
H	-2.299261	0.529774	-2.297924
H	-1.779922	1.949195	-1.335629
H	-3.504174	1.401815	-1.302081
H	-3.506480	1.397380	1.304655
H	-1.782410	1.945017	1.342552
H	-2.302917	0.522466	2.299620
C	4.307808	0.421113	0.001303
C	4.854274	1.709027	0.002455
C	5.156720	-0.691154	-0.000404
C	6.235330	1.882963	0.001899
H	4.178776	2.558830	0.003779
C	6.538008	-0.515512	-0.000969
H	4.716892	-1.683456	-0.001272
C	7.078878	0.770980	0.000185
H	6.656132	2.885562	0.002809
H	7.194628	-1.382128	-0.002310
H	8.157843	0.907138	-0.000248

TS1
E = -1120.203147 a.u.

Ag	-1.015506	1.733936	-2.089919
O	2.096434	3.740067	-1.662986
O	0.767405	2.365848	-2.852671
C	1.735748	2.620269	-2.000551
O	-2.875494	1.065541	-1.257443
S	-2.918152	-0.330624	-0.588486
C	-2.267427	-0.104754	1.085600
C	-4.666788	-0.523921	-0.175730
H	-1.199246	0.108519	0.991477
H	-2.407017	-1.031990	1.650299
H	-2.775685	0.733772	1.570343
H	-5.004562	0.350243	0.387788
H	-4.804504	-1.444350	0.399387
H	-5.211868	-0.591302	-1.120135
C	2.461340	1.409274	-1.440644
C	2.269716	0.122781	-1.957336
C	3.355571	1.590029	-0.380004
C	2.950946	-0.966196	-1.414106
H	1.598522	-0.006284	-2.801852
C	4.029039	0.502723	0.171021
H	3.508315	2.599590	-0.009669
C	3.826836	-0.779242	-0.344085
H	2.806214	-1.960459	-1.831567
H	4.718577	0.653367	0.998669
H	4.357999	-1.628186	0.080627

2
E = -1120.204683 a.u.

Ag	-0.854031	1.995879	-2.212238
O	2.807010	3.686441	-2.236857
O	0.843156	2.887075	-2.963918
C	1.954010	2.810789	-2.280087
O	-2.577124	1.086100	-1.304992
S	-2.402235	-0.352036	-0.754131
C	-1.441116	-0.203945	0.772033
C	-4.019102	-0.696380	-0.023519
H	-0.414061	0.044318	0.489415
H	-1.452054	-1.168701	1.289379
H	-1.866873	0.584658	1.399423
H	-4.280078	0.105113	0.673101
H	-3.989917	-1.666416	0.481594
H	-4.740719	-0.726626	-0.843207
C	2.199096	1.526691	-1.498233
C	1.769540	0.273050	-1.955116
C	2.919529	1.597065	-0.301015
C	2.036720	-0.882721	-1.218037
H	1.259317	0.202602	-2.913736
C	3.159716	0.449887	0.452846
H	3.291720	2.566949	0.016487
C	2.718831	-0.794486	-0.002854
H	1.728730	-1.853376	-1.601603
H	3.707787	0.522116	1.389509
H	2.926322	-1.692915	0.573955

TS2
E = -1120.196963 a.u.

Ag	-0.205187	-0.568853	-0.418421
O	1.717830	2.994130	0.037111
O	0.178214	1.575051	-0.810545
C	1.337096	1.883783	-0.313960
O	-2.265640	-1.252990	0.087929
S	-3.105404	-0.112240	0.718581
C	-3.052402	1.297265	-0.417388
C	-4.811602	-0.634121	0.419105
H	-2.019082	1.671033	-0.454055
H	-3.715427	2.075127	-0.023430
H	-3.372207	0.981282	-1.415225
H	-4.941784	-0.846891	-0.645678
H	-5.494185	0.154800	0.749267
H	-4.981902	-1.540867	1.004285
C	2.274869	0.689237	-0.124495
C	2.291289	-0.393251	-1.029546
C	3.117423	0.645845	0.989473
C	3.106551	-1.507318	-0.791763
H	1.759742	-0.305738	-1.979406
C	3.911625	-0.473270	1.234568
H	3.131329	1.505502	1.653454
C	3.901740	-1.555856	0.352293

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H	3.134429	-2.320066	-1.513940
H	4.546778	-0.501793	2.116887
H	4.528536	-2.422862	0.544357

3

E = -1120.196988 a.u.

Ag	-0.011544	-0.613571	-0.112746
O	1.344191	3.223240	-0.012475
O	0.027835	1.540495	-0.757758
C	1.111014	2.045131	-0.256678
O	-2.039264	-1.391791	0.392512
S	-2.995820	-0.269009	0.871974
C	-3.090107	0.968467	-0.444963
C	-4.635242	-1.006812	0.671211
H	-2.100749	1.440748	-0.537153
H	-3.835360	1.716202	-0.152696
H	-3.369587	0.486598	-1.387085
H	-4.739896	-1.379684	-0.351542
H	-5.399000	-0.256211	0.896208
H	-4.709042	-1.835350	1.379508
C	2.171501	0.997313	0.101014
C	2.373261	-0.154186	-0.693956
C	2.936793	1.154411	1.259964
C	3.294236	-1.136708	-0.302079
H	1.911827	-0.209825	-1.682222
C	3.835877	0.165314	1.656037
H	2.807995	2.065440	1.837509
C	4.009862	-0.986069	0.884583
H	3.465928	-2.000088	-0.940795
H	4.409166	0.292649	2.571381
H	4.717291	-1.750374	1.195521

TS3

E = -1120.168718 a.u.

Ag	-0.122694	-0.390532	0.878596
O	0.738049	2.623470	0.908091
O	0.282906	1.709740	-1.159021
C	0.691779	1.870316	-0.028579
O	-2.226801	-0.911215	1.064522
S	-3.202168	0.276109	0.847911
C	-3.065488	0.756258	-0.891803
C	-4.816134	-0.535301	0.779261
H	-2.067104	1.183171	-1.041781
H	-3.826039	1.515540	-1.102023
H	-3.199889	-0.122244	-1.529967
H	-4.787169	-1.336217	0.035273
H	-5.582465	0.205635	0.532529
H	-5.009652	-0.953172	1.769962
C	1.866597	0.254463	0.450816
C	2.428296	-0.383420	-0.672943
C	2.691248	0.444282	1.578127
C	3.745217	-0.842918	-0.661350
H	1.831398	-0.480458	-1.577591
C	4.005816	-0.016245	1.597276
H	2.300110	0.996059	2.430170
C	4.531673	-0.664730	0.477316
H	4.164222	-1.325437	-1.541787
H	4.627955	0.141555	2.475649
H	5.562156	-1.012827	0.485632

CO_2

E = -188.504221 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.167941
O	0.000000	0.000000	-1.167941

4

E = -931.685530 a.u.

Ag	-0.030557	-0.117260	-0.412044
O	-2.202563	-0.150601	-0.748403
S	-3.099914	-0.277281	0.498226
C	-3.260145	1.394792	1.179411
C	-4.764829	-0.433907	-0.193790
H	-2.279964	1.671502	1.576289
H	-3.998243	1.385961	1.987752
H	-3.550098	2.090494	0.386590
H	-4.945264	0.384862	-0.896028
H	-5.499693	-0.429500	0.616964
H	-4.801515	-1.389564	-0.722017
C	1.988211	-0.029640	-0.049778
C	2.745643	1.111946	-0.373410
C	2.685227	-1.107012	0.528948
C	4.120670	1.176454	-0.134942
H	2.259765	1.975129	-0.825482
C	4.059915	-1.050537	0.771187
H	2.151052	-2.016595	0.798498
C	4.784178	0.093554	0.439734
H	4.674451	2.075790	-0.400099
H	4.566042	-1.904091	1.219583
H	5.854955	0.140513	0.626878

C_6H_5COOH

E = -420.653839 a.u.

C	0.905120	-0.653913	0.880918
C	-0.438067	-1.018962	0.858414
C	-1.323624	-0.375744	-0.007136
C	-0.866745	0.635862	-0.853602
C	0.474193	1.003717	-0.834429
C	1.364652	0.360409	0.032571
H	1.599988	-1.149306	1.551118
H	-0.795348	-1.806353	1.516804
H	-2.371919	-0.663506	-0.021947
H	-1.556904	1.136436	-1.527478
H	0.855041	1.787189	-1.482495
C	2.783851	0.792096	0.012085
O	3.234638	1.664327	-0.701756
O	3.559270	0.109075	0.885163
H	4.454402	0.477434	0.779812

TS4

E = -1352.337665 a.u.

Ag	0.045912	-1.830336	-0.194869
O	2.236919	-1.333668	-0.251282
S	2.594315	0.128318	-0.569987
C	2.168574	1.100165	0.900112
C	4.396590	0.185316	-0.393231
H	1.078346	1.090580	0.984708
H	2.519595	2.128294	0.765114
H	2.616156	0.643826	1.788078
H	4.678557	-0.221877	0.581953
H	4.743699	1.216873	-0.506690
H	4.815239	-0.436447	-1.188123
C	-2.033833	-1.111892	-0.013751
C	-2.353198	-0.603600	1.265505
C	-2.472492	-0.344539	-1.115985
C	-3.059698	0.587400	1.438594
H	-2.063991	-1.171075	2.150200
C	-3.179280	0.848385	-0.958314
H	-2.275680	-0.703070	-2.126230
C	-3.471605	1.317765	0.322957
H	-3.299755	0.942793	2.439135
H	-3.510638	1.408976	-1.830530
H	-4.029396	2.243056	0.451448
O	-0.250473	-4.181515	-0.344157
C	-1.451066	-4.528833	-0.340184
O	-2.456070	-3.724935	-0.241817
H	-2.119327	-2.575111	-0.154139
C	-1.794095	-5.983724	-0.457425
C	-0.764507	-6.923963	-0.566227
C	-3.126119	-6.411069	-0.459867
C	-1.063322	-8.278886	-0.676618
H	0.262211	-6.570973	-0.562337
C	-3.423499	-7.767076	-0.570518
H	-3.914525	-5.669987	-0.374800
C	-2.393379	-8.702173	-0.678958
H	-0.260120	-9.006938	-0.761096
H	-4.459827	-8.096131	-0.572301
H	-2.627084	-9.760820	-0.765301

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C_6H_6

E = -232.155194 a.u.

C	-1.802552	0.136334	0.000075
C	-0.407795	0.136394	0.000581
C	0.289595	1.343988	-0.000086
C	-0.407759	2.551862	-0.001024
C	-1.802319	2.551802	-0.001422
C	-2.499812	1.344048	-0.000981
H	-2.345901	-0.804949	0.000435
H	0.135426	-0.804985	0.001365
H	1.376437	1.343984	0.000172
H	0.135823	3.493001	-0.001452
H	-2.345753	3.493048	-0.002246
H	-3.586662	1.344321	-0.001329

***p*-OMe-C_6H_4COOH**

E = -535.134026 a.u.

C	0.765321	-1.214462	0.001249
C	-0.624299	-1.293770	0.001282
C	-1.384526	-0.117030	0.000290
C	-0.740447	1.131241	-0.000780
C	0.640096	1.197106	-0.000775
C	1.411669	0.024450	0.000299
H	1.354077	-2.126073	0.002105
H	-1.101636	-2.267593	0.002157
C	2.882373	0.155352	0.000311
O	3.490209	1.207702	-0.000522
O	3.525026	-1.037960	0.001345
H	4.473033	-0.817030	0.001246
H	1.151194	2.154985	-0.001561
H	-1.351326	2.028806	-0.001622
O	-2.737236	-0.077771	0.000132
C	-3.445322	-1.302054	-0.000994
H	-4.503447	-1.034911	-0.002742
H	-3.220174	-1.896371	-0.896069
H	-3.223206	-1.895977	0.895114

***m*-OMe-C_6H_4COOH**

E = -535.131167 a.u.

C	-1.221008	1.593693	0.038709
C	-0.029904	2.307439	0.051213
C	1.203972	1.652503	0.026188
C	1.245960	0.254058	-0.012187
C	0.051409	-0.472150	-0.025075
C	-1.172057	0.192762	0.000149
H	-2.177205	2.104187	0.058397
H	-0.050228	3.393755	0.080981
H	2.117791	2.237058	0.036621
C	-2.401136	-0.641203	-0.015813
O	-2.420143	-1.854128	-0.049582
O	-3.537709	0.091967	0.011471
H	-4.263565	-0.556836	-0.002399
H	0.078243	-1.556324	-0.055029
O	2.385400	-0.483971	-0.039070
C	3.621312	0.199221	-0.027631
H	3.743770	0.799992	0.883844
H	4.391222	-0.574036	-0.053489
H	3.733027	0.848844	-0.906273

***o*-OMe-C_6H_4COOH**

E = -535.124294 a.u.

C	0.427687	-1.174963	-0.000049
C	1.812987	-1.280318	-0.000043
C	2.577906	-0.116499	0.000006
C	1.968075	1.134255	0.000046
C	0.570488	1.247380	0.000036
C	-0.218840	0.068605	-0.000010
H	-0.185203	-2.069214	-0.000086
H	2.288281	-2.256640	-0.000076
H	3.663684	-0.174718	0.000013
H	2.586321	2.024651	0.000085
C	-1.701480	0.123239	-0.000020
O	-2.400177	1.113571	-0.000059
O	-2.255412	-1.120808	0.000086
H	-3.215155	-0.959456	0.000079
O	-0.067883	2.432371	0.000074
C	0.697360	3.620236	0.000133
H	1.327621	3.696462	-0.895823
H	-0.028677	4.434793	0.000156
H	1.327597	3.696390	0.896111

***p*-Me-C_6H_4COOH**

E = -459.958413 a.u.

C	0.676851	-1.187435	0.012678
C	-0.713666	-1.195188	0.022616
C	-1.444920	-0.000590	0.016384
C	-0.739378	1.210382	0.006241
C	0.649192	1.228705	-0.003844
C	1.368855	0.028775	-0.001236
H	1.229883	-2.121106	0.019483
H	-1.243623	-2.145176	0.036999
C	2.848117	0.102866	-0.009140
O	3.494158	1.131146	-0.019710
O	3.441608	-1.113819	-0.004120
H	4.398362	-0.933712	-0.010525
H	1.198903	2.165103	-0.010139
H	-1.289104	2.149160	0.007810
C	-2.950016	-0.016373	-0.005334
H	-3.326089	0.001733	-1.036994
H	-3.349842	-0.917423	0.471234
H	-3.368397	0.855835	0.507904

***m*-Me-C_6H_4COOH**

E = -459.957787 a.u.

C	-1.161019	1.570288	-0.000005
C	0.056825	2.241005	0.000045
C	1.254013	1.524229	0.000046
C	1.262883	0.124696	-0.000002
C	0.033887	-0.539235	-0.000054
C	-1.170047	0.169980	-0.000058
H	-2.097408	2.118033	-0.000008
H	0.077370	3.327666	0.000081
H	2.200298	2.061575	0.000084
C	-2.430271	-0.613571	-0.000126
O	-2.496823	-1.825953	0.000008
O	-3.538912	0.161901	0.000104
H	-4.289029	-0.458950	0.000201
H	-0.010815	-1.625318	-0.000096
C	2.554871	-0.650889	0.000016
H	2.630511	-1.298281	0.882019
H	2.630408	-1.298498	-0.881835
H	3.422758	0.015982	-0.000114

***o*-Me-C_6H_4COOH**

E =-459.951204 a.u.

C	-0.480793	-1.458928	0.000037
C	-1.862546	-1.513481	0.000043
C	-2.584754	-0.311046	0.000017
C	-1.936822	0.909467	-0.000017
C	-0.525100	0.988262	-0.000027
C	0.210487	-0.233063	0.000005
H	0.102240	-2.373925	0.000060
H	-2.377952	-2.468918	0.000069
H	-3.672183	-0.331929	0.000022
H	-2.510717	1.833741	-0.000041
C	1.674054	-0.206956	0.000013
O	2.378492	0.798058	-0.000011
O	2.246116	-1.433016	0.000018
H	3.204645	-1.263799	0.000011
C	0.174716	2.360070	-0.000084
H	0.786108	2.448605	0.873564
H	0.786109	2.448533	-0.873739
H	-0.561833	3.136211	-0.000116

***p*-NO_2-C_6H_4COOH**

E = -625.072950 a.u.

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C	0.454238	-1.205989	-0.000115
C	1.843801	-1.244028	-0.000075
C	2.543394	-0.041159	-0.000020
C	1.903306	1.195202	-0.000003
C	0.514982	1.221236	-0.000044
C	-0.211940	0.025288	-0.000105
H	-0.116084	-2.128336	-0.000160
H	2.390009	-2.179844	-0.000086
C	-1.698036	0.121282	-0.000166
O	-2.317012	1.163309	0.000108
O	-2.301056	-1.085111	0.000111
H	-3.258495	-0.905987	0.000293
H	-0.026918	2.161501	-0.000036
H	2.493679	2.103872	0.000042
N	4.013863	-0.077689	0.000024
O	4.604210	0.994293	0.000166
O	4.551031	-1.177478	0.000096

***m*-NO_2-C_6H_4COOH**

E = -625.073020 a.u.

C	0.455079	-1.194616	0.000144
C	1.848316	-1.227971	-0.000005
C	2.578058	-0.042716	-0.000063
C	1.887531	1.166709	0.000032
C	0.501785	1.228334	0.000180
C	-0.219047	0.032731	0.000248
H	-0.115974	-2.116973	0.000195
H	2.369317	-2.180738	-0.000077
H	3.661993	-0.037084	-0.000180
C	-1.704049	0.125553	0.000448
O	-2.327282	1.164420	-0.000076
O	-2.302584	-1.084388	-0.000208
H	-3.260332	-0.907130	-0.000566
H	-0.014615	2.181276	0.000255
N	2.655032	2.420850	-0.000027
O	3.876338	2.332710	-0.000163
O	2.024250	3.468728	0.000064

***o*-NO_2-C_6H_4COOH**

E = -625.058587 a.u.

C	0.797650	1.833154	0.044456
C	-0.271088	2.728239	0.023928
C	-1.580728	2.254412	0.000751
C	-1.822005	0.882745	-0.016317
C	-0.746960	0.003715	-0.011072
C	0.577200	0.453775	0.035933
H	1.818406	2.199721	0.083691
H	-0.077136	3.797033	0.031909
H	-2.416622	2.947652	-0.013381
H	-2.828526	0.480791	-0.049520
C	1.736529	-0.471075	0.237500
O	1.765781	-1.367499	1.045515
O	2.787125	-0.125387	-0.531968
H	3.504424	-0.742106	-0.295722
N	-1.052453	-1.426365	-0.154047
O	-0.276149	-2.099053	-0.815852
O	-2.087887	-1.828602	0.358769

***p*-CN-C_6H_4COOH**

E = -512.852263 a.u.

C	0.657815	-1.191845	0.000039
C	-0.730982	-1.209388	0.000054
C	-1.443155	-0.000160	0.000042
C	-0.756918	1.224833	0.000015
C	0.630325	1.233225	0.000000
C	1.342419	0.028802	0.000012
H	1.214926	-2.122415	0.000048
H	-1.271371	-2.150688	0.000075
C	2.828147	0.104434	-0.000004
O	3.462709	1.137460	-0.000036
O	3.415582	-1.110404	0.000000
H	4.375003	-0.942660	-0.000019
H	1.184626	2.166360	-0.000021
H	-1.316741	2.154669	0.000005
C	-2.874971	-0.016519	0.000057
N	-4.038148	-0.030004	0.000069

***m*-CN-C_6H_4COOH**

E = -512.852054 a.u.

C	-1.134853	1.551564	0.000025
C	0.082587	2.229015	0.000033
C	1.279152	1.520289	0.000017
C	1.259446	0.115700	-0.000008
C	0.038886	-0.567428	-0.000016
C	-1.156417	0.152332	-0.000001
H	-2.070119	2.101266	0.000036
H	0.099255	3.314924	0.000052
H	2.231672	2.041318	0.000024
C	-2.425204	-0.624295	-0.000012
O	-2.489967	-1.834577	0.000019
O	-3.520973	0.163511	0.000048
H	-4.283617	-0.442314	0.000076
H	0.005129	-1.651916	-0.000033
C	2.491744	-0.615252	-0.000024
N	3.495296	-1.203229	-0.000038

***o*-CN-C_6H_4COOH**

E = -512.845768 a.u.

C	-0.462765	-1.449635	0.000045
C	-1.854280	-1.475115	0.000046
C	-2.571390	-0.280012	0.000011
C	-1.896528	0.936199	-0.000026
C	-0.494460	0.972655	-0.000028
C	0.232636	-0.237076	0.000007
H	0.101416	-2.375528	0.000072
H	-2.377009	-2.427370	0.000075
H	-3.657695	-0.291584	0.000012
H	-2.445095	1.872711	-0.000054
C	1.719828	-0.215538	0.000006
O	2.401173	0.784681	-0.000035
O	2.255102	-1.456656	0.000022
H	3.219996	-1.324260	0.000007
C	0.113039	2.271790	-0.000068
N	0.457766	3.382654	-0.000103

***p*-C(O)H-C_6H_4COOH**

E = -533.929315 a.u.

C	3.500256	0.234530	0.000012
C	2.021623	0.396978	-0.000015
O	1.362292	-0.781022	-0.000058
O	1.446248	1.464717	-0.000087
C	4.112277	-1.027579	0.000045
C	5.496529	-1.122271	0.000073
C	6.278283	0.040316	0.000065
C	5.664519	1.297975	0.000033
C	4.278925	1.396851	0.000005
O	8.374288	-1.102428	0.000295
H	3.497831	-1.921664	0.000049
H	5.997820	-2.085809	0.000098
H	6.277587	2.197127	0.000028
H	3.778152	2.359873	-0.000022
C	7.756548	-0.058237	0.000087
H	8.287667	0.919434	0.000253
H	0.415305	-0.553581	-0.000111

***m*-C(O)H-C_6H_4COOH**

E = -533.929639 a.u.

C	-3.616601	-0.697141	0.000032
C	-2.130506	-0.749393	-0.000116
O	-1.560728	0.473215	-0.000276
O	-1.478756	-1.772687	-0.000235
C	-4.321385	0.505049	0.000090
C	-5.720509	0.488417	0.000234
C	-6.405764	-0.731148	0.000320
C	-5.701252	-1.933747	0.000261
C	-4.310562	-1.916117	0.000118
H	-3.806617	1.460314	0.000026
H	-6.233730	-2.880568	0.000328

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H	-3.735458	-2.837149	0.000071
H	-7.494426	-0.733575	0.000432
O	-5.969116	2.862853	0.000177
C	-6.476769	1.760998	0.000299
H	-7.583552	1.642793	0.000357
H	-0.599268	0.318438	-0.000422

***o*-C(O)H-C_6H_4COOH**

E = -533.917158 a.u.

C	3.856964	0.205359	-0.290024
C	2.371563	0.379674	-0.386153
O	1.717554	-0.794609	-0.376485
O	1.828186	1.447326	-0.555295
C	4.497656	-0.458796	0.773967
C	5.886078	-0.624205	0.743898
C	6.644008	-0.122183	-0.310425
C	6.009399	0.563840	-1.343691
C	4.623979	0.730337	-1.328710
O	2.654572	-0.566428	2.298981
H	6.373880	-1.134993	1.572037
H	7.722246	-0.254922	-0.320465
H	6.590714	0.971041	-2.166573
H	4.126113	1.263499	-2.133417
C	3.780004	-0.897291	1.993630
H	4.383448	-1.548834	2.664179
H	0.768718	-0.575024	-0.412533

***p*-C(O)Me-C_6H_4COOH**

E = -573.238538 a.u.

C	-3.166831	0.123568	-0.000015
C	-1.692779	0.315110	-0.000020
O	-1.009161	-0.849803	-0.000227
O	-1.136645	1.393427	-0.000076
C	-3.756956	-1.147237	-0.000076
C	-5.139828	-1.265167	-0.000057
C	-5.953519	-0.124031	0.000012
C	-5.356011	1.143740	0.000069
C	-3.971858	1.266973	0.000059
O	-7.913152	-1.444699	0.000054
H	-3.128949	-2.031948	-0.000135
H	-5.621737	-2.237984	-0.000092
H	-5.967932	2.040998	0.000129
H	-3.492873	2.241148	0.000109
C	-7.441474	-0.320637	0.000041
C	-8.338226	0.898796	-0.000054
H	-8.156295	1.522080	0.883750
H	-8.155957	1.522268	-0.883650
H	-9.378475	0.568675	-0.000269
H	-0.067117	-0.603139	-0.000309

***m*-C(O)Me-C_6H_4COOH**

E = -573.238636 a.u.

C	-3.277009	-0.906971	0.000035
C	-1.790771	-0.894761	0.000035
O	-1.272805	0.351045	-0.000016
O	-1.094636	-1.888877	-0.000312
C	-4.032735	0.264420	0.000194
C	-5.431113	0.203030	0.000208
C	-6.060295	-1.048431	0.000040
C	-5.305699	-2.221263	-0.000129
C	-3.917456	-2.153183	-0.000131
H	-3.556545	1.239049	0.000317
H	-5.803196	-3.187118	-0.000261
H	-3.306928	-3.051052	-0.000255
H	-7.144648	-1.115700	0.000036
O	-5.595632	2.560229	0.000365
C	-6.190207	1.496173	0.000394
C	-7.704013	1.452425	0.000459
H	-8.083864	0.926099	-0.883556
H	-8.083800	0.925683	0.884247
H	-8.083775	2.475607	0.000695
H	-0.306063	0.234582	-0.000191

***o*-C(O)Me-C_6H_4COOH**

E = -573.226262 a.u.

C	-3.680551	0.717343	-0.061239
C	-2.201811	0.830366	0.052124
O	-1.567635	-0.353416	-0.094768
O	-1.597869	1.869180	0.217326
C	-4.391888	-0.496912	0.007291
C	-5.765887	-0.485390	-0.254903
C	-6.435856	0.704087	-0.529438
C	-5.734036	1.908413	-0.560434
C	-4.362218	1.908496	-0.337254
O	-3.985057	-2.799402	-0.343563
H	-6.306858	-1.427108	-0.231263
H	-7.505720	0.688732	-0.720542
H	-6.250289	2.840656	-0.772067
H	-3.784717	2.826428	-0.388073
C	-3.811115	-1.841545	0.383103
C	-3.197999	-1.990503	1.759549
H	-2.722247	-1.079089	2.125913
H	-4.010686	-2.242752	2.454587
H	-2.485850	-2.819123	1.757887
H	-0.615681	-0.161269	-0.015519

***p*-C(O)NMe2-C_6H_4COOH**

E = -667.872944 a.u.

N	4.427383	6.112615	2.067304
O	5.742929	7.647805	3.117857
C	4.243260	4.776138	1.536385
H	4.932278	4.073702	2.004575
H	4.434840	4.773824	0.453994
C	3.740933	7.164647	1.341555
H	4.138049	7.268611	0.321796
H	3.883366	8.106937	1.870128
C	5.403010	6.479542	2.959352
C	6.036911	5.410386	3.808141
C	7.421753	5.470931	4.006799
C	8.049756	4.563176	4.847936
C	7.297009	3.600045	5.530455
C	5.908779	3.556634	5.363522
H	5.323081	2.824267	5.909144
C	5.285470	4.454266	4.502363
H	4.205369	4.426051	4.385410
H	3.215515	4.424684	1.698367
H	2.672148	6.928875	1.275596
H	7.991199	6.244085	3.500129
H	9.124384	4.587818	5.000027
C	8.017603	2.658819	6.423697
O	9.218194	2.652088	6.599450
O	7.195307	1.781492	7.042581
H	7.774680	1.226537	7.594372

***m*-C(O)NMe2-C_6H_4COOH**

E = -667.872264 a.u.

N	4.401464	6.132825	2.065165
O	5.859516	7.599686	3.021317
C	4.126365	4.807557	1.546030
H	4.798033	4.070994	1.986237
H	4.270935	4.793809	0.456366
C	3.732900	7.217141	1.371101
H	4.080648	7.299243	0.331454
H	3.951208	8.151976	1.886828
C	5.448344	6.451397	2.894911
C	6.066292	5.351214	3.715247
C	7.456703	5.322966	3.829692
C	8.079626	4.379280	4.649042
C	7.307893	3.476860	5.391668
H	7.796760	2.753119	6.035290
C	5.919975	3.523365	5.304587
H	5.316089	2.837936	5.893125
C	5.301229	4.450421	4.466688
H	4.216149	4.489768	4.411769
H	3.089707	4.509781	1.753005
H	2.651330	7.036693	1.362291
H	8.063365	6.040466	3.286593
C	9.563915	4.382328	4.705971

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O	10.281709	5.123800	4.069001
O	10.060810	3.454515	5.555776
H	11.028552	3.551885	5.509598

***o*-C(O)NMe2-C$_6$H$_4$COOH**

E = -667.867082 a.u.

N	4.395451	6.132480	2.041720
O	5.096836	7.619893	3.624218
O	7.459608	6.612705	1.783128
O	9.375022	6.025455	2.790076
C	4.577396	4.890757	1.322638
H	5.148663	4.182744	1.923949
H	5.113950	5.058469	0.378155
C	3.605960	7.145733	1.371859
H	4.083525	7.460399	0.433101
H	3.520107	8.008533	2.032698
C	5.130173	6.498783	3.133805
C	5.918582	5.415300	3.839642
C	7.311925	5.255277	3.726143
C	7.978738	4.348682	4.559806
H	9.055382	4.258301	4.453879
C	7.280711	3.589822	5.490472
H	7.810293	2.887285	6.127886
C	5.898426	3.739453	5.599782
H	5.340178	3.154401	6.326232
C	5.228628	4.648679	4.784929
H	4.154704	4.780512	4.888267
C	8.162651	5.992248	2.754082
H	3.602429	4.443322	1.091665
H	2.609131	6.751425	1.140469
H	8.118088	7.083647	1.241329

***p*-Cl-C$_6$H$_4$COOH**

E = -880.194776 a.u.

C	0.666497	-1.189307	0.000050
C	-0.724121	-1.208412	0.000075
C	-1.420088	0.000164	0.000066
C	-0.749859	1.223916	0.000033
C	0.639214	1.230532	0.000008
C	1.355409	0.028724	0.000017
H	1.220262	-2.122219	0.000056
H	-1.267291	-2.147772	0.000101
C	2.836655	0.103813	-0.000009
O	3.477197	1.134508	-0.000055
O	3.427447	-1.112023	-0.000017
H	4.385514	-0.937965	-0.000050
H	1.190216	2.165931	-0.000018
H	-1.312237	2.151880	0.000027
Cl	-3.161423	-0.018707	0.000097

***m*-Cl-C$_6$H$_4$COOH**

E = -880.193777 a.u.

C	-1.147771	1.560130	0.000073
C	0.071205	2.232599	0.000038
C	1.271435	1.523855	-0.000024
C	1.239326	0.129047	-0.000049
C	0.033747	-0.560780	-0.000016
C	-1.163769	0.161619	0.000046
H	-2.082641	2.109734	0.000121
H	0.092614	3.318829	0.000058
H	2.224820	2.042717	-0.000051
C	-2.428577	-0.619157	0.000087
O	-2.493231	-1.830241	-0.000023
O	-3.529898	0.163143	0.000029
H	-4.287036	-0.449342	-0.000023
H	0.001846	-1.644930	-0.000035
Cl	2.738619	-0.761373	-0.000126

***o*-Cl-C$_6$H$_4$COOH**

E = -880.184510 a.u.

C	-0.463099	-1.437059	0.000037
C	-1.849378	-1.504974	0.000045
C	-2.593585	-0.326656	0.000017
C	-1.947117	0.904272	-0.000020
C	-0.552709	0.971534	-0.000028
C	0.217723	-0.207339	-0.000002
H	0.124845	-2.347500	0.000058
H	-2.345273	-2.471245	0.000074
H	-3.679843	-0.360031	0.000024
H	-2.515410	1.828557	-0.000042
C	1.707414	-0.207621	-0.000012
O	2.433352	0.760669	-0.000018
O	2.212125	-1.467287	0.000025
H	3.178466	-1.349578	0.000030
Cl	0.140364	2.563668	-0.000074

***p*-Br-C$_6$H$_4$COOH**

E = -2991.441820 a.u.

C	0.666547	-1.189386	0.000048
C	-0.724385	-1.207965	0.000073
C	-1.419798	0.000179	0.000064
C	-0.750158	1.223526	0.000032
C	0.639234	1.230692	0.000007
C	1.355213	0.028770	0.000016
H	1.220027	-2.122517	0.000055
H	-1.265901	-2.148023	0.000098
C	2.836753	0.103833	-0.000010
O	3.477064	1.134609	-0.000052
O	3.427261	-1.112000	-0.000014
H	4.385389	-0.938254	-0.000044
H	1.189945	2.166316	-0.000018
H	-1.310908	2.152218	0.000025
Br	-3.312883	-0.020603	0.000096

***m*-Br-C$_6$H$_4$COOH**

E = -2991.440907 a.u.

