Supplementary Information

DFT Studies on Copper-Catalyzed Arylation of aromatic C-H bonds

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Cartesian coordinates and electronic energies for all of the calculated structures

Benzoxazole
E_{gas} = −399.715351 a.u.
E_{sol} = −399.720807 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.116307
C	1.335995	0.000000	1.692871
C	−0.299108	0.000000	3.481519
C	2.421527	0.000000	2.557315
C	0.774773	0.000000	4.370887
H	−1.328447	0.000000	3.825117
C	2.108443	0.000000	3.918558
H	3.444936	0.000000	2.197883
H	0.581884	0.000000	5.439854
H	2.915001	0.000000	4.646077
N	−0.828874	0.000000	0.987630
O	1.333102	0.000000	0.317620
H	−0.227961	0.000000	−1.056808

1
E_{gas} = −2327.212868 a.u.
E_{sol} = −2327.227231 a.u.

Cu	−0.005492	0.000431	−0.000618
C	−0.000998	−0.000994	2.704604
H	0.602938	0.020436	3.633298
H	−0.701736	0.863175	2.785432
H	−0.641798	−0.910389	2.787477
O	0.817945	0.025313	1.592565
H	−5.576508	−0.199846	1.562486
C	−4.848284	−0.170989	0.757991
C	−5.239971	−0.176213	−0.566001
C	−3.469875	−0.127102	1.052466
C	−4.260174	−0.137813	−1.582612
H	−6.291847	−0.209564	−0.839252
H	−3.122676	−0.121677	2.083551
C	−2.897830	−0.094961	−1.175591
C	−4.587119	−0.140657	−2.978601
C	−1.857868	−0.054616	−2.183242
C	−3.607646	−0.102930	−3.923613
H	−5.634258	−0.173753	−3.268620
C	−2.219849	−0.059087	−3.556746
H	−3.858638	−0.105359	−4.980989
C	−1.190910	−0.019818	−4.521258
C	0.403114	0.023304	−2.730326
C	0.125785	0.021377	−4.100798
H	−1.444358	−0.022529	−5.577788
H	1.427050	0.055436	−2.374606
H	0.945537	0.052213	−4.810958
N	−0.547334	−0.013088	−1.780584
N	−2.526709	−0.090283	0.124409

2 for benzoxazole
E_{gas} = −2726.950908 a.u.
E_{sol} = −2726.964105 a.u.

Cu	−0.057578	−0.635217	−0.304553
H	0.916142	−0.633736	2.158300
C	1.976994	−0.455046	2.392639
C	4.080118	−0.081537	2.388756
C	3.676291	−0.228533	3.722283
C	5.422035	0.173021	2.093048
C	4.539683	−0.136480	4.804746
C	6.310151	0.269872	3.164679
H	5.755165	0.289703	1.066240
C	5.878218	0.118258	4.495662
H	4.193835	−0.255846	5.826049
H	7.360899	0.466730	2.970550
H	6.601802	0.200811	5.301710
N	2.956306	−0.234027	1.569387
O	2.326312	−0.467880	3.719434
O	−0.726667	−0.982541	1.346253
C	−1.905943	−0.335641	1.694004
H	−2.273051	−0.695064	2.673295
H	−1.808405	0.768445	1.786166
H	−2.734801	−0.504857	0.974729
H	−3.651740	−0.995951	−1.335511
C	−3.106973	−0.795326	−2.255916
C	−3.786007	−0.735397	−3.490064
C	−3.055703	−0.473765	−4.631794
H	−4.859621	−0.890984	−3.529150
C	−1.074620	−0.364716	−3.242668
C	−1.659796	−0.279240	−4.536547
H	−3.537754	−0.415531	−5.604640
C	0.357127	−0.178529	−3.100247
C	−0.835568	−0.004799	−5.677333
C	1.140067	0.091310	−4.253480
C	0.507001	0.174240	−5.539522
H	−1.304857	0.057630	−6.655800
C	2.530922	0.265861	−4.087702
C	2.242991	−0.098432	−1.730281
H	1.129422	0.382387	−6.405754
C	3.078302	0.170833	−2.823730
H	3.151296	0.473102	−4.955774
H	2.640724	−0.168624	−0.719607
H	4.142708	0.301199	−2.658227
N	−1.801465	−0.615347	−2.130448
N	0.918165	−0.272591	−1.856056

TS$_{(2-3)}$ for benzoxazole
E_{gas} = −2726.915105 a.u.
E_{sol} = −2726.934576 a.u.

Cu	0.842539	1.414080	0.545849
H	0.132680	1.027526	2.392586
C	1.408569	0.260196	2.460578
C	3.326834	−0.571957	3.067306
C	2.467505	−1.656146	2.828917
C	4.646214	−0.804625	3.472066
C	2.857628	−2.982236	2.972111
C	5.056183	−2.130536	3.624826
H	5.320009	0.024800	3.668904
C	4.177659	−3.201600	3.378999
H	2.171847	−3.802022	2.781735
H	6.073422	−2.343298	3.943818
H	4.530847	−4.221033	3.510896
N	2.627704	0.608788	2.821884
O	1.261801	−1.150936	2.450859
O	−0.639342	1.698961	1.878471
C	−0.767292	2.946134	2.533706
H	−1.586041	2.926548	3.268305
H	0.156479	3.229480	3.064635
H	−0.992730	3.734088	1.801597
H	−2.173556	2.185330	−0.828574
C	−1.470888	2.221254	−1.657922
C	−1.894648	2.535847	−2.964909
C	−0.961420	2.548803	−3.984689
H	−2.940802	2.751349	−3.157857
C	0.712737	1.961054	−2.347835
C	0.390892	2.255325	−3.696892
H	−1.254351	2.778721	−5.006058
C	2.080324	1.661328	−1.986043
C	1.429426	2.229692	−4.687729
C	3.079883	1.639714	−2.988566
C	2.715170	1.927684	−4.348177
H	1.169632	2.451321	−5.719556
C	4.401442	1.345060	−2.584464
C	3.613020	1.163068	−0.317204
H	3.493750	1.905962	−5.106079
C	4.663955	1.106782	−1.248602

H	5.195699	1.314075	-3.325751
H	3.777656	1.001902	0.745119
H	5.668388	0.885003	-0.903384
N	-0.210987	1.940794	-1.358654
N	2.353558	1.428392	-0.670464

HOMe

E_{gas} = -115.712204 a.u.

E_{sol} = -115.721786 a.u.

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	0.968664
C	1.349511	0.000000	-0.433949
H	1.328213	0.000000	-1.527219
H	1.902967	0.893163	-0.103694
H	1.902967	-0.893163	-0.103694

3 for benzoxazole

E_{gas} = -2611.227664 a.u.

E_{sol} = -2611.241590 a.u.

Cu	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.870941
C	0.674614	0.000000	3.935350
C	-0.728028	-0.003737	3.961487
C	1.390618	0.000970	5.136526
C	-1.470034	-0.006586	5.135602
C	0.664153	-0.001884	6.329330
H	2.477095	0.003845	5.133603
C	-0.742207	-0.005613	6.330389
H	-2.555749	-0.009455	5.124882
H	1.194029	-0.001213	7.278692
H	-1.274980	-0.007801	7.277902
N	1.089415	0.002066	2.605357
O	-1.164842	-0.003995	2.669811
H	3.292959	0.002198	1.074015
C	3.381018	-0.001014	-0.011537
C	4.628314	-0.005178	-0.674657
C	4.654359	-0.009263	-2.056388
H	5.547910	-0.005054	-0.097750
C	2.243426	-0.005291	-2.015710
C	3.437977	-0.009452	-2.778747
H	5.597644	-0.012397	-2.597222
C	0.961589	-0.005844	-2.687281
C	3.356902	-0.013639	-4.211524
C	0.918279	-0.009961	-4.104214
C	2.149475	-0.013758	-4.845364
H	4.279459	-0.016708	-4.786468
C	-0.351806	-0.010267	-4.721622
C	-1.352936	-0.003040	-2.538935
H	2.096196	-0.016871	-5.930736
C	-1.488316	-0.006714	-3.935993
H	-0.421863	-0.013306	-5.806226
H	-2.227882	-0.000382	-1.897316
H	-2.479572	-0.006836	-4.376915
N	2.231860	-0.000921	-0.667950
N	-0.169783	-0.002619	-1.919501

PhI

E_{gas} = -243.027406 a.u.

E_{sol} = -243.029361 a.u.

C	0.000708	0.000000	-0.002373
C	-0.008022	0.000000	1.394760
C	1.207980	0.000000	2.081089
C	2.424036	0.000000	1.394853
C	2.415411	0.000000	-0.002281
C	1.208086	0.000000	-0.702947
H	-0.943917	0.000000	-0.539692
H	-0.947660	0.000000	1.936459
H	3.363633	0.000000	1.936624
H	3.360076	0.000000	-0.539529
H	1.208127	0.000000	-1.789219
I	1.207895	0.000000	4.203938

TS$_{(3-4)}$ for benzoxazole

E_{gas} = -2854.230368 a.u.

E_{sol} = -2854.242379 a.u.

Cu	0.014912	-0.020309	0.011562
C	0.016519	-0.006325	1.950620
C	0.642523	0.025494	4.032043
C	-0.750960	-0.132926	4.024282
C	1.329121	0.077268	5.248421
C	-1.513437	-0.241755	5.179835
C	0.581532	-0.031133	6.423462
H	2.408579	0.197437	5.271418
C	-0.815491	-0.187815	6.391227
H	-2.591759	-0.362859	5.143084
H	1.087780	0.005712	7.384789
H	-1.364614	-0.269514	7.325674
N	1.081076	0.100946	2.709165
O	-1.156292	-0.153397	2.720962
C	-0.694078	-1.997774	-0.356543
C	-1.812950	-2.043427	-1.205827
C	-0.679123	-2.804331	0.797939
C	-2.965287	-2.728833	-0.808463
H	-1.781330	-1.561310	-2.175185
C	-1.828851	-3.485094	1.179092
H	0.207998	-2.845480	1.419095
C	-2.984956	-3.441741	0.388536
H	-3.834890	-2.727285	-1.461458
H	-1.820169	-4.057651	2.102709
H	-3.875751	-3.984787	0.690525
I	1.306016	-1.888395	-1.550157
H	-2.664636	0.414013	-1.746514
C	-1.990213	1.163384	-2.149126
C	-2.409287	2.009974	-3.190677
C	-1.525675	2.947412	-3.688201
H	-3.414010	1.913435	-3.589013
C	0.080316	2.168090	-2.055378
C	-0.241244	3.057177	-3.113716
H	-1.809619	3.609372	-4.502249
C	1.350698	2.305397	-1.382555
C	0.724969	4.033512	-3.533999
C	2.269959	3.299684	-1.800832
C	1.930410	4.147925	-2.907575
H	0.467319	4.692414	-4.358918
C	3.476111	3.404427	-1.071569
C	2.708266	1.624132	0.357843
H	2.648847	4.898075	-3.227698
C	3.691371	2.573541	0.011127
H	4.214656	4.147629	-1.361832
H	2.802778	0.976323	1.227010
H	4.601122	2.643120	0.598774
N	-0.775904	1.208903	-1.608086
N	1.583274	1.488667	-0.333179

Prod for benzoxazole

E_{gas} = -630.778395 a.u.

E_{sol} = -630.782238 a.u.

C	-0.005787	-0.034092	-0.034967
C	-0.014022	-0.022900	2.096784
C	1.326173	-0.007255	1.681960
C	-0.319057	-0.019607	3.461471
C	2.405510	0.011888	2.552147
C	0.749851	-0.000447	4.357061
H	-1.349966	-0.031530	3.800246
C	2.085658	0.015015	3.912938
H	3.430919	0.023719	2.198408
H	0.550284	0.002695	5.424870
H	2.888460	0.029741	4.644423
N	-0.830928	-0.039724	0.970417
O	1.331625	-0.014529	0.310053
C	-0.332673	-0.045391	-1.457356

C	-1.682544	-0.063850	-1.847753
C	0.673488	-0.037677	-2.436628
C	-2.016119	-0.074222	-3.198649
H	-2.449548	-0.069603	-1.080456
C	0.330579	-0.048200	-3.787369
H	1.715324	-0.023367	-2.134728
C	-1.012047	-0.066411	-4.172131
H	-3.061383	-0.088421	-3.494769
H	1.113433	-0.042113	-4.540693
H	-1.275930	-0.074524	-5.226194

4

E_{gas} = -2223.546235 a.u.

E_{sol} = -2854.341118 a.u.

Cu	0.003909	0.004380	0.066864
H	0.034905	-0.005994	3.605108
C	1.085263	-0.004465	3.320229
C	2.104816	-0.006659	4.295134
C	3.422508	-0.004562	3.880657
H	1.846711	-0.009942	5.349417
C	2.616730	0.001637	1.603320
C	3.717968	-0.000285	2.498265
H	4.235724	-0.006156	4.602184
C	2.858285	0.006027	0.175720
C	5.054044	0.002196	1.974758
C	4.191739	0.008428	-0.306827
C	5.280096	0.006389	0.630730
H	5.886780	0.000679	2.673279
C	4.385630	0.012772	-1.705476
C	2.000579	0.011885	-1.979576
H	6.294706	0.008254	0.241602
C	3.285655	0.014502	-2.541959
H	5.395123	0.014702	-2.107739
H	1.118418	0.013145	-2.611703
H	3.397034	0.017835	-3.621149
N	1.331734	-0.000465	2.019825
N	1.779087	0.007765	-0.661370
I	-2.370837	0.001187	0.426519

MeO$^-$

E_{gas} = -115.069054 a.u.

E_{sol} = -115.181126 a.u.

O	-0.000001	0.000000	-0.013637
C	-0.000003	0.000000	1.294423
H	1.030043	0.000000	1.836408
H	-0.515020	0.892031	1.836403
H	-0.515020	-0.892031	1.836403

I$^-$

E_{gas} = -11.472110 a.u.

E_{sol} = -11.560855 a.u.

I	0.000000	0.000000	0.000000

TS$_{(1-5)-}$ for benzoxazole

E_{gas} = -2570.230176 a.u.