C	-1.147486	1.559941	0.000057
C	0.071409	2.232543	0.000037
C	1.271509	1.523106	-0.000014
C	1.239149	0.129048	-0.000044
C	0.034142	-0.560440	-0.000024
C	-1.164062	0.161398	0.000028
H	-2.082400	2.109562	0.000097
H	0.093248	3.318805	0.000060
H	2.223595	2.043530	-0.000030
C	-2.428825	-0.619470	0.000055
O	-2.493707	-1.830473	-0.000015
O	-3.530002	0.163086	0.000043
H	-4.287277	-0.449212	0.000016
H	0.000713	-1.644215	-0.000045
Br	2.869757	-0.837776	-0.000110

***o*-Br-C$_6$H$_4$COOH**

E = -2991.431657 a.u.

C	2.247246	-0.133864	0.028992
C	2.551540	-1.488142	0.060269
C	1.518124	-2.422707	0.077734
C	0.194103	-1.996461	0.062733
C	-0.110261	-0.635216	0.040686
C	0.918609	0.323438	0.024392
H	3.043301	0.601795	0.013965
H	3.588363	-1.811602	0.069874
H	1.736524	-3.487103	0.099868
H	-0.617458	-2.716177	0.066747
C	0.669916	1.792446	0.030393
O	-0.371337	2.347193	0.299062
O	1.784430	2.493575	-0.293736
H	1.522015	3.428798	-0.227871
Br	-1.949940	-0.198653	-0.000976

***p*-NH$_2$-C$_6$H$_4$COOH**

E = -475.990970 a.u.

C	0.009730	-1.188584	-0.013838
C	1.394938	-1.213000	-0.027089
C	2.132449	-0.014063	-0.032903
C	1.432941	1.208094	-0.025083
C	0.049356	1.223521	-0.011541
C	-0.684284	0.029317	-0.004801

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H	-0.545509	-2.121077	-0.007818
H	1.921466	-2.165017	-0.038203
C	-2.154572	0.110958	0.013307
O	-2.801321	1.141144	0.023916
O	-2.758159	-1.104459	0.017523
H	-3.712286	-0.912610	0.028735
H	-0.493413	2.164057	-0.003425
H	1.988623	2.143380	-0.034461
N	3.511659	-0.035574	-0.096387
H	3.991866	0.800549	0.204554
H	3.966136	-0.885860	0.204741

***m*-NH$_2$-C$_6$H$_4$COOH**

E = -475.987715 a.u.

C	-0.264286	1.476850	-0.005826
C	1.072455	1.866590	-0.000983
C	2.093108	0.921263	0.016313
C	1.798881	-0.453267	0.029368
C	0.454577	-0.844261	0.023752
C	-0.563870	0.109928	0.006826
H	-1.061396	2.211291	-0.020635
H	1.327771	2.923153	-0.012218
H	3.132066	1.245204	0.025730
C	-1.960330	-0.392837	-0.002431
O	-2.279913	-1.564690	-0.004100
O	-2.882551	0.596820	-0.009923
H	-3.744594	0.144352	-0.014880
H	0.179168	-1.895493	0.036297
N	2.815499	-1.398666	0.104327
H	2.567442	-2.324610	-0.217210
H	3.712191	-1.101222	-0.255662

***o*-NH$_2$-C$_6$H$_4$COOH**

E = -475.994644 a.u.

C	-0.480088	-1.456267	-0.025770
C	-1.861947	-1.511304	-0.015862
C	-2.584492	-0.310258	0.027995
C	-1.936039	0.910069	0.054591
C	-0.525226	0.989569	0.038164
C	0.210355	-0.230384	0.005089
H	0.103046	-2.370777	-0.052514
H	-2.376954	-2.466703	-0.039029
H	-3.671815	-0.331730	0.040517
H	-2.509849	1.834024	0.080962
C	1.674712	-0.205813	0.027601
O	2.379108	0.796491	0.094985
O	2.245485	-1.431104	-0.025686
H	3.204035	-1.264258	0.003007
N	0.089673	2.202707	0.023615
H	-0.446916	3.026131	0.244236
H	1.096021	2.217223	0.143164

***p*-OH-C$_6$H$_4$COOH**

E = -495.843919 a.u.

C	-0.295986	-1.088819	-0.000457
C	1.087579	-0.964588	-0.000469
C	1.674559	0.306292	-0.000248
C	0.868378	1.452065	-0.000026
C	-0.509572	1.318480	-0.000030
C	-1.108632	0.050308	-0.000256
H	-0.750426	-2.074104	-0.000628
H	1.714923	-1.854604	-0.000662
C	-2.583274	-0.025487	-0.000271
O	-3.332189	0.931365	0.000436
O	-3.051486	-1.297345	0.000179
H	-4.021269	-1.212956	0.000609
H	-1.151731	2.193923	0.000137
H	1.344425	2.427720	0.000147
O	3.017639	0.490570	-0.000271
H	3.457285	-0.372525	-0.000165

***m*-OH-C$_6$H$_4$COOH**

E = -495.840942 a.u.

C	0.826365	1.489080	0.000236
C	-0.464246	2.006792	0.000180
C	-1.570556	1.158284	0.000061
C	-1.389547	-0.228713	0.000000
C	-0.099289	-0.758212	0.000060
C	1.001228	0.098894	0.000184
H	1.689118	2.145397	0.000330
H	-0.618444	3.082527	0.000232
H	-2.576775	1.575379	0.000015
C	2.348973	-0.526332	0.000271
O	2.562057	-1.720874	-0.000196
O	3.352638	0.380338	-0.000277
H	4.173434	-0.143398	-0.000591
H	0.050203	-1.832721	0.000022
O	-2.428003	-1.106873	-0.000116
H	-3.260472	-0.612606	-0.000158

***o*-OH-C$_6$H$_4$COOH**

E = -495.854706 a.u.

C	-0.437466	-1.494275	0.000099
C	-1.819551	-1.556346	0.000113
C	-2.558808	-0.364067	0.000053
C	-1.927991	0.868979	-0.000026
C	-0.526712	0.945253	-0.000048
C	0.228490	-0.254942	0.000022
H	0.156337	-2.402697	0.000150
H	-2.325866	-2.516796	0.000174
H	-3.645412	-0.403750	0.000065
H	-2.490811	1.797213	-0.000077
C	1.687009	-0.163196	0.000024
O	2.319270	0.893778	-0.000010
O	2.329552	-1.342921	0.000056
H	3.279531	-1.127714	0.000046
O	0.036551	2.157991	-0.000138
H	1.016895	2.021505	-0.000172

5

E = -1188.906074 a.u.

Cu	-0.054544	-0.693824	0.000069
C	-4.110686	0.037412	0.000024
C	-2.614300	0.229192	0.000027
O	-1.928270	-0.869553	0.000094
O	-2.151236	1.377893	-0.000037
C	-4.683916	-1.238442	0.000120
C	-6.069234	-1.386888	0.000123
C	-6.893569	-0.260956	0.000024
C	1.683449	3.457986	-0.000032
C	0.753268	2.398774	-0.000008
N	1.136288	1.131248	0.000013
C	2.451654	0.840265	0.000009
C	3.461625	1.828264	-0.000017
C	3.033869	3.174225	-0.000036
C	2.811921	-0.555018	0.000029
C	4.835908	1.422792	-0.000022
N	1.802944	-1.464493	0.000055
C	2.119097	-2.756184	0.000073
C	3.445296	-3.217822	0.000066
C	4.476595	-2.301010	0.000041
C	4.177402	-0.922771	0.000022
C	5.178724	0.103758	-0.000004
C	-6.327031	1.014743	-0.000073
C	-4.942562	1.161573	-0.000070
H	-4.027275	-2.102618	0.000193
H	-6.508208	-2.382172	0.000200
H	-7.975138	-0.377205	0.000025
H	1.326968	4.483518	-0.000048
H	-0.325134	2.547726	-0.000007
H	3.772647	3.972421	-0.000055
H	5.606013	2.190344	-0.000041
H	1.286441	-3.453118	0.000093
H	3.639401	-4.285633	0.000081
H	5.513813	-2.627324	0.000036
H	6.224334	-0.193600	-0.000008
H	-6.967030	1.894297	-0.000149
H	-4.476469	2.142271	-0.000139

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TS5

E = -1188.848817 a.u.

Cu	0.719771	-0.292905	0.098233
C	2.671068	-0.136714	-0.020911
C	3.309418	0.713614	0.899754
C	4.425357	1.467217	0.535792
C	4.939219	1.369632	-0.758958
C	4.344605	0.503667	-1.678144
C	3.231490	-0.250488	-1.305465
H	2.938843	0.753106	1.922595
H	4.907162	2.117603	1.263698
H	5.816306	1.947461	-1.042640
H	4.761677	0.404020	-2.678522
H	2.803932	-0.963112	-2.008088
C	1.998686	-1.906646	0.801626
O	1.901780	-1.741339	2.001749
O	2.018858	-2.766497	-0.058298
C	-1.391656	3.639815	0.230089
C	-0.378431	2.663869	0.230499
N	-0.634363	1.368982	0.124852
C	-1.919681	0.966670	0.008004
C	-3.009997	1.866432	-0.001487
C	-2.707487	3.240168	0.115074
C	-2.161281	-0.449410	-0.111746
C	-4.341661	1.350069	-0.125100
N	-1.083647	-1.266077	-0.106971
C	-1.265281	-2.575941	-0.214224
C	-2.545779	-3.146661	-0.333244
C	-3.653886	-2.324843	-0.342884
C	-3.484956	-0.927622	-0.231232
C	-4.568863	0.010720	-0.233990
H	-1.127888	4.688793	0.320756
H	0.670079	2.937456	0.319081
H	-3.513306	3.970273	0.113047
H	-5.172570	2.050988	-0.129309
H	-0.359802	-3.178952	-0.205494
H	-2.643745	-4.224316	-0.416392
H	-4.654956	-2.739332	-0.435180
H	-5.583455	-0.368695	-0.325805

6

E = -1000.354741 a.u.

Cu	0.743395	-0.174369	-0.333782
C	2.608049	0.187544	-0.398328
C	3.265967	0.845733	0.664241
C	4.627760	1.155732	0.633010
C	5.397041	0.817658	-0.479682
C	4.786231	0.166941	-1.551280
C	3.424289	-0.139424	-1.503240
H	2.700987	1.125282	1.554434
H	5.090242	1.661983	1.479800
H	6.458419	1.056694	-0.510853
H	5.373966	-0.105271	-2.427350
H	2.986467	-0.650770	-2.360600
C	-1.799892	3.814155	0.194747
C	-0.704239	2.940619	0.051314
N	-0.838552	1.630860	-0.053933
C	-2.076579	1.102530	-0.027806
C	-3.247125	1.887413	0.115818
C	-3.072641	3.283441	0.228535
C	-2.191737	-0.331686	-0.154828
C	-4.528633	1.247975	0.141329
N	-1.053081	-1.057170	-0.302841
C	-1.154428	-2.379087	-0.418825
C	-2.382010	-3.058705	-0.397740
C	-3.545381	-2.332868	-0.250807
C	-3.474795	-0.930394	-0.124601
C	-4.636532	-0.104445	0.027706
H	-1.633404	4.883859	0.277941
H	0.315661	3.318594	0.021763
H	-3.943242	3.925620	0.340257
H	-5.417233	1.864340	0.254246
H	-0.218822	-2.918132	-0.532677
H	-2.397628	-4.139273	-0.497511
H	-4.514304	-2.825933	-0.231373
H	-5.611978	-0.583957	0.048603

7

E = -1421.023077 a.u.

C	-0.704020	2.393852	-0.874835
C	-0.938295	2.587794	-2.256205
C	-0.412411	3.572199	-0.148944
C	-0.901927	3.844410	-2.863207
H	-1.162537	1.725384	-2.884883
C	-0.369367	4.837181	-0.739318
H	-0.204498	3.502596	0.919727
C	-0.617559	4.979260	-2.103875
H	-1.093612	3.939678	-3.931256
H	-0.140794	5.713595	-0.134251
H	-0.585020	5.961555	-2.571090
O	0.899996	-0.348573	0.940647
C	1.936427	0.097426	0.453349
O	1.965490	1.091977	-0.418531
H	1.016488	1.411726	-0.562429
C	3.279654	-0.446362	0.796113
C	3.358129	-1.513894	1.697028
C	4.449349	0.084437	0.240099
C	4.596070	-2.048023	2.039184
H	2.437411	-1.907882	2.116477
C	5.686788	-0.452592	0.585040
H	4.378533	0.913523	-0.456334
C	5.761607	-1.517850	1.483168
H	4.654703	-2.877254	2.739566
H	6.594730	-0.039363	0.153358
H	6.729425	-1.934969	1.750837
Cu	-1.069582	0.692081	-0.022001
N	-2.373121	0.070162	1.539560
N	-1.771205	-1.226184	-0.733959
C	-2.648417	0.718384	2.663432
C	-3.069049	-1.056844	1.262386
C	-2.746263	-1.752221	0.042041
C	-1.449622	-1.859455	-1.853454
C	-3.628371	0.291259	3.575072
H	-2.070773	1.620028	2.847735
C	-4.082322	-1.565174	2.110273
C	-3.445798	-2.936183	-0.294576
C	-2.077790	-3.044291	-2.273435
H	-0.659766	-1.407581	-2.447972
C	-4.350756	-0.851520	3.296092
H	-3.807014	0.864088	4.479774
C	-4.775455	-2.762848	1.736232
C	-3.082125	-3.582004	-1.493892
C	-4.470341	-3.420281	0.583245
H	-1.769519	-3.517589	-3.200572
H	-5.120348	-1.207582	3.976860
H	-5.553484	-3.139407	2.395855
H	-3.592989	-4.494981	-1.790570
H	-5.001459	-4.328864	0.310028

TS6

E = -1421.018958 a.u.

C	-0.317710	2.086044	-0.767293
C	-0.822916	2.241566	-2.076659
C	-0.311821	3.253843	0.027528
C	-1.316618	3.457306	-2.551361
H	-0.826760	1.385043	-2.751380
C	-0.800451	4.477828	-0.430034
H	0.105594	3.207395	1.034414
C	-1.311212	4.580882	-1.724306
H	-1.701544	3.533113	-3.567110
H	-0.777292	5.354123	0.215959
H	-1.690450	5.532946	-2.090088
O	1.170924	-0.500563	0.913860
C	2.172588	0.028751	0.385688
O	2.109892	0.977186	-0.489235
H	0.990472	1.313371	-0.593115
C	3.543932	-0.434050	0.758147

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C	3.689060	-1.475161	1.681074
C	4.679421	0.161135	0.197879
C	4.958526	-1.917635	2.040727
H	2.794717	-1.922031	2.104462
C	5.948662	-0.283178	0.559279
H	4.551002	0.969163	-0.515320
C	6.089773	-1.322147	1.480204
H	5.068386	-2.726819	2.758573
H	6.829608	0.181539	0.123458
H	7.081749	-1.667711	1.761640
Cu	-0.655542	0.311870	0.138038
N	-2.214517	0.041247	1.515304
N	-1.644402	-1.373600	-0.701194
C	-2.481181	0.748493	2.606782
C	-3.080113	-0.938589	1.158582
C	-2.772580	-1.698684	-0.025703
C	-1.335974	-2.076399	-1.783988
C	-3.614292	0.528316	3.405829
H	-1.766839	1.528313	2.855511
C	-4.251552	-1.235607	1.896231
C	-3.641197	-2.739568	-0.434639
C	-2.128671	-3.130119	-2.267104
H	-0.419576	-1.790904	-2.293866
C	-4.504042	-0.465705	3.049447
H	-3.776443	1.139984	4.287923
C	-5.113373	-2.290462	1.449976
C	-3.287774	-3.460252	-1.593208
C	-4.820175	-3.012518	0.333383
H	-1.823589	-3.666759	-3.160152
H	-5.392623	-0.661851	3.644627
H	-6.010330	-2.505774	2.025542
H	-3.927695	-4.267288	-1.941879
H	-5.479628	-3.812230	0.005114

1O$_{p\text{-OMe}}$

E = -1234.705198 a.u.

Ag	1.862551	-1.283728	-1.069435
O	-0.255216	-1.294956	-1.103225
O	0.270895	0.037830	0.625777
C	-0.564897	-0.525848	-0.113997
O	3.986243	-0.979446	-0.724513
S	4.293047	-0.546890	0.734412
C	5.981659	0.091051	0.622449
C	3.425062	1.014905	1.014855
H	6.632338	-0.752160	0.379097
H	6.271048	0.517135	1.587879
H	6.031627	0.842231	-0.170692
H	3.693714	1.732114	0.233196
H	3.702655	1.391259	2.005227
H	2.349104	0.798390	0.981352
C	-2.026946	-0.324053	0.128480
C	-2.454384	0.492276	1.185261
C	-2.988829	-0.933739	-0.678873
C	-3.803142	0.692744	1.427100
H	-1.702179	0.963587	1.810188
C	-4.349830	-0.741714	-0.448586
H	-2.658227	-1.566126	-1.496763
C	-4.761898	0.075748	0.609866
H	-4.146599	1.322635	2.242690
H	-5.073399	-1.229101	-1.093591
O	-6.058782	0.333117	0.926214
C	-7.065950	-0.260951	0.135750
H	-8.016002	0.073788	0.557270
H	-7.002320	0.062233	-0.912160
H	-7.019635	-1.357684	0.176620

TS3$_{p\text{-OMe}}$

E = -1234.648860 a.u.

Ag	0.929997	-0.607066	-0.138676
O	0.351660	2.264452	-1.358664
O	0.756232	2.174389	0.909632
C	0.347732	1.930226	-0.204660
O	2.984854	-1.328898	-0.068511
S	4.048413	-0.228902	-0.323133
C	3.997535	0.887787	1.099938
C	5.601438	-1.075702	0.052229
H	3.039714	1.419907	1.069140
H	4.820095	1.604818	1.008081
H	4.080041	0.310892	2.025932
H	5.536223	-1.527128	1.046152
H	6.426534	-0.359224	-0.002805
H	5.735071	-1.854062	-0.702657
C	-0.968859	0.340165	-0.057045
C	-1.596197	0.286855	1.201493
C	-1.800755	0.166899	-1.188472
C	-2.962476	0.045140	1.346939
H	-1.004498	0.482256	2.093594
C	-3.157651	-0.081119	-1.068338
H	-1.369246	0.267812	-2.181773
C	-3.747260	-0.149941	0.204661
H	-3.403665	0.027994	2.338428
H	-3.794801	-0.208402	-1.939385
O	-5.082931	-0.386523	0.219135
C	-5.737294	-0.448333	1.469488
H	-6.786975	-0.651852	1.248857
H	-5.336169	-1.255999	2.096240
H	-5.660110	0.502462	2.013521

1O$_{m\text{-OMe}}$

E = -1234.703160 a.u.

Ag	2.060484	-1.206904	0.053350
O	0.030762	-1.826345	0.045868
O	-0.052034	0.416059	0.006864
C	-0.603518	-0.704680	0.021847
O	3.975338	-0.180793	0.084767
S	3.891067	1.249653	-0.511942
C	2.733598	2.182603	0.518118
C	5.433520	2.012414	0.044644
H	1.743032	1.729348	0.382673
H	2.721626	3.221128	0.170507
H	3.040401	2.123156	1.566804
H	5.522960	1.894150	1.128151
H	5.436050	3.069406	-0.238213
H	6.253196	1.491939	-0.456208
C	-2.103799	-0.797104	0.010232
C	-2.850621	0.377433	-0.016468
C	-2.751957	-2.039912	0.025923
C	-4.247899	0.327501	-0.027643
H	-2.344681	1.336786	-0.029089
C	-4.139894	-2.083974	0.014465
H	-2.156578	-2.946044	0.046375
C	-4.898721	-0.910021	-0.012154
H	-4.652802	-3.042846	0.026233
H	-5.981949	-0.973428	-0.020581
O	-4.882628	1.534097	-0.053765
C	-6.292022	1.537525	-0.067896
H	-6.710163	1.062812	0.830895
H	-6.591443	2.587624	-0.089135
H	-6.692329	1.031721	-0.957791

TS3$_{m\text{-OMe}}$

E = -1234.646052 a.u.

Ag	-0.701527	-0.256764	-0.353630
O	-0.090742	0.789432	2.520666
O	-0.870668	2.362398	1.026473
C	-0.262080	1.438404	1.522642
O	-2.688499	-1.040148	-0.777456
S	-3.750333	-0.690657	0.298498
C	-4.028501	1.094657	0.196928
C	-5.292180	-1.250754	-0.461437
H	-3.114285	1.592219	0.540505
H	-4.860288	1.354445	0.860029
H	-4.247023	1.376669	-0.837381
H	-5.384715	-0.811598	-1.458633
H	-6.134137	-0.964612	0.176009
H	-5.237369	-2.339258	-0.537087
C	1.102486	0.776802	0.131314
C	1.455767	1.755057	-0.822372

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C	2.113264	-0.046470	0.648023
C	2.772733	1.874762	-1.252845
H	0.697888	2.445623	-1.184023
C	3.438774	0.070567	0.212318
H	1.891002	-0.765253	1.432757
C	3.769235	1.035650	-0.745980
H	3.045234	2.636511	-1.980508
H	4.792499	1.156181	-1.086756
O	4.331634	-0.786728	0.781687
C	5.683946	-0.688793	0.394317
H	6.217237	-1.452451	0.964206
H	5.815422	-0.884126	-0.679240
H	6.104690	0.297816	0.633429

1O$_{o\text{-}OMe}$
E = -1234.694558 a.u.

Ag	-1.366414	-0.994975	-0.364629
O	0.015999	1.217712	0.108722
O	0.740294	-0.806340	-0.527196
C	0.929867	0.429075	-0.200400
O	-3.511180	-0.795091	-0.062498
S	-3.992914	0.673880	-0.200514
C	-5.633753	0.635634	0.559673
C	-3.127474	1.636761	1.062641
H	-6.271350	0.013635	-0.072925
H	-6.034557	1.652757	0.605827
H	-5.556713	0.196734	1.558291
H	-3.275512	1.176191	2.044296
H	-3.520575	2.658919	1.045371
H	-2.061882	1.638149	0.797757
C	2.370983	0.857125	-0.172622
C	3.341847	-0.107285	0.111237
C	2.787129	2.190467	-0.393136
C	4.692548	0.214778	0.214019
C	4.147340	2.513248	-0.300615
C	5.088283	1.532291	0.008302
H	5.423894	-0.554081	0.447307
H	4.482141	3.530508	-0.471537
H	6.137635	1.809266	0.079378
H	3.003502	-1.128668	0.253180
O	1.836304	3.098882	-0.720558
C	2.236173	4.425604	-0.974723
H	1.321186	4.969773	-1.217888
H	2.705187	4.887204	-0.094568
H	2.929576	4.489486	-1.825140

TS3$_{o\text{-}OMe}$
E = -1234.648343 a.u.

Ag	0.073131	-0.565376	-0.164605
O	-1.061097	2.473679	-1.086346
O	-0.189323	2.006110	0.986382
C	-0.821821	1.902300	-0.055844
O	2.178367	-1.132471	-0.160517
S	3.151031	0.048334	-0.418887
C	3.045585	1.140598	1.018747
C	4.771401	-0.683538	-0.089539
H	2.044874	1.590568	1.017401
H	3.805703	1.922003	0.914499
H	3.198800	0.562054	1.934775
H	4.761883	-1.151418	0.898819
H	5.538313	0.094491	-0.150376
H	4.947562	-1.439310	-0.858536
C	-1.895663	0.271233	0.019195
C	-2.460274	0.170950	1.305931
C	-2.739885	-0.031095	-1.081942
C	-3.787622	-0.202431	1.512138
H	-1.838476	0.455094	2.152079
C	-4.079858	-0.380626	-0.891455
C	-4.590293	-0.468299	0.405707
H	-4.197323	-0.260784	2.517056
H	-4.729235	-0.598990	-1.733258
H	-5.633562	-0.744379	0.542672
O	-2.154815	0.029657	-2.302946
C	-2.968705	-0.082924	-3.451441
H	-2.309071	0.091125	-4.303302
H	-3.413182	-1.084167	-3.537405
H	-3.766600	0.670586	-3.451922

1O$_{p\text{-}Me}$
E = -1159.530091 a.u.

Ag	-1.845047	-1.155915	0.039132
O	0.259213	-1.389017	0.034872
O	-0.045969	0.835475	0.004102
C	0.690732	-0.173638	0.016446
O	-3.915683	-0.501733	0.069939
S	-4.094532	0.927342	-0.509613
C	-5.743162	1.396198	0.067215
C	-3.112428	2.041407	0.522758
H	-6.460681	0.740233	-0.431265
H	-5.938735	2.437292	-0.207044
H	-5.799631	1.256685	1.150349
H	-3.389295	1.911599	1.573476
H	-3.295711	3.069496	0.192628
H	-2.057131	1.778994	0.370703
C	2.181255	-0.007735	0.007256
C	2.737253	1.274739	-0.015774
C	3.034829	-1.115642	0.025235
C	4.117724	1.444629	-0.022167
H	2.066780	2.128688	-0.024943
C	4.414702	-0.939379	0.018798
H	2.600584	-2.110147	0.047805
C	4.980541	0.341554	-0.008461
H	4.536285	2.449451	-0.036844
H	5.067289	-1.810529	0.036396
C	6.475083	0.525825	-0.048764
H	6.846968	0.513434	-1.082319
H	6.774621	1.482549	0.392563
H	6.993445	-0.274136	0.491151

TS3$_{p\text{-}Me}$
E = -1159.473151 a.u.

Ag	0.690207	-0.573743	-0.145691
O	0.097779	2.240057	-1.417307
O	0.458623	2.203634	0.859446
C	0.073271	1.927387	-0.256361
O	2.748785	-1.274551	-0.036038
S	3.809520	-0.171902	-0.293142
C	3.724814	0.972605	1.106199
C	5.360995	-0.999713	0.127086
H	2.762471	1.494369	1.050073
H	4.541690	1.695815	1.012426
H	3.798460	0.415486	2.044962
H	5.280337	-1.432713	1.128043
H	6.181565	-0.277960	0.073805
H	5.514545	-1.791089	-0.610281
C	-1.231980	0.344103	-0.096303
C	-1.866056	0.270206	1.159287
C	-2.035091	0.131620	-1.235576
C	-3.221766	-0.031356	1.272570
H	-1.290508	0.489754	2.056427
C	-3.387251	-0.173738	-1.123112
H	-1.591858	0.245217	-2.222611
C	-4.003043	-0.261173	0.133943
H	-3.687041	-0.076412	2.256198
H	-3.983395	-0.333997	-2.020398
C	-5.477129	-0.544619	0.249776
H	-6.065550	0.375236	0.130476
H	-5.813205	-1.244808	-0.523138
H	-5.729771	-0.968520	1.227414

1O$_{m\text{-}Me}$
E = -1159.529602 a.u.

Ag	1.457691	-1.172096	0.050870
O	-0.630611	-1.506526	0.041052
O	-0.437847	0.730057	0.001295
C	-1.122540	-0.314585	0.016372
O	3.499716	-0.439168	0.086955
S	3.622872	0.994141	-0.496707

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C	2.590343	2.070258	0.527040
C	5.247547	1.532852	0.087009
H	1.547822	1.761777	0.373658
H	2.729662	3.103546	0.191633
H	2.869288	1.958466	1.579248
H	5.304564	1.397653	1.170689
H	5.400391	2.580802	-0.188220
H	5.994496	0.906855	-0.406753
C	-2.621838	-0.225477	0.004882
C	-3.233889	1.030711	-0.027990
C	-3.411870	-1.379095	0.022133
C	-4.624388	1.161252	-0.041496
H	-2.594575	1.909347	-0.045281
C	-4.798947	-1.263893	0.005340
H	-2.926146	-2.349109	0.043936
C	-5.398640	-0.005526	-0.027479
H	-5.418556	-2.157642	0.013257
H	-6.484386	0.073820	-0.044602
C	-5.274285	2.521518	-0.045894
H	-5.472923	2.870632	0.976402
H	-4.633433	3.269081	-0.525391
H	-6.233348	2.507912	-0.575668

TS3$_{m\text{-Me}}$

E = -1159.472491 a.u.

Ag	-0.576286	-0.405821	-0.388970
O	0.261428	1.010568	2.282176
O	-0.488315	2.385403	0.589987
C	0.080571	1.506554	1.201594
O	-2.626241	-1.095902	-0.627444
S	-3.614288	-0.519263	0.420878
C	-3.766779	1.251382	0.079583
C	-5.223081	-1.056752	-0.205126
H	-2.804679	1.719197	0.318400
H	-4.547134	1.663002	0.728243
H	-4.010732	1.405703	-0.975769
H	-5.324376	-0.752484	-1.250611
H	-6.014963	-0.621207	0.411574
H	-5.250839	-2.146259	-0.129497
C	1.322900	0.524066	-0.117200
C	1.719412	1.323247	-1.205269
C	2.297334	-0.293291	0.489999
C	3.030189	1.279643	-1.680672
H	1.003327	2.012241	-1.648044
C	3.612726	-0.357992	0.024538
H	2.022226	-0.862899	1.376390
C	3.963044	0.441610	-1.073537
H	3.332508	1.910364	-2.514163
H	4.987546	0.421412	-1.442245
C	4.633140	-1.254355	0.678418
H	4.893640	-2.101675	0.030475
H	5.563475	-0.715053	0.893176
H	4.256548	-1.663077	1.621530

1O$_{o\text{-Me}}$

E = -1159.525528 a.u.

Ag	-1.404666	-1.343179	0.352750
O	0.694280	-1.605481	0.314519
O	0.418723	0.611169	0.167874
C	1.149941	-0.401342	0.219127
O	-3.469735	-0.672622	0.392836
S	-3.656444	0.722465	-0.261140
C	-5.288735	1.232230	0.327218
C	-2.645249	1.886094	0.685207
H	-6.020652	0.553824	-0.117387
H	-5.486128	2.257672	0.000381
H	-5.320225	1.152849	1.417410
H	-2.896165	1.813859	1.747913
H	-2.832602	2.896083	0.305345
H	-1.595327	1.610484	0.522044
C	2.649362	-0.277917	0.171178
C	3.313083	0.962349	0.027929
C	3.401197	-1.456960	0.275299
C	4.713707	0.954366	-0.003961
C	4.790439	-1.439411	0.242837
H	2.860547	-2.391217	0.382397
C	5.451293	-0.221504	0.101592
H	5.236007	1.902597	-0.115523
H	5.350957	-2.367206	0.326219
H	6.537933	-0.183467	0.072753
C	2.605815	2.287066	-0.093591
H	1.924055	2.301482	-0.948999
H	1.988943	2.493930	0.785919
H	3.337775	3.094354	-0.210157

TS3$_{o\text{-Me}}$

E = -1159.471616 a.u.

Ag	0.349876	0.173978	-0.564000
O	-0.744881	0.247711	2.513993
O	0.087631	-1.693525	1.608727
C	-0.514011	-0.643783	1.739068
O	2.449259	0.460350	-1.061644
S	3.417675	0.395456	0.148850
C	3.379696	-1.306705	0.760704
C	5.044943	0.365093	-0.638397
H	2.384395	-1.483642	1.185346
H	4.139785	-1.410244	1.542219
H	3.567339	-2.000372	-0.064460
H	5.072638	-0.439077	-1.378939
H	5.814042	0.223834	0.126915
H	5.184056	1.330527	-1.130447
C	-1.628850	-0.352150	0.066705
C	-2.004651	-1.624154	-0.412566
C	-2.591968	0.692487	0.031441
C	-3.273676	-1.872092	-0.932188
H	-1.289814	-2.439093	-0.322742
C	-3.867287	0.424857	-0.474254
C	-4.207515	-0.839071	-0.958797
H	-3.538267	-2.863919	-1.291201
H	-4.609936	1.220879	-0.490392
H	-5.209370	-1.016525	-1.343775
C	-2.263522	2.075754	0.529854
H	-1.725407	2.009669	1.480452
H	-1.621760	2.612953	-0.180880
H	-3.169342	2.675415	0.670892

1O$_{p\text{-NO2}}$

E = -1324.649767 a.u.

Ag	1.866904	0.115538	-0.130816
O	-0.126066	-0.597141	-0.194651
O	-0.395510	1.606564	0.163552
C	-0.841363	0.456283	-0.008654
O	3.730795	1.201974	0.031234
S	3.590664	2.712770	-0.301196
C	2.417362	3.403431	0.889937
C	5.114698	3.417973	0.367842
H	1.438893	2.952694	0.681864
H	2.369542	4.487359	0.741177
H	2.737662	3.161139	1.907791
H	5.223457	3.117114	1.413496
H	5.079888	4.507412	0.271954
H	5.942924	3.020135	-0.223205
C	-2.332144	0.234056	-0.008196
C	-3.188061	1.325313	0.177751
C	-2.867174	-1.046301	-0.191259
C	-4.565881	1.148226	0.182046
H	-2.750034	2.308073	0.317359
C	-4.243344	-1.240050	-0.189170
H	-2.189615	-1.881080	-0.334543
C	-5.071728	-0.136364	-0.002140
H	-5.250410	1.976478	0.323671
H	-4.683790	-2.220477	-0.328481
N	-6.525109	-0.333211	0.001007
O	-6.945280	-1.472563	-0.163552
O	-7.232478	0.653648	0.168065

TS3$_{p\text{-NO2}}$

E = -1324.591437 a.u.