E_{sol} = -2570.241073 a.u.

Cu	0.039064	0.164378	-0.019248
C	0.009620	0.007155	2.172356
C	1.221864	0.276539	2.840124
C	-0.629124	-1.234095	2.386799
C	1.868468	-0.738355	3.553005
H	1.656319	1.269947	2.799486
C	0.028903	-2.231910	3.096638
H	-1.582766	-1.411437	1.904999
C	1.283093	-1.997834	3.679003
H	2.817370	-0.523156	4.039659
H	-0.451090	-3.200871	3.208765
H	1.779203	-2.779675	4.247208
I	-1.294284	1.828651	1.956986
H	2.930656	0.056789	1.098371
C	3.025830	0.641600	0.189557
C	4.277675	1.129836	-0.218198
C	4.366412	1.887056	-1.371047
H	5.156366	0.904261	0.377257
C	1.980672	1.587579	-1.637159
C	3.197699	2.128703	-2.123277
H	5.319092	2.285940	-1.709575
C	0.778660	1.761284	-2.415054
C	3.195409	2.865694	-3.357937
C	0.811303	2.466107	-3.643275
C	2.054867	3.027352	-4.088478
H	4.135779	3.283991	-3.706995
C	-0.407712	2.557132	-4.353703
C	-1.465042	1.264349	-2.616101
H	2.075069	3.577866	-5.025496
C	-1.543492	1.951084	-3.845596
H	-0.438950	3.095524	-5.297805
H	-2.308844	0.746494	-2.166286
H	-2.488584	2.002244	-4.377083
N	1.892562	0.868106	-0.476604
N	-0.338600	1.193164	-1.925113
O	-1.537128	-0.878593	-0.278198
C	-1.356799	-2.135312	-0.825372
H	-2.328300	-2.633625	-1.020795
H	-0.818666	-2.135894	-1.801971
H	-0.791310	-2.837042	-0.167588

5 for benzoxazole

E_{gas} = -2570.254754 a.u.

E_{sol} = -2570.275168 a.u.

Cu	0.214360	-0.095500	-0.081310
C	-0.104138	-0.314135	2.650193
H	0.425872	-0.213281	3.610185
H	-0.894470	0.461734	2.628632
H	-0.594495	-1.300214	2.654690
O	0.845889	-0.174331	1.631906
H	0.860175	4.792046	1.416783
C	0.384794	4.134397	0.696928
C	-0.379013	4.644749	-0.339118
C	0.559357	2.743270	0.811232
C	-0.973172	3.761787	-1.268845
H	-0.515675	5.716981	-0.451618
H	1.162548	2.281075	1.587133
C	-0.753744	2.382813	-1.062329
C	-1.754606	4.164874	-2.405015
C	-1.279296	1.413295	-1.972398
C	-2.247933	3.243133	-3.283330
H	-1.932380	5.224744	-2.564556
C	-2.012033	1.836296	-3.103570
H	-2.821347	3.563207	-4.148888
C	-2.451506	0.832805	-3.994219
C	-1.407873	-0.815258	-2.576073
C	-2.141178	-0.488837	-3.730165
H	-3.016675	1.106725	-4.880982
H	-1.147691	-1.841747	-2.344108
H	-2.454342	-1.282947	-4.399457
N	-0.991319	0.106766	-1.711791
N	-0.000352	1.900169	-0.045823
C	0.153070	-1.986199	0.018184
C	-1.077202	-2.566092	0.325308
C	1.278502	-2.764430	-0.236836
C	-1.192393	-3.963484	0.339190
H	-1.952032	-1.958094	0.545409
C	1.149958	-4.157806	-0.218380
H	2.230710	-2.297174	-0.463113
C	-0.079202	-4.757963	0.066722
H	-2.153022	-4.419658	0.566486
H	2.022795	-4.772078	-0.424886
H	-0.166734	-5.841143	0.081891
I	2.501872	0.392944	-1.931406

$TS_{(5-4)}$ for benzoxazole

E_{gas} = −2969.930040 a.u.

E_{sol} = −2969.948100 a.u.

Cu	1.052634	0.074650	0.079626
C	2.006418	−0.476594	3.448622
H	1.904675	0.118569	4.370508
H	1.655972	−1.496529	3.674817
H	3.074912	−0.528542	3.199597
O	1.298799	0.102428	2.376418
H	0.726059	4.806299	2.131589
C	0.278754	4.120865	1.419650
C	−0.822817	4.485787	0.669606
C	0.826276	2.834900	1.260782
C	−1.386697	3.559616	−0.235241
H	−1.267840	5.471792	0.775679
H	1.671679	2.490337	1.844323
C	−0.763201	2.293350	−0.331593
C	−2.551048	3.824245	−1.033013
C	−1.306775	1.288412	−1.204823
C	−3.075261	2.867770	−1.851827
H	−3.018166	4.802519	−0.959191
C	−2.477895	1.565293	−1.949394
H	−3.966682	3.073082	−2.438228
C	−3.000162	0.517284	−2.739604
C	−1.200951	−0.883697	−1.971663
C	−2.368680	−0.710510	−2.739327
H	−3.901466	0.681944	−3.324076
H	−0.681428	−1.836019	−1.946847
H	−2.758256	−1.544107	−3.313659
N	−0.672327	0.090143	−1.242529
N	0.324373	1.954839	0.402215
C	1.821223	−1.595404	−0.482482
C	1.883643	−2.567377	0.513989
C	1.896333	−1.944074	−1.834083
C	1.932202	−3.914805	0.143608
H	1.858989	−2.294077	1.559170
C	1.948712	−3.295025	−2.189918
H	1.923111	−1.180977	−2.604563
C	1.964955	−4.281727	−1.201720
H	1.938358	−4.674468	0.920385
H	1.997867	−3.567563	−3.241299
H	2.018389	−5.330676	−1.479948
H	−6.528075	−1.316123	0.760337
C	−5.466057	−1.518692	0.874759
C	−4.601072	−0.471400	1.211012
C	−4.989982	−2.829149	0.688507
C	−3.256582	−0.796927	1.347093
H	−4.960986	0.542087	1.362452
C	−3.635088	−3.136967	0.832707
H	−5.694385	−3.616801	0.432650
C	−2.759387	−2.098810	1.167801
O	−2.202569	0.007225	1.654380
H	−3.264657	−4.149140	0.696183
N	−1.380549	−2.076523	1.369086
C	−1.049134	−0.842558	1.657946
H	0.297203	−0.276258	2.271478
I	3.522484	0.585670	−0.297673

1A

E_{gas} = −1870.746513 a.u.

E_{sol} = −1870.824711 a.u.

Cu	−0.167292	0.215545	−0.001443
O	0.036488	0.439220	1.786747
C	1.186289	−0.066545	2.326978
H	1.228080	0.107900	3.431358
H	1.330191	−1.173378	2.211924
H	2.141195	0.375148	1.936890
O	−0.429696	0.064061	−1.789445
C	−0.203258	−1.172675	−2.326664
H	−0.388042	−1.176900	−3.430159
H	0.841857	−1.565768	−2.215498
H	−0.849894	−1.999754	−1.930701

2A for benzoxazole

E_{gas} = −2270.486537 a.u.

E_{sol} = −2270.557979 a.u.

Cu	0.671815	−0.097020	−0.634527
H	1.286019	0.275314	2.578601
C	1.783411	0.198779	3.574400
C	2.849944	0.427873	5.409267
C	2.340708	−0.880014	5.381412
C	3.599195	0.855534	6.509011
C	2.535985	−1.802537	6.400110
C	3.808739	−0.055585	7.546351
H	4.000676	1.864010	6.545124
C	3.287123	−1.361280	7.494254
H	2.128691	−2.807308	6.346814
H	4.388112	0.247593	8.415194
H	3.471918	−2.042493	8.321169
N	2.469434	1.079710	4.236130
O	1.658341	−1.028514	4.209106
O	0.346336	0.303118	1.112149
C	−0.911573	0.789914	1.411432
H	−1.003072	1.006808	2.499624
H	−1.170527	1.741531	0.895173
H	−1.742548	0.087498	1.176116
O	1.026966	−0.556695	−2.345570
C	1.268214	0.479244	−3.209379
H	1.479594	0.102474	−4.239383
H	0.423378	1.204387	−3.340682
H	2.149120	1.123441	−2.956190

$TS_{(2-3)A}$ for benzoxazole

E_{gas} = −2270.447420 a.u.

E_{sol} = −2270.522714 a.u.

Cu	−0.573868	−0.114987	0.416275
H	−0.319971	−0.053815	2.438482
C	1.168600	0.041864	1.905459
C	3.232403	0.732618	1.764530
C	3.275350	−0.674572	1.733254
C	4.425689	1.460467	1.699606
C	4.459486	−1.394144	1.635711
C	5.628190	0.752104	1.605925
H	4.408134	2.547149	1.721997
C	5.647252	−0.652378	1.573715
H	4.461714	−2.480407	1.609380
H	6.568938	1.297199	1.554519
H	6.599245	−1.174073	1.498754
N	1.909152	1.132688	1.880277
O	2.002182	−1.128709	1.827655
O	−1.394227	−0.011325	2.319903
C	−1.820870	1.301039	2.624922
H	−2.162851	1.383149	3.670534
H	−1.014928	2.035462	2.472064
H	−2.662678	1.574630	1.974096
O	−0.567677	−0.243491	−1.394117
C	0.690301	−0.272579	−1.954549
H	1.327849	−1.132388	−1.637421
H	0.627277	−0.350224	−3.065307
H	1.313933	0.631997	−1.759284

3A for benzoxazole

E_{gas} = −2154.771960 a.u.

E_{sol} = −2154.843168 a.u.

Cu	0.073826	0.051164	0.081313
C	0.050934	0.032096	1.926108
C	0.444502	0.020501	4.068929
C	−0.955721	−0.001870	3.921451
C	1.001922	0.019463	5.351807
C	−1.830712	−0.025520	4.999979

C	0.135666	-0.004068	6.450562
H	2.081179	0.036691	5.481297
C	-1.258368	-0.026289	6.279971
H	-2.907704	-0.042429	4.855636
H	0.547651	-0.005256	7.458078
H	-1.905783	-0.044290	7.154442
N	1.025569	0.040893	2.809559
O	-1.230406	0.004761	2.595617
O	0.069128	0.072229	-1.738895
C	1.284392	0.059795	-2.372132
H	1.163930	0.074778	-3.481983
H	1.951430	0.931450	-2.147880
H	1.922446	-0.838315	-2.168682

TS$_{(3-4)A}$ for benzoxazole

E_{gas} = -2397.786129 a.u.

E_{sol} = -2397.848579 a.u.

Cu	0.403315	-0.262163	-0.256507
C	-0.040182	-0.193212	1.704588
C	1.030797	-0.470544	2.571618
C	-1.313528	-0.716055	1.989045
C	0.848727	-1.350344	3.638243
H	1.999671	-0.019596	2.393973
C	-1.479334	-1.588651	3.065646
H	-2.143301	-0.458037	1.344196
C	-0.403428	-1.918077	3.893931
H	1.696919	-1.583595	4.279205
H	-2.465726	-2.008497	3.254954
H	-0.540108	-2.595248	4.733804
I	-0.163201	2.304804	1.248748
C	2.316644	-0.444151	-0.383832
N	2.993733	-1.430216	-0.921712
O	3.189167	0.549343	0.146380
C	4.342493	-1.124533	-0.771267
C	4.449014	0.108132	-0.105043
C	5.501842	-1.807455	-1.151868
C	5.665004	0.703752	0.204846
C	6.736114	-1.225643	-0.848185
H	5.434725	-2.761685	-1.667548
C	6.817961	0.009377	-0.181237
H	5.714721	1.658540	0.720150
H	7.653758	-1.736250	-1.132861
H	7.794780	0.434006	0.039636
O	-1.278940	-0.402898	-0.989389
C	-1.764337	-1.681460	-1.176826
H	-2.745086	-1.660651	-1.695742
H	-1.109068	-2.342372	-1.785503
H	-1.945833	-2.226605	-0.220181

4A for benzoxazole

E_{gas} = -2397.835070 a.u.

E_{sol} = -2397.897016 a.u.

Cu	-0.099167	-0.141365	-0.204915
C	0.286774	-0.682714	1.596919
C	1.092875	-1.780612	1.900962
C	-0.352086	0.008582	2.631126
C	1.246867	-2.195791	3.230268
H	1.627917	-2.297512	1.109519
C	-0.173737	-0.388907	3.959235
H	-1.021051	0.830595	2.397757
C	0.621786	-1.497344	4.263407
H	1.871632	-3.058980	3.454258
H	-0.672793	0.159106	4.757033
H	0.752294	-1.811956	5.297109
I	-0.492828	0.467551	-2.738276
C	1.761568	0.047531	-0.458451
N	2.652971	-0.860582	-0.728835
O	2.298464	1.330236	-0.318025
C	3.866703	-0.182594	-0.807274
C	3.635995	1.178619	-0.550290
C	5.164994	-0.622880	-1.077554
C	4.636041	2.139120	-0.547109
C	6.190077	0.327771	-1.078081
H	5.361175	-1.671785	-1.280816
C	5.932846	1.684658	-0.817984
H	4.421885	3.184562	-0.347209
H	7.210322	0.012810	-1.285887
H	6.754791	2.396560	-0.828759
O	-1.881536	-0.222060	0.194974
C	-2.485362	-1.452182	-0.030939
H	-3.559683	-1.379382	0.220250
H	-2.427965	-1.785024	-1.085621
H	-2.073131	-2.270507	0.596288

TS$_{(4-5)A}$ for benzoxazole

E_{gas} = -2397.826701 a.u.

E_{sol} = -2397.892984 a.u.

Cu	-0.008506	-0.041060	-0.129312
C	0.035874	-0.085204	1.794818
C	1.284419	-0.010095	2.433345
C	-1.037287	-0.691130	2.466402
C	1.467788	-0.585070	3.689846
H	2.100909	0.520674	1.953645
C	-0.849276	-1.259554	3.726210
H	-2.018552	-0.721088	2.002305
C	0.404139	-1.215871	4.342161
H	2.444654	-0.532013	4.166333
H	-1.687302	-1.738687	4.228576
H	0.547488	-1.655830	5.326424
I	-0.323272	0.878697	-2.542209
C	-0.434986	1.531561	0.819522
N	0.330646	2.569322	1.044070
O	-1.801667	1.803319	0.966110
C	-0.536801	3.618130	1.295147
C	-1.858642	3.137040	1.251640
C	-0.306494	4.969810	1.573944
C	-2.973215	3.930593	1.469785
C	-1.416721	5.787933	1.799008
H	0.706101	5.360703	1.606974
C	-2.726642	5.281384	1.748731
H	-3.979315	3.525940	1.421679
H	-1.266060	6.843231	2.014995
H	-3.565852	5.949448	1.926079
O	0.431461	-1.808978	-0.449873
C	1.785302	-2.043013	-0.561140
H	1.984418	-3.125005	-0.704985
H	2.267459	-1.526734	-1.421807
H	2.376731	-1.754772	0.343049

5A

E_{gas} = -1767.088012 a.u.

E_{sol} = -1767.157500 a.u.

Cu	0.002234	0.000000	-0.091810
O	0.058875	0.000000	1.733936
C	1.309583	0.000000	2.293217
H	1.250889	0.000000	3.408944
H	1.949926	-0.884946	2.043026
H	1.949927	0.884945	2.043026
I	-0.120897	0.000000	-2.513790

For oxazole (Table 1 entry 2)

Oxazole

E_{gas} = -246.065112 a.u.

E_{sol} = -246.070741 a.u.

C	0.011190	0.000000	0.006578
C	0.006420	0.000000	2.124509
C	1.303490	0.000000	1.727672
N	-0.816185	0.000000	1.001814
O	1.323075	0.000000	0.357688
H	-0.206767	0.000000	-1.051431

H	-0.401585	0.000000	3.125055
H	2.260924	0.000000	2.223340

2 for oxazole (Table 1 entry 2)

E_{gas} = -2573.299968 a.u.

E_{sol} = -2573.313128 a.u.

Cu	-0.012992	-0.033866	0.007330
H	0.016571	0.013608	2.666682
C	0.941872	0.029476	3.258339
C	2.942707	0.025733	4.007645
C	2.115294	0.099531	5.077721
N	2.176645	-0.018254	2.846250
O	0.828629	0.102684	4.610391
O	-1.280758	-0.144082	1.299507
C	-2.390322	0.679704	1.166811
H	-3.126845	0.472548	1.965637
H	-2.162085	1.766518	1.231649
H	-2.934441	0.544356	0.207688
H	-2.982004	0.263595	-2.289201
C	-2.110570	0.294377	-2.940273
C	-2.265372	0.411517	-4.336694
C	-1.132285	0.451454	-5.123984
H	-3.258255	0.469979	-4.771642
C	0.183348	0.251063	-3.100061
C	0.140778	0.370808	-4.517189
H	-1.203576	0.543425	-6.205054
C	1.470263	0.159611	-2.436552
C	1.361192	0.405015	-5.269118
C	2.656772	0.196231	-3.215537
C	2.567192	0.322443	-4.642889
H	1.303943	0.498116	-6.350627
C	3.896030	0.102825	-2.546290
C	2.701932	-0.044898	-0.466239
H	3.490946	0.348740	-5.214838
C	3.913713	-0.017026	-1.170933
H	4.817871	0.127916	-3.121626
H	2.682100	-0.122043	0.619698
H	4.847094	-0.088415	-0.622208
N	-0.933740	0.218458	-2.338802
N	1.507853	0.037103	-1.074428
H	4.022999	0.000844	3.981398
H	2.245285	0.152939	6.146764

TS$_{(2-3)}$ for oxazole (Table 1 entry 2)

E_{gas} = -2573.261885 a.u.

E_{sol} = -2573.280405 a.u.

Cu	0.038021	-0.022700	-0.016222
H	0.017866	0.004055	1.958250
C	1.416654	-0.041676	1.708659
C	3.549354	0.341907	1.877019
C	3.370393	-0.978911	2.133564
N	2.317920	0.922509	1.612451
O	2.040166	-1.248554	2.038078
O	-1.143168	0.030103	1.655414
C	-1.772554	1.229533	2.042565
H	-2.298080	1.118226	3.004776
H	-1.054522	2.061605	2.152582
H	-2.520290	1.534182	1.293737
H	-2.990301	-1.334354	-0.260206
C	-2.644878	-1.249361	-1.287754
C	-3.453009	-1.633024	-2.375928
C	-2.945834	-1.529815	-3.659659
H	-4.450006	-2.023088	-2.197016
C	-0.920824	-0.643241	-2.695461
C	-1.641434	-1.022874	-3.854656
H	-3.537430	-1.835522	-4.518971
C	0.405074	-0.088710	-2.820613
C	-1.011908	-0.890663	-5.138939
C	1.002869	0.019189	-4.099066
C	0.258012	-0.404992	-5.253090
H	-1.566050	-1.194265	-6.023344
C	2.302463	0.568808	-4.162373
C	2.239826	0.861929	-1.771143
H	0.726545	-0.317650	-6.229909
C	2.918938	0.984875	-2.994860
H	2.800080	0.666179	-5.123730
H	2.675059	1.198098	-0.833045
H	3.912122	1.422055	-3.011076
N	-1.413741	-0.779969	-1.440957
N	1.013904	0.341841	-1.678770
H	4.026549	-1.799230	2.382668
H	4.468378	0.913553	1.868491

3 for oxazole (Table 1 entry 2)

E_{gas} = -2457.573484 a.u.

E_{sol} = -2457.587008 a.u.

Cu	-0.017962	-0.002556	-0.002459
C	-0.003524	-0.001046	1.869432
C	0.687411	0.001077	3.929263
C	-0.666121	-0.000732	3.975639
N	1.094309	0.000524	2.600834
O	-1.129073	-0.002185	2.689542
H	3.271931	-0.001412	1.082660
C	3.367019	-0.003632	-0.002553
C	4.616496	-0.006228	-0.661765
C	4.647267	-0.008919	-2.043632
H	5.534505	-0.006036	-0.082214
C	2.236425	-0.006556	-2.010900
C	3.433552	-0.009145	-2.770238
H	5.592456	-0.010885	-2.581200
C	0.956287	-0.006898	-2.685286
C	3.356333	-0.011809	-4.203109
C	0.916922	-0.009494	-4.102430
C	2.150392	-0.011906	-4.839921
H	4.280277	-0.013739	-4.775901
C	-0.350996	-0.009641	-4.724008
C	-1.358535	-0.005004	-2.543908
H	2.099983	-0.013882	-5.925467
C	-1.489576	-0.007342	-3.941072
H	-0.417933	-0.011564	-5.808783
H	-2.235427	-0.003273	-1.905076
H	-2.479619	-0.007369	-4.384846
N	2.220618	-0.003751	-0.663636
N	-0.177259	-0.004787	-1.919522
H	-1.402057	-0.001207	4.765345
H	1.395286	0.002526	4.748097

TS$_{(3-4)}$ for oxazole (Table 1 entry 2)

E_{gas} = -2700.576352 a.u.

E_{sol} = -2700.587814 a.u.

Cu	-0.015106	0.017621	0.032423
C	0.024704	-0.000608	1.971144
C	0.688231	0.017848	4.041350
C	-0.653412	-0.159794	4.066903
N	1.103548	0.116775	2.716733
O	-1.097893	-0.174459	2.772783
C	-0.770000	-1.938567	-0.365958
C	-1.851238	-1.955367	-1.264604
C	-0.831931	-2.744602	0.788107
C	-3.040439	-2.605457	-0.919358
H	-1.760956	-1.477995	-2.232640
C	-2.016523	-3.391505	1.116652
H	0.024671	-2.810446	1.448244
C	-3.135104	-3.315536	0.275657
H	-3.878787	-2.580435	-1.611731
H	-2.065530	-3.964000	2.039170
H	-4.053916	-3.832378	0.537263
I	1.277585	-1.915957	-1.486276
H	-2.664026	0.500074	-1.728854
C	-1.973357	1.234471	-2.131598

C	-2.372942	2.089496	-3.173607
C	-1.467307	3.004018	-3.674729
H	-3.380381	2.016806	-3.570210
C	0.120894	2.189537	-2.041722
C	-0.179975	3.083442	-3.102115
H	-1.736030	3.670808	-4.490039
C	1.393296	2.299461	-1.368330
C	0.809709	4.034788	-3.525356
C	2.336692	3.269508	-1.789673
C	2.017811	4.121776	-2.899468
H	0.567761	4.697343	-4.352134
C	3.544201	3.346930	-1.059236
C	2.729283	1.593147	0.378443
H	2.754112	4.853350	-3.222156
C	3.736603	2.515695	0.027624
H	4.301766	4.069913	-1.351762
H	2.801481	0.948655	1.252783
H	4.647338	2.565014	0.615932
N	-0.757348	1.251275	-1.591852
N	1.602848	1.482767	-0.314732
H	-1.392685	-0.280147	4.844114
H	1.383440	0.078695	4.868479

For benzothiazole (Table 1 entry 3)

benzothiazole

E_{gas} = -722.689910 a.u.

E_{sol} = -722.694940 a.u.

C	-0.183162	0.000000	-0.098254
C	0.099693	0.000000	2.085925
C	1.466619	0.000000	1.711814
C	-0.247107	0.000000	3.445126
C	2.483896	0.000000	2.670600
C	0.764303	0.000000	4.397683
H	-1.295690	0.000000	3.725251
C	2.117564	0.000000	4.013831
H	3.530030	0.000000	2.380145
H	0.508546	0.000000	5.453406
H	2.891358	0.000000	4.776373
N	-0.805938	0.000000	1.032126
H	-0.682355	0.000000	-1.061494
S	1.583515	0.000000	-0.037703

2 for benzothiazole (Table 1 entry 3)

E_{gas} = -3049.923917 a.u.

E_{sol} = -3049.936910 a.u.

Cu	-0.009429	-0.280099	-0.005706
H	-0.014778	-0.024125	2.589750
C	0.821816	0.029046	3.304539
C	2.888541	0.049515	4.115442
C	2.197193	0.203576	5.342086
C	4.290695	0.002903	4.113790
C	2.884550	0.310363	6.554999
C	4.973230	0.109015	5.319702
H	4.819656	-0.115693	3.172781
C	4.275796	0.261507	6.531356
H	2.349622	0.427800	7.492727
H	6.059138	0.073618	5.328618
H	4.828890	0.342383	7.463065
N	2.078417	-0.044598	2.989285
O	-1.329250	-0.260878	1.238435
C	-2.372086	0.633303	1.030293
H	-3.160600	0.496308	1.793995
H	-2.072229	1.702998	1.084478
H	-2.874158	0.512239	0.047076
H	-2.871191	-0.221790	-2.441889
C	-1.972026	-0.242117	-3.054482
C	-2.065389	-0.249106	-4.461278
C	-0.898916	-0.271287	-5.199017
H	-3.038283	-0.235272	-4.942589
C	0.326639	-0.284628	-3.110160
C	0.346463	-0.290560	-4.532528
H	-0.922906	-0.274891	-6.286024
C	1.583079	-0.310366	-2.385459
C	1.599144	-0.315157	-5.229980
C	2.803087	-0.335709	-3.111122
C	2.776546	-0.335472	-4.546644
H	1.589749	-0.317355	-6.316930
C	4.010954	-0.364155	-2.381316
C	2.724774	-0.337323	-0.352221
H	3.724450	-0.354067	-5.077898
C	3.967143	-0.364591	-1.001243
H	4.957870	-0.384355	-2.914463
H	2.657211	-0.322429	0.734027
H	4.875390	-0.383831	-0.407842
N	-0.822482	-0.256884	-2.398175
N	1.559553	-0.313721	-1.017792
S	0.474477	0.224548	5.027596

TS$_{(2-3)}$ for benzothiazole (Table 1 entry 3)

E_{gas} = -3049.887859 a.u.

E_{sol} = -3049.906430 a.u.

Cu	-0.086492	-0.182756	0.020355
H	-0.163328	-0.249483	2.036655
C	1.310716	-0.329253	1.825690
C	3.488466	0.297546	1.937113
C	3.726656	-1.101024	2.018552
C	4.576803	1.186837	1.960268
C	5.029641	-1.601367	2.117542
C	5.868963	0.683032	2.062542
H	4.385903	2.254912	1.906410
C	6.094744	-0.702583	2.140038
H	5.210336	-2.670743	2.181531
H	6.714105	1.366316	2.086679
H	7.111260	-1.078925	2.222349
N	2.157357	0.673120	1.828915
O	-1.242682	-0.124860	1.674666
C	-1.777800	1.117122	2.092906
H	-2.326924	1.014015	3.040552
H	-0.990631	1.874501	2.237649
H	-2.480838	1.496294	1.338070
H	-3.339442	-0.939856	-0.432542
C	-2.918948	-0.903272	-1.434767
C	-3.712105	-1.148654	-2.573676
C	-3.119477	-1.110624	-3.822113
H	-4.767379	-1.375396	-2.459492
C	-1.036559	-0.577589	-2.725340
C	-1.740400	-0.820706	-3.931405
H	-3.699384	-1.305028	-4.720849
C	0.375029	-0.268625	-2.767382
C	-1.030087	-0.776823	-5.178204
C	1.047849	-0.243664	-4.012610
C	0.306578	-0.508546	-5.214721
H	-1.578466	-0.969888	-6.096460
C	2.428531	0.057029	-4.000266
C	2.302240	0.292400	-1.608174
H	0.836987	-0.484842	-6.162969
C	3.053218	0.320921	-2.796051
H	2.981799	0.081477	-4.935429
H	2.755382	0.516766	-0.647580
H	4.110426	0.560280	-2.750038
N	-1.624249	-0.629769	-1.506961
N	0.999517	0.006125	-1.586678
S	2.195049	-1.938775	1.978135

3 for benzothiazole (Table 1 entry 3)

E_{gas} = -2934.199527 a.u.

E_{sol} = -2934.212663 a.u.