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Ag	0.093575	-0.592586	-0.036346
O	-0.711430	2.013027	-1.538083
O	-0.293380	2.204285	0.720480
C	-0.700247	1.802301	-0.351529
O	2.185203	-1.148938	0.079008
S	3.187995	-0.035660	-0.332089
C	3.106540	1.234054	0.953895
C	4.786019	-0.763156	0.094299
H	2.121447	1.709346	0.886616
H	3.887280	1.976447	0.758731
H	3.238111	0.774105	1.937792
H	4.765845	-1.096597	1.135527
H	5.574471	-0.022276	-0.068521
H	4.937695	-1.617894	-0.568969
C	-1.895682	0.235322	-0.018477
C	-2.473878	0.208000	1.266411
C	-2.692450	-0.162323	-1.111804
C	-3.777633	-0.236821	1.467895
H	-1.898764	0.578232	2.111789
C	-3.994873	-0.615467	-0.933630
H	-2.288588	-0.075636	-2.117411
C	-4.512845	-0.649537	0.359917
H	-4.233998	-0.261694	2.451084
H	-4.615694	-0.929217	-1.765275
N	-5.887993	-1.122884	0.559121
O	-6.323496	-1.137898	1.704344
O	-6.515464	-1.477673	-0.431621

1O$_{m\text{-}NO2}$

E = -1324.650252 a.u.

Ag	-1.758810	-0.175140	0.139893
O	0.055758	0.922678	-0.045577
O	0.717455	-1.207437	0.229753
C	0.950843	0.005015	0.060240
O	-3.343849	-1.631232	0.394259
S	-2.929314	-3.069726	-0.018831
C	-1.573375	-3.557804	1.073875
C	-4.242052	-4.087785	0.694081
H	-0.720144	-2.909519	0.839566
H	-1.317834	-4.601861	0.864336
H	-1.874110	-3.429257	2.118044
H	-4.345570	-3.849615	1.756363
H	-3.998410	-5.144470	0.548379
H	-5.166170	-3.843447	0.165032
C	2.379422	0.470610	-0.034663
C	3.406501	-0.467283	0.074503
C	2.692098	1.820326	-0.229771
C	4.723097	-0.033380	-0.013814
H	3.172389	-1.513988	0.225257
C	4.021266	2.233974	-0.316104
H	1.878290	2.533470	-0.312192
C	5.052837	1.306483	-0.208311
H	4.256359	3.283703	-0.468092
H	6.095464	1.595731	-0.270993
N	5.805247	-1.017118	0.101475
O	5.494308	-2.189094	0.274569
O	6.957380	-0.606225	0.017732

TS3$_{m\text{-}NO2}$

E = -1324.591925 a.u.

Ag	0.098462	-0.596639	-0.052168
O	-0.707770	2.043752	-1.492408
O	-0.304193	2.190912	0.772388
C	-0.702559	1.811625	-0.310693
O	2.189991	-1.151443	0.065796
S	3.190738	-0.037285	-0.348017
C	3.103339	1.237986	0.932444
C	4.789814	-0.757270	0.086903
H	2.111903	1.700918	0.872018
H	3.872812	1.989351	0.726921
H	3.248695	0.785359	1.917780
H	4.764896	-1.089277	1.128419
H	5.575638	-0.012831	-0.072317
H	4.949238	-1.612072	-0.574457
C	-1.890475	0.225001	-0.012155
C	-2.480260	0.178227	1.266708
C	-2.676729	-0.160606	-1.113411
C	-3.791635	-0.264476	1.453916
H	-1.905630	0.535090	2.118703
C	-3.975808	-0.610120	-0.909200
H	-2.293062	-0.077455	-2.124977
C	-4.550409	-0.668760	0.360230
H	-4.229614	-0.283814	2.448506
H	-5.574008	-1.009928	0.464713
N	-4.781391	-1.026305	-2.064922
O	-4.247853	-1.005444	-3.166723
O	-5.937912	-1.374295	-1.854859

1O$_{o\text{-}NO2}$

E = -1324.638060 a.u.

Ag	-1.037588	1.704943	-0.841273
O	1.092042	1.661315	-0.872205
O	0.500375	-0.350165	-0.053428
C	1.339423	0.517072	-0.348253
O	-3.156334	1.412404	-0.477331
S	-3.419921	0.627961	0.838265
C	-5.173470	0.206325	0.712501
C	-2.720184	-1.024191	0.613573
H	-5.737321	1.140532	0.766370
H	-5.448600	-0.442595	1.549452
H	-5.357551	-0.287109	-0.245893
H	-3.128796	-1.480454	-0.293088
H	-2.959291	-1.622998	1.498665
H	-1.633055	-0.909031	0.522216
C	2.803225	0.208720	-0.152622
C	3.313473	-0.387022	1.005663
C	3.690399	0.418397	-1.211543
C	4.639532	-0.794337	1.109352
C	5.024849	0.028130	-1.121661
H	3.310457	0.888765	-2.113120
C	5.501214	-0.583362	0.037455
H	4.978152	-1.256364	2.030269
H	5.693952	0.200977	-1.960461
H	6.541153	-0.887932	0.113245
N	2.477221	-0.545838	2.200621
O	2.676501	-1.535483	2.896054
O	1.670255	0.338264	2.450077

TS3$_{o\text{-}NO2}$

E = -1324.595135 a.u.

Ag	0.137997	-0.633186	-0.276917
O	-0.941804	2.246655	-1.369683
O	-0.177966	2.015930	0.787356
C	-0.757207	1.800784	-0.265799
O	2.256856	-1.129296	-0.014325
S	3.240291	0.024960	-0.337835
C	3.104734	1.215069	1.017161
C	4.850727	-0.683935	0.076624
H	2.103904	1.659103	0.962164
H	3.864201	1.990863	0.874643
H	3.239379	0.703080	1.974694
H	4.819221	-1.082080	1.094665
H	5.621035	0.086809	-0.022337
H	5.040415	-1.491345	-0.634494
C	-1.879650	0.241387	-0.059532
C	-2.461995	0.229013	1.218159
C	-2.708774	-0.199015	-1.104587
C	-3.773904	-0.202494	1.431034
H	-1.874903	0.622580	2.044787
C	-4.030102	-0.591248	-0.938044
C	-4.560862	-0.602453	0.352466
H	-4.190605	-0.202454	2.435303
H	-4.617423	-0.899454	-1.796695
H	-5.587543	-0.921885	0.508326
N	-2.163758	-0.286293	-2.468752
O	-0.976643	-0.596960	-2.602610
O	-2.924547	-0.088583	-3.400715

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$1O_{p\text{-}CN}$

E = -1212.428550 a.u.

Ag	-1.823231	-1.124408	0.044631
O	0.283445	-1.344648	0.033549
O	0.006171	0.886523	0.007911
C	0.720929	-0.134261	0.015770
O	-3.894515	-0.495914	0.082223
S	-4.111574	0.924730	-0.506774
C	-5.766045	1.358016	0.078898
C	-3.147300	2.066423	0.512543
H	-6.470857	0.681642	-0.410310
H	-5.988166	2.392061	-0.201622
H	-5.811720	1.224822	1.163297
H	-3.411898	1.935102	1.566153
H	-3.355870	3.088811	0.180046
H	-2.087922	1.828714	0.353961
C	2.219653	0.012976	0.002728
C	2.783664	1.292572	-0.024313
C	3.052843	-1.110824	0.016869
C	4.162345	1.455041	-0.037163
H	2.118422	2.149829	-0.035275
C	4.433685	-0.961874	0.004522
H	2.600570	-2.096668	0.037274
C	4.995036	0.324593	-0.022627
H	4.604640	2.446485	-0.058415
H	5.084932	-1.830651	0.015459
C	6.417523	0.484442	-0.035425
N	7.573900	0.615219	-0.045789

$TS3_{p\text{-}CN}$

E = -1212.370409 a.u.

Ag	0.656210	-0.532306	-0.128381
O	0.092035	2.245477	-1.427515
O	0.443309	2.220264	0.850517
C	0.048627	1.939038	-0.263202
O	2.698344	-1.250355	-0.001000
S	3.789232	-0.180663	-0.282237
C	3.747318	0.978976	1.105641
C	5.317383	-1.052662	0.129639
H	2.799870	1.526817	1.049628
H	4.583191	1.678150	0.999313
H	3.811475	0.429779	2.049675
H	5.234990	-1.471747	1.136300
H	6.159460	-0.357761	0.058349
H	5.436701	-1.856112	-0.600935
C	-1.266719	0.431503	-0.097687
C	-1.893177	0.347297	1.161488
C	-2.053687	0.191439	-1.242420
C	-3.234017	-0.002091	1.284327
H	-1.322079	0.598479	2.052383
C	-3.392761	-0.164270	-1.140382
H	-1.608202	0.325686	-2.225168
C	-3.986106	-0.268311	0.129346
H	-3.709800	-0.061558	2.259060
H	-3.991042	-0.351370	-2.027535
C	-5.366825	-0.628030	0.243919
N	-6.488418	-0.924240	0.337075

$1O_{m\text{-}CN}$

E = -1212.428736 a.u.

Ag	1.792210	-1.158436	0.036298
O	-0.274068	-1.645731	0.019569
O	-0.248335	0.601659	0.018058
C	-0.845084	-0.492693	0.013963
O	3.773792	-0.287361	0.081540
S	3.818773	1.151492	-0.501646
C	2.737932	2.169279	0.531791
C	5.416813	1.771687	0.072588
H	1.713204	1.805850	0.385583
H	2.816965	3.209041	0.197129
H	3.029745	2.071913	1.581840
H	5.488280	1.636352	1.155383
H	5.512884	2.826890	-0.200417
H	6.191487	1.186694	-0.428643
C	-2.350336	-0.510726	-0.000009
C	-3.043052	0.699294	-0.009520
C	-3.061014	-1.715345	-0.003580
C	-4.443357	0.704062	-0.022381
H	-2.481151	1.627058	-0.007036
C	-4.454920	-1.711337	-0.016451
H	-2.503838	-2.646520	0.003661
C	-5.152554	-0.508142	-0.025819
H	-5.001624	-2.650377	-0.019233
H	-6.238281	-0.494328	-0.035867
C	-5.154818	1.947146	-0.031834
N	-5.735355	2.955660	-0.039344

$TS3_{m\text{-}CN}$

E = -1212.370545 a.u.

Ag	-0.559442	-0.392860	-0.371926
O	0.257346	1.004491	2.291381
O	-0.463185	2.383623	0.590317
C	0.103709	1.504157	1.206481
O	-2.601931	-1.065455	-0.642423
S	-3.615225	-0.535371	0.409118
C	-3.784156	1.242032	0.115654
C	-5.203558	-1.077930	-0.259847
H	-2.828679	1.713049	0.372838
H	-4.572245	1.628499	0.770261
H	-4.022941	1.423132	-0.936560
H	-5.291125	-0.744503	-1.297598
H	-6.011743	-0.671521	0.355540
H	-5.216378	-2.169429	-0.215484
C	1.343785	0.559770	-0.063966
C	1.746780	1.339390	-1.165630
C	2.302161	-0.274269	0.536905
C	3.044518	1.266622	-1.674628
H	1.035468	2.039687	-1.598275
C	3.604826	-0.359368	0.025683
H	2.042686	-0.832350	1.432678
C	3.973923	0.414183	-1.088435
H	3.338371	1.882564	-2.520805
H	4.988899	0.352263	-1.469825
C	4.565835	-1.225058	0.641178
N	5.344338	-1.933618	1.137234

$1O_{o\text{-}CN}$

E = -1212.424596 a.u.

Ag	-1.440474	-1.412125	0.374408
O	0.675150	-1.719154	0.344694
O	0.389274	0.500485	0.188849
C	1.109729	-0.513068	0.250207
O	-3.470352	-0.650741	0.413768
S	-3.608287	0.748454	-0.249634
C	-5.243380	1.292525	0.296997
C	-2.596913	1.895780	0.714530
H	-5.977942	0.626305	-0.161346
H	-5.411965	2.319853	-0.039804
H	-5.302073	1.220856	1.386602
H	-2.868480	1.829591	1.772437
H	-2.761021	2.907660	0.329331
H	-1.548119	1.610707	0.568655
C	2.604960	-0.353901	0.211027
C	3.208774	0.919152	0.154940
C	3.422121	-1.486443	0.228130
C	4.608563	1.026177	0.116808
C	4.808825	-1.374479	0.188225
H	2.938717	-2.456534	0.273216
C	5.403539	-0.114317	0.132276
H	5.059340	2.013060	0.075257
H	5.425310	-2.269519	0.201153
H	6.485396	-0.017051	0.101331
C	2.475313	2.153705	0.139987
N	2.041568	3.233840	0.127054

$TS3_{o\text{-}CN}$

E = -1212.369003 a.u.

Ag	0.331331	0.026740	-0.621481

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O	-0.759522	0.111033	2.470418
O	0.103839	-1.794101	1.514144
C	-0.531185	-0.761437	1.673931
O	2.426117	0.289463	-1.123074
S	3.362754	0.409598	0.111144
C	3.450003	-1.238491	0.851172
C	5.005692	0.468070	-0.638236
H	2.455905	-1.471696	1.250412
H	4.180112	-1.214080	1.666798
H	3.733059	-1.972313	0.090667
H	5.124227	-0.381202	-1.316821
H	5.762633	0.451744	0.151652
H	5.072283	1.405033	-1.196113
C	-1.649639	-0.469832	0.113043
C	-2.126334	-1.694201	-0.387188
C	-2.539806	0.637715	0.054558
C	-3.408673	-1.826546	-0.922621
H	-1.478742	-2.563761	-0.301207
C	-3.828618	0.510348	-0.476924
C	-4.259854	-0.723865	-0.961790
H	-3.749390	-2.790454	-1.292760
H	-4.484659	1.375576	-0.510837
H	-5.264802	-0.821006	-1.363988
C	-2.118528	1.934680	0.504111
N	-1.798275	3.012112	0.806122

$5_{p\text{-OMe}}$

E = -1303.384654 a.u.

Cu	-0.645835	-0.702003	0.000994
C	3.409373	-0.003376	0.000526
C	1.920020	0.199231	0.000753
O	1.224666	-0.895358	0.001028
O	1.461925	1.350995	0.000675
C	3.983533	-1.282369	0.000565
C	5.360466	-1.443193	0.000345
C	6.199336	-0.319892	0.000083
C	-2.350633	3.464624	0.000450
C	-1.429104	2.397799	0.000675
N	-1.822826	1.133623	0.000709
C	-3.140470	0.853583	0.000495
C	-4.142398	1.849768	0.000257
C	-3.703420	3.192109	0.000247
C	-3.511860	-0.538681	0.000497
C	-5.519914	1.455345	0.000039
N	-2.510032	-1.456043	0.000714
C	-2.836554	-2.745187	0.000722
C	-4.166390	-3.196213	0.000510
C	-5.190436	-2.271282	0.000285
C	-4.880249	-0.895506	0.000273
C	-5.873270	0.139073	0.000049
C	5.640913	0.963119	0.000043
C	4.254713	1.106349	0.000266
O	7.536186	-0.580521	-0.000122
C	8.422995	0.515828	-0.000355
H	3.327393	-2.146868	0.000768
H	5.816701	-2.429226	0.000373
H	-1.985823	4.487246	0.000434
H	-0.349274	2.536907	0.000811
H	-4.435560	3.996424	0.000072
H	-6.283889	2.229023	-0.000136
H	-2.009432	-3.448684	0.000898
H	-4.368961	-4.262461	0.000525
H	-6.230223	-2.589350	0.000117
H	-6.921242	-0.149903	-0.000118
H	6.269614	1.847626	-0.000164
H	3.802061	2.093450	0.000237
H	8.296315	1.141436	0.893980
H	8.296055	1.141263	-0.894773
H	9.429014	0.090587	-0.000461

$TS5_{p\text{-OMe}}$

E = -1303.327593 a.u.

Cu	0.128352	-0.483580	0.200642
C	2.078050	-0.548273	0.260640
C	2.736151	0.187862	1.267878
C	3.972731	0.781177	1.054216
C	4.612223	0.636590	-0.185601
C	4.007263	-0.121976	-1.192820
C	2.762996	-0.710424	-0.953239
O	5.823118	1.251420	-0.301387
C	6.527751	1.098204	-1.513087
H	2.274292	0.266939	2.250468
H	4.479143	1.344375	1.834159
H	4.499033	-0.276079	-2.148501
H	2.326970	-1.339189	-1.727129
H	5.968994	1.511331	-2.364489
H	6.760726	0.044152	-1.717134
H	7.459928	1.654661	-1.393026
C	1.141531	-2.289919	0.951576
O	0.975433	-2.155660	2.145009
O	1.133172	-3.103211	0.049546
C	-1.552431	3.670921	0.427638
C	-0.655339	2.587189	0.446045
N	-1.039974	1.337757	0.237312
C	-2.345913	1.091678	-0.007416
C	-3.327440	2.108572	-0.046967
C	-2.888854	3.430592	0.181490
C	-2.728812	-0.279521	-0.234176
C	-4.691590	1.754391	-0.308848
N	-1.750971	-1.213117	-0.194420
C	-2.066511	-2.486739	-0.393509
C	-3.386767	-2.900676	-0.647821
C	-4.393037	-1.958114	-0.696337
C	-4.081770	-0.597140	-0.487010
C	-5.052852	0.457129	-0.518306
H	-1.185143	4.676422	0.607400
H	0.405092	2.734818	0.635590
H	-3.607477	4.246474	0.161975
H	-5.437909	2.544366	-0.335604
H	-1.237494	-3.189646	-0.347359
H	-3.594625	-3.954543	-0.802794
H	-5.421997	-2.249891	-0.892758
H	-6.090971	0.200519	-0.713996

$5_{m\text{-OMe}}$

E = -1303.383076 a.u.

Cu	0.613578	-0.665205	0.000147
C	-3.439283	0.101612	0.000557
C	-1.940399	0.285016	0.000350
O	-1.260640	-0.817003	0.000350
O	-1.473067	1.431781	0.000113
C	-4.004739	-1.170349	0.000759
C	-5.394943	-1.327053	0.000955
C	-6.223651	-0.201430	0.000942
C	2.397439	3.462810	-0.000297
C	1.455638	2.413929	-0.000184
N	1.825346	1.142511	-0.000082
C	3.137324	0.837075	-0.000075
C	4.158245	1.813703	-0.000180
C	3.744733	3.164377	-0.000297
C	3.481329	-0.562272	0.000055
C	5.527784	1.391604	-0.000161
N	2.461450	-1.459389	0.000160
C	2.761629	-2.754782	0.000277
C	4.082262	-3.232369	0.000301
C	5.124718	-2.328150	0.000200
C	4.842233	-0.946406	0.000072
C	5.855206	0.068624	-0.000040
C	-5.646434	1.072607	0.000738
C	-4.267623	1.232001	0.000547
H	-3.366669	-2.047171	0.000768
H	2.052324	4.492227	-0.000381
H	0.378766	2.574590	-0.000166
H	4.491922	3.954729	-0.000382
H	6.307045	2.149890	-0.000244
H	1.920313	-3.441265	0.000358
H	4.263479	-4.302454	0.000400
H	6.157938	-2.666781	0.000217

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H	6.897347	-0.240745	-0.000026
H	-6.295853	1.945272	0.000729
H	-3.804614	2.213120	0.000386
H	-7.304360	-0.300015	0.001081
O	-5.844257	-2.616499	0.001141
C	-7.236711	-2.827678	0.001406
H	-7.378995	-3.910737	0.001563
H	-7.714555	-2.402758	0.895670
H	-7.714863	-2.402978	-0.892799

TS5$_{m\text{-}OMe}$
E = -1303.326148 a.u.

Cu	0.138932	-0.465529	0.310516
C	2.096753	-0.569904	0.387198
C	2.744194	0.168886	1.397663
C	3.969874	0.776783	1.149622
C	4.591586	0.655680	-0.098148
C	3.974180	-0.100751	-1.099009
C	2.741302	-0.716883	-0.845585
H	2.293262	0.225751	2.385853
H	4.470118	1.342940	1.933556
H	2.311838	-1.345252	-1.622233
C	1.120948	-2.258044	1.062829
O	0.925231	-2.114452	2.253707
O	1.114268	-3.087968	0.174149
C	-1.489223	3.682341	0.490260
C	-0.608515	2.586594	0.541687
N	-1.000796	1.343659	0.307497
C	-2.298700	1.116846	0.003906
C	-3.262532	2.148014	-0.073755
C	-2.816319	3.462276	0.182443
C	-2.691021	-0.247472	-0.246168
C	-4.618355	1.814805	-0.399229
N	-1.729657	-1.194516	-0.165105
C	-2.051518	-2.462680	-0.384569
C	-3.364478	-2.857104	-0.701501
C	-4.354577	-1.900549	-0.791655
C	-4.035228	-0.544556	-0.561929
C	-4.988446	0.523980	-0.632183
H	-1.116600	4.681527	0.692616
H	0.444397	2.717583	0.778879
H	-3.521864	4.288362	0.135376
H	-5.351117	2.615811	-0.455705
H	-1.233535	-3.175572	-0.304365
H	-3.579560	-3.907211	-0.871451
H	-5.377155	-2.177614	-1.036725
H	-6.020155	0.283852	-0.876575
H	5.554399	1.128054	-0.264860
O	4.497684	-0.304708	-2.343677
C	5.760213	0.251997	-2.626214
H	5.998106	-0.039698	-3.651649
H	5.747753	1.349524	-2.559463
H	6.536952	-0.136301	-1.952382

5$_{o\text{-}OMe}$
E = -1303.373951 a.u.

Cu	0.270147	-0.518978	-0.139186
C	-3.716447	0.555285	-0.147425
C	-2.206054	0.593276	-0.069343
O	-1.607507	-0.542925	-0.195097
O	-1.656452	1.697005	0.061878
C	-4.521905	-0.546409	0.222092
C	-5.913642	-0.467019	0.073354
C	-6.508650	0.687436	-0.432948
C	2.314345	3.455025	0.429764
C	1.308402	2.479200	0.276914
N	1.596848	1.196777	0.118640
C	2.886257	0.808457	0.100181
C	3.966770	1.707355	0.243900
C	3.639747	3.070965	0.413734
C	3.140636	-0.598525	-0.079598
C	5.306307	1.199382	0.208507
N	2.065936	-1.418365	-0.213639
C	2.283393	-2.719316	-0.382882
C	3.570655	-3.278698	-0.428589
C	4.668279	-2.453323	-0.292877
C	4.474090	-1.068194	-0.111926
C	5.549046	-0.130852	0.037653
C	-5.729058	1.785022	-0.782538
C	-4.347911	1.705883	-0.625272
O	-3.904083	-1.635803	0.744030
C	-4.696059	-2.728910	1.142063
H	-6.543802	-1.303985	0.354070
H	-7.590319	0.721177	-0.543355
H	2.035083	4.496391	0.557958
H	0.243923	2.708314	0.276760
H	4.435227	3.803691	0.529128
H	6.131994	1.897999	0.320214
H	1.400251	-3.342486	-0.486674
H	3.683570	-4.348893	-0.569699
H	5.677645	-2.856437	-0.323868
H	6.569218	-0.505528	0.011734
H	-6.187955	2.691037	-1.169312
H	-3.707836	2.547840	-0.870638
H	-3.999126	-3.475212	1.529504
H	-5.251770	-3.161851	0.298117
H	-5.407181	-2.455288	1.934754

TS5$_{o\text{-}OMe}$
E = -1303.325850 a.u.

Cu	0.442366	-0.366127	-0.085147
C	2.409283	-0.491058	-0.341847
C	3.104401	0.574643	0.281831
C	4.244148	1.137579	-0.301304
C	4.688486	0.668622	-1.539605
C	4.015190	-0.360546	-2.192181
C	2.902280	-0.935911	-1.579330
O	2.569537	1.033796	1.447087
C	3.345673	1.894270	2.250508
H	4.783664	1.944561	0.185369
H	5.575359	1.113317	-1.986239
H	4.372165	-0.731299	-3.149810
H	2.415003	-1.799161	-2.025776
H	2.794249	2.011680	3.185568
H	3.480563	2.882397	1.786103
H	4.331788	1.462468	2.464917
C	1.781694	-1.985814	0.675142
O	1.891705	-1.770367	1.866738
O	1.511119	-2.912690	-0.083698
C	-1.546914	3.606501	-0.272683
C	-0.563509	2.602203	-0.227497
N	-0.859277	1.312749	-0.158697
C	-2.161104	0.946109	-0.127267
C	-3.224099	1.877713	-0.167038
C	-2.877918	3.243497	-0.243191
C	-2.451444	-0.463744	-0.043483
C	-4.575080	1.400113	-0.124379
N	-1.400165	-1.311475	-0.009583
C	-1.622348	-2.616342	0.074874
C	-2.924094	-3.149319	0.129326
C	-4.007419	-2.295851	0.091286
C	-3.792999	-0.902989	0.001826
C	-4.847363	0.067251	-0.042701
H	-1.248752	4.648706	-0.328868
H	0.494525	2.848600	-0.245373
H	-3.662071	3.996156	-0.275884
H	-5.383645	2.126063	-0.156010
H	-0.729558	-3.239414	0.097051
H	-3.057556	-4.224155	0.199936
H	-5.023522	-2.681405	0.130360
H	-5.876330	-0.282065	-0.008617

5$_{p\text{-}Me}$
E = -1228.209835 a.u.

Cu	0.291874	-0.691907	-0.013197
C	-3.751421	0.096087	-0.010051
C	-2.254558	0.266427	-0.015062
O	-1.583433	-0.842250	-0.012874

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O	-1.774202	1.408377	-0.019915
C	-4.348299	-1.168046	-0.001991
C	-5.734692	-1.293454	0.000884
C	-6.562931	-0.164673	-0.001931
C	2.081306	3.438281	0.016459
C	1.138245	2.390540	0.005890
N	1.505965	1.118496	-0.000340
C	2.817565	0.811564	0.003052
C	3.839525	1.787087	0.013175
C	3.428198	3.138136	0.020105
C	3.160515	-0.588069	-0.004520
C	5.208654	1.364570	0.015704
N	2.140138	-1.484746	-0.013888
C	2.440302	-2.780247	-0.021365
C	3.760653	-3.258387	-0.019921
C	4.803368	-2.354579	-0.010166
C	4.521299	-0.972747	-0.002081
C	5.535157	0.041406	0.008313
C	-5.956756	1.098124	-0.014538
C	-4.572094	1.227885	-0.016991
C	-8.062955	-0.302867	0.034887
H	-3.709450	-2.045583	-0.001899
H	-6.185012	-2.284884	0.004060
H	1.737370	4.468087	0.021476
H	0.061601	2.551986	0.001871
H	4.176599	3.927286	0.028125
H	5.988219	2.122483	0.023568
H	1.599031	-3.466720	-0.028746
H	3.941404	-4.328526	-0.026366
H	5.836432	-2.693807	-0.008663
H	6.577030	-0.268815	0.010208
H	-6.581583	1.989886	-0.023788
H	-4.097784	2.204673	-0.028258
H	-8.437529	-0.288675	1.067587
H	-8.391196	-1.245728	-0.416147
H	-8.555834	0.517479	-0.498717

TS5$_{p\text{-Me}}$

E = -1228.152646 a.u.

Cu	0.415980	-0.428028	0.124495
C	2.373396	-0.432620	0.081644
C	3.052274	0.333488	1.045551
C	4.246297	0.986871	0.746084
C	4.823844	0.882701	-0.525861
C	4.172297	0.094313	-1.482726
C	2.980898	-0.562375	-1.179711
C	6.136679	1.552802	-0.838520
H	2.646503	0.391265	2.054185
H	4.749873	1.575029	1.512898
H	4.616206	-0.018133	-2.471470
H	2.522520	-1.208660	-1.925864
H	6.286293	2.449445	-0.226702
H	6.197550	1.846868	-1.892489
H	6.983300	0.881050	-0.641116
C	1.526515	-2.167981	0.837919
O	1.403457	-2.020955	2.037155
O	1.506451	-3.004703	-0.043901
C	-1.383672	3.662561	0.296557
C	-0.450631	2.609605	0.296683
N	-0.804655	1.341799	0.153683
C	-2.114230	1.045433	-0.002194
C	-3.130146	2.028501	-0.014685
C	-2.723599	3.371061	0.141684
C	-2.463429	-0.344125	-0.160419
C	-4.494951	1.621783	-0.179100
N	-1.453614	-1.243298	-0.151276
C	-1.735139	-2.532171	-0.292469
C	-3.053364	-2.997378	-0.452010
C	-4.093015	-2.090567	-0.466035
C	-3.817421	-0.713748	-0.318730
C	-4.824045	0.307112	-0.323064
H	-1.040661	4.685082	0.418977
H	0.613570	2.797144	0.416746
H	-3.469360	4.162436	0.138989
H	-5.267946	2.386100	-0.184958
H	-0.880024	-3.204581	-0.277499
H	-3.233541	-4.061921	-0.562130
H	-5.121207	-2.422515	-0.588887
H	-5.862898	0.011043	-0.445209

5$_{m\text{-Me}}$

E = -1228.209490 a.u.

Cu	-0.180911	-0.592614	-0.007817
C	3.812985	0.433748	-0.003857
C	2.306583	0.517071	-0.004750
O	1.700504	-0.628074	-0.010222
O	1.762323	1.629659	0.000201
C	4.473020	-0.798044	-0.006551
C	5.868791	-0.875053	-0.006972
C	6.599816	0.318635	-0.011452
C	-2.209053	3.421760	0.008503
C	-1.206474	2.430816	0.003912
N	-1.499577	1.139502	-0.000170
C	-2.790945	0.756670	0.000190
C	-3.868137	1.670818	0.004610
C	-3.536161	3.043742	0.008762
C	-3.050985	-0.660778	-0.004165
C	-5.209997	1.168041	0.004567
N	-1.979279	-1.495453	-0.008102
C	-2.202282	-2.806323	-0.012092
C	-3.492127	-3.361796	-0.012417
C	-4.586577	-2.521255	-0.008384
C	-4.386611	-1.125110	-0.004034
C	-5.458170	-0.172077	0.000458
C	5.952002	1.553985	-0.009091
C	4.561925	1.614109	-0.004485
H	3.872142	-1.703194	-0.010079
H	-1.925673	4.469856	0.011732
H	-0.141036	2.654715	0.003487
H	-4.329146	3.788112	0.012202
H	-6.032928	1.878671	0.007879
H	-1.321875	-3.441894	-0.015121
H	-3.609225	-4.440777	-0.015793
H	-5.597840	-2.920711	-0.008509
H	-6.480065	-0.542880	0.000557
H	6.537392	2.470875	-0.015345
H	4.031408	2.561195	-0.005633
H	7.688012	0.279426	-0.018815
C	6.567794	-2.210754	0.022423
H	6.739383	-2.548242	1.053687
H	5.973190	-2.983865	-0.476328
H	7.545397	-2.165311	-0.470571

TS5$_{m\text{-Me}}$

E = -1228.152364 a.u.

Cu	0.419859	-0.405455	0.170370
C	2.379190	-0.435981	0.124279
C	3.062832	0.346862	1.070544
C	4.262666	0.976071	0.740880
C	4.807099	0.819041	-0.533966
C	4.171473	0.019431	-1.492225
C	2.971888	-0.608517	-1.137616
H	2.664219	0.426675	2.080170
H	4.790219	1.573788	1.482293
H	2.497801	-1.281612	-1.851072
C	1.506488	-2.141294	0.909511
O	1.375855	-1.970130	2.105352
O	1.482148	-2.996431	0.045217
C	-1.351772	3.688874	0.382374
C	-0.426945	2.628786	0.383325
N	-0.787388	1.366450	0.210106
C	-2.095848	1.083204	0.021576
C	-3.103348	2.074723	0.003379
C	-2.690123	3.410935	0.192688
C	-2.452837	-0.300765	-0.165478
C	-4.467302	1.682389	-0.199014
N	-1.451271	-1.208699	-0.145055
C	-1.740104	-2.493251	-0.308663

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C	-3.058075	-2.944577	-0.505570
C	-4.089341	-2.028513	-0.532935
C	-3.805945	-0.656269	-0.360183
C	-4.803678	0.373135	-0.372376
H	-1.003736	4.706204	0.530945
H	0.635894	2.805825	0.528597
H	-3.429492	4.208256	0.187773
H	-5.233707	2.453255	-0.210090
H	-0.891074	-3.173039	-0.280098
H	-3.244921	-4.006007	-0.633357
H	-5.116999	-2.350018	-0.684750
H	-5.841786	0.087962	-0.523313
H	5.752348	1.300602	-0.780497
C	4.764745	-0.157596	-2.867314
H	4.425072	-1.090849	-3.329111
H	4.474601	0.662960	-3.538021
H	5.860180	-0.175955	-2.835065

$5_{o\text{-}Me}$

E = -1228.205054 a.u.