Cu	0.006243	-0.004183	-0.050772
C	-0.022171	-0.002907	1.820625

C	0.815459	-0.001848	3.922297
C	-0.551774	-0.001545	4.299501
C	1.803838	-0.001400	4.919230
C	-0.928660	-0.000813	5.646149
C	1.426450	-0.000676	6.257840
H	2.849985	-0.001628	4.625929
C	0.068339	-0.000385	6.620104
H	-1.977199	-0.000581	5.930939
H	2.188361	-0.000331	7.033304
H	-0.209224	0.000184	7.671196
N	1.061226	-0.002595	2.556097
H	3.312141	-0.005592	1.026934
C	3.400360	-0.007072	-0.058204
C	4.648876	-0.009417	-0.718741
C	4.676879	-0.011174	-2.100363
H	5.567542	-0.009794	-0.140394
C	2.265506	-0.008321	-2.062907
C	3.461471	-0.010653	-2.824103
H	5.620845	-0.012965	-2.639909
C	0.985017	-0.007799	-2.737357
C	3.383515	-0.012342	-4.256983
C	0.944956	-0.009478	-4.154564
C	2.177485	-0.011745	-4.893274
H	4.307289	-0.014107	-4.829908
C	-0.323422	-0.008855	-4.775296
C	-1.329878	-0.005203	-2.595561
H	2.126344	-0.013010	-5.978720
C	-1.461988	-0.006690	-3.992770
H	-0.390597	-0.010085	-5.860046
H	-2.206378	-0.003538	-1.956156
H	-2.452059	-0.006146	-4.436298
N	2.251686	-0.006528	-0.715239
N	-0.148351	-0.005731	-1.973010
S	-1.524520	-0.002240	2.846479

$TS_{(3-4)}$ for benzothiazole (Table 1 entry 3)

E_{gas} = -3177.202754 a.u.

E_{sol} = -3177.213824 a.u.

Cu	-0.137471	-0.018945	-0.056417
C	-0.286903	-0.004165	1.879841
C	0.443021	-0.048497	4.024548
C	-0.935862	0.070445	4.330604
C	1.378599	-0.124051	5.067126
C	-1.377038	0.117399	5.656689
C	0.936698	-0.077477	6.385606
H	2.433589	-0.219595	4.825957
C	-0.432254	0.042715	6.679076
H	-2.434401	0.209336	5.888996
H	1.656430	-0.135599	7.198164
H	-0.760321	0.076875	7.714899
N	0.750188	-0.083548	2.668498
C	-0.785665	-2.017429	-0.485206
C	-1.845852	-2.051606	-1.408698
C	-0.857105	-2.823986	0.668020
C	-3.029805	-2.722915	-1.089187
H	-1.742174	-1.569816	-2.373223
C	-2.037379	-3.491980	0.970337
H	-0.014852	-2.871933	1.348291
C	-3.137364	-3.435376	0.104010
H	-3.854294	-2.711409	-1.798182
H	-2.097795	-4.063876	1.892314
H	-4.052522	-3.968028	0.345402
I	1.284215	-1.918565	-1.514097
H	-2.640848	0.412268	-2.037878
C	-1.939371	1.171904	-2.368504
C	-2.277599	2.038702	-3.422189
C	-1.361953	2.990032	-3.827458
H	-3.246724	1.947129	-3.901636
C	0.113464	2.178906	-2.089780
C	-0.127592	3.090039	-3.150857
H	-1.583367	3.668928	-4.646946
C	1.329312	2.301431	-1.320603
C	0.865127	4.077061	-3.473357
C	2.276782	3.304139	-1.646224
C	2.019187	4.178473	-2.754791
H	0.668960	4.753774	-4.300747
C	3.427432	3.387530	-0.829983
C	2.560891	1.569593	0.490384
H	2.757969	4.936189	-3.002650
C	3.566259	2.525772	0.241420
H	4.184990	4.136543	-1.046915
H	2.599427	0.891347	1.340208
H	4.433368	2.575871	0.892157
N	-0.772499	1.209329	-1.729808
N	1.485654	1.457548	-0.278947
S	-1.836037	0.137235	2.831262

For thiazole (Table 1 entry 4)

thiazole

E_{gas} = -569.040508 a.u.

E_{sol} = -569.045620 a.u.

C	0.008015	0.000000	-0.000400
C	0.022058	0.000000	2.199084
C	1.374790	0.000000	2.010123
N	-0.748145	0.000000	1.057252
H	-0.367333	0.000000	-1.017185
S	1.729363	0.000000	0.313875
H	-0.469702	0.000000	3.165260
H	2.161253	0.000000	2.751783

2 for thiazole (Table 1 entry 4)

E_{gas} = -2896.274344 a.u.

E_{sol} = -2896.287157 a.u.

Cu	-0.011375	-0.011601	0.009476
H	-0.020444	-0.012775	2.628327
C	0.828939	0.001821	3.327202
C	2.909293	0.008002	4.093611
C	2.276312	0.041902	5.301770
N	2.090133	-0.013874	2.984312
O	-1.333076	-0.157883	1.242421
C	-2.407581	0.712472	1.114320
H	-3.189875	0.478245	1.860888
H	-2.147593	1.783408	1.265967
H	-2.907277	0.663262	0.123320
H	-2.874597	0.280618	-2.415686
C	-1.974769	0.329744	-3.025703
C	-2.067036	0.460705	-4.426479
C	-0.899777	0.523656	-5.160590
H	-3.039645	0.511935	-4.905875
C	0.324315	0.316688	-3.080834
C	0.345147	0.452057	-4.496931
H	-0.922719	0.627176	-6.242707
C	1.580511	0.233290	-2.359930
C	1.598351	0.510712	-5.191293
C	2.801109	0.295018	-3.082588
C	2.775396	0.436991	-4.511113
H	1.589607	0.615665	-6.273192
C	4.009108	0.209873	-2.357419
C	2.722144	0.020012	-0.337242
H	3.723885	0.482440	-5.039745
C	3.964856	0.073201	-0.984146
H	4.956263	0.254484	-2.888737
H	2.653682	-0.071633	0.745650
H	4.872877	0.007586	-0.393751
N	-0.825738	0.261838	-2.371891
N	1.556665	0.093515	-0.999303
S	0.560192	0.045266	5.055898
H	3.985221	-0.002464	3.956579
H	2.713256	0.063530	6.290334

$TS_{(2-3)}$ for thiazole (Table 1 entry 4)

E_{gas} = −2896.236368 a.u.

E_{sol} = −2896.254335 a.u.

Cu	0.021318	−0.022017	−0.015046
H	0.006574	−0.003584	1.969925
C	1.413636	−0.037729	1.696557
C	3.552484	0.682124	1.808955
C	3.841855	−0.650568	1.922451
N	2.222874	1.010916	1.684327
O	−1.142336	0.070736	1.667515
C	−1.697895	1.309135	2.052501
H	−2.215998	1.234588	3.021741
H	−0.930294	2.096475	2.144527
H	−2.436698	1.646994	1.309618
H	−3.099986	−1.030814	−0.236624
C	−2.753128	−0.983934	−1.266034
C	−3.599594	−1.291275	−2.349177
C	−3.090151	−1.245843	−3.635258
H	−4.629437	−1.579927	−2.164308
C	−0.982868	−0.560138	−2.684075
C	−1.742180	−0.873913	−3.837963
H	−3.712713	−1.496721	−4.490405
C	0.393479	−0.148951	−2.816319
C	−1.106364	−0.819534	−5.124687
C	0.997346	−0.123789	−4.096003
C	0.208322	−0.475026	−5.245083
H	−1.691962	−1.070738	−6.005185
C	2.351239	0.273033	−4.165514
C	2.323381	0.601142	−1.778775
H	0.681654	−0.448932	−6.223088
C	3.013096	0.626866	−3.002819
H	2.855692	0.302365	−5.127760
H	2.800235	0.901074	−0.849987
H	4.050642	0.944207	−3.022703
N	−1.482127	−0.639369	−1.426943
N	1.045854	0.229171	−1.680047
S	2.370892	−1.561124	1.896483
H	4.294334	1.476159	1.816809
H	4.815584	−1.110806	2.024326

3 for thiazole (Table 1 entry 4)

E_{gas} = −2780.547779 a.u.

E_{sol} = −2780.560195 a.u.

Cu	−0.022618	−0.000385	−0.006780
C	−0.013913	−0.000118	1.865399
C	0.871403	−0.000071	3.942375
C	−0.432265	0.000146	4.344512
N	1.095716	−0.000216	2.581887
H	3.291627	−0.001487	1.040051
C	3.372516	−0.001947	−0.045918
C	4.614478	−0.002944	−0.718946
C	4.629014	−0.003465	−2.100954
H	5.539013	−0.003279	−0.149908
C	2.218271	−0.002045	−2.039963
C	3.406754	−0.003018	−2.813016
H	5.567728	−0.004219	−2.649711
C	0.930797	−0.001594	−2.700905
C	3.314152	−0.003490	−4.244960
C	0.876345	−0.002070	−4.117676
C	2.101530	−0.003023	−4.868708
H	4.231964	−0.004228	−4.827486
C	−0.398010	−0.001587	−4.725953
C	−1.382568	−0.000299	−2.535966
H	2.039271	−0.003377	−5.953619
C	−1.528542	−0.000691	−3.931607
H	−0.476068	−0.001926	−5.809982
H	−2.252637	0.000386	−1.887874
H	−2.523120	−0.000295	−4.365054
N	2.218010	−0.001507	−0.692536
N	−0.194886	−0.000735	−1.924307
S	−1.449050	0.000228	2.938621
H	−0.821264	0.000281	5.353648
H	1.723643	−0.000142	4.616130

$TS_{(3-4)}$ for thiazole (Table 1 entry 4)

E_{gas} = −3023.550729 a.u.

E_{sol} = −3023.561463 a.u.

Cu	−0.011827	0.008073	0.019730
C	0.004517	0.004338	1.961186
C	0.918034	0.031123	4.029174
C	−0.379419	0.028228	4.446574
N	1.118282	0.020208	2.661887
C	−0.552667	−2.032541	−0.385580
C	−1.653016	−2.139356	−1.255657
C	−0.513574	−2.843243	0.766509
C	−2.772883	−2.887472	−0.879862
H	−1.630601	−1.654196	−2.223904
C	−1.629761	−3.589039	1.124180
H	0.362263	−2.833837	1.404369
C	−2.773721	−3.605623	0.314537
H	−3.630018	−2.931481	−1.547807
H	−1.605486	−4.164319	2.045812
H	−3.638075	−4.198457	0.599247
I	1.450654	−1.806697	−1.523467
H	−2.666593	0.247797	−1.766098
C	−2.048907	1.055444	−2.146348
C	−2.527893	1.895062	−3.166691
C	−1.715596	2.908093	−3.637713
H	−3.522488	1.734927	−3.569946
C	−0.056848	2.205979	−2.022147
C	−0.442886	3.095921	−3.058149
H	−2.047237	3.568253	−4.434993
C	1.202238	2.415986	−1.347455
C	0.450257	4.149952	−3.452133
C	2.049412	3.481713	−1.741783
C	1.646336	4.333606	−2.824191
H	0.144140	4.810288	−4.259179
C	3.251001	3.646260	−1.016335
C	2.616149	1.775857	0.362359
H	2.308582	5.141029	−3.125722
C	3.531150	2.798524	0.038680
H	3.935991	4.445514	−1.288500
H	2.762981	1.103939	1.205754
H	4.440672	2.909801	0.620345
N	−0.841401	1.175739	−1.599515
N	1.495639	1.588248	−0.322841
S	−1.419639	0.010253	3.055690
H	−0.755023	0.036516	5.460868
H	1.781478	0.037181	4.688058

For benzothiophene (Table 1 entry 5)

benzothiophene

E_{gas} = −706.644454 a.u.

E_{sol} = −706.648570 a.u.

H	−0.010839	−0.011011	0.015133
C	0.006974	0.003336	1.097193
C	0.742904	−0.000649	3.487499
C	−0.664908	0.067980	3.331968
C	1.342143	−0.013481	4.751568
C	−1.471432	0.124536	4.484256
C	0.521178	0.043177	5.872947
H	2.422044	−0.066268	4.856249
C	−0.878098	0.111943	5.739216
H	−2.552631	0.177543	4.384997
H	0.967177	0.034297	6.863607
H	−1.499257	0.155473	6.629559
S	1.548307	−0.062442	1.926470
C	−1.052793	0.068122	1.943622

H	-2.084116	0.115251	1.610110

2 for benzothiophene (Table 1 entry 5)

E_{gas} = -3033.873805 a.u.

E_{sol} = -3033.885993 a.u.

Cu	0.340930	1.546331	0.429922
H	0.505944	1.991291	3.195548
C	1.304100	1.292034	3.418616
C	3.270819	0.252755	4.151090
C	2.569831	-0.859842	3.614368
C	4.547002	0.048182	4.708953
C	3.125920	-2.144267	3.628114
C	5.095615	-1.227869	4.722852
H	5.094483	0.888568	5.129174
C	4.389184	-2.319560	4.184490
H	2.580143	-2.989006	3.216548
H	6.079573	-1.387424	5.155925
H	4.833009	-3.311332	4.206179
O	-0.950490	1.761436	1.682841
C	-2.278392	1.704454	1.291499
H	-2.948326	1.830631	2.162856
H	-2.569653	2.498790	0.568491
H	-2.570183	0.741872	0.818265
H	-2.494578	2.059576	-1.942096
C	-1.626606	1.872343	-2.570818
C	-1.752232	1.834177	-3.974579
C	-0.622754	1.594859	-4.731534
H	-2.720720	1.991288	-4.439005
C	0.632850	1.449999	-2.666069
C	0.618381	1.395189	-4.087218
H	-0.672899	1.557880	-5.817025
C	1.883915	1.247668	-1.962007
C	1.834906	1.145650	-4.804170
C	3.069314	1.009455	-2.706585
C	3.009506	0.962286	-4.140506
H	1.800894	1.107171	-5.889954
C	4.276357	0.826672	-1.998478
C	3.054563	1.122778	0.045279
H	3.930365	0.775521	-4.686538
C	4.264967	0.887074	-0.618349
H	5.196683	0.641847	-2.545978
H	3.019528	1.171273	1.128374
H	5.171233	0.751944	-0.037539
N	-0.479753	1.687878	-1.935647
N	1.887243	1.295492	-0.593713
S	1.009683	-0.374749	2.966138
C	2.508676	1.472198	4.023441
H	2.858237	2.435137	4.382582

TS$_{(2-3)}$ for benzothiophene (Table 1 entry 5)

E_{gas} = -3033.838608 a.u.

E_{sol} = -3033.854595 a.u.

Cu	0.050713	-0.066721	-0.023681
H	-0.007273	-0.024992	1.953550
C	1.369499	0.028765	1.654706
C	3.607027	0.872277	1.802722
C	3.882970	-0.521918	1.811593
C	4.689772	1.774909	1.867892
C	5.194364	-1.006055	1.876760
C	5.989704	1.291847	1.936270
H	4.499949	2.846026	1.868044
C	6.243602	-0.093183	1.939840
H	5.390678	-2.075007	1.884345
H	6.822275	1.988897	1.989722
H	7.267486	-0.453478	1.997096
O	-1.192558	-0.014044	1.667576
C	-1.816411	1.184756	2.049556
H	-2.329726	1.091341	3.021136
H	-1.100828	2.024022	2.141702
H	-2.575505	1.486834	1.309386
H	-3.017033	-0.991627	-0.183041
C	-2.701623	-0.943784	-1.222209
C	-3.580594	-1.226058	-2.286104
C	-3.104315	-1.182556	-3.585073
H	-4.610923	-1.495337	-2.076562
C	-0.960563	-0.546041	-2.685843
C	-1.754196	-0.838276	-3.821085
H	-3.754210	-1.415822	-4.424710
C	0.422401	-0.170973	-2.847348
C	-1.146065	-0.795118	-5.121861
C	1.000301	-0.165196	-4.138889
C	0.175427	-0.488432	-5.270972
H	-1.757643	-1.027472	-5.989764
C	2.366905	0.181586	-4.232050
C	2.393614	0.501656	-1.844187
H	0.627176	-0.474810	-6.259398
C	3.063390	0.504326	-3.080739
H	2.855185	0.194178	-5.203028
H	2.902143	0.777366	-0.923904
H	4.112689	0.778582	-3.117708
N	-1.428499	-0.622634	-1.416405
N	1.105597	0.183223	-1.724055
S	2.382070	-1.430223	1.740079
C	2.194314	1.135407	1.719492
H	1.802841	2.150471	1.721626

3 for benzothiophene (Table 1 entry 5)

E_{gas} = -2918.147098 a.u.

E_{sol} = -2918.160691 a.u.

Cu	-0.199572	-0.027045	-0.002686
C	-0.033798	-0.048435	1.861784
C	0.695578	0.092245	4.134223
C	-0.664836	-0.241665	4.360474
C	1.534489	0.278981	5.250313
C	-1.179057	-0.387547	5.652572
C	1.024254	0.135831	6.535149
H	2.581267	0.535544	5.101008
C	-0.327613	-0.196435	6.738280
H	-2.223716	-0.645143	5.808581
H	1.675297	0.281384	7.393890
H	-0.711527	-0.305139	7.749623
H	-3.749147	0.329435	0.766493
C	-3.709519	0.301858	-0.320653
C	-4.888160	0.386484	-1.091882
C	-4.785898	0.347632	-2.468230
H	-5.851853	0.479371	-0.601046
C	-2.391789	0.148784	-2.198646
C	-3.511780	0.226936	-3.068286
H	-5.670258	0.409361	-3.097662
C	-1.062882	0.028371	-2.762130
C	-3.312963	0.182220	-4.488382
C	-0.903441	-0.008771	-4.171923
C	-2.062265	0.068975	-5.016754
H	-4.182682	0.241198	-5.137736
C	0.406531	-0.120123	-4.686295
C	1.228164	-0.144821	-2.433351
H	-1.917498	0.036586	-6.093254
C	1.474789	-0.187115	-3.812903
H	0.559550	-0.150818	-5.761821
H	2.045805	-0.197069	-1.722216
H	2.494858	-0.272048	-4.172435
N	-2.503280	0.184894	-0.853309
N	0.002271	-0.040740	-1.909856
S	-1.488931	-0.422692	2.819208
C	1.001620	0.187603	2.728120
H	2.003806	0.438099	2.386860

TS$_{(3-4)}$ for benzothiophene (Table 1 entry 5)

E_{gas} = -3161.148046 a.u.

E_{sol} = -3161.159420 a.u.

Cu	-0.076127	0.131000	0.569167
C	0.008011	0.421568	2.669341
C	1.281783	0.831096	3.101279
C	-0.668845	-0.587263	3.382236
C	1.939036	0.118402	4.110032
H	1.755841	1.697087	2.653851
C	-0.004754	-1.284861	4.383801
H	-1.680720	-0.860593	3.107955
C	1.305619	-0.946127	4.748431
H	2.936166	0.427611	4.414874
H	-0.518579	-2.098819	4.888155
H	1.809904	-1.488540	5.542979
I	-1.272212	2.205298	1.942447
H	3.032287	0.115132	1.370281
C	3.053287	0.513937	0.360438
C	4.278589	0.750640	-0.285771
C	4.271867	1.271765	-1.565063
H	5.207929	0.524804	0.227009
C	1.853759	1.243130	-1.466114
C	3.037060	1.526947	-2.197846
H	5.199752	1.477512	-2.092501
C	0.570460	1.433718	-2.099846
C	2.934865	2.035243	-3.537197
C	0.505234	1.918445	-3.431693
C	1.721853	2.224654	-4.128736
H	3.852171	2.257032	-4.076134
C	-0.777826	2.061227	-4.003824
C	-1.720745	1.241327	-1.950440
H	1.657144	2.601243	-5.146215
C	-1.893373	1.719947	-3.262814
H	-0.873549	2.431350	-5.021396
H	-2.574830	0.951704	-1.344315
H	-2.892855	1.812964	-3.675106
N	1.868468	0.766562	-0.191502
N	-0.528643	1.107348	-1.383542
C	-0.865362	-1.632577	0.365039
S	-2.637247	-1.797724	0.326176
C	-0.314288	-2.871451	0.178347
C	-2.588205	-3.537321	0.061342
C	-1.237907	-3.967893	0.005294
H	0.761283	-3.039009	0.167135
C	-3.651806	-4.432860	-0.082423
C	-0.979723	-5.336859	-0.200292
C	-3.367995	-5.781758	-0.285506
H	-4.680856	-4.085444	-0.036170
C	-2.035968	-6.229394	-0.343712
H	0.047958	-5.691277	-0.245962
H	-4.182756	-6.492491	-0.398832
H	-1.832096	-7.285647	-0.502302

For thiophene (Table 1 entry 6)

thiophene

E_{gas} = -552.996668 a.u.

E_{sol} = -553.000344 a.u.

C	0.005188	-0.000077	-0.006476
C	0.007980	0.000145	2.323415
C	1.354632	-0.000032	2.082760
H	-0.313840	-0.000108	-1.040038
S	1.696652	-0.000474	0.381687
C	-0.767843	0.000113	1.122014
H	-1.852359	0.000287	1.102005
H	-0.419737	0.000340	3.320216
H	2.164799	-0.000021	2.799398

2 for thiophene (Table 1 entry 6)

E_{gas} = -2880.224845 a.u.

E_{sol} = -2880.236981 a.u.

Cu	0.012802	-0.039638	0.001402
H	0.001626	0.011012	2.799171
C	1.073668	0.016683	2.956778
C	3.269728	0.494486	3.598298
C	3.464232	-0.682458	2.925739
O	-1.006767	-0.959839	1.182372
C	-1.991036	-1.805384	0.699499
H	-2.515373	-2.311989	1.532019
H	-2.783994	-1.288013	0.113806
H	-1.609740	-2.616251	0.040816
H	-2.576874	-1.196681	-2.430777
C	-1.856823	-0.637878	-3.024924
C	-2.022382	-0.509273	-4.419164
C	-1.083319	0.210013	-5.131051
H	-2.873284	-0.969836	-4.911322
C	0.082305	0.600223	-3.044484
C	0.009171	0.793559	-4.451838
H	-1.171264	0.335338	-6.207517
C	1.186221	1.181147	-2.305752
C	1.021748	1.557315	-5.120827
C	2.166208	1.936902	-3.002189
C	2.054922	2.105437	-4.423864
H	0.947143	1.691379	-6.196970
C	3.224416	2.502966	-2.259711
C	2.266787	1.547891	-0.276700
H	2.819783	2.685675	-4.933163
C	3.268876	2.307751	-0.892724
H	3.986957	3.084640	-2.770704
H	2.280670	1.381116	0.795198
H	4.064114	2.728557	-0.286433
N	-0.844598	-0.105403	-2.358254
N	1.249706	0.988789	-0.951232
S	1.972276	-1.317471	2.303470
C	1.893143	0.892352	3.617610
H	1.531329	1.789538	4.109881
H	4.395441	-1.209642	2.763243
H	4.069671	1.057601	4.068710

TS$_{(2-3)}$ for thiophene (Table 1 entry 6)

E_{gas} = -2880.189719 a.u.

E_{sol} = -2880.204934 a.u.

Cu	0.004183	-0.013234	-0.010725
H	-0.005299	-0.008825	1.957663
C	1.339792	-0.011068	1.614685
C	3.611795	0.706041	1.775707
C	3.813015	-0.651521	1.761111
O	-1.223612	0.067390	1.724724
C	-1.760386	1.291269	2.147123
H	-2.245683	1.214627	3.135557
H	-0.993942	2.087145	2.228486
H	-2.526044	1.655680	1.440924
H	-3.045131	-0.804585	-0.060811
C	-2.776843	-0.741129	-1.112255
C	-3.711571	-0.952150	-2.143429
C	-3.290204	-0.897133	-3.461935
H	-4.742846	-1.182313	-1.895447
C	-1.085111	-0.373216	-2.643288
C	-1.938366	-0.604244	-3.748750
H	-3.985265	-1.082492	-4.276959
C	0.301276	-0.045457	-2.854097
C	-1.380881	-0.558423	-5.072434
C	0.829715	-0.042692	-4.166907
C	-0.053430	-0.309170	-5.269841
H	-2.036415	-0.745004	-5.919099
C	2.204769	0.248632	-4.306007
C	2.331797	0.533527	-1.915521
H	0.358277	-0.296871	-6.275709
C	2.956136	0.522690	-3.175260
H	2.657479	0.258134	-5.294117
H	2.883192	0.774022	-1.009585
H	4.013846	0.754649	-3.249351
N	-1.498079	-0.473658	-1.355032

N	1.035380	0.271853	-1.752154
S	2.296783	-1.488986	1.674328
C	2.229961	1.055856	1.700385
H	1.891038	2.088925	1.721202
H	4.420381	1.428300	1.847678
H	4.753474	-1.186351	1.804155

3 for thiophene (Table 1 entry 6)

E_{gas} = -2764.496602 a.u.

E_{sol} = -2764.509552 a.u.

Cu	0.003851	0.034964	0.004773
C	0.015177	0.036607	1.875978
C	0.547543	-0.095739	4.197199
C	-0.766637	0.264588	4.312952
H	-3.368301	1.416267	0.431738
C	-3.242131	1.336746	-0.646099
C	-4.275656	1.722151	-1.525807
C	-4.068720	1.603733	-2.885788
H	-5.211577	2.103092	-1.129330
C	-1.864230	0.743984	-2.388355
C	-2.835384	1.103398	-3.360820
H	-4.839743	1.889887	-3.596942
C	-0.583098	0.226679	-2.822910
C	-2.535750	0.949514	-4.755232
C	-0.320334	0.090342	-4.211230
C	-1.329624	0.464150	-5.162070
H	-3.292160	1.229223	-5.484036
C	0.939647	-0.413213	-4.600129
C	1.522015	-0.587079	-2.280205
H	-1.107378	0.350456	-6.219690
C	1.862960	-0.751802	-3.629601
H	1.168817	-0.528071	-5.656216
H	2.224995	-0.845148	-1.495320
H	2.841222	-1.141215	-3.891172
N	-2.077168	0.863402	-1.060001
N	0.338597	-0.113799	-1.873582
S	-1.469974	0.445676	2.732268
C	0.973863	-0.220744	2.835567
H	1.993236	-0.500685	2.578516
H	1.195366	-0.268425	5.052564
H	-1.343283	0.426219	5.214680

TS$_{(3-4)}$ for thiophene (Table 1 entry 6)

E_{gas} = -3007.497282 a.u.

E_{sol} = -3007.507852 a.u.

Cu	-0.035102	-0.009241	-0.006849
C	-0.042333	-0.016572	2.100305
C	1.255585	0.109377	2.626712
C	-0.916766	-0.975507	2.649471
C	1.723903	-0.821412	3.561189
H	1.896863	0.921849	2.304183
C	-0.439344	-1.890459	3.579340
H	-1.940262	-1.035409	2.300359
C	0.884906	-1.827411	4.036108
H	2.739484	-0.728215	3.939226
H	-1.110274	-2.658259	3.955383
H	1.243350	-2.538120	4.775285
I	-0.970760	2.050592	1.607960
H	2.878200	-0.963252	0.946062
C	3.087549	-0.475968	-0.001564
C	4.377012	-0.522468	-0.557933
C	4.614982	0.124196	-1.755736
H	5.165052	-1.060348	-0.040858
C	2.284002	0.773431	-1.762431
C	3.552948	0.793434	-2.399145
H	5.601988	0.117608	-2.211061
C	1.157862	1.398309	-2.413634
C	3.699645	1.466285	-3.659557
C	1.332746	2.038765	-3.667537
C	2.636575	2.064770	-4.267148
H	4.681071	1.479298	-4.126211
C	0.188338	2.612198	-4.263295
C	-1.100153	1.853665	-2.380624
H	2.757747	2.563726	-5.225090
C	-1.031343	2.517343	-3.619580
H	0.277282	3.115305	-5.222822
H	-2.044739	1.749537	-1.853894
H	-1.930664	2.942756	-4.053049
N	2.065282	0.163773	-0.565742
N	-0.039564	1.316301	-1.791076
C	-1.241235	-1.450413	-0.502108
S	-2.962883	-1.142674	-0.708410
C	-1.027851	-2.775388	-0.818062
C	-3.330415	-2.772968	-1.203559
C	-2.187652	-3.522544	-1.210083
H	-0.043175	-3.236758	-0.767430
H	-2.167154	-4.574645	-1.482523
H	-4.339188	-3.078334	-1.450885

For benzofuran (Table 1 entry 7)

benzofuran

E_{gas} = -383.666048 a.u.