Cu	-0.099438	-0.606489	0.000018
C	3.948499	0.234329	0.000013
C	2.439017	0.355299	-0.000004
O	1.779945	-0.759344	0.000126
O	1.928852	1.485079	-0.000232
C	4.663236	-0.985501	-0.000011
C	6.063877	-0.923767	0.000018
C	6.755085	0.284424	0.000072
C	-1.942177	3.487213	-0.000167
C	-0.986443	2.451089	-0.000141
N	-1.338562	1.174552	-0.000088
C	-2.646505	0.851716	-0.000058
C	-3.680098	1.814763	-0.000084
C	-3.285304	3.170790	-0.000139
C	-2.972218	-0.551945	0.000001
C	-5.043960	1.375470	-0.000055
N	-1.940674	-1.435401	0.000031
C	-2.224357	-2.734243	0.000081
C	-3.538690	-3.229285	0.000107
C	-4.592729	-2.338701	0.000080
C	-4.328097	-0.953297	0.000026
C	-5.354320	0.048367	-0.000004
C	6.044512	1.482461	0.000090
C	4.655545	1.444282	0.000054
C	4.017492	-2.347635	-0.000072
H	6.624290	-1.856970	-0.000006
H	7.842960	0.286641	0.000095
H	-1.610653	4.521079	-0.000209
H	0.087890	2.626237	-0.000165
H	-4.043230	3.950818	-0.000159
H	-5.832671	2.123882	-0.000076
H	-1.374561	-3.410304	0.000104
H	-3.705832	-4.301660	0.000149
H	-5.621454	-2.690861	0.000101
H	-6.392336	-0.274529	0.000017
H	6.566838	2.436284	0.000128
H	4.068162	2.356970	0.000053
H	3.373423	-2.486278	-0.873388
H	3.373560	-2.486413	0.873325
H	4.786769	-3.128627	-0.000192

$TS5_{o\text{-}Me}$

E = -1228.151214 a.u.

Cu	0.425342	-0.493094	-0.117949
C	2.379034	-0.424091	-0.330556
C	3.081719	0.565460	0.403847
C	4.176584	1.203102	-0.190165
C	4.590472	0.885932	-1.484706
C	3.917777	-0.097748	-2.206019
C	2.835582	-0.752363	-1.618617
H	4.719949	1.959782	0.374664
H	5.448821	1.395145	-1.918077
H	4.246683	-0.367831	-3.207285
H	2.344210	-1.568526	-2.143633
C	1.719245	-2.118462	0.578234
O	1.806887	-1.994029	1.784264
O	1.534520	-2.974171	-0.273725
C	-1.474846	3.540075	-0.536273
C	-0.514127	2.515172	-0.461193
N	-0.839004	1.242271	-0.294447
C	-2.146005	0.911320	-0.198644
C	-3.187878	1.865111	-0.259133
C	-2.811797	3.214388	-0.432604
C	-2.464986	-0.485229	-0.035073
C	-4.547103	1.424406	-0.144948
N	-1.433259	-1.358597	0.000231
C	-1.687221	-2.653880	0.134715
C	-2.998298	-3.150986	0.251685
C	-4.060252	-2.270838	0.221385
C	-3.814389	-0.888719	0.070012
C	-4.846800	0.104492	0.014273
H	-1.154785	4.568234	-0.672775
H	0.548709	2.731096	-0.537999
H	-3.578380	3.983821	-0.484799
H	-5.339668	2.167124	-0.188589
H	-0.816310	-3.305713	0.141160
H	-3.155403	-4.219000	0.363372
H	-5.083562	-2.627913	0.309597
H	-5.881632	-0.217503	0.099325
C	2.678339	0.934361	1.808352
H	1.652539	1.325476	1.844111
H	2.691134	0.046379	2.448017
H	3.344140	1.696415	2.228847

$5_{p\text{-}NO2}$

E = -1393.331537 a.u.

Cu	-0.861117	-0.655084	0.000019
C	3.187787	0.169828	0.000043
C	1.683673	0.338073	0.000109
O	1.023954	-0.772067	0.000161
O	1.213259	1.481802	-0.000126
C	3.778649	-1.098844	0.000220
C	5.162056	-1.233040	0.000175
C	5.943943	-0.080264	-0.000057
C	-4.288866	-3.277250	-0.000113
C	-2.975022	-2.781635	-0.000049
N	-2.692147	-1.482455	-0.000005
C	-3.723680	-0.598203	-0.000022
C	-5.079004	-1.001348	-0.000089
C	-5.342819	-2.386910	-0.000134
C	-3.400090	0.806234	0.000013
C	-6.107297	-0.001999	-0.000125
N	-2.092697	1.134215	0.000089
C	-1.746389	2.412344	0.000081
C	-2.704804	3.445589	0.000006
C	-4.046448	3.124113	-0.000053
C	-4.436259	1.766685	-0.000049
C	-5.799388	1.325400	-0.000111
C	5.382684	1.194994	-0.000240
C	3.998601	1.310215	-0.000186
N	7.402629	-0.212667	-0.000109
O	8.069007	0.816765	-0.000139
O	7.873411	-1.345030	0.000227
H	3.135992	-1.972586	0.000393
H	5.643794	-2.203998	0.000314
H	-4.455508	-4.349627	-0.000148
H	-2.124999	-3.457260	-0.000031
H	-6.371393	-2.739326	-0.000187
H	-7.144540	-0.327108	-0.000172
H	-0.673568	2.594639	0.000137
H	-2.376521	4.480412	-0.000002
H	-4.807278	3.901196	-0.000103
H	-6.589051	2.072686	-0.000148
H	6.031212	2.063416	-0.000419
H	3.515994	2.282114	-0.000315

$TS5_{p\text{-}NO2}$

E = -1393.275370 a.u.

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Cu	-0.085536	-0.570122	0.212194
C	1.871002	-0.846285	0.235364
C	2.582445	-0.183465	1.253778
C	3.815499	0.411278	1.009546
C	4.354846	0.319432	-0.273314
C	3.709147	-0.369949	-1.298709
C	2.478853	-0.960618	-1.029405
N	5.644190	0.953219	-0.546546
O	6.106070	0.846836	-1.678108
O	6.187614	1.561900	0.370006
H	2.163249	-0.163428	2.257162
H	4.368879	0.931732	1.783461
H	4.181176	-0.439216	-2.272519
H	1.985443	-1.545144	-1.802069
C	0.834851	-2.433248	0.856384
O	0.652278	-2.321718	2.055409
O	0.753152	-3.233013	-0.057890
C	-1.353769	3.675675	0.404377
C	-0.559967	2.515066	0.422274
N	-1.060063	1.303551	0.227077
C	-2.388150	1.175713	-0.000538
C	-3.270493	2.279385	-0.035567
C	-2.709348	3.557003	0.176031
C	-2.901539	-0.154619	-0.212096
C	-4.665354	2.053073	-0.276743
N	-2.016011	-1.175780	-0.178252
C	-2.449305	-2.415472	-0.364972
C	-3.805983	-2.705946	-0.598666
C	-4.720210	-1.673594	-0.639703
C	-4.281351	-0.345687	-0.444738
C	-5.149995	0.794340	-0.471143
H	-0.892740	4.644005	0.570595
H	0.510832	2.568793	0.600897
H	-3.349966	4.435321	0.157725
H	-5.334014	2.909699	-0.299747
H	-1.688579	-3.192074	-0.328026
H	-4.113720	-3.736389	-0.744124
H	-5.774373	-1.869760	-0.820171
H	-6.210154	0.635352	-0.650925

$5_{m\text{-}NO2}$

E = -1393.331808 a.u.

Cu	0.853048	-0.640425	0.000156
C	-3.196149	0.173686	0.000062
C	-1.694192	0.354271	0.000248
O	-1.028211	-0.751323	0.000173
O	-1.232878	1.501842	0.000149
C	-3.770128	-1.097942	0.000009
C	-5.156205	-1.208636	-0.000151
C	-5.993019	-0.094257	-0.000264
C	4.255794	-3.292041	-0.000050
C	2.946450	-2.784398	0.000020
N	2.676872	-1.482357	0.000058
C	3.716179	-0.608040	0.000028
C	5.067780	-1.023586	-0.000042
C	5.318217	-2.411650	-0.000081
C	3.404689	0.799113	0.000075
C	6.104539	-0.032990	-0.000065
N	2.100059	1.137722	0.000140
C	1.763261	2.418325	0.000196
C	2.730139	3.443686	0.000185
C	4.069364	3.111240	0.000114
C	4.448932	1.750813	0.000056
C	5.808303	1.297158	-0.000018
C	-5.410803	1.169535	-0.000214
C	-4.022845	1.301668	-0.000053
H	-3.143130	-1.980682	0.000096
H	4.412492	-4.365919	-0.000078
H	2.089728	-3.451518	0.000045
H	6.343338	-2.773982	-0.000135
H	7.139013	-0.366834	-0.000120
H	0.691861	2.609965	0.000251
H	2.410766	4.481302	0.000234
H	4.836190	3.882453	0.000104
H	6.604810	2.037200	-0.000034
H	-6.043810	2.052778	-0.000301
H	-3.547516	2.277743	-0.000008
H	-7.067705	-0.233479	-0.000388
N	-5.762823	-2.543496	-0.000203
O	-5.012830	-3.512211	-0.000087
O	-6.987667	-2.612839	-0.000331

$TS5_{m\text{-}NO2}$

E = -1393.275041 a.u.

Cu	-0.070783	-0.491508	0.303864
C	1.880514	-0.819329	0.276877
C	2.674480	-0.176216	1.243512
C	3.936644	0.335793	0.933898
C	4.443294	0.208668	-0.356022
C	3.669504	-0.452995	-1.308795
C	2.418561	-0.984348	-1.009486
H	2.298426	-0.111039	2.262535
H	4.534902	0.824367	1.699321
H	1.882968	-1.544792	-1.768559
C	0.823263	-2.362643	0.999457
O	0.665135	-2.184189	2.193134
O	0.714977	-3.200759	0.125629
C	-1.412430	3.728528	0.552099
C	-0.605473	2.577549	0.581100
N	-1.079646	1.363714	0.340389
C	-2.394936	1.224823	0.051483
C	-3.288894	2.318734	-0.001731
C	-2.754787	3.598336	0.260892
C	-2.881855	-0.106709	-0.209597
C	-4.668210	2.081554	-0.311747
N	-1.986478	-1.117973	-0.154398
C	-2.395678	-2.358339	-0.385698
C	-3.736251	-2.659112	-0.689601
C	-4.660099	-1.636663	-0.753375
C	-4.246956	-0.308432	-0.510341
C	-5.127480	0.821745	-0.554400
H	-0.971853	4.698798	0.757884
H	0.456123	2.641582	0.804905
H	-3.405349	4.469000	0.231030
H	-5.345495	2.930888	-0.349060
H	-1.627542	-3.126423	-0.326043
H	-4.023812	-3.689704	-0.871013
H	-5.701983	-1.840463	-0.988466
H	-6.175934	0.654402	-0.787522
H	5.420258	0.588374	-0.631934
N	4.205401	-0.601604	-2.666245
O	3.501728	-1.158634	-3.500605
O	5.325031	-0.152673	-2.890383

$5_{o\text{-}NO2}$

E = -1393.319282 a.u.

Cu	-0.310231	-0.429079	-0.361709
C	3.673648	0.617003	-0.211726
C	2.163537	0.744989	-0.255119
O	1.564581	-0.368572	-0.493454
O	1.665920	1.866782	-0.126984
C	4.357158	-0.478109	0.326392
C	5.738405	-0.614406	0.230425
C	6.478337	0.385466	-0.393926
C	-3.543742	-3.261485	-0.510361
C	-2.270159	-2.670667	-0.540437
N	-2.073878	-1.369024	-0.351510
C	-3.154367	-0.579952	-0.116607
C	-4.474741	-1.083516	-0.069266
C	-4.647865	-2.468034	-0.275711
C	-2.921536	0.827248	0.092745
C	-5.559279	-0.180266	0.183817
N	-1.643538	1.251076	0.039416
C	-1.378125	2.534358	0.228121
C	-2.394749	3.476361	0.484532
C	-3.707919	3.056431	0.540779
C	-4.011429	1.691246	0.342134
C	-5.337701	1.149842	0.380937

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C	5.827131	1.503009	-0.915277
C	4.441457	1.611171	-0.822609
N	3.650953	-1.512476	1.092793
O	3.990176	-2.675584	0.905270
O	2.818956	-1.142048	1.906914
H	6.214156	-1.491405	0.656486
H	7.558566	0.292714	-0.464416
H	-3.640483	-4.330408	-0.671005
H	-1.381839	-3.268178	-0.721276
H	-5.647000	-2.895879	-0.246549
H	-6.569138	-0.581231	0.216890
H	-0.323269	2.797151	0.170598
H	-2.133254	4.519254	0.635172
H	-4.512001	3.761996	0.736945
H	-6.169954	1.822617	0.572989
H	6.399399	2.289706	-1.400223
H	3.917645	2.470546	-1.229914

TS5$_{o\text{-}NO2}$
E = -1393.279505 a.u.

Cu	0.397321	-0.110173	-0.132022
C	2.381775	-0.170547	-0.705848
C	3.134582	0.105899	0.449142
C	4.323635	0.826797	0.456822
C	4.780651	1.359332	-0.746172
C	4.053069	1.142924	-1.919164
C	2.889695	0.374313	-1.896007
N	2.608256	-0.320357	1.740155
O	3.382102	-0.586795	2.642910
O	1.372378	-0.335678	1.866977
H	4.853053	0.984840	1.390898
H	5.699357	1.939034	-0.765993
H	4.414067	1.551243	-2.860391
H	2.369527	0.120912	-2.816488
C	1.602823	-1.798491	-1.004521
O	1.820970	-2.562455	-0.071415
O	1.129784	-1.837643	-2.133731
C	-1.843178	3.625858	-0.759756
C	-0.790787	2.703565	-0.634316
N	-0.986417	1.420601	-0.360444
C	-2.258264	0.978345	-0.196303
C	-3.383547	1.828825	-0.303564
C	-3.140892	3.187795	-0.593631
C	-2.451314	-0.421057	0.095034
C	-4.696070	1.283126	-0.116724
N	-1.349144	-1.195761	0.180917
C	-1.481570	-2.489023	0.436637
C	-2.740956	-3.086657	0.629973
C	-3.877021	-2.308209	0.547758
C	-3.758070	-0.929057	0.270618
C	-4.875536	-0.038977	0.158804
H	-1.622749	4.664500	-0.984778
H	0.242614	3.013846	-0.762015
H	-3.977924	3.875828	-0.684527
H	-5.550904	1.949290	-0.201102
H	-0.555287	-3.057875	0.478306
H	-2.801815	-4.150283	0.837067
H	-4.863175	-2.743565	0.690717
H	-5.876179	-0.440763	0.297211

5$_{p\text{-}CN}$
E = -1281.110098 a.u.

Cu	0.645613	-0.703674	0.000041
C	-3.426128	-0.015634	0.000143
C	-1.929396	0.201720	0.000165
O	-1.232607	-0.886171	0.000083
O	-1.495222	1.360026	0.000139
C	-3.976039	-1.301780	0.000094
C	-5.353867	-1.479788	0.000075
C	-6.200561	-0.359922	0.000106
C	2.355262	3.454714	0.000197
C	1.431572	2.390231	0.000157
N	1.820695	1.124397	0.000099
C	3.138046	0.840363	0.000082
C	4.141968	1.834469	0.000118
C	3.707028	3.178140	0.000177
C	3.507398	-0.552792	0.000028
C	5.518798	1.437795	0.000097
N	2.504941	-1.469399	0.000000
C	2.829328	-2.758928	-0.000050
C	4.158558	-3.211844	-0.000073
C	5.183440	-2.287992	-0.000044
C	4.875155	-0.911633	0.000009
C	5.870019	0.121079	0.000044
C	-5.653695	0.933631	0.000156
C	-4.275008	1.095921	0.000173
H	-3.305149	-2.154281	0.000071
H	-5.784646	-2.476708	0.000037
H	1.992906	4.478118	0.000244
H	0.353166	2.536369	0.000172
H	4.441396	3.980294	0.000206
H	6.283802	2.210322	0.000124
H	2.001581	-3.461666	-0.000072
H	4.359806	-4.278279	-0.000114
H	6.222790	-2.607273	-0.000060
H	6.917437	-0.169617	0.000028
H	-6.315084	1.794966	0.000180
H	-3.824845	2.083499	0.000211
C	-7.620895	-0.537066	0.000088
N	-8.775900	-0.681641	0.000072

TS5$_{p\text{-}CN}$
E = -1281.053646 a.u.

Cu	0.123331	-0.487303	0.262403
C	2.090491	-0.635868	0.326289
C	2.744250	0.071169	1.352527
C	3.950598	0.724844	1.129526
C	4.546376	0.665212	-0.141994
C	3.936372	-0.075785	-1.167957
C	2.732908	-0.727457	-0.922305
H	2.302594	0.077945	2.346705
H	4.446001	1.272805	1.926585
H	4.419292	-0.141352	-2.139154
H	2.288823	-1.342656	-1.701421
C	1.136607	-2.288841	0.947544
O	0.928514	-2.176664	2.141662
O	1.122511	-3.099004	0.039386
C	-1.429576	3.670547	0.416758
C	-0.561794	2.564670	0.456698
N	-0.975960	1.322824	0.252093
C	-2.286370	1.107990	-0.008541
C	-3.238580	2.150948	-0.068419
C	-2.768260	3.462911	0.154680
C	-2.705154	-0.253565	-0.230147
C	-4.608748	1.832573	-0.344692
N	-1.754982	-1.213638	-0.171448
C	-2.100420	-2.479447	-0.366210
C	-3.428495	-2.859363	-0.633631
C	-4.407803	-1.889889	-0.700560
C	-4.062831	-0.535727	-0.497537
C	-5.003920	0.544400	-0.548744
H	-1.037641	4.667267	0.592336
H	0.498618	2.688838	0.660579
H	-3.464569	4.297201	0.118502
H	-5.331920	2.642954	-0.386770
H	-1.290720	-3.203513	-0.307659
H	-3.663428	-3.908079	-0.784312
H	-5.441710	-2.155422	-0.907516
H	-6.046289	0.315529	-0.755306
C	5.781171	1.345003	-0.385755
N	6.781036	1.907116	-0.585653

5$_{m\text{-}CN}$
E = -1281.110270 a.u.

Cu	0.643761	-0.684612	0.000025
C	-3.429270	0.005629	0.000098
C	-1.933537	0.230741	0.000160
O	-1.233950	-0.854795	0.000084

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O	-1.505309	1.391029	0.000067
C	-3.964855	-1.281629	0.000093
C	-5.354964	-1.461824	0.000042
C	-6.212259	-0.349816	-0.000006
C	2.377558	3.460196	0.000219
C	1.447411	2.401394	0.000157
N	1.829384	1.133494	0.000094
C	3.144989	0.841279	0.000093
C	4.155097	1.829118	0.000150
C	3.727687	3.175444	0.000214
C	3.505218	-0.554218	0.000030
C	5.529420	1.422912	0.000141
N	2.496688	-1.463995	-0.000017
C	2.811729	-2.755771	-0.000078
C	4.137962	-3.217627	-0.000094
C	5.169189	-2.300837	-0.000043
C	4.870437	-0.922409	0.000022
C	5.871886	0.103875	0.000079
C	-5.670972	0.931687	-0.000001
C	-4.288786	1.108297	0.000049
H	-3.294989	-2.134296	0.000131
H	2.021621	4.485857	0.000269
H	0.369763	2.554257	0.000160
H	4.466656	3.973388	0.000260
H	6.299731	2.190179	0.000184
H	1.978925	-3.452520	-0.000115
H	4.331934	-4.285408	-0.000144
H	6.206345	-2.627066	-0.000052
H	6.917410	-0.193628	0.000072
H	-6.331593	1.794688	-0.000038
H	-3.844059	2.098710	0.000054
H	-7.287691	-0.500685	-0.000045
C	-5.904617	-2.784472	0.000039
N	-6.354190	-3.858035	0.000036

TS5$_{m\text{-}CN}$
E = -1281.053404 a.u.

Cu	0.124112	-0.440839	0.316234
C	2.092978	-0.622847	0.338668
C	2.803955	0.099277	1.313702
C	4.029036	0.703022	1.025755
C	4.580974	0.588942	-0.246547
C	3.906810	-0.157024	-1.227633
C	2.681927	-0.772555	-0.925256
H	2.394947	0.154767	2.320588
H	4.564355	1.253840	1.795750
H	2.200525	-1.395543	-1.674591
C	1.127681	-2.235658	1.057853
O	0.939248	-2.058781	2.246844
O	1.091066	-3.086274	0.189753
C	-1.495549	3.689115	0.476169
C	-0.614676	2.594582	0.532075
N	-1.005583	1.348455	0.308066
C	-2.305671	1.118262	0.009837
C	-3.269358	2.149496	-0.070514
C	-2.823399	3.465756	0.175023
C	-2.700845	-0.246870	-0.231809
C	-4.626820	1.816244	-0.388624
N	-1.741224	-1.195610	-0.150477
C	-2.065658	-2.464308	-0.362047
C	-3.380481	-2.858402	-0.671460
C	-4.369018	-1.900494	-0.762271
C	-4.046723	-0.543761	-0.540436
C	-4.999426	0.524778	-0.612746
H	-1.122114	4.689675	0.669364
H	0.438236	2.731840	0.764082
H	-3.529579	4.290952	0.124438
H	-5.358380	2.618053	-0.446984
H	-1.249050	-3.178630	-0.281622
H	-3.597889	-3.908879	-0.835663
H	-5.392897	-2.176976	-1.002174
H	-6.032182	0.284390	-0.851933
H	5.535480	1.049561	-0.483856
C	4.477805	-0.294170	-2.533885
N	4.935437	-0.397210	-3.599268

5$_{o\text{-}CN}$
E = -1281.105753 a.u.

Cu	0.276376	-0.459026	-0.064824
C	-3.713086	0.643892	-0.145229
C	-2.203592	0.755608	-0.098249
O	-1.599004	-0.379540	-0.116095
O	-1.690510	1.879628	-0.048563
C	-4.398921	-0.586795	-0.202844
C	-5.804040	-0.602983	-0.243943
C	-6.524987	0.585056	-0.228303
C	2.419918	3.501238	0.118283
C	1.386098	2.545061	0.059406
N	1.635640	1.245270	0.026381
C	2.913084	0.817489	0.049482
C	4.019248	1.694665	0.107964
C	3.732931	3.077460	0.142500
C	3.127693	-0.607777	0.011636
C	5.343747	1.148078	0.128718
N	2.031716	-1.408524	-0.044156
C	2.210634	-2.725913	-0.079650
C	3.482458	-3.321621	-0.061897
C	4.601994	-2.517056	-0.005332
C	4.446866	-1.115460	0.033448
C	5.548152	-0.198859	0.092980
C	-5.849422	1.804280	-0.171324
C	-4.459008	1.824006	-0.130511
H	-6.317152	-1.559060	-0.288089
H	-7.610965	0.557140	-0.260550
H	2.171986	4.557951	0.143853
H	0.330087	2.809173	0.037554
H	4.549994	3.793849	0.187812
H	6.188769	1.830745	0.173770
H	1.310246	-3.331261	-0.123854
H	3.565331	-4.403242	-0.092859
H	5.599774	-2.948795	0.009689
H	6.557081	-0.603224	0.109157
H	-6.406888	2.737546	-0.158794
H	-3.905031	2.756328	-0.085819
C	-3.754837	-1.870665	-0.223457
N	-3.402948	-2.980262	-0.246481

TS5$_{o\text{-}CN}$
E = -1281.052167 a.u.

Cu	0.445668	-0.238539	0.199250
C	2.405638	-0.509129	-0.202181
C	3.170137	0.643397	0.110261
C	4.248328	1.051496	-0.691444
C	4.579403	0.321040	-1.827966
C	3.837833	-0.812625	-2.164381
C	2.783334	-1.221612	-1.350472
H	4.812418	1.940107	-0.421348
H	5.418789	0.632187	-2.444375
H	4.099256	-1.389239	-3.048747
H	2.256583	-2.148109	-1.563188
C	1.746465	-1.698736	1.164532
O	1.726254	-1.126936	2.242348
O	1.606169	-2.808819	0.678607
C	-1.613775	3.646020	0.268775
C	-0.612622	2.661804	0.349566
N	-0.869697	1.368399	0.200199
C	-2.150366	0.978508	-0.012464
C	-3.223609	1.893019	-0.111037
C	-2.917019	3.263324	0.030356
C	-2.411738	-0.436282	-0.112166
C	-4.550196	1.396628	-0.332138
N	-1.358374	-1.273383	0.013866
C	-1.561077	-2.582707	-0.029557
C	-2.840975	-3.135295	-0.221023
C	-3.924009	-2.293123	-0.367358
C	-3.733331	-0.895328	-0.310020
C	-4.795222	0.059747	-0.427885
H	-1.346750	4.689785	0.398934

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H	0.419805	2.925983	0.558997
H	-3.712052	4.001919	-0.038718
H	-5.364133	2.112476	-0.414171
H	-0.674046	-3.198863	0.101817
H	-2.959337	-4.213816	-0.249220
H	-4.924272	-2.692142	-0.518192
H	-5.807004	-0.304351	-0.587454
C	2.810910	1.495813	1.208447
N	2.528196	2.280672	2.021670

1O$_{p\text{-C(O)Me}}$
E = -1272.812856 a.u.

Ag	1.293708	-0.930852	-0.750809
O	-0.807785	-1.175471	-0.837880
O	-0.545224	0.658959	0.432986
C	-1.256634	-0.193579	-0.134792
O	3.355541	-0.333046	-0.455345
S	3.558064	0.522705	0.824721
C	5.186769	1.263174	0.564097
C	2.543279	2.007364	0.629910
H	5.918902	0.452501	0.583467
H	5.394546	1.970620	1.372584
H	5.205695	1.760462	-0.409623
H	2.783080	2.497413	-0.318641
H	2.739156	2.673911	1.476530
H	1.493433	1.687388	0.638538
C	-2.754128	-0.108497	-0.015438
C	-3.330827	0.923426	0.735117
C	-3.579237	-1.046405	-0.643908
C	-4.709955	1.015416	0.854715
C	-4.961896	-0.953720	-0.523696
H	-3.120596	-1.841662	-1.222326
C	-5.542994	0.077949	0.226702
H	-5.587196	-1.691507	-1.018883
H	-2.673718	1.641378	1.215723
H	-5.175260	1.808447	1.432531
C	-7.022777	0.225424	0.389236
O	-7.490366	1.139086	1.049825
C	-7.934027	-0.782887	-0.282679
H	-7.786806	-0.784508	-1.369327
H	-7.729623	-1.798821	0.075903
H	-8.970109	-0.522379	-0.058849

TS3$_{p\text{-C(O)Me}}$
E = -1272.754829 a.u.

Ag	-0.221778	-0.093768	-0.577546
O	0.599749	0.243392	2.412361
O	0.053127	2.171656	1.274082
C	0.522583	1.088346	1.557819
O	-2.311126	-0.458737	-1.050062
S	-3.288549	-0.222208	0.132930
C	-3.319918	1.562073	0.430869
C	-4.909540	-0.401066	-0.646398
H	-2.336760	1.848866	0.821073
H	-4.089749	1.775562	1.179629
H	-3.524013	2.090376	-0.505193
H	-4.966791	0.256831	-1.518025
H	-5.689172	-0.160278	0.082494
H	-5.003210	-1.443732	-0.958821
C	1.737994	0.514325	0.045580
C	2.249618	1.589418	-0.705973
C	2.612551	-0.551917	0.345037
C	3.562623	1.586473	-1.172072
H	1.615152	2.453908	-0.889319
C	3.919087	-0.564709	-0.124274
C	4.407721	0.504032	-0.891828
H	3.928264	2.434652	-1.745163
H	2.260744	-1.357517	0.985554
H	4.594557	-1.385976	0.097966
C	5.827700	0.442629	-1.362672
O	6.527974	-0.522120	-1.102204
C	6.380102	1.600198	-2.169974
H	5.801824	1.752383	-3.089222
H	6.336884	2.534841	-1.598062
H	7.418097	1.382692	-2.428182

1O$_{m\text{-C(O)Me}}$
E = -1272.812540 a.u.

Ag	1.256265	-0.954034	-0.808117
O	-0.850118	-1.268126	-0.844118
O	-0.551060	0.558576	0.426480
C	-1.279766	-0.296476	-0.116221
O	3.298287	-0.268687	-0.525382
S	3.484040	0.558390	0.775405
C	5.098649	1.335044	0.531802
C	2.442147	2.027972	0.618121
H	5.846396	0.538506	0.534920
H	5.292619	2.030542	1.353921
H	5.107374	1.851638	-0.432026
H	2.673493	2.547426	-0.316774
H	2.624145	2.675076	1.482691
H	1.399491	1.686264	0.618468
C	-2.770188	-0.222279	0.070602
C	-3.316361	0.803950	0.838897
C	-3.618254	-1.169732	-0.515849
C	-4.699713	0.898835	1.030759
C	-4.996070	-1.085720	-0.331029
H	-3.179682	-1.963806	-1.111822
C	-5.536635	-0.057280	0.438062
H	-5.651750	-1.823122	-0.787121
H	-6.613496	-0.004190	0.573391
H	-2.663142	1.539962	1.295224
C	-5.222749	2.024806	1.865178
O	-4.463989	2.839682	2.364337
C	-6.719816	2.137763	2.081597
H	-7.249540	2.250329	1.127985
H	-7.116751	1.241104	2.572597
H	-6.917284	3.009251	2.708475

TS3$_{m\text{-C(O)Me}}$
E = -1272.754505 a.u.

Ag	-0.206887	-0.136949	-0.568588
O	0.640135	0.309639	2.391824
O	0.099212	2.204573	1.196417
C	0.562490	1.127156	1.511819
O	-2.300813	-0.504371	-1.018483
S	-3.269424	-0.233523	0.164270
C	-3.279341	1.556726	0.427732
C	-4.896403	-0.406408	-0.603860
H	-2.287825	1.843044	0.796651
H	-4.035318	1.791820	1.184161
H	-3.493236	2.069034	-0.515011
H	-4.947379	0.233488	-1.489073
H	-5.669173	-0.138416	0.122841
H	-5.006699	-1.454080	-0.893244
C	1.758969	0.500213	0.001327
C	2.267367	1.559904	-0.777335
C	2.626499	-0.562115	0.304617
C	3.577611	1.543802	-1.254343
H	1.631859	2.421554	-0.970930
C	3.941848	-0.600597	-0.176752
C	4.409472	0.465689	-0.959284
H	3.957203	2.374602	-1.844667
H	5.430862	0.465371	-1.330585
H	2.298310	-1.369273	0.954217
C	4.795222	-1.778012	0.178184
O	4.336448	-2.713524	0.812385
C	6.245359	-1.789014	-0.266331
H	6.323608	-1.751801	-1.359763
H	6.787471	-0.922396	0.130588
H	6.714256	-2.705953	0.095339

1O$_{o\text{-C(O)Me}}$
E = -1272.803892 a.u.

Ag	-1.766865	-1.514184	-0.436740
O	0.314035	-1.963978	-0.461240
O	0.201602	0.201289	0.113497
C	0.845688	-0.849647	-0.104879

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O	-3.755699	-0.701614	-0.147846
S	-3.787496	0.850824	-0.099470
C	-5.399483	1.198191	0.642131
C	-2.733420	1.360180	1.279089
H	-6.161667	0.863893	-0.065582
H	-5.494468	2.275335	0.809524
H	-5.491767	0.643973	1.580255
H	-3.036839	0.836431	2.190692
H	-2.824136	2.444706	1.401440
H	-1.701015	1.101274	1.013674
C	2.333329	-0.836318	0.076560
C	2.999298	0.368703	0.359014
C	3.051975	-2.035799	0.050148
C	4.367992	0.340325	0.642086
C	4.419635	-2.049782	0.305965
H	2.510678	-2.952505	-0.161402
C	5.077554	-0.858269	0.609753
H	4.875510	1.269649	0.888068
H	4.968166	-2.987952	0.281861
H	6.143023	-0.861206	0.826641
C	2.328866	1.724476	0.366293
O	2.294134	2.387395	1.385618
C	1.929718	2.298254	-0.977140
H	2.838061	2.672280	-1.470307
H	1.474182	1.550364	-1.628350
H	1.246341	3.138013	-0.828482

TS3$_{o\text{-C(O)Me}}$
E = -1272.759560 a.u.

Ag	0.271282	0.320917	-0.675305
O	-0.962428	0.663567	2.284334
O	-0.078623	-1.397210	1.753532
C	-0.667288	-0.340180	1.690734
O	2.432576	0.382197	-1.105584
S	3.347929	0.386543	0.141351
C	3.249935	-1.268960	0.866197
C	5.009200	0.272266	-0.565591
H	2.238630	-1.389923	1.270279
H	3.983352	-1.338626	1.676320
H	3.442307	-2.021244	0.095273
H	5.053596	-0.580713	-1.248587
H	5.741167	0.170767	0.241363
H	5.189328	1.199113	-1.115277
C	-1.724108	-0.296163	-0.060549
C	-2.173023	-1.590610	-0.355782
C	-2.640981	0.769931	-0.230282
C	-3.466259	-1.829217	-0.828792
H	-1.505017	-2.427164	-0.161154
C	-3.947105	0.531197	-0.665822
C	-4.353341	-0.766560	-0.983096
H	-3.788547	-2.843527	-1.053988
H	-4.646549	1.353572	-0.798111
H	-5.364428	-0.943798	-1.341285
C	-2.157752	2.160960	0.029349
O	-1.036500	2.506608	-0.330324
C	-3.051876	3.116017	0.776154
H	-4.072376	3.129086	0.380186
H	-3.111222	2.773764	1.816859
H	-2.627418	4.121574	0.749203

1O$_{p\text{-C(O)H}}$
E = -1233.504460 a.u.