E_{sol} = -383.670254 a.u.

C	0.185080	-0.009451	0.055712
C	-0.156756	-0.007889	2.266626
C	1.223306	-0.002122	1.985076
C	-0.571929	-0.007678	3.607517
C	2.210909	0.003733	2.963340
C	0.400987	-0.001833	4.603278
H	-1.627929	-0.012007	3.863206
C	1.773430	0.003781	4.287252
H	3.264004	0.008035	2.701853
H	0.098137	-0.001560	5.646721
H	2.505699	0.008257	5.089613
H	0.181586	-0.010532	-1.024252
C	-0.808881	-0.012431	0.977894
H	-1.870957	-0.018028	0.775627
O	1.431890	-0.003125	0.630993

2 for benzofuran (Table 1 entry 7)

E_{gas} = -2710.894683 a.u.

E_{sol} = -2710.908070 a.u.

Cu	-0.138735	0.740966	0.354835
H	-0.596674	0.601314	2.921845
C	0.375364	0.423584	3.383332
C	2.384643	0.392729	4.399136
C	2.066869	-0.889363	3.905181
C	3.609534	0.573579	5.061950
C	2.901057	-1.993843	4.035490
C	4.459626	-0.521233	5.203112
H	3.887786	1.545833	5.460193
C	4.112076	-1.788516	4.697613
H	2.614906	-2.963993	3.641925
H	5.409388	-0.397959	5.716899
H	4.796686	-2.622132	4.827505
O	-1.652881	1.009398	1.315761
C	-2.829743	0.468951	0.820845
H	-3.682165	0.721894	1.479018
H	-3.106139	0.846245	-0.188383
H	-2.823562	-0.640284	0.738423
H	-2.533165	0.113698	-2.448364
C	-1.545689	-0.060588	-2.870558
C	-1.401821	-0.465772	-4.213287
C	-0.129567	-0.675199	-4.706250
H	-2.279494	-0.606680	-4.836309
C	0.727973	-0.074241	-2.522633
C	0.985445	-0.481049	-3.861051
H	0.028552	-0.987870	-5.735501
C	1.842671	0.133735	-1.619383

C	2.336193	-0.677663	-4.300228
C	3.166656	-0.067940	-2.091215
C	3.381022	-0.478760	-3.450278
H	2.509711	-0.989332	-5.327030
C	4.234953	0.145678	-1.193872
C	2.627853	0.723213	0.490416
H	4.403733	-0.628310	-3.785980
C	3.960737	0.543822	0.099958
H	5.256764	-0.005839	-1.531313
H	2.386042	1.034471	1.500957
H	4.752200	0.715146	0.821726
N	-0.522987	0.129951	-2.051520
N	1.587069	0.524495	-0.332367
C	1.257795	1.222697	4.042678
H	1.119669	2.273527	4.257929
O	0.846400	-0.869801	3.289420

TS$_{(2-3)}$ for benzofuran (Table 1 entry 7)

E_{gas} = -2710.858901 a.u.

E_{sol} = -2710.875759 a.u.

Cu	-0.081199	0.000546	0.094652
H	-0.108298	-0.022548	2.050887
C	1.244087	0.007425	1.732113
C	3.477233	0.480127	1.969792
C	3.276063	-0.917391	1.975200
C	4.786942	0.975933	2.099204
C	4.314186	-1.836434	2.099018
C	5.836200	0.069035	2.226955
H	4.977515	2.046449	2.104355
C	5.604491	-1.320233	2.226559
H	4.118976	-2.904381	2.100556
H	6.853666	0.437282	2.331536
H	6.444391	-2.001952	2.331312
O	-1.325187	0.036077	1.819422
C	-1.888293	1.237598	2.272163
H	-2.392274	1.119294	3.246813
H	-1.134628	2.040122	2.397380
H	-2.644149	1.616047	1.562913
H	-3.139111	-0.850125	0.021721
C	-2.863938	-0.783598	-1.027793
C	-3.784765	-1.023058	-2.066336
C	-3.354455	-0.957065	-3.380716
H	-4.811800	-1.279236	-1.826474
C	-1.169424	-0.379354	-2.545171
C	-2.007778	-0.630295	-3.657530
H	-4.038180	-1.159264	-4.201315
C	0.212663	-0.023024	-2.745331
C	-1.443667	-0.566592	-4.977319
C	0.746748	0.002475	-4.055430
C	-0.122476	-0.279988	-5.165236
H	-2.088600	-0.767520	-5.828784
C	2.115431	0.327431	-4.186891
C	2.227430	0.591013	-1.794512
H	0.295154	-0.251455	-6.168253
C	2.855895	0.610723	-3.052274
H	2.571442	0.354063	-5.173147
H	2.771282	0.833048	-0.884385
H	3.908240	0.867386	-3.119080
N	-1.592448	-0.481364	-1.261702
N	0.938300	0.294500	-1.637498
C	2.160900	1.037061	1.817464
H	1.909858	2.090606	1.790906
O	1.954779	-1.207381	1.843517

3 for benzofuran (Table 1 entry 7)

E_{gas} = -2595.168389 a.u.

E_{sol} = -2595.181736 a.u.

Cu	0.312091	-0.037594	-0.026152
C	0.374607	-0.039248	1.845042
C	0.663917	-0.130607	4.117866
C	-0.628670	0.352383	3.826123
C	1.044447	-0.263122	5.462781
C	-1.549950	0.706487	4.805780
C	0.133333	0.086985	6.458874
H	2.033127	-0.632288	5.725600
C	-1.149154	0.566436	6.136927
H	-2.536991	1.075425	4.541401
H	0.417116	-0.011326	7.503979
H	-1.838719	0.831867	6.934281
H	-2.921412	1.121711	0.832492
C	-2.930862	1.099597	-0.254986
C	-4.072442	1.477230	-0.994414
C	-4.020768	1.426998	-2.374125
H	-4.970745	1.800445	-0.477774
C	-1.746084	0.643528	-2.174215
C	-2.833417	1.000712	-3.012681
H	-4.880306	1.710665	-2.976472
C	-0.502834	0.198134	-2.765888
C	-2.683387	0.915998	-4.437204
C	-0.388937	0.127608	-4.177716
C	-1.511561	0.498038	-4.994223
H	-3.524639	1.192786	-5.067484
C	0.839849	-0.309991	-4.718144
C	1.673783	-0.551074	-2.480172
H	-1.404606	0.436813	-6.073890
C	1.872664	-0.649174	-3.865167
H	0.959825	-0.374987	-5.796309
H	2.466356	-0.811609	-1.786776
H	2.830323	-0.989029	-4.245229
N	-1.807831	0.697379	-0.827489
N	0.525598	-0.141600	-1.931695
C	1.267005	-0.366650	2.832009
H	2.267767	-0.743600	2.659064
O	-0.815518	0.412110	2.478254

TS$_{(3-4)}$ for benzofuran (Table 1 entry 7)

E_{gas} = -2838.170130 a.u.

E_{sol} = -2838.181543 a.u.

Cu	0.046762	-0.230144	0.010867
C	0.103345	-0.219428	2.128072
C	1.406483	-0.074466	2.637934
C	-0.758319	-1.165798	2.717496
C	1.892915	-0.978815	3.588038
H	2.034813	0.739514	2.295701
C	-0.264555	-2.054107	3.665696
H	-1.785657	-1.241723	2.385011
C	1.065891	-1.976700	4.100259
H	2.912830	-0.870727	3.949940
H	-0.928940	-2.811137	4.074190
H	1.437912	-2.667344	4.851547
I	-0.835074	1.848305	1.616862
H	3.082619	-0.894072	0.890832
C	3.219667	-0.351522	-0.039707
C	4.502660	-0.202206	-0.594285
C	4.646707	0.509317	-1.769463
H	5.358153	-0.642694	-0.092608
C	2.247659	0.821811	-1.766146
C	3.500346	1.040605	-2.397222
H	5.624587	0.655391	-2.221046
C	1.043072	1.286617	-2.410868
C	3.549157	1.762088	-3.638172
C	1.123571	1.977213	-3.646836
C	2.410758	2.214071	-4.236051
H	4.518875	1.931423	-4.098622
C	-0.093423	2.382917	-4.237452
C	-1.260327	1.382454	-2.387260
H	2.459588	2.750997	-5.179769
C	-1.286668	2.082256	-3.608643
H	-0.078775	2.918833	-5.183098
H	-2.176428	1.106662	-1.875509

H	−2.238353	2.373685	−4.041068
N	2.118278	0.158620	−0.585179
N	−0.130517	1.004708	−1.802700
C	−1.127266	−1.725784	−0.387259
C	−1.196108	−3.056684	−0.069416
C	−2.818902	−2.619933	−1.579048
C	−2.271051	−3.666747	−0.810137
H	−0.548781	−3.556838	0.640408
C	−3.894478	−2.786438	−2.443867
C	−2.834111	−4.947806	−0.923596
C	−4.437849	−4.070121	−2.540769
H	−4.289561	−1.952439	−3.016864
C	−3.911779	−5.135894	−1.788765
H	−2.438507	−5.781082	−0.347474
H	−5.278564	−4.246718	−3.206750
H	−4.355793	−6.123813	−1.884798
O	−2.143466	−1.458901	−1.336362

For furan (Table 1 entry 8)

furan

E_{gas} = −230.016371 a.u.

E_{sol} = −230.020184 a.u.

C	0.039936	0.003869	0.046119
C	−0.007347	−0.000748	2.281073
C	1.283274	0.000288	1.848690
C	−0.822650	0.001517	1.098985
H	−1.902524	0.001318	1.047326
O	1.330887	0.003349	0.485854
H	−0.342927	−0.002904	3.308775
H	2.239454	−0.000629	2.349388
H	−0.088332	0.006142	−1.025563

2 for furan (Table 1 entry 8)

E_{gas} = −2557.243655 a.u.

E_{sol} = −2557.257585 a.u.

Cu	−0.013151	−0.037979	−0.005424
H	0.040006	−0.006862	2.599812
C	1.084667	0.025370	2.905852
C	3.197560	0.396417	3.582218
C	3.042691	−0.918934	3.264086
O	−1.366885	0.088499	1.191921
C	−2.509494	−0.659598	0.958714
H	−3.266914	−0.470390	1.742881
H	−3.011278	−0.425598	−0.006597
H	−2.342892	−1.759670	0.952746
H	−2.712787	−1.171497	−2.337653
C	−1.791778	−1.233861	−2.913609
C	−1.809002	−1.699351	−4.244293
C	−0.616282	−1.761870	−4.936608
H	−2.745541	−1.999277	−4.703958
C	0.485115	−0.910736	−2.954770
C	0.579833	−1.362008	−4.300516
H	−0.582502	−2.114325	−5.964644
C	1.688204	−0.492968	−2.262093
C	1.855746	−1.396889	−4.953817
C	2.933301	−0.537858	−2.943343
C	2.983334	−1.000939	−4.301596
H	1.904678	−1.746305	−5.981952
C	4.088769	−0.118796	−2.249831
C	2.708146	0.333417	−0.339288
H	3.948948	−1.027543	−4.799536
C	3.970784	0.318760	−0.944804
H	5.053256	−0.145229	−2.749917
H	2.589767	0.670828	0.685167
H	4.834699	0.648505	−0.377450
N	−0.689367	−0.852756	−2.287216
N	1.588955	−0.060135	−0.966909
C	1.919417	1.010814	3.349448
H	1.654247	2.048070	3.502405
O	1.766127	−1.161373	2.851851
H	3.701872	−1.773981	3.278807
H	4.099870	0.869719	3.945408

TS$_{(2-3)}$ for furan (Table 1 entry 8)

E_{gas} = −2557.207479 a.u.

E_{sol} = −2557.223641 a.u.

Cu	0.023548	−0.017328	−0.019926
H	0.004315	−0.001036	1.923534
C	1.324975	−0.014500	1.592327
C	3.558571	0.375822	1.918474
C	3.317253	−0.967137	1.964962
O	−1.248828	0.090593	1.727861
C	−1.748551	1.323220	2.159401
H	−2.245142	1.254939	3.144149
H	−0.957452	2.094876	2.258416
H	−2.496674	1.726980	1.453633
H	−2.981104	−0.827113	0.015665
C	−2.747501	−0.773824	−1.044721
C	−3.706884	−1.005293	−2.048178
C	−3.323636	−0.957093	−3.379055
H	−4.727734	−1.246665	−1.769638
C	−1.104839	−0.394306	−2.627683
C	−1.985184	−0.646673	−3.706633
H	−4.038763	−1.159798	−4.172311
C	0.268353	−0.043427	−2.877921
C	−1.464161	−0.602560	−5.045296
C	0.761505	−0.042036	−4.204742
C	−0.146764	−0.333369	−5.280914
H	−2.139115	−0.806460	−5.872538
C	2.126143	0.274458	−4.383142
C	2.310263	0.581747	−1.999562
H	0.236979	−0.322547	−6.297820
C	2.901855	0.573323	−3.274616
H	2.552340	0.284337	−5.382966
H	2.880902	0.839765	−1.110161
H	3.952067	0.827063	−3.379077
N	−1.479032	−0.493375	−1.327392
N	1.024489	0.297333	−1.797681
C	2.284833	0.981300	1.687249
H	2.085873	2.043633	1.614336
O	2.002125	−1.226837	1.782426
H	3.956819	−1.825739	2.116456
H	4.516777	0.862885	2.044100

3 for furan (Table 1 entry 8)

E_{gas} = −2441.514160 a.u.

E_{sol} = −2441.526910 a.u.