Ag	1.253680	-0.945160	-0.712976
O	-0.847595	-1.200701	-0.751453
O	-0.575727	0.665338	0.471313
C	-1.289547	-0.205623	-0.063611
O	3.319995	-0.344033	-0.470541
S	3.550326	0.536685	0.787891
C	5.173405	1.270273	0.478114
C	2.532326	2.018186	0.584904
H	5.905241	0.459337	0.497638
H	5.398856	1.992972	1.268161
H	5.171919	1.748578	-0.505248
H	2.753655	2.490227	-0.377161
H	2.744680	2.700495	1.414819
H	1.482766	1.699471	0.619978
C	-2.786383	-0.128208	0.080933
C	-3.352333	0.919143	0.821425
C	-3.613660	-1.086923	-0.513927
C	-4.728542	1.008931	0.966740
C	-4.993587	-0.997159	-0.368697
H	-3.157554	-1.890347	-1.082726
C	-5.558340	0.048689	0.370697
H	-5.642526	-1.740309	-0.829465
H	-2.686541	1.648321	1.272094
H	-5.189075	1.811506	1.536151
C	-7.025301	0.133361	0.517906
O	-7.613288	0.996897	1.138250
H	-7.588817	-0.678038	0.003339

TS3$_{p\text{-C(O)H}}$
E = -1233.446391 a.u.

Ag	-0.210778	-0.125343	-0.545393
O	0.628937	0.291719	2.430088
O	0.088040	2.187009	1.234755
C	0.553556	1.110586	1.550093
O	-2.299308	-0.483646	-1.016891
S	-3.288029	-0.206618	0.148137
C	-3.294555	1.583492	0.410004
C	-4.901083	-0.375068	-0.649121
H	-2.310722	1.864219	0.802773
H	-4.067127	1.822984	1.148067
H	-3.483328	2.096270	-0.537809
H	-4.936557	0.267027	-1.533582
H	-5.686175	-0.108424	0.064773
H	-5.007382	-1.421873	-0.943154
C	1.757940	0.485257	0.057325
C	2.269266	1.531247	-0.735626
C	2.621296	-0.583421	0.386433
C	3.576071	1.492971	-1.215710
H	1.639888	2.394912	-0.938598
C	3.921961	-0.632015	-0.095217
C	4.403699	0.408239	-0.904432
H	3.965637	2.307681	-1.824988
H	2.262686	-1.359473	1.058755
H	4.591359	-1.453255	0.147194
C	5.789843	0.375380	-1.416161
O	6.586641	-0.516488	-1.203809
H	6.074415	1.254463	-2.037836

1O$_{m\text{-C(O)H}}$
E = -1233.504321 a.u.

Ag	1.251215	-0.931516	-0.779290
O	-0.854215	-1.222912	-0.800697
O	-0.546804	0.598095	0.477753
C	-1.277539	-0.252648	-0.067469
O	3.309649	-0.292319	-0.540396
S	3.536093	0.539057	0.751667
C	5.152983	1.296598	0.467160
C	2.507292	2.019952	0.611141
H	5.891844	0.491889	0.456579
H	5.373114	1.992914	1.281957
H	5.145515	1.809595	-0.498601
H	2.725483	2.535028	-0.329277
H	2.713319	2.667019	1.470352
H	1.460827	1.690789	0.632826
C	-2.768094	-0.175565	0.121808
C	-3.311133	0.843949	0.900019
C	-3.619850	-1.116073	-0.474420
C	-4.695869	0.927679	1.084323
C	-4.999449	-1.037796	-0.294082
H	-3.179186	-1.903750	-1.077374
C	-5.537912	-0.016752	0.484681
H	-5.651456	-1.771848	-0.760280
H	-6.614498	0.053990	0.632206
H	-2.658431	1.575604	1.365186
C	-5.278740	2.006372	1.907644
O	-4.644602	2.876097	2.470446

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H	-6.389994	1.975247	1.986773

TS3$_{m\text{-}C(O)H}$

E = -1233.446219 a.u.

Ag	-0.227077	-0.159981	-0.540563
O	0.614148	0.305402	2.413613
O	0.105642	2.196332	1.197662
C	0.553517	1.116094	1.525616
O	-2.319245	-0.514081	-0.998331
S	-3.297895	-0.212945	0.169284
C	-3.280243	1.580055	0.412421
C	-4.917705	-0.367688	-0.617043
H	-2.288879	1.853957	0.790973
H	-4.041585	1.836773	1.156337
H	-3.473115	2.085426	-0.538555
H	-4.947741	0.262911	-1.509878
H	-5.694499	-0.078922	0.097304
H	-5.041837	-1.416630	-0.896009
C	1.745815	0.460944	0.032456
C	2.268616	1.501950	-0.764550
C	2.597852	-0.609207	0.349410
C	3.576006	1.465855	-1.251138
H	1.642668	2.368852	-0.966001
C	3.907589	-0.663098	-0.144232
C	4.391765	0.379745	-0.944814
H	3.960524	2.284886	-1.854182
H	5.416243	0.340783	-1.312464
H	2.262774	-1.402058	1.013828
C	4.788589	-1.804603	0.180025
O	4.463730	-2.770094	0.840648
H	5.818041	-1.727245	-0.240395

1O$_{o\text{-}C(O)H}$

E = -1233.493195 a.u.

Ag	-1.541982	-1.224543	0.684761
O	0.569720	-1.513008	0.794665
O	0.266260	-0.082893	-0.915817
C	0.980044	-0.693719	-0.101800
O	-3.536003	-0.389525	0.450408
S	-3.641673	0.620282	-0.724744
C	-5.099706	1.597450	-0.287151
C	-2.376935	1.885437	-0.457875
H	-5.963400	0.929670	-0.327956
H	-5.221768	2.407444	-1.012628
H	-4.979189	1.991035	0.725942
H	-2.455874	2.278215	0.560298
H	-2.524322	2.679499	-1.197920
H	-1.398774	1.411172	-0.609423
C	2.479070	-0.543053	-0.186075
C	3.143855	0.648731	0.166238
C	3.230305	-1.612392	-0.675798
C	4.530749	0.747899	-0.007669
C	4.609948	-1.500930	-0.844245
H	2.724163	-2.539570	-0.930120
C	5.267985	-0.316284	-0.513392
H	5.030110	1.674476	0.271532
H	5.173205	-2.345540	-1.233626
H	6.343207	-0.228350	-0.642771
C	2.455186	1.808595	0.766278
O	1.297420	1.852142	1.131076
H	3.113429	2.699449	0.891560

TS3$_{o\text{-}C(O)H}$

E = -1233.449052 a.u.

Ag	0.402459	0.175208	-0.589667
O	-0.724285	0.217406	2.409370
O	0.264647	-1.705662	1.628106
C	-0.418361	-0.697009	1.685648
O	2.548229	0.386134	-1.046494
S	3.464357	0.434120	0.200963
C	3.534090	-1.250075	0.857355
C	5.124587	0.519931	-0.511121
H	2.536782	-1.489035	1.244962
H	4.265364	-1.276018	1.671970
H	3.808475	-1.946632	0.059364
H	5.252474	-0.293697	-1.230692
H	5.866322	0.457627	0.290870
H	5.207689	1.483491	-1.019332
C	-1.549204	-0.592889	0.084092
C	-1.967747	-1.887160	-0.252252
C	-2.509961	0.442985	-0.036005
C	-3.270799	-2.149917	-0.688650
H	-1.268752	-2.707966	-0.106935
C	-3.827174	0.178965	-0.418447
C	-4.206069	-1.119448	-0.762059
H	-3.564788	-3.166407	-0.940971
H	-4.549028	0.992656	-0.478077
H	-5.225859	-1.324682	-1.077202
C	-2.120329	1.848505	0.185455
O	-0.997364	2.292191	0.001079
H	-2.931589	2.534365	0.502134

1O$_{p\text{-}C(O)NMe2}$

E = -1367.446529 a.u.

Ag	-1.542754	-0.710882	-0.830753
O	0.563104	-0.901403	-0.937411
O	0.258748	1.100675	0.035459
C	0.991271	0.190010	-0.401754
O	-3.612910	-0.167571	-0.479354
S	-3.812367	1.365698	-0.335095
C	-5.456841	1.492561	0.405820
C	-2.825787	1.893212	1.086041
H	-6.175158	1.129810	-0.333114
H	-5.665393	2.540056	0.643691
H	-5.497054	0.868975	1.303255
H	-3.089312	1.293683	1.962694
H	-3.018660	2.956324	1.265190
H	-1.770856	1.741950	0.822799
C	2.485031	0.334297	-0.320012
C	3.039864	1.491847	0.236754
C	3.332172	-0.677612	-0.782117
C	4.418469	1.637424	0.327573
H	2.368428	2.262838	0.601460
C	4.713215	-0.523549	-0.709753
H	2.892548	-1.580758	-1.192830
C	5.269601	0.641000	-0.165247
H	4.855814	2.518605	0.787966
H	5.364607	-1.321811	-1.057102
C	6.747908	0.814755	0.038217
O	7.170763	1.223160	1.116078
N	7.593386	0.461003	-0.987396
C	7.217160	0.380103	-2.384678
C	9.020324	0.509895	-0.737188
H	7.474780	-0.600057	-2.808461
H	6.147055	0.543985	-2.507522
H	7.751475	1.148669	-2.961801
H	9.468184	1.425466	-1.150422
H	9.188634	0.494955	0.339432
H	9.506439	-0.354627	-1.205582

TS3$_{p\text{-}C(O)NMe2}$

E = -1367.389241 a.u.

Ag	0.359707	-0.623716	0.081341
O	-0.232038	1.226634	-2.376236
O	0.074605	2.287433	-0.352384
C	-0.282599	1.503569	-1.206377
O	2.410914	-1.156182	0.564502
S	3.483451	-0.318180	-0.181209
C	3.393831	1.359049	0.492005
C	5.023276	-0.847894	0.603550
H	2.436661	1.790449	0.177987
H	4.217573	1.946077	0.072709
H	3.451935	1.323320	1.583916
H	4.931459	-0.743852	1.688257
H	5.851444	-0.246227	0.217236
H	5.173526	-1.897653	0.340954
C	-1.574620	0.179809	-0.341338
C	-2.224708	0.692865	0.797514

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C	-2.343465	-0.586704	-1.241517
C	-3.574759	0.443250	1.036141
H	-1.667806	1.328033	1.483311
C	-3.682715	-0.865619	-0.994116
H	-1.882235	-0.942923	-2.159981
C	-4.314337	-0.338005	0.139528
H	-4.055891	0.846075	1.924799
H	-4.258479	-1.488230	-1.673626
C	-5.740071	-0.733642	0.402561
O	-6.066329	-1.913786	0.311729
N	-6.626666	0.242633	0.786964
C	-6.453749	1.662072	0.549857
C	-7.969096	-0.163193	1.153758
H	-6.544259	2.232120	1.484390
H	-5.478207	1.864810	0.108933
H	-7.226873	2.023565	-0.143247
H	-8.680880	0.029713	0.338135
H	-7.965247	-1.231486	1.369292
H	-8.295909	0.397621	2.037961

1O$_{m\text{-C(O)NMe2}}$

E = -1367.446064 a.u.

Ag	1.384291	-1.113269	0.695226
O	-0.698041	-1.519186	0.615053
O	-0.532839	0.663794	0.115067
C	-1.198101	-0.377257	0.288784
O	3.393909	-0.291277	0.648073
S	3.513101	0.924663	-0.310578
C	2.421082	2.213435	0.335323
C	5.103425	1.650398	0.151807
H	1.391845	1.845088	0.237799
H	2.555578	3.115388	-0.271139
H	2.658309	2.407544	1.385830
H	5.120213	1.822585	1.231574
H	5.246993	2.584893	-0.398994
H	5.880530	0.933718	-0.123942
C	-2.690623	-0.342489	0.111266
C	-3.311770	0.855814	-0.243691
C	-3.462374	-1.497963	0.278134
C	-4.698451	0.920743	-0.399411
H	-2.704217	1.740104	-0.404085
C	-4.841025	-1.448953	0.090317
H	-2.963920	-2.424459	0.544291
C	-5.459709	-0.244510	-0.241378
H	-5.437553	-2.351475	0.198337
H	-6.534910	-0.212457	-0.400669
C	-5.297299	2.218993	-0.861589
O	-4.760139	2.856796	-1.761888
N	-6.476914	2.631755	-0.283531
C	-6.949160	2.219784	1.023025
C	-7.116667	3.815597	-0.821934
H	-7.972034	1.822704	0.967770
H	-6.298469	1.454558	1.444969
H	-6.957699	3.079944	1.708310
H	-6.900884	4.702397	-0.208005
H	-6.740749	3.990311	-1.829851
H	-8.203397	3.668489	-0.846328

TS3$_{m\text{-C(O)NMe2}}$

E = -1367.389285 a.u.

Ag	-0.347975	-0.567428	-0.470979
O	0.695901	0.972495	2.050169
O	0.076516	2.271655	0.249370
C	0.554082	1.388493	0.930270
O	-2.474344	-1.002461	-0.622405
S	-3.354170	-0.246970	0.408658
C	-3.345585	1.495082	-0.080860
C	-5.033358	-0.670222	-0.109083
H	-2.332784	1.879205	0.085547
H	-4.054152	2.037963	0.553310
H	-3.615116	1.583459	-1.137559
H	-5.152894	-0.444808	-1.172498
H	-5.750534	-0.108657	0.497083
H	-5.162229	-1.741575	0.061749
C	1.649484	0.178462	-0.298118
C	2.113750	0.840451	-1.452035
C	2.527406	-0.711368	0.346337
C	3.391513	0.600856	-1.955946
H	1.470918	1.574173	-1.933873
C	3.817708	-0.946446	-0.137259
H	2.214091	-1.211693	1.259014
C	4.240526	-0.290268	-1.301133
H	3.733412	1.112700	-2.852789
H	5.236091	-0.481622	-1.695274
C	4.655877	-1.989599	0.546174
O	4.172650	-3.088881	0.801340
N	5.968028	-1.687699	0.823577
C	6.503283	-0.345280	0.932522
C	6.802262	-2.731716	1.385174
H	7.384353	-0.219181	0.288703
H	5.753658	0.393661	0.650828
H	6.810153	-0.144524	1.969113
H	6.916373	-2.610015	2.472052
H	6.334788	-3.696511	1.189159
H	7.798052	-2.696093	0.926590

1O$_{o\text{-C(O)NMe2}}$

E = -1367.442437 a.u.

Ag	-1.752559	1.718865	0.077248
O	0.361125	1.571992	0.032809
O	-0.264588	-0.069366	1.430391
C	0.601059	0.552041	0.782403
O	-3.894607	1.489260	0.326990
S	-4.272346	0.678959	1.596389
C	-5.988473	0.205726	1.278871
C	-3.502174	-0.949478	1.432052
H	-6.582613	1.122532	1.272993
H	-6.333956	-0.455957	2.078944
H	-6.052240	-0.287012	0.304711
H	-3.778946	-1.394090	0.471201
H	-3.837616	-1.575768	2.265626
H	-2.415798	-0.802536	1.486654
C	2.040330	0.130391	0.867524
C	2.993263	0.516841	-0.089975
C	2.434075	-0.664372	1.948946
C	4.320539	0.101709	0.062272
C	3.758479	-1.061239	2.100482
H	1.672774	-0.959748	2.664385
C	4.705756	-0.674585	1.152949
H	5.053897	0.386690	-0.688174
H	4.050986	-1.671839	2.951039
H	5.743243	-0.983087	1.256878
C	2.627417	1.223871	-1.376728
O	2.249561	0.562588	-2.336976
N	2.879419	2.567307	-1.448041
C	3.050473	3.402962	-0.280205
H	2.114201	3.918422	-0.023745
H	3.354917	2.799264	0.575294
H	3.826696	4.154831	-0.471001
C	2.532339	3.259202	-2.671150
H	3.302377	4.002394	-2.911257
H	2.458392	2.525827	-3.474403
H	1.566169	3.776078	-2.571916

TS3$_{o\text{-C(O)NMe2}}$

E = -1367.399309 a.u.

Ag	0.376276	0.144359	-0.565034
O	-0.847673	0.209588	2.415527
O	0.171933	-1.767704	1.802383
C	-0.472295	-0.747201	1.795368
O	2.522821	0.459718	-0.980617
S	3.457340	0.340084	0.243912
C	3.456004	-1.401523	0.739163
C	5.111343	0.404398	-0.487841
H	2.462737	-1.625721	1.143096
H	4.212224	-1.543697	1.518353
H	3.663941	-2.032356	-0.130436
H	5.185798	-0.347249	-1.278767

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H	5.860653	0.233687	0.291063
H	5.237100	1.403553	-0.911482
C	-1.549639	-0.687723	-0.010096
C	-1.901339	-1.992977	-0.382682
C	-2.541944	0.311308	-0.122678
C	-3.169544	-2.296859	-0.885359
H	-1.173037	-2.789132	-0.241465
C	-3.814483	0.014059	-0.616430
C	-4.125007	-1.290342	-1.006939
H	-3.414979	-3.317282	-1.172051
H	-4.556702	0.803305	-0.720258
H	-5.112963	-1.515956	-1.401188
C	-2.146991	1.729918	0.170230
O	-1.125306	2.200537	-0.354072
N	-2.960400	2.496230	0.946900
C	-3.874504	1.952616	1.935819
H	-3.499280	2.164035	2.945804
H	-4.869195	2.404141	1.830352
H	-3.957376	0.872773	1.825668
C	-2.606011	3.890561	1.137871
H	-1.968047	4.020187	2.023202
H	-2.062753	4.247122	0.263060
H	-3.520883	4.478014	1.274151

$5_{p\text{-}C(O)Me}$

E = -1341.493614 a.u.

Cu	0.878377	-0.666073	-0.000077
C	-3.163245	0.170593	-0.000102
C	-1.660507	0.331804	-0.000146
O	-1.002387	-0.781178	-0.000177
O	-1.179100	1.472201	-0.000065
C	-3.765143	-1.093893	-0.000134
C	-5.148344	-1.211262	-0.000062
C	-5.961807	-0.068622	0.000008
C	4.302436	-3.292843	-0.000050
C	2.989781	-2.793819	-0.000081
N	2.710539	-1.493738	-0.000048
C	3.744673	-0.612909	0.000020
C	5.099067	-1.019221	0.000057
C	5.359116	-2.405497	0.000018
C	3.424171	0.792220	0.000061
C	6.129211	-0.021631	0.000132
N	2.117569	1.121347	0.000023
C	1.771742	2.399609	0.000058
C	2.731768	3.431601	0.000136
C	4.073317	3.108780	0.000175
C	4.461908	1.750975	0.000136
C	5.824084	1.306579	0.000170
C	-5.355491	1.196167	0.000034
C	-3.970134	1.312189	-0.000010
O	-7.937479	-1.371566	0.000538
H	-3.128366	-1.972561	-0.000204
H	-5.632070	-2.183688	-0.000060
H	4.466184	-4.365693	-0.000080
H	2.137875	-3.467077	-0.000135
H	6.386679	-2.760943	0.000044
H	7.165907	-0.348610	0.000158
H	0.698514	2.581143	0.000020
H	2.404981	4.466949	0.000164
H	4.834845	3.885245	0.000234
H	6.615615	2.051953	0.000228
H	-5.963907	2.096664	0.000125
H	-3.483904	2.282766	0.000026
C	-7.444120	-0.254505	0.000134
C	-8.332745	0.975043	-0.000070
H	-8.145331	1.596623	0.883592
H	-8.144172	1.597415	-0.882909
H	-9.375660	0.652827	-0.000840

$TS5_{p\text{-}C(O)Me}$

E = -1341.437195 a.u.

Cu	-0.112321	-0.583600	0.192223
C	1.837907	-0.839639	0.209327
C	2.548075	-0.167058	1.223333
C	3.787874	0.407739	0.974922
C	4.378646	0.302536	-0.294607
C	3.704939	-0.408847	-1.298748
C	2.460216	-0.979158	-1.043574
O	6.248563	1.587172	0.376554
H	2.119619	-0.124140	2.222850
H	4.334214	0.937921	1.750418
H	4.155382	-0.528752	-2.281137
H	1.968517	-1.568002	-1.814824
C	0.788323	-2.454265	0.836902
O	0.625962	-2.350509	2.038216
O	0.699755	-3.247127	-0.082536
C	-1.346994	3.683130	0.435557
C	-0.562825	2.515380	0.434536
N	-1.076226	1.310757	0.234237
C	-2.407067	1.196665	0.020865
C	-3.280791	2.307580	0.004490
C	-2.706056	3.578415	0.220844
C	-2.932948	-0.128118	-0.194566
C	-4.679961	2.093857	-0.223055
N	-2.054654	-1.156019	-0.177288
C	-2.499990	-2.391041	-0.367412
C	-3.861341	-2.669380	-0.588255
C	-4.768114	-1.629855	-0.612356
C	-4.316765	-0.306881	-0.413148
C	-5.176474	0.840316	-0.421591
H	-0.876074	4.646042	0.605900
H	0.510508	2.556485	0.602231
H	-3.339131	4.462441	0.217390
H	-5.342415	2.955635	-0.231957
H	-1.744773	-3.173579	-0.343359
H	-4.178669	-3.696477	-0.736997
H	-5.825744	-1.816724	-0.782347
H	-6.239832	0.690925	-0.590689
C	5.709637	0.941906	-0.510181
C	6.388181	0.779822	-1.857417
H	6.565492	-0.278223	-2.084462
H	5.767862	1.186733	-2.665080
H	7.342589	1.309291	-1.834163

$5_{m\text{-}C(O)Me}$

E = -1341.492974 a.u.

Cu	0.613594	0.436456	0.000003
C	-3.287867	-0.907796	0.000011
C	-1.776803	-0.880973	0.000000
O	-1.262784	0.304459	0.000046
O	-1.158354	-1.953607	-0.000096
C	-4.040160	0.265200	0.000087
C	-5.440750	0.220332	0.000143
C	-6.084255	-1.025513	0.000065
C	3.645408	3.505748	0.000080
C	2.413135	2.832168	0.000060
N	2.315061	1.506117	0.000024
C	3.459556	0.774856	0.000005
C	4.745737	1.362420	0.000024
C	4.813549	2.771242	0.000062
C	3.333416	-0.660717	-0.000037
C	5.902148	0.514431	0.000002
N	2.083651	-1.164608	-0.000054
C	1.914242	-2.477830	-0.000093
C	3.005742	-3.369634	-0.000118
C	4.291039	-2.867283	-0.000101
C	4.491997	-1.469274	-0.000059
C	5.780984	-0.842997	-0.000037
C	-5.337278	-2.201681	-0.000049
C	-3.946291	-2.142901	-0.000061
H	-3.540778	1.227819	0.000121
H	3.661006	4.590920	0.000109
H	1.476727	3.381914	0.000073
H	5.782807	3.263958	0.000078
H	6.884654	0.979580	0.000018
H	0.875617	-2.804094	-0.000102
H	2.823108	-4.439862	-0.000150
H	5.150959	-3.533187	-0.000119

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H	6.666895	-1.473360	-0.000053
H	-5.842575	-3.164470	-0.000123
H	-3.340249	-3.043926	-0.000128
H	-7.169374	-1.084214	0.000056
O	-5.604583	2.582827	-0.000234
C	-6.191455	1.512610	0.000215
C	-7.708945	1.474254	0.000606
H	-8.091084	0.949809	-0.883430
H	-8.090807	0.947967	0.883644
H	-8.083812	2.499458	0.001667

TS5$_{m\text{-}C(O)Me}$

E = -1341.435907 a.u.

Cu	-0.087418	-0.283142	-0.555060
C	-2.044540	-0.230914	-0.781943
C	-2.588391	0.562109	-1.809219
C	-3.781748	1.262001	-1.630141
C	-4.464085	1.174966	-0.418161
C	-3.962810	0.373312	0.618245
C	-2.769387	-0.335195	0.413551
H	-2.077291	0.595027	-2.769546
H	-4.190179	1.865491	-2.438196
H	-2.428403	-0.994833	1.207317
C	-1.179732	-1.930267	-1.478624
O	-0.856303	-1.736381	-2.635847
O	-1.329385	-2.810284	-0.653439
C	1.980747	3.646716	-0.338622
C	0.999153	2.660353	-0.541489
N	1.228053	1.370823	-0.341985
C	2.455528	0.985702	0.077408
C	3.509912	1.898400	0.309665
C	3.236637	3.264839	0.086637
C	2.672324	-0.423449	0.290170
C	4.780801	1.402315	0.749804
N	1.629857	-1.253177	0.062621
C	1.788979	-2.557250	0.245939
C	3.011628	-3.108796	0.671530
C	4.083093	-2.273432	0.910686
C	3.936265	-0.881711	0.722726
C	4.985162	0.069380	0.946486
H	1.739834	4.689650	-0.518310
H	-0.001773	2.922488	-0.874458
H	4.017396	4.003313	0.252085
H	5.583995	2.113724	0.924149
H	0.912447	-3.170395	0.047103
H	3.093826	-4.182399	0.807230
H	5.038555	-2.672787	1.242410
H	5.953754	-0.294741	1.279623
H	-5.395753	1.719861	-0.290511
O	-4.162405	-0.412579	2.843091
C	-4.658407	0.232691	1.933139
C	-6.003037	0.911283	2.124118
H	-5.916832	1.998673	2.009132
H	-6.731496	0.561102	1.383147
H	-6.368870	0.684767	3.127392

5$_{o\text{-}C(O)Me}$

E = -1341.484315 a.u.

Cu	-0.240117	-0.506763	0.227381
C	3.747296	0.548313	0.167927
C	2.248229	0.636080	0.028614
O	1.640929	-0.492094	0.219828
O	1.714621	1.722727	-0.221514
C	4.417502	-0.681462	0.288339
C	5.793059	-0.688169	0.543444
C	6.507358	0.503878	0.638215
C	-3.475004	-3.273235	0.918759
C	-2.198271	-2.706371	0.773450
N	-2.008069	-1.428420	0.459106
C	-3.098149	-0.639523	0.274657
C	-4.422200	-1.119945	0.397531
C	-4.588562	-2.480666	0.729629
C	-2.871527	0.744802	-0.056535
C	-5.516212	-0.217917	0.183647
N	-1.589505	1.149153	-0.151845
C	-1.328482	2.412879	-0.448848
C	-2.354665	3.352768	-0.672607
C	-3.671916	2.952374	-0.579014
C	-3.970434	1.609046	-0.260203
C	-5.300155	1.089996	-0.132627
C	5.846426	1.723142	0.490409
C	4.473479	1.738625	0.265527
O	3.790699	-2.844284	1.037283
H	6.300836	-1.641833	0.664377
H	7.577364	0.479693	0.830809
H	-3.566818	-4.323353	1.176862
H	-1.302700	-3.303540	0.916442
H	-5.590019	-2.890913	0.834438
H	-6.528918	-0.601115	0.279879
H	-0.269786	2.660768	-0.501861
H	-2.097347	4.379426	-0.914345
H	-4.482945	3.657496	-0.745953
H	-6.139703	1.762319	-0.291513
H	6.397602	2.657527	0.564124
H	3.924153	2.670808	0.173562
C	3.754992	-2.030224	0.133405
C	3.268957	-2.401982	-1.252985
H	2.805712	-1.562141	-1.772976
H	4.140070	-2.728110	-1.838853
H	2.567887	-3.237608	-1.184464

TS5$_{o\text{-}C(O)Me}$

E = -1341.441939 a.u.

Cu	0.437486	-0.049764	-0.004105
C	2.383580	0.204174	-0.461563
C	3.119023	0.226366	0.751413
C	4.297127	0.971899	0.871701
C	4.744021	1.746866	-0.197557
C	4.028758	1.748061	-1.396095
C	2.878417	0.968680	-1.526447
H	4.852382	0.983322	1.807031
H	5.650118	2.339411	-0.097897
H	4.387259	2.335818	-2.238923
H	2.369651	0.896472	-2.485223
C	1.734648	-1.510139	-1.138353
O	2.001557	-2.389238	-0.333344
O	1.363444	-1.368842	-2.288624
C	-1.956790	3.676530	0.046956
C	-0.870845	2.784310	0.033257
N	-1.022087	1.467366	0.029323
C	-2.277971	0.959598	0.036511
C	-3.435193	1.772975	0.049640
C	-3.240517	3.170047	0.055291
C	-2.416819	-0.475206	0.028852
C	-4.727674	1.152531	0.058305
N	-1.282389	-1.208199	0.007862
C	-1.368316	-2.530939	0.000518
C	-2.604625	-3.202068	0.014516
C	-3.771904	-2.466381	0.031980
C	-3.704870	-1.056735	0.038865
C	-4.856682	-0.203827	0.054016
H	-1.773145	4.746367	0.050232
H	0.153516	3.147242	0.022373
H	-4.102215	3.833227	0.065470
H	-5.608688	1.789384	0.068425
H	-0.421005	-3.064264	-0.024927
H	-2.623951	-4.287245	0.005707
H	-4.741783	-2.958173	0.038542
H	-5.842482	-0.662272	0.061022
C	2.532498	-0.505586	1.899754
O	1.305905	-0.567240	2.011021
C	3.420503	-1.194311	2.900242
H	3.885728	-2.056532	2.406403
H	4.229443	-0.546996	3.254143
H	2.826106	-1.541424	3.747829

5$_{p\text{-}C(O)H}$

E = -1302.185559 a.u.

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Cu	0.864382	-0.669862	0.000092
C	-3.182431	0.153235	0.000045
C	-1.679354	0.321659	0.000115
O	-1.017325	-0.788396	0.000072
O	-1.205064	1.464623	0.000130
C	-3.773816	-1.118190	-0.000007
C	-5.155290	-1.247630	-0.000067
C	-5.966397	-0.103870	-0.000076
C	4.296083	-3.287704	0.000002
C	2.981898	-2.792615	0.000035
N	2.698739	-1.493445	0.000051
C	3.730144	-0.609436	0.000036
C	5.085733	-1.011608	0.000002
C	5.350044	-2.397122	-0.000015
C	3.405225	0.794751	0.000057
C	6.112708	-0.010767	-0.000012
N	2.097587	1.119812	0.000090
C	1.747868	2.397049	0.000113
C	2.704555	3.432064	0.000104
C	4.047067	3.113456	0.000069
C	4.439886	1.756795	0.000045
C	5.803413	1.316476	0.000009
C	-5.376264	1.166234	-0.000030
C	-3.992455	1.293465	0.000033
O	-8.049755	-1.277279	-0.000203
H	-3.127479	-1.989734	0.000004
H	-5.634374	-2.222949	-0.000103
H	4.463083	-4.360047	-0.000010
H	2.132103	-3.468543	0.000048
H	6.378704	-2.749317	-0.000041
H	7.150426	-0.334465	-0.000038
H	0.674233	2.575740	0.000141
H	2.374436	4.466342	0.000124
H	4.806107	3.892334	0.000061
H	6.592632	2.064282	-0.000001
H	-6.010020	2.052008	-0.000039
H	-3.508631	2.265082	0.000073
C	-7.436232	-0.227736	-0.000126
H	-7.980450	0.744719	-0.000169

TS5$_{p\text{-C(O)H}}$
E = -1302.129240 a.u.

Cu	-0.092522	-0.583838	0.216276
C	1.858501	-0.848649	0.241371
C	2.564429	-0.177124	1.261595
C	3.800188	0.406761	1.017977
C	4.379643	0.307200	-0.256853
C	3.716017	-0.401264	-1.267052
C	2.476787	-0.982882	-1.015048
O	6.338378	1.576791	0.259755
H	2.132394	-0.144413	2.259853
H	4.346613	0.935410	1.795242
H	4.184254	-0.500486	-2.246115
H	1.985314	-1.572857	-1.785356
C	0.806357	-2.454354	0.865721
O	0.637001	-2.346544	2.065995
O	0.718975	-3.249362	-0.051950
C	-1.321877	3.680905	0.451198
C	-0.539801	2.511935	0.460120
N	-1.052090	1.308191	0.251088
C	-2.380110	1.196554	0.018311
C	-3.251411	2.309108	-0.009824
C	-2.677735	3.578787	0.216223
C	-2.905532	-0.127058	-0.205707
C	-4.647451	2.098148	-0.258221
N	-2.029571	-1.156642	-0.176554
C	-2.474145	-2.390791	-0.373532
C	-3.832829	-2.666640	-0.613276
C	-4.737211	-1.625351	-0.650063
C	-4.286298	-0.303146	-0.444255
C	-5.143516	0.845723	-0.464841
H	-0.851732	4.642773	0.629298
H	0.531097	2.551774	0.642603
H	-3.309086	4.463946	0.204254
H	-5.307992	2.961217	-0.276539
H	-1.720385	-3.174375	-0.339775
H	-4.149923	-3.693127	-0.766583
H	-5.792642	-1.810134	-0.835170
H	-6.204552	0.698559	-0.649672
C	5.686927	0.926687	-0.535772
H	6.062777	0.762177	-1.572009

5$_{m\text{-C(O)H}}$
E = -1302.185218 a.u.

Cu	0.615337	0.454092	-0.000181
C	-3.294122	-0.873041	-0.000102
C	-1.782350	-0.857322	-0.000314
O	-1.262707	0.325175	-0.000252
O	-1.172299	-1.934347	-0.000144
C	-4.037115	0.305049	-0.000077
C	-5.437042	0.255202	0.000111
C	-6.093223	-0.981802	0.000279
C	3.665421	3.506024	0.000064
C	2.428985	2.840012	-0.000025
N	2.322654	1.514614	-0.000066
C	3.462700	0.776304	-0.000019
C	4.752392	1.355960	0.000072
C	4.828990	2.764306	0.000114
C	3.327884	-0.658547	-0.000066
C	5.903558	0.500902	0.000116
N	2.075077	-1.154654	-0.000153
C	1.897525	-2.466802	-0.000204
C	2.983312	-3.365460	-0.000167
C	4.271689	-2.871224	-0.000076
C	4.481402	-1.474346	-0.000023
C	5.774146	-0.855764	0.000070
C	-5.354611	-2.162264	0.000255
C	-3.962647	-2.104582	0.000066
H	-3.533277	1.265876	-0.000207
H	3.687717	4.591070	0.000095
H	1.496135	3.395756	-0.000065
H	5.801357	3.250792	0.000184
H	6.888885	0.960054	0.000186
H	0.856964	-2.786681	-0.000275
H	2.793864	-4.434499	-0.000211
H	5.127324	-3.542603	-0.000047
H	6.656236	-1.491426	0.000104
H	-5.860987	-3.124270	0.000383
H	-3.359587	-3.007673	0.000041
H	-7.181888	-1.011900	0.000426
O	-5.777740	2.624350	0.000288
C	-6.233205	1.497869	0.000131
H	-7.336440	1.335728	0.000586

TS5$_{m\text{-C(O)H}}$
E = -1302.128198 a.u.

Cu	-0.084419	-0.291444	-0.543544
C	-2.044428	-0.258788	-0.765866
C	-2.589691	0.558236	-1.776083
C	-3.781229	1.260648	-1.588437
C	-4.461726	1.149233	-0.378342
C	-3.959003	0.322057	0.634390
C	-2.768993	-0.390311	0.426292
H	-2.077024	0.608285	-2.734911
H	-4.184768	1.880098	-2.386499
H	-2.431942	-1.069279	1.206006
C	-1.171003	-1.934766	-1.486879
O	-0.854304	-1.721823	-2.642488
O	-1.305772	-2.826873	-0.672031
C	1.969547	3.644776	-0.337762
C	0.990008	2.655384	-0.535064
N	1.223410	1.366532	-0.335502
C	2.454204	0.985311	0.078373
C	3.506714	1.901592	0.305311
C	3.228402	3.266998	0.082292
C	2.677296	-0.423045	0.289971
C	4.781305	1.410322	0.740067
N	1.637615	-1.257275	0.065736

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C	1.803281	-2.560954	0.245997
C	3.029915	-3.107676	0.666173
C	4.098434	-2.267787	0.902590
C	3.944994	-0.876550	0.716581
C	4.991347	0.078244	0.936195
H	1.724622	4.686771	-0.517320
H	-0.013066	2.915013	-0.863368
H	4.007630	4.007969	0.243667
H	5.582605	2.124743	0.910573
H	0.929049	-3.177652	0.048104
H	3.117581	-4.181110	0.799680
H	5.056911	-2.663398	1.230006
H	5.962686	-0.282310	1.265069
H	-5.395629	1.686530	-0.218335
O	-4.345995	-0.454506	2.865063
C	-4.698022	0.203506	1.905940
H	-5.647223	0.788318	1.941896

$5_{o\text{-}C(O)H}$

E = -1302.172280 a.u.

Cu	-0.177061	-0.626502	-0.381476
C	3.844792	0.213326	-0.291890
C	2.342245	0.384235	-0.386617
O	1.700273	-0.725874	-0.491156
O	1.888384	1.531550	-0.430785
C	4.491852	-0.433743	0.780303
C	5.883194	-0.600108	0.755604
C	6.645095	-0.122064	-0.304281
C	-3.607632	-3.235785	-0.331602
C	-2.298030	-2.736615	-0.419290
N	-2.008051	-1.443814	-0.306246
C	-3.027435	-0.570959	-0.095575
C	-4.377609	-0.978443	0.007594
C	-4.649532	-2.356676	-0.118010
C	-2.695043	0.826154	0.027396
C	-5.391746	0.010060	0.232776
N	-1.393501	1.156539	-0.080469
C	-1.036787	2.427077	0.027874
C	-1.980431	3.449456	0.254535
C	-3.317126	3.125443	0.364766
C	-3.717082	1.775743	0.250967
C	-5.075347	1.330454	0.349853
C	6.006760	0.541131	-1.352466
C	4.623192	0.711701	-1.338176
O	2.646827	-0.631618	2.313760
H	6.367233	-1.100815	1.593046
H	7.723493	-0.256614	-0.311579
H	-3.780649	-4.302530	-0.431733
H	-1.457120	-3.403302	-0.584703
H	-5.674353	-2.712538	-0.044535
H	-6.425333	-0.317752	0.310103
H	0.031465	2.611129	-0.072647
H	-1.644707	4.478458	0.339380
H	-4.066194	3.894612	0.538589
H	-5.854764	2.068781	0.521985
H	6.588449	0.928608	-2.185713
H	4.128319	1.235673	-2.151315
C	3.786842	-0.896529	1.994475
H	4.424891	-1.519852	2.664953

$TS5_{o\text{-}C(O)H}$

E = -1302.131442 a.u.

Cu	0.429894	-0.115950	-0.112340
C	2.409080	0.075959	-0.591687
C	3.116167	0.093355	0.639703
C	4.310480	0.804745	0.796450
C	4.802197	1.574232	-0.255551
C	4.105594	1.602644	-1.465823
C	2.942523	0.847745	-1.632703
H	4.833916	0.781915	1.751602
H	5.722256	2.140787	-0.137106
H	4.492440	2.190807	-2.295648
H	2.455079	0.792266	-2.603253
C	1.695564	-1.512507	-1.285457
O	1.936646	-2.453322	-0.538975
O	1.273570	-1.320595	-2.418255
C	-1.881422	3.625472	0.242329
C	-0.814023	2.717893	0.133749
N	-0.990224	1.406102	0.055769
C	-2.254763	0.918799	0.080265
C	-3.394473	1.749918	0.185990
C	-3.173054	3.140733	0.268541
C	-2.423047	-0.510784	-0.009236
C	-4.697836	1.152771	0.204505
N	-1.305860	-1.261112	-0.114422
C	-1.415469	-2.578381	-0.204431
C	-2.664248	-3.227257	-0.190988
C	-3.815362	-2.473976	-0.084101
C	-3.721090	-1.068663	0.010190
C	-4.854225	-0.198140	0.120583
H	-1.677334	4.689835	0.302941
H	0.215621	3.064328	0.106813
H	-4.021035	3.816387	0.351050
H	-5.564849	1.803408	0.286657
H	-0.478555	-3.123563	-0.295561
H	-2.705545	-4.309053	-0.268811
H	-4.793916	-2.948174	-0.073922
H	-5.848285	-0.638233	0.134907
C	2.517099	-0.558234	1.805232
H	3.194585	-0.859038	2.627623
O	1.308500	-0.732406	1.923145

$5_{p\text{-}C(O)NMe2}$

E = -1436.126870 a.u.

Cu	0.868380	-0.601295	-0.050869
C	-3.142725	0.302143	0.269454
C	-1.641175	0.435155	0.184618
O	-1.011195	-0.683524	0.023759
O	-1.130123	1.559664	0.270395
C	-3.775299	-0.942703	0.179417
C	-5.159347	-1.037260	0.268948
C	-5.941187	0.114157	0.419491
C	4.224535	-3.285446	-0.441176
C	2.925385	-2.760068	-0.350725
N	2.679293	-1.461706	-0.202406
C	3.735079	-0.609689	-0.135855
C	5.078377	-1.043933	-0.216870
C	5.303104	-2.427409	-0.374060
C	3.450189	0.793733	0.025703
C	6.132984	-0.075520	-0.137077
N	2.152723	1.149394	0.099163
C	1.838816	2.427031	0.249180
C	2.824112	3.431498	0.333367
C	4.156789	3.081304	0.259362
C	4.511371	1.723466	0.100672
C	5.861518	1.251327	0.014798
C	-5.306330	1.359167	0.523978
C	-3.920072	1.449057	0.454028
O	-7.856284	-0.951699	1.314224
H	-3.162937	-1.828905	0.048232
H	-5.654155	-2.003614	0.231159
H	4.361048	-4.355347	-0.561706
H	2.056869	-3.409942	-0.399318
H	6.321003	-2.803878	-0.440446
H	7.160822	-0.423644	-0.200641
H	0.770728	2.630181	0.302822
H	2.523535	4.467519	0.456105
H	4.937182	3.836237	0.322055
H	6.671430	1.974308	0.073865
H	-5.899944	2.256254	0.683951
H	-3.411553	2.404124	0.543543
C	-7.422523	-0.059670	0.590279
N	-8.261387	0.828893	-0.044349
C	-9.681688	0.730000	0.225310
H	-10.112564	1.735550	0.306884
H	-10.206218	0.192955	-0.578809
H	-9.824668	0.185241	1.158307
C	-7.912398	1.610851	-1.213189

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H	-8.109941	2.679011	-1.048521
H	-6.859411	1.484047	-1.462116
H	-8.512527	1.286014	-2.075908

TS5$_{p\text{-C(O)NMe2}}$

E = -1436.069355 a.u.

Cu	-0.165914	-0.427185	0.288760
C	1.791606	-0.610795	0.320456
C	2.473963	-0.029710	1.406083
C	3.714895	0.577284	1.240792
C	4.313866	0.629559	-0.025080
C	3.675112	0.003311	-1.104389
C	2.442444	-0.621408	-0.925392
O	6.513748	1.018792	0.760427
H	2.032531	-0.093463	2.398903
H	4.250512	0.999594	2.087009
H	4.164559	-0.028664	-2.075615
H	1.987236	-1.158877	-1.754518
C	0.785046	-2.327837	0.771477
O	0.582265	-2.337840	1.970220
O	0.758244	-3.032349	-0.219736
C	-1.705226	3.672205	1.092903
C	-0.845177	2.566667	0.965495
N	-1.264352	1.377890	0.558398
C	-2.572051	1.219213	0.251402
C	-3.516910	2.266558	0.345641
C	-3.041355	3.521556	0.782514
C	-2.996459	-0.087248	-0.185527
C	-4.884848	2.007676	0.003912
N	-2.053593	-1.053085	-0.261651
C	-2.405733	-2.271080	-0.651804
C	-3.732145	-2.592829	-0.993780
C	-4.703488	-1.615459	-0.926084
C	-4.352074	-0.312253	-0.511544
C	-5.284968	0.771165	-0.406238
H	-1.310049	4.624079	1.433274
H	0.213272	2.645379	1.200664
H	-3.731775	4.356857	0.871704
H	-5.602169	2.820774	0.080899
H	-1.602326	-3.003738	-0.689282
H	-3.972214	-3.604131	-1.305949
H	-5.735958	-1.836315	-1.186120
H	-6.325699	0.586697	-0.660372
C	5.686881	1.225782	-0.123490
N	6.001540	1.964646	-1.244173
C	7.369390	2.420745	-1.389306
H	7.671013	2.350284	-2.441577
H	7.481598	3.466447	-1.066071
H	8.015603	1.796184	-0.772898
C	5.039616	2.640901	-2.090019
H	5.171712	2.361721	-3.144472
H	4.021564	2.395530	-1.788969
H	5.170215	3.730620	-2.011317

5$_{m\text{-C(O)NMe2}}$

E = -1436.126211 a.u.

Cu	0.522219	0.395223	-0.035225
C	-3.326595	-1.049982	-0.329176
C	-1.824565	-0.973436	-0.189610
O	-1.349298	0.228175	-0.143176
O	-1.171997	-2.024274	-0.131251
C	-4.111066	0.102048	-0.403404
C	-5.502019	0.011206	-0.510884
C	-6.103344	-1.251333	-0.591168
C	3.469414	3.549967	0.061908
C	2.256864	2.842656	0.019071
N	2.194501	1.514621	0.033044
C	3.357291	0.815591	0.090510
C	4.626060	1.437916	0.137347
C	4.655958	2.848011	0.121429
C	3.269460	-0.622865	0.101292
C	5.803431	0.621384	0.196776
N	2.034565	-1.159743	0.051580
C	1.900209	-2.477112	0.056359
C	3.013896	-3.339183	0.113600
C	4.284321	-2.802698	0.165375
C	4.447868	-1.399895	0.159727
C	5.718411	-0.738786	0.207818
C	-5.321588	-2.404774	-0.542340
C	-3.940685	-2.304787	-0.400037
H	-3.632167	1.074872	-0.380663
H	3.455742	4.635086	0.047136
H	1.306924	3.366544	-0.028798
H	5.610666	3.367279	0.155468
H	6.772429	1.112773	0.232596
H	0.871784	-2.831183	0.011163
H	2.859695	-4.413879	0.115599
H	5.160653	-3.445330	0.209593
H	6.620013	-1.344830	0.252701
H	-5.793514	-3.381535	-0.618912
H	-3.308832	-3.186314	-0.350202
H	-7.181070	-1.329266	-0.714487
O	-5.894583	2.162633	-1.425041
C	-6.285652	1.283220	-0.663698
N	-7.468803	1.402862	0.033257
C	-7.797677	0.669439	1.238572
H	-8.767651	0.162396	1.141764
H	-7.033302	-0.075620	1.456655
H	-7.861291	1.358497	2.093707
C	-8.283044	2.575896	-0.211956
H	-8.140497	3.334708	0.571780
H	-7.995762	3.007903	-1.170442
H	-9.342893	2.292970	-0.229474

TS5$_{m\text{-C(O)NMe2}}$

E = -1436.068161 a.u.

Cu	-0.058956	-0.360785	-0.730773
C	-1.961412	-0.418296	-1.236090
C	-2.378083	0.358533	-2.332566
C	-3.622217	0.987914	-2.340381
C	-4.473758	0.860226	-1.243240
C	-4.095297	0.076177	-0.144915
C	-2.862075	-0.586270	-0.172312
H	-1.728033	0.427073	-3.202775
H	-3.941777	1.563185	-3.207121
H	-2.620910	-1.268145	0.639521
C	-0.910794	-2.075916	-1.781704
O	-0.440974	-1.869919	-2.884717
O	-1.118689	-2.954742	-0.968437
C	1.774112	3.679684	-0.350206
C	0.871398	2.641563	-0.641870
N	1.137332	1.368992	-0.387629
C	2.325458	1.053704	0.177319
C	3.300946	2.022255	0.508398
C	2.989295	3.369239	0.225334
C	2.585678	-0.339409	0.441066
C	4.535689	1.598238	1.100534
N	1.619171	-1.224759	0.110884
C	1.822416	-2.516788	0.332131
C	3.014416	-2.998964	0.903901
C	4.007542	-2.106230	1.250014
C	3.813250	-0.726274	1.022525
C	4.781385	0.280404	1.345611
H	1.506168	4.705869	-0.581038
H	-0.094996	2.846560	-1.095449
H	3.709280	4.148943	0.462128
H	5.277949	2.352251	1.349783
H	1.007810	-3.177007	0.041518
H	3.135208	-4.065402	1.064915
H	4.937836	-2.451535	1.694696
H	5.722548	-0.029013	1.793099
H	-5.453776	1.331845	-1.257746
O	-5.161395	-1.341696	1.427862
C	-5.024498	-0.199596	1.001948
N	-5.747823	0.854528	1.521611
C	-6.733000	0.557880	2.542024
H	-6.338081	0.749206	3.551060
H	-7.619155	1.187058	2.392911

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H	-7.006238	-0.494754	2.470875
C	-5.360976	2.247232	1.432938
H	-6.181567	2.862455	1.038397
H	-5.101613	2.632316	2.430737
H	-4.493193	2.364931	0.784515

5$_{o\text{-}C(O)NMe2}$

E = -1436.122676 a.u.

Cu	0.264564	-0.423256	-0.531835
C	-3.753201	0.450567	-0.320342
C	-2.253342	0.615508	-0.380932
O	-1.608743	-0.454009	-0.717946
O	-1.754276	1.716037	-0.115483
C	-4.397865	-0.782063	-0.522253
C	-5.792921	-0.848244	-0.426580
C	-6.546939	0.289494	-0.151635
C	3.590489	-3.165018	-0.754542
C	2.299765	-2.611958	-0.773503
N	2.061438	-1.326010	-0.534050
C	3.115039	-0.516579	-0.252498
C	4.450161	-0.980570	-0.212658
C	4.667794	-2.349018	-0.476203
C	2.835907	0.870945	0.019356
C	5.503471	-0.056016	0.090703
N	1.544749	1.254573	-0.021705
C	1.235928	2.517825	0.227966
C	2.220399	3.479214	0.533166
C	3.546551	3.100366	0.577420
C	3.895399	1.756661	0.317737
C	5.238013	1.256481	0.344009
C	-5.908342	1.514052	0.043974
C	-4.522300	1.584699	-0.036833
O	-3.489161	-2.841786	0.227475
H	-6.286806	-1.807022	-0.564305
H	-7.629996	0.217430	-0.084839
H	3.721461	-4.222982	-0.958047
H	1.431847	-3.228493	-0.986837
H	5.679224	-2.747531	-0.455192
H	6.525247	-0.426175	0.116116
H	0.172495	2.745766	0.182806
H	1.924176	4.504668	0.731670
H	4.326055	3.821725	0.811668
H	6.046764	1.945903	0.573742
H	-6.488887	2.407004	0.262898
H	-3.991962	2.518805	0.120836
C	-3.680032	-2.097904	-0.727815
N	-3.428622	-2.477078	-2.022280
C	-3.418937	-1.551853	-3.132809
H	-4.056599	-0.693978	-2.916322
H	-2.402960	-1.185712	-3.337846
H	-3.803966	-2.050999	-4.031110
C	-2.732815	-3.725480	-2.238265
H	-2.837135	-4.336700	-1.341303
H	-3.161020	-4.249916	-3.101601
H	-1.662183	-3.554817	-2.431685

TS5$_{o\text{-}C(O)NMe2}$

E = -1436.080669 a.u.

Cu	0.467537	-0.159046	-0.123631
C	2.365912	0.200573	-0.594148
C	3.134909	0.172877	0.589956
C	4.259285	0.989241	0.747104
C	4.648959	1.841398	-0.286801
C	3.923146	1.859083	-1.478641
C	2.805201	1.036313	-1.629327
H	4.813462	0.981901	1.683986
H	5.518108	2.483056	-0.162640
H	4.238247	2.507012	-2.294446
H	2.270590	1.008226	-2.576521
C	1.726098	-1.586303	-1.349680
O	2.027482	-2.461611	-0.558099
O	1.378660	-1.403888	-2.495775
C	-1.834364	3.647574	0.226903
C	-0.773117	2.729943	0.132528
N	-0.961074	1.421075	0.056877
C	-2.227134	0.946117	0.069974
C	-3.362614	1.784770	0.161523
C	-3.130604	3.174030	0.241103
C	-2.400367	-0.482657	-0.013626
C	-4.669293	1.195448	0.171932
N	-1.284421	-1.240732	-0.108269
C	-1.408221	-2.559275	-0.180527
C	-2.659976	-3.199920	-0.166227
C	-3.806996	-2.437922	-0.077311
C	-3.702059	-1.033145	0.002825
C	-4.831488	-0.155282	0.097289
H	-1.622565	4.710567	0.287390
H	0.260773	3.065257	0.115889
H	-3.973670	3.857146	0.312928
H	-5.533990	1.850707	0.242163
H	-0.478849	-3.117743	-0.258600
H	-2.707066	-4.282323	-0.231681
H	-4.789007	-2.904958	-0.069552
H	-5.827632	-0.590795	0.107227
C	2.577863	-0.638914	1.714327
O	1.357419	-0.569838	1.949307
N	3.404871	-1.380252	2.499606
C	4.686591	-1.894187	2.050082
H	4.951621	-1.462557	1.086373
H	5.474835	-1.665083	2.778742
H	4.628035	-2.984387	1.931353
C	2.827457	-2.074504	3.635257
H	2.501545	-3.086839	3.358079
H	3.578326	-2.151756	4.429758
H	1.962356	-1.518077	3.995322

1O$_{p\text{-}NH2}$

E = -1175.560858 a.u.

Ag	-1.831748	-1.162218	0.010191
O	0.270925	-1.400714	0.028463
O	-0.045736	0.821933	-0.018553
C	0.700467	-0.182525	0.010034
O	-3.903323	-0.503090	0.033306
S	-4.068083	0.937029	-0.521597
C	-5.715881	1.409112	0.055966
C	-3.082675	2.025875	0.534253
H	-6.436591	0.768298	-0.457416
H	-5.901626	2.456633	-0.200054
H	-5.778527	1.250473	1.136140
H	-3.363764	1.877678	1.581450
H	-3.259747	3.060979	0.223048
H	-2.028255	1.759960	0.379925
C	2.182852	-0.009472	0.022741
C	2.739118	1.274532	-0.006006
C	3.048024	-1.109707	0.061146
C	4.113793	1.459934	0.000691
H	2.066585	2.126428	-0.037361
C	4.424494	-0.935282	0.068634
H	2.621379	-2.107619	0.081818
C	4.981591	0.354744	0.037887
H	4.529146	2.466098	-0.018056
H	5.083087	-1.801480	0.102938
N	6.358956	0.534965	0.097880
H	6.910681	-0.249176	-0.223248
H	6.696069	1.411918	-0.275834

TS3$_{p\text{-}NH2}$

E = -1175.505402 a.u.

Ag	0.700629	-0.636712	-0.142765
O	0.044916	2.209330	-1.412883
O	0.414319	2.177891	0.863762
C	0.038201	1.901053	-0.252515
O	2.777107	-1.296332	-0.041340
S	3.809482	-0.168476	-0.297134
C	3.695950	0.975552	1.101252
C	5.381966	-0.954604	0.127014
H	2.722271	1.475472	1.043630
H	4.496693	1.716788	1.008626

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H	3.780229	0.420769	2.040533
H	5.311212	-1.387811	1.128636
H	6.183857	-0.212152	0.073432
H	5.556931	-1.743331	-0.608434
C	-1.224374	0.238866	-0.090778
C	-1.874044	0.189763	1.161956
C	-2.041718	0.046964	-1.227144
C	-3.234347	-0.060752	1.282480
H	-1.299019	0.396031	2.062551
C	-3.400688	-0.208331	-1.126268
H	-1.599319	0.142611	-2.216409
C	-4.020085	-0.272223	0.136085
H	-3.704992	-0.081253	2.264464
H	-4.002282	-0.347236	-2.023514
N	-5.369928	-0.564799	0.245904
H	-5.817248	-0.268994	1.102673
H	-5.931396	-0.369180	-0.571496

1O$_{m\text{-NH2}}$
E = -1175.558642 a.u.

Ag	1.796587	-1.164215	-0.063640
O	-0.261603	-1.644386	-0.042283
O	-0.228590	0.600067	-0.025225
C	-0.837912	-0.490922	-0.021565
O	3.783093	-0.290790	-0.022346
S	3.792998	1.179369	-0.520305
C	2.697799	2.114305	0.574647
C	5.381135	1.801795	0.080864
H	1.677936	1.742630	0.408708
H	2.760880	3.173661	0.303672
H	2.995093	1.957647	1.616076
H	5.461619	1.607317	1.153991
H	5.453043	2.872625	-0.132315
H	6.165801	1.263148	-0.455577
C	-2.340181	-0.509804	0.006652
C	-3.028405	0.703711	0.014864
C	-3.044448	-1.718524	0.020181
C	-4.428086	0.735722	0.036499
H	-2.450140	1.623929	0.006141
C	-4.436101	-1.690973	0.043575
H	-2.494997	-2.653206	0.010611
C	-5.126580	-0.481738	0.051824
H	-4.997143	-2.622689	0.053439
H	-6.215028	-0.475100	0.075471
N	-5.113228	1.952518	0.099940
H	-6.049872	1.925043	-0.281889
H	-4.593974	2.738845	-0.268664

TS3$_{m\text{-NH2}}$
E = -1175.502168 a.u.

Ag	-0.573651	-0.429255	-0.379408
O	0.300264	0.906763	2.330319
O	-0.465950	2.336220	0.690920
C	0.103505	1.437113	1.269516
O	-2.628151	-1.103013	-0.638295
S	-3.623027	-0.529896	0.404454
C	-3.743502	1.249040	0.092990
C	-5.230611	-1.028013	-0.256949
H	-2.779385	1.698623	0.357059
H	-4.529907	1.660514	0.734462
H	-3.965983	1.424561	-0.963780
H	-5.311111	-0.698928	-1.296732
H	-6.025074	-0.593812	0.357371
H	-5.276332	-2.118362	-0.206338
C	1.331542	0.481675	-0.106763
C	1.706778	1.298846	-1.190684
C	2.302741	-0.348725	0.476286
C	3.011291	1.253416	-1.682181
H	0.988204	1.998755	-1.609813
C	3.616377	-0.403495	-0.010970
H	2.038410	-0.932866	1.356928
C	3.956157	0.409176	-1.105760
H	3.306814	1.892140	-2.512160
H	4.973743	0.386903	-1.492677
N	4.552626	-1.277308	0.544835
H	4.357056	-1.540431	1.502313
H	5.516355	-0.988680	0.435648

1O$_{o\text{-NH2}}$
E = -1175.564703 a.u.

Ag	1.106638	-0.042518	0.035022
O	-0.825681	-0.883743	-0.077291
O	-1.218445	1.300000	0.204602
C	-1.627497	0.115565	0.057677
O	2.908999	1.140019	0.284415
S	2.675519	2.653918	0.038081
C	1.426145	3.190934	1.231566
C	4.127943	3.419368	0.796364
H	0.487685	2.689129	0.963810
H	1.309769	4.276767	1.148780
H	1.733622	2.905352	2.242179
H	4.228680	3.061858	1.824860
H	4.019978	4.507808	0.765398
H	4.998097	3.116253	0.209363
C	-3.084853	-0.196513	0.016454
C	-4.078811	0.803134	0.201394
C	-3.485915	-1.515568	-0.246534
C	-5.433781	0.426382	0.090274
C	-4.822186	-1.872438	-0.345536
H	-2.702763	-2.254722	-0.380399
C	-5.797005	-0.882738	-0.178416
H	-6.199266	1.187421	0.231825
H	-5.105380	-2.900476	-0.552925
H	-6.852198	-1.136341	-0.256445
N	-3.754121	2.097457	0.525539
H	-4.435265	2.806462	0.297734
H	-2.772760	2.321465	0.379444

TS3$_{o\text{-NH2}}$
E = -1175.512056 a.u.

Ag	0.160611	-0.656597	-0.124239
O	-0.763070	2.051845	-1.618215
O	-0.326430	2.245242	0.639101
C	-0.700228	1.850571	-0.433905
O	2.272703	-1.181093	-0.001360
S	3.240090	-0.012246	-0.314939
C	3.080754	1.177483	1.040349
C	4.857315	-0.697054	0.116888
H	2.085602	1.629068	0.966451
H	3.845908	1.951103	0.917226
H	3.192299	0.662770	1.999317
H	4.821557	-1.094375	1.135115
H	5.618525	0.083324	0.023500
H	5.064162	-1.503712	-0.590246
C	-1.827837	0.055437	-0.083830
C	-2.400821	0.117900	1.203478
C	-2.679067	-0.299281	-1.167355
C	-3.730625	-0.211338	1.445310
H	-1.779078	0.463986	2.026806
C	-4.024288	-0.627743	-0.922956
C	-4.534722	-0.596027	0.368448
H	-4.142035	-0.157425	2.449864
H	-4.669772	-0.901216	-1.756665
H	-5.579699	-0.850514	0.532963
N	-2.166387	-0.343180	-2.456573
H	-1.445269	0.360993	-2.595371
H	-2.870702	-0.302104	-3.183652

1O$_{p\text{-OH}}$
E = -1195.415412 a.u.

Ag	-1.271679	-1.248486	0.113323
O	0.520319	0.740339	0.060530
O	0.832758	-1.483096	0.108877
C	1.261777	-0.265999	0.080518
O	-3.342369	-0.593034	0.145823
S	-3.520321	0.833574	-0.440028
C	-5.168139	1.306602	0.135831
C	-2.536502	1.951389	0.586587

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H	-5.886688	0.649213	-0.359279
H	-5.362826	2.346694	-0.142830
H	-5.224022	1.171923	1.219610
H	-2.812012	1.825711	1.638170
H	-2.719930	2.978235	0.252707
H	-1.481560	1.687881	0.433912
C	2.747720	-0.095359	0.070289
C	3.605185	-1.199632	0.094402
C	3.303186	1.189961	0.035766
C	4.984787	-1.026852	0.084510
C	4.678225	1.375642	0.025492
C	5.525579	0.262732	0.049972
H	5.645050	-1.893449	0.103346
H	3.174891	-2.195584	0.120695
H	2.629427	2.040962	0.016706
H	5.117120	2.368711	-0.001445
O	6.867162	0.493383	0.038737
H	7.328220	-0.357755	0.057834

TS3$_{p\text{-OH}}$
E = -1195.359143 a.u.

Ag	-0.237113	-0.540950	-0.327764
O	0.691741	1.305087	2.071556
O	0.157519	2.382002	0.103652
C	0.599572	1.591828	0.908420
O	-2.351307	-1.021787	-0.530782
S	-3.285442	-0.149573	0.348353
C	-3.218324	1.530165	-0.322541
C	-4.933912	-0.608191	-0.235873
H	-2.212587	1.923004	-0.134181
H	-3.957513	2.143324	0.203517
H	-3.419605	1.507425	-1.397743
H	-4.976188	-0.497724	-1.323032
H	-5.680082	0.023924	0.254810
H	-5.094461	-1.653239	0.039204
C	1.739133	0.211750	-0.131969
C	2.279915	0.747448	-1.318425
C	2.612813	-0.545485	0.680998
C	3.600629	0.519826	-1.693702
H	1.660154	1.391164	-1.939101
C	3.930673	-0.788858	0.321854
C	4.426763	-0.258331	-0.875730
H	3.999237	0.957150	-2.609285
H	2.251059	-0.917604	1.636881
H	4.598636	-1.366680	0.954649
O	5.725916	-0.512313	-1.181693
H	5.940362	-0.075051	-2.018829

1O$_{m\text{-OH}}$
E = -1195.413263 a.u.

Ag	-1.258716	-1.230371	0.123449
O	0.541439	0.760662	0.049869
O	0.844666	-1.463165	0.107531
C	1.275690	-0.248645	0.070769
O	-3.331414	-0.590206	0.163588
S	-3.522683	0.830530	-0.433082
C	-5.169024	1.298144	0.151040
C	-2.538447	1.963277	0.576819
H	-5.887289	0.633084	-0.334130
H	-5.371589	2.335066	-0.133680
H	-5.216343	1.171041	1.236159
H	-2.807997	1.848046	1.631096
H	-2.727570	2.985716	0.232711
H	-1.483051	1.703412	0.421883
C	2.770535	-0.085886	0.051533
C	3.615156	-1.202481	0.080495
C	3.307921	1.200336	0.004230
C	4.993529	-1.018237	0.061901
C	4.691306	1.377332	-0.014419
C	5.537650	0.265336	0.014589
H	5.658813	-1.877983	0.084136
H	6.618574	0.402331	0.000131
H	3.177815	-2.194011	0.116657
H	2.646296	2.059425	-0.018389
O	5.163749	2.657327	-0.061012
H	6.131108	2.629076	-0.069702

TS3$_{m\text{-OH}}$
E = -1195.356059 a.u.

Ag	-0.210808	-0.506157	-0.273205
O	0.680244	1.312586	2.112612
O	0.153284	2.399362	0.148549
C	0.597764	1.604006	0.948877
O	-2.313551	-1.017988	-0.495357
S	-3.273938	-0.145151	0.355358
C	-3.208462	1.527806	-0.332150
C	-4.904633	-0.626019	-0.259807
H	-2.210462	1.932477	-0.127948
H	-3.963890	2.139278	0.172431
H	-3.388382	1.491135	-1.410726
H	-4.924817	-0.523673	-1.348397
H	-5.667775	0.001569	0.210116
H	-5.059677	-1.670669	0.019783
C	1.770555	0.267153	-0.086229
C	2.275279	0.782424	-1.297256
C	2.615166	-0.520556	0.713809
C	3.576924	0.492777	-1.700952
H	1.654976	1.447748	-1.892600
C	3.917509	-0.815628	0.305052
C	4.397473	-0.308262	-0.907257
H	3.969285	0.900286	-2.630223
H	5.419255	-0.522904	-1.219622
H	2.279379	-0.877967	1.683885
O	4.680697	-1.593889	1.125089
H	5.555713	-1.703965	0.725992

1O$_{o\text{-OH}}$
E = -1195.430102 a.u.