Cu	0.025237	−0.061505	−0.002354
C	0.014031	−0.021650	1.869363
C	0.205709	0.060924	4.150510
C	−1.100260	−0.132809	3.822582
H	−3.405487	−0.541293	0.763871
C	−3.376705	−0.554379	−0.323531
C	−4.545279	−0.730292	−1.095376
C	−4.440105	−0.736339	−2.473245
H	−5.505523	−0.857743	−0.605280
C	−2.064347	−0.398184	−2.207361
C	−3.173054	−0.567297	−3.077031
H	−5.318357	−0.869265	−3.100313
C	−0.739921	−0.219813	−2.761729
C	−2.963208	−0.559218	−4.496348
C	−0.568775	−0.217564	−4.169622
C	−1.715149	−0.391672	−5.018300
H	−3.821035	−0.689540	−5.151210
C	0.737723	−0.041945	−4.674921
C	1.530421	0.105886	−2.413527
H	−1.563274	−0.386748	−6.094368
C	1.788519	0.119776	−3.791577
H	0.902463	−0.035914	−5.749098

H	2.335748	0.231242	-1.697611
H	2.805636	0.256925	-4.143524
N	-2.179453	-0.394304	-0.863183
N	0.307477	-0.058111	-1.896782
C	0.909393	0.130808	2.902325
H	1.976006	0.279658	2.782268
O	-1.248157	-0.186588	2.469317
H	0.613543	0.143138	5.150080
H	-2.002893	-0.247096	4.407154

TS$_{(3-4)}$ for furan (Table 1 entry 8)

E_{gas} = -2684.516225 a.u.

E_{sol} = -2684.526864 a.u.

Cu	0.028645	-0.169404	-0.069053
C	0.037546	-0.163894	2.043489
C	1.333466	-0.036219	2.577581
C	-0.846474	-1.098337	2.620199
C	1.790735	-0.945158	3.538119
H	1.979826	0.767875	2.245266
C	-0.381816	-1.990590	3.578876
H	-1.867196	-1.162229	2.266277
C	0.941708	-1.930539	4.037915
H	2.805465	-0.849336	3.917990
H	-1.063662	-2.737759	3.976951
H	1.290715	-2.624187	4.797527
I	-0.867506	1.933160	1.552813
H	2.984307	-0.981900	0.882162
C	3.173246	-0.439473	-0.039218
C	4.475788	-0.349454	-0.558983
C	4.687270	0.367366	-1.721128
H	5.294247	-0.838637	-0.040858
C	2.308222	0.802589	-1.774947
C	3.586564	0.964197	-2.370767
H	5.683030	0.468481	-2.145137
C	1.146474	1.336776	-2.443062
C	3.703881	1.697576	-3.600224
C	1.293374	2.037654	-3.666990
C	2.605850	2.214864	-4.220491
H	4.692603	1.822431	-4.033747
C	0.113569	2.512960	-4.280562
C	-1.148592	1.550133	-2.472382
H	2.706524	2.760107	-5.155349
C	-1.108710	2.265760	-3.684289
H	0.178676	3.059858	-5.217825
H	-2.088860	1.313520	-1.985496
H	-2.033230	2.611987	-4.135021
N	2.113374	0.132404	-0.606498
N	-0.053940	1.108016	-1.866479
C	-1.265485	-1.554039	-0.489699
C	-1.462692	-2.882080	-0.193756
C	-3.021698	-2.307620	-1.678233
C	-2.585229	-3.367267	-0.946814
H	-0.871189	-3.458934	0.506908
O	-2.248343	-1.210579	-1.426890
H	-3.832384	-2.169322	-2.380179
H	-3.006583	-4.364606	-0.944308

For N-methylindole (Table 1 entry 9)

N-methylindole

E_{gas} = -403.120864 a.u.

E_{sol} = -403.125044 a.u.

C	0.180612	-0.009610	-0.046652
C	-0.097211	-0.007375	2.190362
C	1.297601	-0.003254	1.899386
C	-0.507349	-0.006638	3.534906
C	2.271139	0.001829	2.905658
C	0.455827	-0.001993	4.536541
H	-1.565165	-0.009710	3.786088
C	1.831462	0.002232	4.225213
H	3.331841	0.005211	2.669809
H	0.147533	-0.001403	5.578623
H	2.561149	0.005985	5.030454
H	0.079641	-0.010848	-1.123893
C	-0.781928	-0.010919	0.928312
H	-1.851132	-0.016064	0.766527
N	1.442612	-0.005148	0.524257
C	2.702892	0.000348	-0.187899
H	3.287979	0.896956	0.050577
H	3.301573	-0.883811	0.062664
H	2.504996	-0.008637	-1.262118

2 for N-methylindole (Table 1 entry 9)

E_{gas} = -2730.356158 a.u.

E_{sol} = -2730.366670 a.u.

Cu	0.087787	-0.512270	0.019746
H	0.079858	0.272650	2.607541
C	1.125653	0.176948	2.877231
C	3.309420	0.413991	3.424189
C	2.983479	-0.975862	3.401675
C	4.627788	0.794856	3.734251
C	3.932868	-1.966974	3.681708
C	5.571340	-0.188024	4.010745
H	4.902391	1.846916	3.763053
C	5.227085	-1.555815	3.984762
H	3.669352	-3.020991	3.669649
H	6.590803	0.098720	4.256153
H	5.984999	-2.301665	4.209827
O	-1.239276	-0.710147	1.247452
C	-2.520509	-0.981396	0.787864
H	-3.224529	-1.084504	1.634450
H	-2.941301	-0.186427	0.135612
H	-2.600237	-1.926380	0.207021
H	-2.667890	-1.379787	-2.339705
C	-1.769690	-1.334935	-2.951844
C	-1.825200	-1.629052	-4.329612
C	-0.660786	-1.554087	-5.067068
H	-2.768743	-1.905271	-4.789786
C	0.492030	-0.920267	-3.033732
C	0.546255	-1.190851	-4.428980
H	-0.657309	-1.770079	-6.132658
C	1.707989	-0.548251	-2.336452
C	1.793836	-1.089354	-5.128337
C	2.923395	-0.453802	-3.063976
C	2.932669	-0.734374	-4.472016
H	1.812099	-1.301250	-6.194286
C	4.093055	-0.085575	-2.364359
C	2.779226	0.061766	-0.361624
H	3.876897	-0.657137	-5.004433
C	4.016166	0.174858	-1.010922
H	5.035936	-0.010369	-2.899544
H	2.692929	0.278485	0.697888
H	4.889621	0.461367	-0.435003
N	-0.655838	-0.993292	-2.322916
N	1.650103	-0.293829	-0.992248
C	2.104869	1.120302	3.088606
H	1.975552	2.192549	3.024263
N	1.649876	-1.090658	3.063308
C	0.898717	-2.327425	2.923241
H	1.462906	-3.040052	2.309865
H	0.708033	-2.786748	3.901377
H	-0.047689	-2.088540	2.425713

TS$_{(2-3)}$ for N-methylindole (Table 1 entry 9)

E_{gas} = -2730.313548 a.u.

E_{sol} = -2730.328415 a.u.

Cu	0.105138	-0.058709	-0.105501
H	0.061185	-0.003618	1.828059
C	1.367705	-0.062397	1.509896
C	3.626137	0.339869	1.718665

C	3.375707	-1.037648	2.001723
C	4.950511	0.815332	1.781552
C	4.408505	-1.925603	2.335412
C	5.973291	-0.063956	2.114518
H	5.167760	1.861640	1.577339
C	5.704379	-1.422549	2.388298
H	4.207570	-2.972648	2.546207
H	6.997752	0.295971	2.168228
H	6.525074	-2.087067	2.646439
O	-1.217921	-0.062505	1.707954
C	-1.874858	1.043226	2.253243
H	-2.322097	0.828780	3.242104
H	-1.201240	1.912578	2.395527
H	-2.700572	1.390666	1.604270
H	-2.840927	-0.838763	-0.004595
C	-2.654861	-0.757753	-1.072857
C	-3.652332	-0.963380	-2.044903
C	-3.323507	-0.869333	-3.386558
H	-4.661961	-1.211579	-1.733513
C	-1.073927	-0.334534	-2.708665
C	-1.997982	-0.548875	-3.758212
H	-4.070814	-1.042581	-4.156812
C	0.293919	0.012018	-3.005785
C	-1.536550	-0.452042	-5.115808
C	0.724048	0.073016	-4.352915
C	-0.231694	-0.168418	-5.399229
H	-2.248170	-0.622750	-5.919430
C	2.083243	0.388212	-4.577486
C	2.380982	0.560948	-2.192867
H	0.105428	-0.112356	-6.431025
C	2.913036	0.622366	-3.495302
H	2.462563	0.444576	-5.594660
H	2.996090	0.754814	-1.316419
H	3.960816	0.868432	-3.635435
N	-1.400184	-0.462311	-1.398913
N	1.106142	0.276071	-1.950072
C	2.353167	0.920721	1.422499
H	2.168429	1.964817	1.198708
N	2.022461	-1.247814	1.878027
C	1.343971	-2.501442	2.137765
H	1.579167	-3.257427	1.375731
H	1.630125	-2.901357	3.118247
H	0.267856	-2.312207	2.135459

3 for N-methylindole (Table 1 entry 9)

E_{gas} = -2614.618067 a.u.

E_{sol} = -2614.632364 a.u.

Cu	0.018846	0.016879	-0.029895
C	-0.231260	0.042029	1.831612
C	0.099783	0.208914	4.108104
C	-1.241941	-0.216346	3.873438
C	0.526872	0.380791	5.436518
C	-2.136778	-0.468583	4.918891
C	-0.361144	0.131524	6.479384
H	1.543674	0.706157	5.648200
C	-1.681220	-0.289735	6.224440
H	-3.156062	-0.794340	4.725291
H	-0.033839	0.263175	7.508225
H	-2.354686	-0.478144	7.057079
H	3.354933	-0.590052	1.136657
C	3.458328	-0.509577	0.056445
C	4.719742	-0.626461	-0.564695
C	4.795882	-0.522655	-1.939947
H	5.607439	-0.793881	0.037078
C	2.400910	-0.204208	-1.962163
C	3.616417	-0.307175	-2.688437
H	5.749472	-0.606304	-2.455335
C	1.159615	0.005934	-2.675099
C	3.597672	-0.191751	-4.118377
C	1.177452	0.110172	-4.089859
C	2.428414	0.009518	-4.788775
H	4.537045	-0.268904	-4.659769
C	-0.053338	0.306841	-4.752569
C	-1.143406	0.271668	-2.614909
H	2.420625	0.095254	-5.872029
C	-1.216331	0.386403	-4.010342
H	-0.072716	0.391714	-5.835793
H	-2.040478	0.332426	-2.008033
H	-2.180256	0.536103	-4.485224
N	2.338528	-0.300133	-0.616720
N	0.002761	0.086284	-1.951413
C	0.697181	0.356903	2.814659
H	1.709979	0.695356	2.626176
N	-1.412401	-0.304258	2.505843
C	-2.640768	-0.704076	1.864867
H	-2.476173	-0.637822	0.786006
H	-2.921146	-1.736488	2.118022
H	-3.475972	-0.044828	2.139880

TS$_{(3-4)}$ for N-methylindole (Table 1 entry 9)

E_{gas} = -2857.619061 a.u.

E_{sol} = -2857.630741 a.u.

Cu	0.098839	-0.254584	-0.021254
C	0.060395	-0.104386	2.100227
C	1.328858	0.034380	2.690997
C	-0.876812	-0.973888	2.693676
C	1.715195	-0.816223	3.733539
H	2.008566	0.804529	2.345528
C	-0.482050	-1.808051	3.732745
H	-1.879302	-1.042025	2.290343
C	0.818916	-1.747570	4.252610
H	2.711003	-0.714410	4.159128
H	-1.201423	-2.511903	4.143286
H	1.112667	-2.396549	5.072673
I	-0.742965	1.982861	1.383239
H	3.036647	-0.884456	1.063885
C	3.240644	-0.350064	0.141249
C	4.564104	-0.147132	-0.284348
C	4.793998	0.557932	-1.450056
H	5.383284	-0.541648	0.307935
C	2.394361	0.754586	-1.694857
C	3.693714	1.024517	-2.199396
H	5.804848	0.745802	-1.802646
C	1.243447	1.142792	-2.473957
C	3.835564	1.726260	-3.444880
C	1.417459	1.805450	-3.715689
C	2.745471	2.102717	-4.171510
H	4.838645	1.939422	-3.804541
C	0.248906	2.120484	-4.444017
C	-1.049203	1.087237	-2.701629
H	2.866778	2.622513	-5.118285
C	-0.985340	1.755051	-3.940264
H	0.333601	2.635147	-5.397797
H	-1.994926	0.751287	-2.283880
H	-1.899932	1.971948	-4.482648
N	2.175594	0.101845	-0.519218
N	0.030785	0.806630	-1.985404
C	-1.297861	-1.575917	-0.356960
C	-2.664563	-1.341310	-0.448640
C	-2.322416	-3.551750	-0.908961
C	-3.339870	-2.560757	-0.791741
H	-3.146014	-0.388326	-0.256873
C	-2.610405	-4.880542	-1.238046
C	-4.674981	-2.938062	-1.016609
C	-3.944515	-5.222896	-1.455564
H	-1.824101	-5.626712	-1.322900
C	-4.966105	-4.259554	-1.345294
H	-5.474440	-2.204519	-0.933033
H	-4.199115	-6.248172	-1.712773
H	-5.998032	-4.555712	-1.519137

N	-1.112309	-2.933411	-0.645696
C	0.155830	-3.623133	-0.651367
H	0.939714	-2.893020	-0.437685
H	0.192695	-4.412089	0.112598
H	0.360496	-4.083191	-1.628025

For caffeine (Table 1 entry 10)

caffeine

E_{gas} = -680.364051 a.u.

E_{sol} = -680.374036 a.u.