Ag	-1.256140	-1.175184	0.134369
O	0.577641	0.816275	0.042655
O	0.846452	-1.404613	0.120488
C	1.317503	-0.214551	0.070850
O	-3.335398	-0.573780	0.172344
S	-3.579307	0.836131	-0.430050
C	-5.245930	1.239580	0.142366
C	-2.646162	2.004540	0.588304
H	-5.933404	0.545387	-0.346550
H	-5.487460	2.266854	-0.146830
H	-5.295659	1.112675	1.227319
H	-2.913328	1.873862	1.641293
H	-2.871050	3.021013	0.248741
H	-1.582511	1.785927	0.436892
C	2.792570	-0.055261	0.044014
C	3.631577	-1.179037	0.077740
C	3.370391	1.236808	-0.017383
C	5.011650	-1.046514	0.052346
C	4.767839	1.363816	-0.043172
C	5.573153	0.235336	-0.008585
H	5.648967	-1.925894	0.079032
H	5.190775	2.363024	-0.090730
H	6.654447	0.352831	-0.029371
H	3.163792	-2.157631	0.124134
O	2.628553	2.352481	-0.052469
H	1.682546	2.032168	-0.026679

TS3$_{o\text{-OH}}$
E = -1195.371574 a.u.

Ag	-0.257272	-0.504052	-0.303026
O	0.720485	1.206950	2.183043
O	0.282369	2.480990	0.304871
C	0.639559	1.620383	1.054617
O	-2.366223	-0.967268	-0.559937
S	-3.338448	-0.133998	0.312222
C	-3.311213	1.552255	-0.347467
C	-4.964261	-0.635395	-0.299113
H	-2.325671	1.974860	-0.128300
H	-4.083611	2.139825	0.159396
H	-3.478951	1.530170	-1.428315

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H	-4.994558	-0.517545	-1.385887
H	-5.735918	-0.030442	0.186331
H	-5.096322	-1.687121	-0.034640
C	1.739363	0.152455	-0.139611
C	2.271543	0.711009	-1.321583
C	2.620237	-0.594767	0.676110
C	3.584390	0.479397	-1.718756
H	1.635614	1.352569	-1.928904
C	3.941911	-0.838318	0.284081
C	4.410191	-0.313748	-0.914822
H	3.967617	0.914329	-2.638312
H	4.585644	-1.419597	0.938586
H	5.439358	-0.501480	-1.212956
O	2.216258	-1.093521	1.870658
H	1.487954	-0.514050	2.176222

$5_{p\text{-}NH2}$

E = -1244.239955 a.u.

Cu	0.168987	-0.846178	-0.021893
C	-3.903802	-0.281067	-0.022858
C	-2.424519	-0.032578	-0.032185
O	-1.692344	-1.104621	-0.023985
O	-2.000821	1.132911	-0.046899
C	-4.439082	-1.573839	-0.004999
C	-5.812337	-1.780444	-0.000372
C	-6.698198	-0.690479	-0.013017
C	1.721993	3.379197	-0.004751
C	0.840111	2.279342	-0.014736
N	1.280284	1.030533	-0.013728
C	2.607065	0.799183	-0.003040
C	3.571815	1.831319	0.007077
C	3.083894	3.156637	0.006017
C	3.028714	-0.578688	-0.002181
C	4.962662	1.487083	0.017718
N	2.060398	-1.531396	-0.011525
C	2.433544	-2.807871	-0.010800
C	3.778773	-3.210574	-0.000864
C	4.768874	-2.249328	0.008794
C	4.409077	-0.885684	0.008392
C	5.363676	0.184495	0.018250
C	-6.162853	0.608399	-0.029416
C	-4.788786	0.802503	-0.033742
H	-3.756745	-2.418072	0.002270
H	-6.211563	-2.793446	0.018210
H	1.319917	4.387767	-0.005698
H	-0.244274	2.377474	-0.023955
H	3.785925	3.987347	0.013736
H	5.698058	2.287964	0.025446
H	1.632388	-3.540775	-0.018215
H	4.019699	-4.268834	-0.000730
H	5.819434	-2.529669	0.016802
H	6.421471	-0.066091	0.026396
H	-6.835927	1.464425	-0.033946
H	-4.369458	1.804192	-0.048843
N	-8.076357	-0.891992	0.045720
H	-8.631553	-0.132713	-0.326387
H	-8.388971	-1.786697	-0.307778

$TS5_{p\text{-}NH2}$

E = -1244.182245 a.u.

Cu	-0.587650	-0.351113	-0.097731
C	-2.521241	-0.243207	-0.302747
C	-3.074136	-0.546801	-1.561503
C	-4.227303	0.072192	-2.032057
C	-4.903131	1.013441	-1.238555
C	-4.393791	1.299958	0.039077
C	-3.237031	0.673889	0.490615
H	-2.600241	-1.307656	-2.178859
H	-4.631243	-0.189518	-3.009636
H	-4.929310	1.996950	0.683295
C	-1.861251	-1.937910	0.778621
O	-1.827234	-2.881255	0.016129
O	-1.831383	-1.621693	1.947423
C	1.514001	3.627937	-0.213145
C	0.505941	2.646798	-0.181456
N	0.770999	1.350553	-0.144603
C	2.061541	0.951102	-0.141546
C	3.148488	1.855177	-0.169187
C	2.835667	3.230921	-0.205717
C	2.313593	-0.467827	-0.108104
C	4.486645	1.341327	-0.156008
N	1.239896	-1.290306	-0.094273
C	1.434205	-2.602909	-0.060467
C	2.721296	-3.170254	-0.040193
C	3.825014	-2.342834	-0.057930
C	3.643842	-0.943340	-0.093957
C	4.723385	-0.000172	-0.117991
H	1.242336	4.678556	-0.240636
H	-0.547077	2.917919	-0.184729
H	3.638218	3.964376	-0.227382
H	5.314445	2.045762	-0.174985
H	0.532592	-3.211538	-0.048426
H	2.827439	-4.249961	-0.011065
H	4.831499	-2.754298	-0.043975
H	5.742627	-0.378142	-0.106296
H	-2.890189	0.878656	1.502223
N	-6.096624	1.586659	-1.674796
H	-6.329194	2.470422	-1.241551
H	-6.210854	1.620846	-2.679109

$5_{m\text{-}NH2}$

E = -1244.238378 a.u.

Cu	0.154396	-0.823896	-0.031047
C	-3.929620	-0.291750	-0.024547
C	-2.443382	-0.029988	-0.048974
O	-1.706277	-1.095030	-0.023279
O	-2.030725	1.137682	-0.090961
C	-4.440849	-1.593174	0.017098
C	-5.820343	-1.781979	0.034762
C	-6.690589	-0.694792	0.011213
C	1.723583	3.390089	-0.016724
C	0.837356	2.293964	-0.030615
N	1.272062	1.043297	-0.026352
C	2.598191	0.806259	-0.008840
C	3.567201	1.834380	0.005014
C	3.084474	3.161699	0.000849
C	3.014381	-0.573209	-0.004867
C	4.956759	1.484149	0.022172
N	2.042540	-1.521765	-0.017267
C	2.409428	-2.799908	-0.014401
C	3.752863	-3.208354	0.000985
C	4.746968	-2.251355	0.014313
C	4.393373	-0.886150	0.011707
C	5.352329	0.179950	0.025135
C	-6.187083	0.614478	-0.031509
C	-4.799312	0.798306	-0.048745
H	-3.752753	-2.430997	0.033340
H	-6.230501	-2.789210	0.065702
H	-7.767339	-0.855701	0.031738
H	1.325932	4.400372	-0.020129
H	-0.246190	2.399140	-0.046068
H	3.789774	3.989568	0.011500
H	5.695550	2.281840	0.032787
H	1.604867	-3.529050	-0.024360
H	3.989439	-4.267590	0.002608
H	5.796227	-2.536306	0.026865
H	6.409022	-0.074995	0.038083
H	-4.367575	1.795595	-0.079137
N	-7.052749	1.713795	0.000881
H	-6.652887	2.560516	-0.383047
H	-7.966266	1.534505	-0.396107

$TS5_{m\text{-}NH2}$

E = -1244.180632 a.u.

Cu	-0.602788	-0.331273	-0.051190
C	-2.546345	-0.220847	-0.275618
C	-3.005218	-0.447846	-1.585489
C	-4.105179	0.257350	-2.072872

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C	-4.782775	1.167135	-1.264000
C	-4.372328	1.377960	0.062055
C	-3.253133	0.676618	0.536451
H	-2.518786	-1.197092	-2.205507
H	-4.456394	0.088670	-3.089434
H	-5.658190	1.691158	-1.644841
C	-1.882480	-1.886279	0.777869
O	-1.847897	-2.835674	0.019081
O	-1.848558	-1.586506	1.954789
C	1.484013	3.610699	-0.347018
C	0.477079	2.631566	-0.267257
N	0.743811	1.337336	-0.184087
C	2.035491	0.938520	-0.179806
C	3.120612	1.841879	-0.253065
C	2.806101	3.214944	-0.338237
C	2.290101	-0.477806	-0.097736
C	4.459553	1.330218	-0.235821
N	1.217788	-1.299302	-0.042823
C	1.411427	-2.609826	0.030379
C	2.699332	-3.175854	0.055391
C	3.802353	-2.349156	-0.001138
C	3.620678	-0.951454	-0.082730
C	4.698700	-0.008871	-0.152290
H	1.211063	4.659225	-0.412989
H	-0.576100	2.901452	-0.270528
H	3.607574	3.947520	-0.396619
H	5.285940	2.034418	-0.289765
H	0.509055	-3.216521	0.067178
H	2.806739	-4.254002	0.117951
H	4.808980	-2.760213	0.015462
H	5.718591	-0.384985	-0.138874
H	-2.951554	0.792986	1.577473
N	-5.106028	2.215566	0.907739
H	-4.590195	2.558622	1.707284
H	-5.603424	2.961979	0.439938

$5_{o\text{-}NH2}$

E = -1244.245091 a.u.

Cu	0.066310	-0.605533	-0.006018
C	4.123076	0.105892	0.004633
C	2.638530	0.301773	-0.030527
O	1.938322	-0.783270	0.031460
O	2.145483	1.448099	-0.126956
C	4.638342	-1.198111	0.001788
C	6.002305	-1.454240	-0.016761
C	6.889253	-0.372990	-0.034639
C	-1.780384	3.481833	-0.036166
C	-0.824150	2.446678	-0.037744
N	-1.173535	1.169696	-0.026959
C	-2.481385	0.845103	-0.015523
C	-3.516233	1.806937	-0.015084
C	-3.123215	3.163267	-0.025231
C	-2.805217	-0.558780	-0.004435
C	-4.879659	1.365791	-0.004788
N	-1.772319	-1.440117	-0.003134
C	-2.053300	-2.739629	0.005921
C	-3.366839	-3.236552	0.014365
C	-4.422513	-2.347835	0.014083
C	-4.160394	-0.962058	0.004630
C	-5.187951	0.038285	0.004228
C	6.412979	0.927914	-0.023813
C	5.029239	1.201749	0.003075
H	3.920796	-2.012098	0.005355
H	6.372962	-2.475696	-0.021504
H	7.963414	-0.546364	-0.054792
H	-1.450749	4.516255	-0.044012
H	0.249063	2.625789	-0.049351
H	-3.882025	3.942379	-0.024522
H	-5.669499	2.112968	-0.004510
H	-1.202089	-3.413881	0.006965
H	-3.532391	-4.309147	0.021576
H	-5.450497	-2.702058	0.021169
H	-6.225531	-0.285900	0.011685
H	7.109603	1.764771	-0.024219
N	4.589193	2.501223	0.072142
H	5.210557	3.210046	-0.288472
H	3.593668	2.599473	-0.119645

$TS5_{o\text{-}NH2}$

E = -1244.190871 a.u.

Cu	0.719348	-0.415726	0.024862
C	2.632243	-0.102356	-0.077858
C	3.237266	0.661606	0.930695
C	4.369425	1.442016	0.692140
C	4.938800	1.432155	-0.582440
C	4.399103	0.638147	-1.589783
C	3.257403	-0.143975	-1.348356
H	2.812691	0.624510	1.932775
H	4.811529	2.034502	1.489774
H	5.827451	2.025306	-0.789120
H	4.871131	0.610165	-2.571660
C	1.982866	-2.047357	0.679571
O	1.907647	-1.951564	1.882122
O	2.062090	-2.851802	-0.233752
C	-1.299213	3.593462	0.028143
C	-0.309660	2.592584	0.038836
N	-0.603184	1.302901	0.009046
C	-1.898995	0.928340	-0.037008
C	-2.967963	1.852936	-0.050086
C	-2.627774	3.222681	-0.015173
C	-2.174264	-0.486013	-0.077524
C	-4.314395	1.363612	-0.097449
N	-1.114728	-1.328759	-0.073380
C	-1.335129	-2.636619	-0.121554
C	-2.631143	-3.180419	-0.169671
C	-3.719061	-2.332269	-0.171381
C	-3.512251	-0.936736	-0.127471
C	-4.574518	0.026339	-0.133700
H	-1.007719	4.638730	0.054499
H	0.748868	2.839332	0.073641
H	-3.415296	3.972487	-0.023368
H	-5.129641	2.082714	-0.104222
H	-0.450051	-3.267652	-0.127165
H	-2.756454	-4.257811	-0.205085
H	-4.732484	-2.724690	-0.208188
H	-5.599732	-0.333321	-0.169835
N	2.702668	-0.936376	-2.356197
H	3.357449	-1.155129	-3.098907
H	2.308156	-1.788526	-1.958673

$5_{p\text{-}OH}$

E = -1264.094975 a.u.

Cu	0.148054	-0.814743	0.000037
C	-3.924402	-0.217305	0.000101
C	-2.440802	0.023769	0.000076
O	-1.717452	-1.052222	0.000032
O	-2.013771	1.187472	0.000121
C	-4.464125	-1.509632	0.000067
C	-5.838267	-1.712096	0.000091
C	-6.699899	-0.610854	0.000149
C	1.744796	3.393376	-0.000044
C	0.851178	2.303101	-0.000007
N	1.277527	1.049503	0.000004
C	2.601884	0.803591	-0.000019
C	3.577661	1.825353	-0.000055
C	3.104185	3.155905	-0.000067
C	3.009009	-0.578733	-0.000005
C	4.964847	1.466477	-0.000075
N	2.030953	-1.521412	0.000028
C	2.390503	-2.801756	0.000043
C	3.731497	-3.218503	0.000026
C	4.731521	-2.267601	-0.000009
C	4.386075	-0.900215	-0.000025
C	5.352025	0.159745	-0.000061
C	-6.175447	0.685749	0.000183
C	-4.797808	0.873469	0.000159
H	-6.264580	-2.711228	0.000065
H	1.353717	4.406243	-0.000052

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H	-0.231905	2.414024	0.000017
H	3.815248	3.978903	-0.000095
H	5.708662	2.259548	-0.000102
H	1.581748	-3.526290	0.000069
H	3.961354	-4.279200	0.000039
H	5.779108	-2.558912	-0.000024
H	6.407118	-0.102030	-0.000076
H	-6.847090	1.544207	0.000228
H	-3.783808	-2.355227	0.000022
H	-4.370926	1.871813	0.000185
O	-8.040837	-0.858050	0.000170
H	-8.509126	-0.010832	0.000211

TS5$_{p\text{-OH}}$

E = -1264.037911 a.u.

Cu	0.600087	-0.396995	-0.062601
C	2.540330	-0.265246	-0.235935
C	3.208046	0.689046	0.557209
C	4.340659	1.361375	0.110372
C	4.855802	1.072419	-1.157474
C	4.242555	0.101064	-1.954220
C	3.109286	-0.561930	-1.486656
H	4.853022	2.092832	0.730046
C	1.891001	-1.948534	0.825472
O	1.837060	-1.634526	1.995134
O	1.879707	-2.897032	0.066929
C	-1.514971	3.557946	-0.261666
C	-0.501403	2.583444	-0.209386
N	-0.759755	1.286119	-0.156917
C	-2.048264	0.879010	-0.157336
C	-3.139752	1.776431	-0.205184
C	-2.834300	3.153395	-0.258326
C	-2.292996	-0.540682	-0.105380
C	-4.475124	1.255255	-0.194515
N	-1.215154	-1.357024	-0.070685
C	-1.401608	-2.669990	-0.019592
C	-2.685599	-3.244462	-0.001615
C	-3.793681	-2.423523	-0.039774
C	-3.620491	-1.023529	-0.094500
C	-4.705002	-0.086887	-0.139700
H	-1.248786	4.609507	-0.301680
H	0.549867	2.861133	-0.208625
H	-3.640727	3.881908	-0.295757
H	-5.306524	1.954792	-0.229075
H	-0.496553	-3.272896	0.008350
H	-2.786099	-4.324194	0.042172
H	-4.797844	-2.840632	-0.027618
H	-5.722245	-0.470183	-0.130123
H	2.842752	0.883825	1.564005
H	2.672059	-1.350342	-2.095859
H	4.665646	-0.147502	-2.928329
O	5.969917	1.750986	-1.556906
H	6.231622	1.422142	-2.429079

5$_{m\text{-OH}}$

E = -1264.093085 a.u.

Cu	0.144046	-0.802655	0.000004
C	-3.935066	-0.231799	0.000053
C	-2.444787	0.014582	0.000008
O	-1.720865	-1.059301	-0.000007
O	-2.021939	1.178105	0.000053
C	-4.458422	-1.530588	0.000039
C	-5.837045	-1.716134	0.000079
C	-6.700769	-0.620487	0.000135
C	1.746815	3.399860	-0.000057
C	0.851451	2.311083	-0.000035
N	1.275508	1.056682	-0.000018
C	2.599848	0.808608	-0.000022
C	3.577340	1.828770	-0.000043
C	3.105756	3.160122	-0.000061
C	3.005141	-0.574173	-0.000003
C	4.964133	1.467515	-0.000044
N	2.026018	-1.515352	0.000015
C	2.382948	-2.796323	0.000033
C	3.723190	-3.215265	0.000034
C	4.724685	-2.265944	0.000015
C	4.381777	-0.898029	-0.000005
C	5.349374	0.160252	-0.000025
C	-6.175354	0.674650	0.000150
C	-4.793998	0.866722	0.000109
H	-6.252653	-2.721247	0.000067
H	-7.780070	-0.771738	0.000168
H	1.357229	4.413257	-0.000071
H	-0.231048	2.426285	-0.000029
H	3.818055	3.982031	-0.000077
H	5.709244	2.259364	-0.000059
H	1.572723	-3.519227	0.000047
H	3.951567	-4.276294	0.000049
H	5.771783	-2.559004	0.000014
H	6.404057	-0.103154	-0.000026
H	-3.774648	-2.372128	-0.000005
H	-4.378800	1.868864	0.000119
O	-6.969622	1.786680	0.000205
H	-7.894708	1.502581	0.000211

TS5$_{m\text{-OH}}$

E = -1264.037788 a.u.

Cu	0.602738	-0.416524	0.020772
C	2.551117	-0.290170	-0.159041
C	3.186098	0.702034	0.608216
C	4.285659	1.395278	0.100084
C	4.786779	1.102676	-1.166926
C	4.187835	0.092481	-1.924982
C	3.086024	-0.600772	-1.418353
H	4.774193	2.161144	0.699867
H	5.652490	1.620786	-1.569797
C	1.886317	-1.942574	0.892760
O	1.814787	-1.629712	2.064095
O	1.883586	-2.900658	0.143072
C	-1.460732	3.532693	-0.239689
C	-0.457982	2.549416	-0.156087
N	-0.730862	1.254543	-0.110144
C	-2.022966	0.858991	-0.147748
C	-3.103541	1.766484	-0.230747
C	-2.783325	3.140436	-0.276399
C	-2.282503	-0.558078	-0.098380
C	-4.443417	1.257416	-0.261040
N	-1.213820	-1.383411	-0.025864
C	-1.412198	-2.694261	0.025216
C	-2.701227	-3.257515	0.005114
C	-3.800391	-2.427268	-0.072611
C	-3.613909	-1.028922	-0.127863
C	-4.687576	-0.082459	-0.210788
H	-1.183702	4.581631	-0.273049
H	0.595695	2.815951	-0.124724
H	-3.581104	3.876603	-0.339637
H	-5.266794	1.964413	-0.323636
H	-0.513299	-3.304280	0.083077
H	-2.812947	-4.336072	0.050821
H	-4.807824	-2.836176	-0.090968
H	-5.708188	-0.456088	-0.232815
H	2.834539	0.899696	1.618469
H	2.657448	-1.425721	-1.989142
O	4.728550	-0.181612	-3.149733
H	4.244790	-0.928608	-3.531097

5$_{o\text{-OH}}$

E = -1264.111669 a.u.

Cu	-0.099329	-0.508518	0.000074
C	3.942849	0.317564	0.000004
C	2.458771	0.445878	0.000119
O	1.783577	-0.646369	0.000038
O	1.942749	1.596005	0.000187
C	4.555451	-0.943113	-0.000111
C	5.936863	-1.074778	-0.000219
C	6.731442	0.078337	-0.000224
C	-2.071194	3.513215	0.000046
C	-1.082878	2.508998	0.000072

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N	-1.390055	1.220906	0.000066
C	-2.687492	0.854302	0.000039
C	-3.752018	1.783149	0.000014
C	-3.402859	3.151503	0.000016
C	-2.968194	-0.559094	0.000041
C	-5.101197	1.300058	-0.000010
N	-1.909561	-1.408907	0.000065
C	-2.149884	-2.716344	0.000073
C	-3.447567	-3.253470	0.000057
C	-4.529615	-2.397235	0.000030
C	-4.310363	-1.003941	0.000021
C	-5.368504	-0.036227	-0.000006
C	6.153260	1.339125	-0.000115
C	4.756169	1.477713	0.000005
H	6.395919	-2.059698	-0.000305
H	7.815914	-0.009911	-0.000312
H	-1.773966	4.557333	0.000050
H	-0.017363	2.727318	0.000102
H	-4.186292	3.905756	-0.000004
H	-5.913499	2.022659	-0.000031
H	-1.278424	-3.364248	0.000092
H	-3.580385	-4.330596	0.000065
H	-5.546283	-2.782739	0.000015
H	-6.395535	-0.392352	-0.000024
H	6.757720	2.241656	-0.000121
H	3.909598	-1.815807	-0.000109
O	4.235918	2.712133	0.000080
H	3.243580	2.565207	0.000124

TS5$_{o\text{-}OH}$

E = -1264.051495 a.u.

Cu	0.596029	-0.537166	-0.011816
C	2.484433	-0.185979	-0.217361
C	3.076584	0.787303	0.603832
C	4.193122	1.515020	0.190283
C	4.755561	1.249897	-1.061056
C	4.231423	0.246935	-1.870895
C	3.116001	-0.482034	-1.441463
H	4.626844	2.273346	0.838294
H	5.627446	1.807836	-1.396142
H	4.684975	-0.003452	-2.826503
C	1.820406	-2.098100	0.804125
O	1.785883	-1.883936	1.988010
O	1.905793	-2.974632	-0.042664
C	-1.378549	3.483745	-0.325706
C	-0.398996	2.476392	-0.242601
N	-0.707097	1.192867	-0.154330
C	-2.006905	0.830174	-0.148113
C	-3.066367	1.762184	-0.226919
C	-2.711305	3.125762	-0.316589
C	-2.296197	-0.579063	-0.062876
C	-4.418160	1.285994	-0.213839
N	-1.245160	-1.431532	-0.000837
C	-1.481400	-2.736443	0.061105
C	-2.783278	-3.267106	0.073729
C	-3.861726	-2.409095	0.016198
C	-3.639257	-1.017320	-0.058248
C	-4.691886	-0.046530	-0.132436
H	-1.076271	4.523877	-0.395722
H	0.662911	2.711727	-0.246819
H	-3.491066	3.881044	-0.379110
H	-5.226242	2.010780	-0.271696
H	-0.605076	-3.378145	0.096146
H	-2.920163	-4.342245	0.127632
H	-4.879641	-2.791244	0.024343
H	-5.720863	-0.396844	-0.124975
H	2.652344	0.974744	1.589673
O	2.657874	-1.478014	-2.247890
H	2.222527	-2.127790	-1.653804

1O$_{p\text{-}Cl}$

E = -1579.768717 a.u.

Ag	2.128976	-0.747371	-1.619591
O	0.013865	-0.669364	-1.595375
O	0.587639	-0.005509	0.473486
C	-0.261607	-0.266148	-0.402779
O	4.265407	-0.663884	-1.262648
S	4.628209	-0.770186	0.243461
C	6.341714	-0.194925	0.289870
C	3.841823	0.631718	1.073079
H	6.944830	-0.926912	-0.252379
H	6.674541	-0.137432	1.330658
H	6.408528	0.780470	-0.199962
H	4.126572	1.563348	0.574671
H	4.157984	0.635064	2.121640
H	2.756518	0.480995	1.007776
C	-1.722330	-0.114622	-0.088398
C	-2.114443	0.311169	1.184101
C	-2.700547	-0.392839	-1.048247
C	-3.460625	0.459491	1.501588
H	-1.344340	0.523058	1.919118
C	-4.051452	-0.249232	-0.746742
H	-2.388601	-0.723386	-2.033602
C	-4.418186	0.176607	0.528769
H	-3.769617	0.789515	2.488378
H	-4.814674	-0.463785	-1.488063
Cl	-6.112472	0.359641	0.916518

TS3$_{p\text{-}Cl}$

E = -1579.711363 a.u.

Ag	0.868956	-0.552123	-0.154289
O	0.373405	2.278590	-1.404509
O	0.714039	2.209910	0.874412
C	0.323620	1.956520	-0.246000
O	2.901482	-1.311039	-0.038274
S	4.003597	-0.245804	-0.284882
C	3.963172	0.881629	1.129633
C	5.521636	-1.140010	0.119178
H	3.022358	1.441567	1.079163
H	4.807861	1.573399	1.046559
H	4.013405	0.309397	2.060781
H	5.426869	-1.582359	1.114774
H	6.370037	-0.450755	0.072086
H	5.641056	-1.927006	-0.629088
C	-1.025431	0.441097	-0.109136
C	-1.664832	0.364914	1.143867
C	-1.822865	0.253291	-1.256246
C	-3.024156	0.080461	1.259307
H	-1.090810	0.572877	2.044326
C	-3.181063	-0.036597	-1.165766
H	-1.372825	0.377299	-2.238593
C	-3.766560	-0.126124	0.097822
H	-3.509289	0.031966	2.229589
H	-3.787425	-0.177694	-2.055439
Cl	-5.472065	-0.476684	0.224618

1O$_{m\text{-}Cl}$

E = -1579.768336 a.u.

Ag	2.041313	-1.177151	0.029331
O	-0.000539	-1.756599	0.015029
O	-0.061172	0.488832	0.011874
C	-0.618893	-0.627328	0.009195
O	3.979270	-0.205437	0.070837
S	3.943075	1.234107	-0.509906
C	2.812807	2.190682	0.528920
C	5.507413	1.939958	0.059210
H	1.808963	1.770898	0.386690
H	2.833499	3.233234	0.194146
H	3.114595	2.109180	1.577533
H	5.590296	1.806365	1.141432
H	5.544653	2.999446	-0.211549
H	6.311036	1.399162	-0.446088
C	-2.121243	-0.703744	-0.003228
C	-2.855881	0.485418	-0.012231
C	-2.784785	-1.934114	-0.005846
C	-4.243994	0.426720	-0.023545
H	-2.328661	1.432762	-0.010528
C	-4.176716	-1.973260	-0.017352

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H	-2.196549	-2.845499	0.000943
C	-4.918985	-0.792888	-0.026230
H	-4.695102	-2.928698	-0.019542
H	-6.004214	-0.813352	-0.035261
Cl	-5.167044	1.914249	-0.034722

TS3$_{m\text{-Cl}}$
E = -1579.711012 a.u.

Ag	-0.727207	-0.284040	-0.466298
O	0.079241	0.577170	2.431969
O	-0.726011	2.241938	1.054892
C	-0.118023	1.279712	1.475176
O	-2.754109	-0.963667	-0.848602
S	-3.762687	-0.675513	0.296140
C	-3.988641	1.118887	0.350426
C	-5.347652	-1.130798	-0.443266
H	-3.044336	1.561513	0.687424
H	-4.780038	1.347349	1.071890
H	-4.245240	1.490817	-0.645981
H	-5.464244	-0.609958	-1.397727
H	-6.155652	-0.874097	0.248325
H	-5.328601	-2.210768	-0.607103
C	1.141569	0.652020	0.007644
C	1.493441	1.655721	-0.914639
C	2.140648	-0.247044	0.429627
C	2.788347	1.742452	-1.424993
H	0.748743	2.396520	-1.196529
C	3.426460	-0.154436	-0.091501
H	1.916782	-0.987140	1.192871
C	3.763189	0.832293	-1.019353
H	3.051876	2.527404	-2.130200
H	4.778385	0.894198	-1.399113
Cl	4.659941	-1.282277	0.432600

1O$_{o\text{-Cl}}$
E = -1579.758863 a.u.

Ag	-1.493852	-1.305371	-0.172712
O	0.610577	-1.587520	-0.258882
O	0.354170	0.536724	0.416429
C	1.062485	-0.436080	0.103695
O	-3.537918	-0.603811	0.033526
S	-3.665815	0.932852	-0.151984
C	-5.316252	1.281837	0.499111
C	-2.684637	1.706466	1.155568
H	-6.037137	0.802603	-0.167356
H	-5.479386	2.363766	0.507216
H	-5.401529	0.862804	1.505559
H	-2.992411	1.314689	2.129883
H	-2.833923	2.790168	1.102906
H	-1.632470	1.463210	0.960935
C	2.566121	-0.346764	0.170887
C	3.306393	0.829605	-0.023176
C	3.276042	-1.516806	0.479216
C	4.696973	0.831467	0.097361
C	4.658541	-1.521391	0.618774
H	2.702370	-2.429040	0.606167
C	5.371894	-0.339446	0.427426
H	5.239971	1.755844	-0.072287
H	5.176744	-2.443332	0.868486
H	6.454335	-0.324292	0.526014
Cl	2.563368	2.341905	-0.479426

TS3$_{o\text{-Cl}}$
E = -1579.709077 a.u.

Ag	0.400901	-0.052781	-0.606472
O	-0.797551	0.055196	2.529890
O	0.248496	-1.766763	1.599113
C	-0.476170	-0.790347	1.739369
O	2.494897	0.242472	-1.118101
S	3.438787	0.374884	0.107634
C	3.516993	-1.257544	0.881944
C	5.079572	0.403549	-0.649679
H	2.524801	-1.470429	1.298044
H	4.258556	-1.223150	1.686895
H	3.782549	-2.010227	0.133569
H	5.187140	-0.460414	-1.311340
H	5.840082	0.395831	0.136911
H	5.152641	1.327983	-1.227310
C	-1.561466	-0.594979	0.131964
C	-1.957332	-1.876107	-0.310718
C	-2.517973	0.431127	-0.008614
C	-3.215963	-2.121928	-0.855709
H	-1.255436	-2.694682	-0.167848
C	-3.786035	0.208222	-0.536241
C	-4.131001	-1.076236	-0.960242
H	-3.488782	-3.123215	-1.179047
H	-4.492358	1.028590	-0.621274
H	-5.123192	-1.253166	-1.368194
Cl	-2.124390	2.069475	0.471081

1O$_{p\text{-Br}}$
E = -3691.015818 a.u.

Ag	-1.822588	-1.487018	0.149367
O	0.238280	-1.966643	0.146384
O	0.221384	0.269335	0.371471
C	0.817305	-0.822567	0.274952
O	-3.805147	-0.615897	0.229174
S	-3.819868	0.880353	-0.186318
C	-5.421489	1.455646	0.424349
C	-2.747567	1.758431	0.976161
H	-6.193108	0.940776	-0.152799
H	-5.499829	2.535855	0.268395
H	-5.516149	1.202328	1.483915
H	-3.059764	1.542738	2.002520
H	-2.811652	2.830901	0.763622
H	-1.723333	1.401973	0.806604
C	2.318808	-0.853350	0.304320
C	3.031547	0.342375	0.432968
C	3.018575	-2.060007	0.204648
C	4.422588	0.341647	0.462281
C	4.410049	-2.077204	0.232778
H	2.458540	-2.984093	0.104533
C	5.098317	-0.872740	0.361498
H	4.956585	-3.011443	0.155824
H	2.475483	1.271519	0.508990
H	4.978617	1.268172	0.561562
Br	6.997091	-0.886398	0.399995

TS3$_{p\text{-Br}}$
E = -3690.958413 a.u.

Ag	-0.553784	0.236275	-0.663634
O	0.479426	-0.377900	2.225877
O	-0.376199	1.733705	1.875210
C	0.233345	0.693843	1.736559
O	-2.623505	-0.209505	-1.152430
S	-3.532056	-0.493047	0.074013
C	-3.706769	1.072308	0.964379
C	-5.181034	-0.577450	-0.661550
H	-2.730287	1.316711	1.397908
H	-4.441356	0.936432	1.764910
H	-4.020641	1.858934	0.271761
H	-5.359734	0.324428	-1.253595
H	-5.925961	-0.682751	0.132852
H	-5.200769	-1.458137	-1.307708
C	1.364864	0.853683	0.056132
C	1.685037	2.182089	-0.286301
C	2.385161	-0.111271	-0.064960
C	2.946982	2.534448	-0.761992
H	0.940497	2.961435	-0.138235
C	3.651261	0.216752	-0.541906
C	3.914851	1.540819	-0.892384
H	3.183970	3.562912	-1.016237
H	2.190497	-1.130909	0.259842
H	4.429849	-0.534616	-0.629677
Br	5.639966	2.003272	-1.533210

1O$_{m\text{-Br}}$
E = -3691.015672 a.u.

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Ag	-1.829794	-1.527553	0.201939
O	0.238067	-2.016493	0.181656
O	0.199827	0.221311	0.373473
C	0.805672	-0.865781	0.285468
O	-3.796897	-0.614753	0.287271
S	-3.798345	0.868324	-0.172053
C	-5.397731	1.471929	0.416725
C	-2.723331	1.771916	0.967619
H	-6.171260	0.947309	-0.148961
H	-5.467683	2.548183	0.232187
H	-5.497061	1.247084	1.482266
H	-3.039435	1.588296	1.999022
H	-2.779288	2.838134	0.723759
H	-1.701837	1.403431	0.809736
C	2.310152	-0.877000	0.295791
C	2.992567	0.338105	0.407382
C	3.027374	-2.072850	0.195837
C	4.381364	0.338577	0.417710
C	4.419668	-2.052399	0.207368
H	2.479120	-3.004960	0.109848
C	5.109370	-0.845339	0.318628
H	4.979604	-2.980854	0.129172
H	6.194346	-0.820874	0.328491
H	2.423619	1.257677	0.483460
Br	5.313735	1.989769	0.570346

TS3$_{m\text{-}Br}$

E = -3690.958351 a.u.

Ag	-0.541905	0.223380	-0.642158
O	0.485431	-0.389274	2.245359
O	-0.373415	1.721041	1.891938
C	0.238871	0.682289	1.756732
O	-2.612141	-0.196527	-1.147631
S	-3.531853	-0.490615	0.068220
C	-3.708300	1.066066	0.973514
C	-5.174916	-0.560989	-0.681319
H	-2.732640	1.306626	1.410892
H	-4.443862	0.922042	1.771726
H	-4.021609	1.859281	0.288193
H	-5.344199	0.346988	-1.266637
H	-5.926669	-0.669793	0.106150
H	-5.193606	-1.435899	-1.335325
C	1.376705	0.849872	0.081077
C	1.679253	2.177681	-0.276365
C	2.387069	-0.123394	-0.049739
C	2.933881	2.520547	-0.779133
H	0.930533	2.950058	-0.115848
C	3.631634	0.230326	-0.557280
C	3.918243	1.544390	-0.927528
H	3.159841	3.550809	-1.044647
H	4.902692	1.799075	-1.306859
H	2.203689	-1.141022	0.282542
Br	4.988227	-1.093450	-0.737881

1O$_{o\text{-}Br}$

E = -3691.006188 a.u.

Ag	-1.415579	-1.234090	-0.248586
O	0.691020	-1.502619	-0.320765
O	0.409735	0.623051	0.339647
C	1.129262	-0.344086	0.034731
O	-3.475459	-0.585828	-0.046219
S	-3.646253	0.944759	-0.247108
C	-5.297618	1.257447	0.419764
C	-2.670025	1.758285	1.039996
H	-6.013232	0.753177	-0.233825
H	-5.489015	2.334763	0.419790
H	-5.360344	0.845706	1.430842
H	-2.958725	1.373235	2.022778
H	-2.844154	2.837522	0.974347
H	-1.614268	1.536161	0.839517
C	2.631158	-0.234901	0.104388
C	3.360391	0.942169	-0.115599
C	3.350507	-1.390894	0.442809
C	4.749930	0.960668	0.007375
C	4.732621	-1.378873	0.586201
H	2.785537	-2.305640	0.589713
C	5.435484	-0.195481	0.367531
H	5.286133	1.884443	-0.183754
H	5.258779	-2.289424	0.860021
H	6.517472	-0.167033	0.468335
Br	2.550304	2.573764	-0.655566

TS3$_{o\text{-}Br}$

E = -3690.957402 a.u.

Ag	0.334080	0.137369	-0.576505
O	-0.834143	0.121106	2.531070
O	0.129364	-1.714146	1.539402
C	-0.552480	-0.712460	1.711594
O	2.432148	0.426689	-1.074954
S	3.390568	0.411358	0.146435
C	3.402899	-1.282927	0.778970
C	5.024713	0.430874	-0.625665
H	2.406102	-1.487898	1.188089
H	4.151324	-1.349066	1.575648
H	3.630009	-1.980244	-0.033041
H	5.086605	-0.377606	-1.359420
H	5.790565	0.321415	0.148047
H	5.135591	1.396852	-1.123780
C	-1.639198	-0.425723	0.125671
C	-2.079175	-1.678360	-0.352979
C	-2.557612	0.635419	0.015970
C	-3.349274	-1.863284	-0.895822
H	-1.402751	-2.522441	-0.239781
C	-3.833798	0.476920	-0.511940
C	-4.227677	-0.783737	-0.965854
H	-3.659209	-2.844678	-1.245755
H	-4.509425	1.324057	-0.576018
H	-5.227966	-0.914065	-1.371591
Br	-2.053385	2.392342	0.566244

5$_{p\text{-}Cl}$

E = -1648.449375 a.u.

Cu	0.055872	-0.698278	-0.000179
C	4.113393	0.038245	-0.000138
C	2.617386	0.232854	-0.000306
O	1.932778	-0.865222	-0.000289
O	2.160670	1.383522	-0.000064
C	4.686288	-1.236916	-0.000127
C	6.069437	-1.396347	0.000027
C	6.879856	-0.262866	0.000172
C	-1.690310	3.447023	0.000038
C	-0.757776	2.390067	-0.000043
N	-1.137278	1.121384	-0.000052
C	-2.452050	0.827013	0.000014
C	-3.464198	1.812740	0.000099
C	-3.039932	3.159815	0.000111
C	-2.809347	-0.569170	-0.000010
C	-4.837568	1.404245	0.000166
N	-1.798579	-1.476669	-0.000098
C	-2.111921	-2.768977	-0.000123
C	-3.437158	-3.233475	-0.000063
C	-4.470283	-2.318763	0.000027
C	-4.173977	-0.939823	0.000055
C	-5.177534	0.084515	0.000145
C	6.332684	1.019096	0.000164
C	4.948518	1.159107	0.000008
H	4.031976	-2.102567	-0.000243
H	6.518298	-2.384860	0.000036
H	-1.336266	4.473371	0.000043
H	0.319919	2.542841	-0.000103
H	-3.780675	3.956141	0.000174
H	-5.609258	2.170154	0.000233
H	-1.277944	-3.464324	-0.000193
H	-3.629004	-4.301670	-0.000087
H	-5.506807	-2.647178	0.000075
H	-6.222478	-0.215080	0.000196
H	4.487957	2.142186	-0.000003
H	6.983731	1.887825	0.000277

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Cl	8.619683	-0.452326	0.000368

TS5$_{p\text{-}Cl}$
E = -1648.392544 a.u.

Cu	0.715563	-0.284946	0.093845
C	2.673209	-0.150790	-0.017973
C	3.315438	0.690555	0.907763
C	4.425108	1.457718	0.557021
C	4.917551	1.369483	-0.744357
C	4.338108	0.516136	-1.681574
C	3.232259	-0.244815	-1.304650
H	2.953292	0.717894	1.933666
H	4.914922	2.104014	1.279768
C	2.008305	-1.907010	0.783569
O	1.904535	-1.748783	1.984186
O	2.024314	-2.760593	-0.082448
C	-1.391958	3.643382	0.219703
C	-0.378324	2.668174	0.221069
N	-0.632755	1.372494	0.117232
C	-1.918391	0.969012	0.002099
C	-3.008961	1.868445	-0.007592
C	-2.707459	3.242646	0.106003
C	-2.160620	-0.447446	-0.113304
C	-4.340850	1.351905	-0.127004
N	-1.083383	-1.264687	-0.109169
C	-1.265473	-2.575008	-0.209475
C	-2.546458	-3.146075	-0.321240
C	-3.654199	-2.323762	-0.331220
C	-3.484606	-0.925945	-0.226620
C	-4.568583	0.012220	-0.230163
H	-1.128402	4.692517	0.308611
H	0.669361	2.944555	0.309177
H	-3.513798	3.972115	0.103414
H	-5.171571	2.052964	-0.131694
H	-0.360317	-3.178401	-0.201160
H	-2.644936	-4.224056	-0.398905
H	-4.655675	-2.738287	-0.418369
H	-5.583369	-0.367527	-0.317895
H	2.809281	-0.949668	-2.017213
H	4.759187	0.440855	-2.679941
Cl	6.309848	2.328102	-1.201047

5$_{m\text{-}Cl}$
E = -1648.449021 a.u.

Cu	0.057579	-0.686196	0.000044
C	4.118020	0.032270	0.000064
C	2.620072	0.233813	0.000152
O	1.932931	-0.861908	0.000073
O	2.168063	1.385431	0.000109
C	4.685431	-1.245046	0.000007
C	6.070072	-1.393813	-0.000068
C	6.903520	-0.275534	-0.000088
C	-1.703145	3.455861	0.000122
C	-0.766805	2.402275	0.000117
N	-1.141625	1.132268	0.000074
C	-2.455503	0.833234	0.000037
C	-3.471474	1.815134	0.000040
C	-3.051694	3.163787	0.000083
C	-2.807976	-0.564163	-0.000005
C	-4.843430	1.400818	0.000000
N	-1.794077	-1.467710	-0.000006
C	-2.101591	-2.761360	-0.000042
C	-3.424824	-3.231248	-0.000080
C	-4.461636	-2.320690	-0.000080
C	-4.171130	-0.940606	-0.000042
C	-5.178449	0.079859	-0.000038
C	6.324262	0.992257	-0.000032
C	4.944892	1.159096	0.000042
H	4.027038	-2.107060	0.000024
H	6.512284	-2.387228	-0.000111
H	7.983874	-0.380237	-0.000146
H	-1.352842	4.483460	0.000157
H	0.309931	2.561292	0.000150
H	-3.795147	3.957591	0.000087
H	-5.618272	2.163559	0.000002
H	-1.264445	-3.452868	-0.000042
H	-3.612500	-4.300204	-0.000109
H	-5.496841	-2.653178	-0.000109
H	-6.222256	-0.223672	-0.000068
H	4.489986	2.143532	0.000087
Cl	7.362136	2.404265	-0.000056

TS5$_{m\text{-}Cl}$
E = -1648.392619 a.u.

Cu	0.718243	-0.253959	0.161231
C	2.680755	-0.149586	0.016897
C	3.349389	0.718808	0.896963
C	4.452583	1.460522	0.476607
C	4.923491	1.341620	-0.831520
C	4.281932	0.457015	-1.697136
C	3.186486	-0.296875	-1.286209
H	3.013176	0.779738	1.929822
H	4.965055	2.126346	1.168113
H	5.787366	1.904830	-1.170816
C	2.006383	-1.863000	0.886999
O	1.901678	-1.655428	2.080397
O	2.016099	-2.749707	0.055477
C	-1.414200	3.646665	0.305066
C	-0.395430	2.677221	0.320220
N	-0.638872	1.381814	0.188006
C	-1.918678	0.973142	0.028553
C	-3.013206	1.867326	-0.000517
C	-2.723282	3.240905	0.144892
C	-2.150088	-0.442430	-0.115279
C	-4.338030	1.346585	-0.170077
N	-1.069636	-1.254569	-0.087908
C	-1.241369	-2.564013	-0.213015
C	-2.515137	-3.139220	-0.375628
C	-3.626123	-2.322035	-0.409840
C	-3.467377	-0.925218	-0.278165
C	-4.555466	0.007747	-0.302042
H	-1.159574	4.695562	0.419024
H	0.647698	2.957641	0.442073
H	-3.533383	3.966017	0.129353
H	-5.171651	2.043913	-0.190277
H	-0.333354	-3.162527	-0.182641
H	-2.605580	-4.216310	-0.473056
H	-4.621990	-2.739893	-0.536486
H	-5.564943	-0.375143	-0.428648
H	2.743112	-1.021356	-1.963796
Cl	4.889191	0.282572	-3.335215

5$_{o\text{-}Cl}$
E = -1648.439033 a.u.

Cu	0.375031	-0.853638	0.065430
C	-3.716895	-0.465711	-0.020227
C	-2.237578	-0.141898	-0.040976
O	-1.482253	-1.183258	0.106994
O	-1.859474	1.017310	-0.223954
C	-4.125543	-1.711301	-0.518683
C	-5.466350	-2.068346	-0.600969
C	-6.442627	-1.178468	-0.156428
C	1.818616	3.383445	-0.301243
C	0.964893	2.265110	-0.215110
N	1.435477	1.032594	-0.099011
C	2.768275	0.836785	-0.064147
C	3.706399	1.890006	-0.145284
C	3.185342	3.197292	-0.266367
C	3.225723	-0.524206	0.059690
C	5.105696	1.583750	-0.103157
N	2.283112	-1.498948	0.134895
C	2.687900	-2.760343	0.247625
C	4.043024	-3.126224	0.291473
C	5.007806	-2.142519	0.215859
C	4.613469	-0.793681	0.096237
C	5.540290	0.297186	0.011959
C	-6.066974	0.055129	0.365839
C	-4.718109	0.409695	0.425649

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H	-3.348171	-2.395992	-0.841848
H	-5.747840	-3.037878	-1.003796
H	-7.496329	-1.441389	-0.206580
H	1.390690	4.376835	-0.394525
H	-0.120617	2.340291	-0.240271
H	3.866211	4.042879	-0.331683
H	5.820189	2.400909	-0.165775
H	1.905626	-3.511222	0.305775
H	4.311189	-4.173772	0.384389
H	6.065201	-2.393829	0.247558
H	6.604131	0.075741	0.042235
H	-6.813124	0.753052	0.732750
Cl	-4.353639	1.964654	1.134105

TS5$_{o\text{-Cl}}$
E = -1648.390704 a.u.

Cu	0.696454	-0.145680	0.258754
C	2.689191	-0.179476	0.013332
C	3.475929	0.592457	0.889877
C	4.604288	1.288990	0.462750
C	4.991170	1.216082	-0.874911
C	4.245735	0.457420	-1.777138
C	3.118290	-0.223173	-1.323713
H	3.191763	0.597151	1.939791
H	5.190224	1.870470	1.170709
H	5.878105	1.740582	-1.222307
H	4.533597	0.395874	-2.822562
C	2.011137	-1.720368	0.973994
O	1.762282	-1.379857	2.127197
O	2.101824	-2.718905	0.290711
C	-1.496037	3.665794	0.335235
C	-0.461808	2.715606	0.388266
N	-0.675172	1.414259	0.248171
C	-1.943000	0.981619	0.043667
C	-3.050268	1.858311	-0.024935
C	-2.790974	3.236647	0.128279
C	-2.148556	-0.437818	-0.104453
C	-4.360307	1.316843	-0.238857
N	-1.058308	-1.232422	-0.038667
C	-1.204063	-2.543976	-0.162541
C	-2.463123	-3.140356	-0.363151
C	-3.584852	-2.340730	-0.439092
C	-3.452433	-0.941000	-0.309349
C	-4.553225	-0.025289	-0.373637
H	-1.263816	4.718951	0.457221
H	0.569814	3.017220	0.547626
H	-3.613080	3.946800	0.082484
H	-5.202675	2.002002	-0.289568
H	-0.288770	-3.128827	-0.100383
H	-2.534081	-4.219209	-0.457803
H	-4.569432	-2.774515	-0.596947
H	-5.552073	-0.423629	-0.533176
Cl	2.197897	-1.126712	-2.517807

5$_{p\text{-Br}}$
E = -3759.696544 a.u.

Cu	0.055806	-0.698076	-0.000113
C	4.113781	0.039022	-0.000081
C	2.617527	0.234125	-0.000177
O	1.932990	-0.863832	-0.000186
O	2.161533	1.385011	-0.000020
C	4.685872	-1.236485	-0.000124
C	6.069281	-1.396134	-0.000035
C	6.879244	-0.263110	0.000097
C	-1.690143	3.446707	0.000047
C	-0.757742	2.389649	-0.000009
N	-1.137410	1.121007	-0.000023
C	-2.452179	0.826775	0.000016
C	-3.464210	1.812600	0.000073
C	-3.039793	3.159658	0.000088
C	-2.809528	-0.569422	-0.000005
C	-4.837580	1.404072	0.000112
N	-1.798714	-1.476859	-0.000063
C	-2.112000	-2.769155	-0.000084
C	-3.437241	-3.233717	-0.000049
C	-4.470417	-2.319045	0.000010
C	-4.174130	-0.940078	0.000033
C	-5.177608	0.084348	0.000093
C	6.333505	1.018815	0.000141
C	4.949122	1.159745	0.000051
H	4.031477	-2.102117	-0.000228
H	6.516149	-2.385197	-0.000068
H	-1.335966	4.473010	0.000057
H	0.319962	2.542334	-0.000042
H	-3.780422	3.956086	0.000131
H	-5.609261	2.169989	0.000157
H	-1.278012	-3.464494	-0.000130
H	-3.629028	-4.301923	-0.000068
H	-5.506936	-2.647456	0.000038
H	-6.222574	-0.215175	0.000122
H	4.489088	2.143101	0.000083
H	6.983464	1.887920	0.000244
Br	8.769363	-0.469834	0.000218

TS5$_{p\text{-Br}}$
E = -3759.639772 a.u.

Cu	0.715680	-0.288427	0.090867
C	2.674252	-0.153290	-0.017936
C	3.313424	0.685081	0.912557
C	4.421210	1.457136	0.565738
C	4.913531	1.376721	-0.735501
C	4.337636	0.527174	-1.677411
C	3.233777	-0.239356	-1.304886
H	2.950923	0.706771	1.938482
H	4.907013	2.100993	1.292826
C	2.010120	-1.912432	0.770786
O	1.904775	-1.763056	1.972538
O	2.027186	-2.760237	-0.100975
C	-1.385279	3.641528	0.207039
C	-0.372971	2.664929	0.208987
N	-0.629537	1.369260	0.109644
C	-1.916070	0.967046	-0.000834
C	-3.005292	1.868096	-0.009948
C	-2.701628	3.242125	0.098558
C	-2.160646	-0.449219	-0.112046
C	-4.338418	1.353504	-0.123778
N	-1.084769	-1.268367	-0.109239
C	-1.269503	-2.578523	-0.207111
C	-2.551723	-3.147528	-0.314666
C	-3.658021	-2.323403	-0.322461
C	-3.485849	-0.925783	-0.220553
C	-4.568464	0.013960	-0.222815
H	-1.120066	4.690577	0.291813
H	0.675289	2.939972	0.294514
H	-3.507077	3.972584	0.095953
H	-5.167928	2.056007	-0.127596
H	-0.365754	-3.183943	-0.200697
H	-2.652326	-4.225417	-0.390796
H	-4.660410	-2.736498	-0.406024
H	-5.584073	-0.364447	-0.306575
H	2.813184	-0.941788	-2.021318
H	4.756944	0.457931	-2.676598
Br	6.421982	2.427371	-1.225541

5$_{m\text{-Br}}$
E = -3759.696300 a.u.

Cu	0.055845	-0.685737	-0.000009
C	4.117042	0.032196	-0.000005
C	2.618847	0.231768	-0.000007
O	1.932598	-0.864298	-0.000021
O	2.166676	1.383433	0.000034
C	4.688324	-1.243327	-0.000024
C	6.073631	-1.388296	-0.000021
C	6.903279	-0.267249	0.000001
C	-1.695139	3.450504	0.000107
C	-0.761316	2.394724	0.000075
N	-1.139329	1.125510	0.000040
C	-2.453960	0.829585	0.000034

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C	-3.467232	1.814027	0.000062
C	-3.044389	3.161722	0.000100
C	-2.809740	-0.567024	-0.000006
C	-4.840089	1.403319	0.000051
N	-1.797768	-1.472897	-0.000032
C	-2.108525	-2.765542	-0.000069
C	-3.433018	-3.232436	-0.000082
C	-4.467656	-2.319389	-0.000056
C	-4.173695	-0.939875	-0.000017
C	-5.178502	0.083151	0.000013
C	6.320311	0.998113	0.000019
C	4.941395	1.161303	0.000016
H	4.032412	-2.107336	-0.000041
H	6.519334	-2.380130	-0.000035
H	7.983437	-0.371054	0.000004
H	-1.342131	4.477173	0.000136
H	0.315949	2.550155	0.000077
H	-3.786015	3.957242	0.000123
H	-5.612816	2.168194	0.000073
H	-1.272934	-3.459004	-0.000089
H	-3.623129	-4.300957	-0.000112
H	-5.503660	-2.649372	-0.000065
H	-6.223092	-0.217650	0.000004
Br	7.445543	2.534671	0.000049
H	4.481987	2.143305	0.000031

TS5$_{m\text{-}Br}$

E = -3759.640037 a.u.

Cu	0.718098	-0.287640	0.118416
C	2.680679	-0.162876	0.003082
C	3.328864	0.674008	0.927856
C	4.425658	1.448633	0.553156
C	4.910604	1.394077	-0.754513
C	4.289539	0.540602	-1.664102
C	3.201146	-0.245823	-1.300313
H	2.980580	0.684085	1.958431
H	4.922322	2.089914	1.278621
H	5.769085	1.984474	-1.058377
C	2.012954	-1.913489	0.794232
O	1.910163	-1.760083	1.995952
O	2.022372	-2.763412	-0.075324
C	-1.376608	3.639327	0.209641
C	-0.365687	2.661520	0.223745
N	-0.623130	1.365942	0.125406
C	-1.909142	0.964953	0.003020
C	-2.996878	1.867503	-0.018907
C	-2.692366	3.241379	0.089495
C	-2.154556	-0.451159	-0.108923
C	-4.329421	1.354376	-0.145478
N	-1.079795	-1.271422	-0.094972
C	-1.264413	-2.581210	-0.196035
C	-2.546128	-3.148985	-0.316344
C	-3.651506	-2.323768	-0.334483
C	-3.479000	-0.926212	-0.230913
C	-4.560250	0.014974	-0.245204
H	-1.110914	4.688294	0.293883
H	0.682302	2.934764	0.317493
H	-3.496727	3.972917	0.077049
H	-5.157907	2.057960	-0.159203
H	-0.360813	-3.186761	-0.182690
H	-2.646949	-4.226704	-0.394468
H	-4.653434	-2.735773	-0.428295
H	-5.575461	-0.362087	-0.339297
H	2.771563	-0.943537	-2.013349
Br	4.967899	0.442224	-3.444733

5$_{o\text{-}Br}$

E = -3759.686529 a.u.

Cu	0.064703	-0.636316	0.071019
C	4.105768	0.125419	0.028996
C	2.603595	0.313219	-0.005218
O	1.944377	-0.794422	0.112675
O	2.125924	1.437863	-0.170382
C	4.630571	-1.058893	-0.508992
C	5.999097	-1.291421	-0.581051
C	6.885270	-0.336750	-0.085287
C	-1.753456	3.453187	-0.281196
C	-0.802677	2.416125	-0.194589
N	-1.160612	1.145558	-0.085986
C	-2.470465	0.830183	-0.057174
C	-3.499232	1.794943	-0.138550
C	-3.097926	3.144227	-0.253655
C	-2.803879	-0.566659	0.063316
C	-4.865406	1.364229	-0.099823
N	-1.777550	-1.452899	0.138382
C	-2.067560	-2.745377	0.252391
C	-3.384436	-3.231250	0.297260
C	-4.433573	-2.338209	0.220445
C	-4.161880	-0.959478	0.099791
C	-5.182838	0.043793	0.014396
C	6.392489	0.836973	0.476803
C	5.017240	1.067048	0.524711
H	3.922540	-1.797486	-0.870686
H	6.372099	-2.215409	-1.015432
H	7.959013	-0.502175	-0.126200
H	-1.416524	4.481524	-0.368534
H	0.271732	2.589133	-0.212082
H	-3.852131	3.925084	-0.319166
H	-5.650241	2.114009	-0.163271
H	-1.221106	-3.423089	0.310681
H	-3.557554	-4.298521	0.391414
H	-5.464122	-2.683488	0.252299
H	-6.222525	-0.272306	0.043148
H	7.068673	1.581547	0.884006
Br	4.471747	2.687715	1.355893

TS5$_{o\text{-}Br}$

E = -3759.638943 a.u.

Cu	0.697265	-0.154203	0.216652
C	2.694325	-0.184358	0.012189
C	3.474353	0.571149	0.909019
C	4.605224	1.275348	0.501352
C	5.000787	1.228635	-0.835012
C	4.259586	0.488885	-1.756944
C	3.131649	-0.200126	-1.320874
H	3.182011	0.556176	1.956535
H	5.186574	1.843468	1.223837
H	5.890245	1.758884	-1.166897
H	4.553039	0.450602	-2.801601
C	2.005310	-1.734717	0.937841
O	1.759167	-1.419455	2.098289
O	2.089700	-2.720553	0.233662
C	-1.487474	3.666015	0.285163
C	-0.453532	2.714977	0.329739
N	-0.670826	1.412809	0.205748
C	-1.942261	0.979915	0.026770
C	-3.049741	1.857060	-0.030472
C	-2.786259	3.236499	0.105059
C	-2.151672	-0.440595	-0.105930
C	-4.363784	1.314910	-0.216569
N	-1.061258	-1.235513	-0.052911
C	-1.209057	-2.547744	-0.165448
C	-2.471691	-3.144717	-0.340509
C	-3.594269	-2.345005	-0.402065
C	-3.459127	-0.944377	-0.284543
C	-4.560130	-0.028164	-0.336633
H	-1.252062	4.720016	0.392953
H	0.580941	3.016628	0.469420
H	-3.608240	3.947260	0.066844
H	-5.206448	2.000333	-0.258182
H	-0.292366	-3.131648	-0.114997
H	-2.544807	-4.224141	-0.426675
H	-4.581590	-2.779474	-0.539623
H	-5.561971	-0.426736	-0.475387
Br	2.131108	-1.145133	-2.649576

1O$_{o\text{-}NH2\text{-}6\text{-}mem}$

E = -1175.542773 a.u.

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O	-0.320007	-0.473271	0.142672
O	-1.322861	1.275616	1.127645
C	-1.326077	0.129334	0.501258
C	-2.688731	-0.487946	0.204902
C	-3.898219	-0.082281	0.810455
C	-2.734140	-1.523946	-0.734519
C	-5.101381	-0.697061	0.438707
C	-3.928014	-2.130992	-1.107420
H	-1.783011	-1.834631	-1.157242
C	-5.118917	-1.707459	-0.516086
H	-6.029544	-0.379574	0.912274
H	-3.932530	-2.928975	-1.845214
H	-6.064532	-2.171105	-0.787351
N	-3.926404	0.969482	1.757949
H	-3.094050	0.973879	2.342911
H	-4.776464	0.977044	2.312500
Ag	-2.705646	2.796589	0.514632
O	-3.273850	4.641145	-0.526313
S	-2.095121	5.477855	-1.074709
C	-1.317827	4.491276	-2.380163
C	-2.906435	6.706288	-2.127055
H	-0.836388	3.635952	-1.897322
H	-0.560669	5.101503	-2.883088
H	-2.077930	4.144361	-3.086288
H	-3.563286	6.197954	-2.838510
H	-2.147061	7.300388	-2.644392
H	-3.496623	7.350305	-1.470922

1O$_{o\text{-}OH\text{-}6\text{-}mem}$

E =-1195.388863 a.u.

O	0.856523	-1.855853	-0.339683
O	2.873100	-2.624623	0.202500
C	2.106293	-1.695429	-0.022763
C	2.662012	-0.282607	0.126480
C	3.642994	-0.097619	1.108723
C	2.321258	0.830617	-0.658447
C	4.237751	1.137660	1.344758
C	2.923612	2.073516	-0.443362
C	3.874568	2.230992	0.560043
H	4.987694	1.244206	2.123870
H	2.649159	2.919215	-1.074387
H	4.333630	3.203984	0.716736
H	3.934988	-0.976059	1.676546
O	1.392590	0.683304	-1.663786
H	1.314309	1.527515	-2.132670
Ag	-0.650382	-0.458063	-0.418507
O	-2.457811	0.730324	-0.327724
S	-3.735428	0.009644	0.162461
C	-3.564750	-0.161738	1.957285
C	-4.982106	1.319725	0.139804
H	-2.757300	-0.877033	2.135861
H	-4.500270	-0.552814	2.369777
H	-3.311394	0.805893	2.400175
H	-4.617008	2.179248	0.708827
H	-5.918543	0.937202	0.556747
H	-5.130289	1.600771	-0.905525

1O$_{o\text{-}OMe\text{-}6\text{-}mem}$

E = -1234.677085 a.u.

O	0.872252	-1.892804	-0.638721
O	2.910509	-2.591380	-0.083126
C	2.095911	-1.691462	-0.246445
C	2.543917	-0.272853	0.090675
C	3.349141	-0.128635	1.224046
C	2.272128	0.879919	-0.673838
C	3.837984	1.109769	1.633224
C	2.777864	2.124990	-0.284825
C	3.549183	2.237702	0.871838
H	4.452919	1.188374	2.525817
H	2.580796	3.010976	-0.879488
H	3.932240	3.213211	1.161991
H	3.597950	-1.033501	1.771037
O	1.512067	0.714293	-1.803712
Ag	-0.645285	-0.512740	-0.630162
O	-2.432381	0.689475	-0.453883
S	-3.628224	0.022247	0.266345
C	-3.242416	0.060627	2.035608
C	-4.894170	1.313709	0.246859
H	-2.404628	-0.623175	2.196536
H	-4.113925	-0.286459	2.599690
H	-2.958163	1.074780	2.330443
H	-4.480081	2.234421	0.667421
H	-5.765862	0.975365	0.815177
H	-5.172375	1.473157	-0.797473
C	1.393298	1.802858	-2.696717
H	2.378523	2.150724	-3.032572
H	0.831471	1.424978	-3.553144
H	0.845539	2.642934	-2.248232

5$_{o\text{-}OH\text{-}6\text{-}mem}$

E = -1264.073693 a.u.

C	-1.379199	-0.084794	-0.362828
C	-2.062747	-0.179573	0.997795
O	-1.886608	-1.204106	1.647863
O	-2.803479	0.814878	1.378314
C	-1.180615	-1.281818	-1.059878
C	-0.574215	-1.323321	-2.312159
C	-0.115873	-0.139080	-2.886748
C	-0.272052	1.064496	-2.204937
C	-0.897561	1.095607	-0.954383
H	-0.447165	-2.271109	-2.828500
H	0.372618	-0.146325	-3.858245
H	0.104850	1.991230	-2.639286
H	-1.515229	-2.190779	-0.568475
O	-1.032850	2.285602	-0.283466
H	-0.616904	2.979774	-0.816158
Cu	-3.574434	2.167453	0.362884
N	-4.179409	3.986151	1.612608
N	-4.573090	3.208893	-0.948426
C	-4.926953	4.789264	0.829810
C	-3.977085	4.331214	2.872744
C	-4.758637	2.825025	-2.211228
C	-5.135050	4.378252	-0.538478
C	-5.503887	5.995898	1.293647
C	-4.506854	5.508608	3.434663
H	-3.371484	3.647239	3.462910
C	-5.507864	3.570342	-3.133497
H	-4.293519	1.887087	-2.497773
C	-5.909366	5.191898	-1.399163
C	-5.269581	6.341364	2.641910
C	-6.283157	6.794941	0.395734
H	-4.311051	5.746214	4.475725
C	-6.086742	4.755329	-2.728149
H	-5.623461	3.202197	-4.147831
C	-6.476191	6.408863	-0.895771
H	-5.693715	7.259180	3.042338
H	-6.720527	7.718992	0.765709
H	-6.676899	5.354445	-3.417163
H	-7.069326	7.020133	-1.571207

5$_{o\text{-}OMe\text{-}6\text{-}mem}$

E = -1303.362668 a.u.

C	3.380360	-0.447530	0.089651
C	2.896361	-1.868504	-0.173522
O	3.728536	-2.712053	-0.477905
O	1.615270	-2.081676	-0.100752
C	4.209108	0.147035	-0.862407
C	4.696448	1.445240	-0.707030
C	4.381656	2.154948	0.447007
C	3.586790	1.572398	1.437832
C	3.087529	0.276422	1.264076
H	5.330277	1.887410	-1.471248
H	4.765237	3.161580	0.597528
H	3.377101	2.129030	2.345862
H	4.473369	-0.442185	-1.736338
O	2.315527	-0.358652	2.193505
Cu	0.325389	-0.757303	-0.036440
N	-1.825027	-1.570868	0.069859

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N	-0.705895	0.888467	-0.107237
C	-2.657911	-0.514348	-0.013779
C	-2.340675	-2.785633	0.148921
C	-0.146854	2.095855	-0.188006
C	-2.063033	0.798071	-0.105857
C	-4.067663	-0.644475	-0.015537
C	-3.728009	-3.026081	0.152858
H	-1.626779	-3.603805	0.211351
C	-0.899348	3.276666	-0.276896
H	0.938690	2.122120	-0.177572
C	-2.898771	1.936385	-0.192568
C	-4.590621	-1.952486	0.071639
C	-4.884098	0.529095	-0.105225
H	-4.100201	-4.043739	0.219419
C	-2.276679	3.198879	-0.280766
H	-0.386550	4.230781	-0.343281
C	-4.322364	1.766648	-0.189254
H	-5.667965	-2.100644	0.072638
H	-5.965142	0.413469	-0.105967
H	-2.887736	4.095425	-0.350999
H	-4.948057	2.652927	-0.257711
C	2.117966	0.268973	3.439440
H	1.535406	-0.433346	4.038908
H	3.071567	0.473035	3.945181
H	1.556214	1.209263	3.342088