C	-0.010173	-0.004234	-0.003703
C	0.073572	0.005205	2.108544
C	1.386761	-0.006789	1.678609
C	2.516605	-0.009153	2.560716
C	0.779075	0.012293	4.396689
N	-0.799811	0.006962	1.066321
H	-0.362761	-0.006547	-1.026830
N	1.313716	-0.012231	0.292708
C	2.435430	-0.027192	-0.637113
H	3.068503	0.848596	-0.478592
H	3.041440	-0.923065	-0.483950
H	2.039832	-0.018334	-1.655112
O	3.699634	-0.017937	2.229192
O	0.535303	0.021062	5.594973
N	2.103069	0.000133	3.917085
N	-0.240434	0.013904	3.448350
C	3.140294	-0.001280	4.953196
H	3.046243	0.890180	5.578211
H	3.030622	-0.881832	5.590918
H	4.103076	-0.013187	4.445779
C	-1.623384	0.028222	3.923041
H	-1.814005	-0.848139	4.547806
H	-1.806141	0.925104	4.520755
H	-2.274091	0.018258	3.049173

2 for caffeine (Table 1 entry 10)

E_{gas} = -3007.603451 a.u.

E_{sol} = -3007.619190 a.u.

Cu	0.059264	0.219390	0.034834
H	0.699891	0.660830	2.206230
C	1.306336	0.490618	3.089015
C	2.921771	0.261010	4.440205
C	1.780422	-0.061249	5.151352
C	1.795649	-0.464519	6.525485
C	4.305849	-0.156414	6.352952
N	2.637980	0.602824	3.155533
O	-1.270677	0.302039	1.278450
C	-2.272116	1.235729	1.029058
H	-3.077779	1.153138	1.782177
H	-1.926211	2.291574	1.063816
H	-2.764639	1.113710	0.041232
H	-2.805501	-0.212304	-2.159594
C	-1.939053	-0.189939	-2.816925
C	-2.094601	-0.291203	-4.214525
C	-0.966080	-0.262418	-5.009308
H	-3.086019	-0.389411	-4.645311
C	0.350128	-0.037300	-2.991328
C	0.306418	-0.135740	-4.408390
H	-1.041136	-0.337391	-6.091290
C	1.632065	0.090793	-2.327240
C	1.525998	-0.104485	-5.162217
C	2.817666	0.110996	-3.106047
C	2.729546	0.013582	-4.535961
H	1.470940	-0.178271	-6.245187
C	4.052219	0.224454	-2.430891
C	2.847686	0.282992	-0.351715
H	3.651966	0.035095	-5.109992
C	4.062528	0.308200	-1.053165
H	4.976288	0.243075	-3.002634
H	2.845748	0.353942	0.733193
H	4.990673	0.395424	-0.498399
N	-0.762280	-0.063739	-2.223127
N	1.657831	0.179499	-0.961691
N	0.738975	0.091541	4.247277
C	-0.688803	-0.145364	4.458261
H	-0.830785	-1.131453	4.904977
H	-1.096375	0.605517	5.141149
H	-1.169823	-0.084517	3.476041
O	0.827105	-0.771419	7.214280
O	5.395456	-0.211044	6.910057
N	3.123711	-0.476635	7.040941
N	4.171643	0.224154	5.017416
C	3.308355	-0.869680	8.440713
H	3.951135	-1.751552	8.501582
H	3.783854	-0.058893	8.998283
H	2.321962	-1.086549	8.846329
C	5.357540	0.570361	4.241724
H	6.202336	0.594194	4.927853
H	5.534906	-0.175677	3.459439
H	5.217199	1.546813	3.770066

TS$_{(2-3)}$ for caffeine (Table 1 entry 10)

E_{gas} = -3007.563580 a.u.

E_{sol} = -3007.584230 a.u.

Cu	0.109037	-0.011646	-0.068365
H	0.096813	0.030574	1.900230
C	1.489235	-0.086096	1.638784
C	3.611464	0.316663	1.804629
C	3.466949	-1.024512	2.116723
C	4.560453	-1.885816	2.440963
C	5.989582	0.176969	2.117867
N	2.428326	0.899773	1.512229
O	-1.070898	0.006280	1.630411
C	-1.798417	1.131275	2.067789
H	-2.295724	0.941976	3.032621
H	-1.156382	2.020193	2.195428
H	-2.581775	1.391817	1.339418
H	-2.940313	-1.271818	-0.231163
C	-2.622298	-1.192305	-1.267885
C	-3.462532	-1.571856	-2.333198
C	-2.989463	-1.474274	-3.629801
H	-4.458292	-1.951265	-2.126971
C	-0.930379	-0.606677	-2.722371
C	-1.685518	-0.980548	-3.860946
H	-3.607160	-1.774468	-4.472437
C	0.399871	-0.070348	-2.884010
C	-1.091384	-0.855010	-5.162455
C	0.961244	0.031921	-4.179192
C	0.179320	-0.381494	-5.312254
H	-1.673189	-1.152875	-6.030765
C	2.267226	0.561368	-4.279610
C	2.280456	0.844128	-1.887704
H	0.621182	-0.298212	-6.301642
C	2.925227	0.962895	-3.130823
H	2.737807	0.653107	-5.254962
H	2.750276	1.166786	-0.962152
H	3.925522	1.381268	-3.174629
N	-1.392711	-0.732181	-1.455671
N	1.051098	0.342256	-1.759523
N	2.105996	-1.257816	2.011612
C	1.431329	-2.516508	2.287779
H	1.716477	-3.280339	1.557395
H	1.702101	-2.882507	3.281314
H	0.355291	-2.335032	2.237341
O	4.503144	-3.084896	2.712263
O	7.105135	0.686726	2.127858
N	5.800555	-1.181784	2.415083
N	4.856137	0.919733	1.811014
C	7.019817	-1.926070	2.734952

H	7.713572	-1.895633	1.890422
H	7.516463	-1.480993	3.601132
H	6.722673	-2.951232	2.948677
C	5.019587	2.343809	1.537012
H	5.568554	2.819603	2.353349
H	5.585315	2.498095	0.612264
H	4.023300	2.776473	1.445629

3 for caffeine (Table 1 entry 10)

E_{gas} = -2891.876375 a.u.

E_{sol} = -2891.893577 a.u.

Cu	-0.046255	-0.005792	-0.020438
C	-0.135118	-0.009699	1.855968
C	0.548457	-0.006945	3.910293
C	-0.832092	-0.021999	3.985501
C	-1.556372	-0.032947	5.212410
C	0.730272	-0.010169	6.306499
N	0.986677	0.000570	2.631341
H	3.191197	0.015392	1.137903
C	3.310342	0.016128	0.055782
C	4.576094	0.023220	-0.570826
C	4.642769	0.023737	-1.951184
H	5.478445	0.028220	0.032563
C	2.231958	0.010160	-1.980523
C	3.447922	0.017121	-2.708347
H	5.601491	0.029192	-2.463872
C	0.970698	0.002991	-2.687703
C	3.407566	0.017187	-4.142926
C	0.967021	0.003526	-4.105089
C	2.218666	0.010773	-4.810963
H	4.345971	0.022557	-4.691414
C	-0.285560	-0.003267	-4.757062
C	-1.345295	-0.010418	-2.602039
H	2.196463	0.010970	-5.897335
C	-1.442766	-0.010132	-4.002268
H	-0.326400	-0.003011	-5.843071
H	-2.238437	-0.015929	-1.986258
H	-2.421609	-0.015424	-4.469994
N	2.179900	0.009861	-0.633207
N	-0.180180	-0.004157	-1.949783
N	-1.246752	-0.023424	2.660896
C	-2.619797	-0.036694	2.197703
H	-2.574960	-0.033110	1.104703
H	-3.145784	-0.929576	2.548841
H	-3.164564	0.842851	2.553830
O	-2.779614	-0.046762	5.356829
O	1.383443	-0.005008	7.346146
N	-0.671879	-0.026125	6.335029
N	1.330278	-0.000859	5.049307
C	-1.266331	-0.036327	7.672342
H	-0.935099	-0.918691	8.226520
H	-0.957927	0.852022	8.230191
H	-2.346919	-0.049849	7.541329
C	2.783227	0.015975	4.944104
H	3.131660	-0.867568	4.399582
H	3.111332	0.909630	4.403473
H	3.185109	0.018344	5.955940

$TS_{(3-4)}$ for caffeine (Table 1 entry 10)

E_{gas} = -3134.877667 a.u.

E_{sol} = -3134.893112 a.u.

Cu	-0.078593	0.000057	0.003505
C	-0.214900	-0.004192	1.943088
C	0.468523	0.046950	4.000242
C	-0.900314	-0.121981	4.073759
C	-1.616732	-0.226327	5.301513
C	0.655835	0.034942	6.394457
N	0.898174	0.121350	2.718329
C	-0.486121	-2.080325	-0.394023
C	-1.569376	-2.281288	-1.267143
C	-0.382009	-2.882102	0.760331
C	-2.618743	-3.129867	-0.898186
H	-1.588034	-1.795676	-2.235092
C	-1.427999	-3.727055	1.112062
H	0.487534	-2.796852	1.401587
C	-2.560927	-3.847498	0.294706
H	-3.464539	-3.250408	-1.570863
H	-1.355023	-4.302354	2.031207
H	-3.368185	-4.518553	0.572941
I	1.502323	-1.673760	-1.517489
H	-2.681493	0.061807	-1.942914
C	-2.092268	0.900707	-2.300004
C	-2.559187	1.689973	-3.365587
C	-1.785586	2.746281	-3.804581
H	-3.513520	1.458251	-3.827063
C	-0.189472	2.178109	-2.076951
C	-0.566103	3.025418	-3.151587
H	-2.108077	3.370880	-4.633574
C	1.012334	2.476168	-1.334127
C	0.280260	4.128701	-3.511469
C	1.811676	3.588863	-1.696966
C	1.421580	4.397951	-2.816313
H	-0.017161	4.755768	-4.347650
C	2.954746	3.842758	-0.905715
C	2.362714	1.953783	0.465795
H	2.048477	5.241817	-3.092138
C	3.226186	3.030400	0.178518
H	3.601130	4.681627	-1.151453
H	2.503388	1.305932	1.328372
H	4.089755	3.209906	0.810818
N	-0.932754	1.108271	-1.681494
N	1.298858	1.681920	-0.280284
N	-1.315768	-0.146726	2.746392
C	-2.686524	-0.317023	2.301852
H	-3.317246	0.501085	2.662425
H	-2.678644	-0.327673	1.210026
H	-3.100671	-1.257995	2.673441
O	-2.830669	-0.374450	5.447216
O	1.307500	0.105076	7.432195
N	-0.735638	-0.138268	6.423593
N	1.249562	0.116884	5.136696
C	-1.322666	-0.228513	7.761439
H	-0.888876	-1.070312	8.307649
H	-1.119591	0.685402	8.326293
H	-2.394509	-0.367181	7.631519
C	2.691944	0.298872	5.033052
H	3.096809	-0.410055	4.306311
H	2.931396	1.315570	4.700340
H	3.118974	0.127758	6.019884

For N-benzimidazole (Table 1 entry 11)

N-benzimidazole

E_{gas} = -419.170748 a.u.

E_{sol} = -419.179283 a.u.

C	-0.001598	0.000000	-0.028621
C	0.026487	0.000000	2.101897
C	1.382201	0.000000	1.689795
C	-0.284022	0.000000	3.467640
C	2.444382	0.000000	2.597811
C	0.767903	0.000000	4.378810
H	-1.320183	0.000000	3.791858
C	2.111337	0.000000	3.950519
H	3.481333	0.000000	2.273555
H	0.553993	0.000000	5.444055
H	2.905433	0.000000	4.692171
N	-0.814218	0.000000	0.995889
H	-0.309219	0.000000	-1.068074
N	1.336232	0.000000	0.304557
C	2.465531	0.000000	-0.602345

H	3.086081	0.890977	-0.453463
H	3.086081	-0.890977	-0.453463
H	2.095632	0.000000	-1.630421

2 for N-benzimidazole (Table 1 entry 11)

E_{gas} = -2746.411171 a.u.

E_{sol} = -2746.423643 a.u.

Cu	-0.006627	0.346333	0.086068
H	0.827260	0.793391	2.170692
C	1.505291	0.573234	2.987945
C	3.228942	0.227947	4.202822
C	2.099464	-0.079883	5.004836
C	4.516262	0.095472	4.738149
C	2.216481	-0.515498	6.327202
C	4.639845	-0.339037	6.055028
H	5.387373	0.329655	4.132959
C	3.506791	-0.640325	6.837958
H	1.344940	-0.746422	6.933215
H	5.628644	-0.448787	6.492540
H	3.642680	-0.975992	7.862598
N	2.818439	0.633668	2.938696
O	-1.279446	0.434451	1.390042
C	-2.280287	1.379714	1.195341
H	-3.059060	1.291387	1.976527
H	-1.924701	2.432588	1.235611
H	-2.811513	1.280864	0.224543
H	-2.998024	-0.083839	-1.931464
C	-2.173918	-0.051162	-2.640843
C	-2.415432	-0.132169	-4.027437
C	-1.337491	-0.092890	-4.889227
H	-3.431559	-0.223930	-4.398001
C	0.100748	0.105715	-2.952925
C	-0.030386	0.025387	-4.365995
H	-1.478595	-0.153222	-5.965577
C	1.421074	0.226594	-2.366596
C	1.140345	0.065493	-5.193034
C	2.556114	0.254441	-3.217021
C	2.379968	0.174721	-4.639827
H	1.018790	0.005545	-6.271474
C	3.830677	0.358046	-2.618598
C	2.757346	0.392602	-0.466991
H	3.265757	0.202447	-5.268813
C	3.926125	0.423761	-1.243658
H	4.717297	0.382708	-3.246798
H	2.828602	0.448029	0.617759
H	4.886093	0.501796	-0.744453
N	-0.962872	0.067108	-2.118919
N	1.531290	0.300474	-1.003967
N	1.004437	0.149002	4.189069
C	-0.406256	-0.053357	4.485245
H	-0.563055	-1.063633	4.879226
H	-0.755398	0.673389	5.228266
H	-0.959467	0.066914	3.545582

TS$_{(2-3)}$ for N-benzimidazole (Table 1 entry 11)

E_{gas} = -2746.366878 a.u.

E_{sol} = -2746.384123 a.u.

Cu	0.158626	-0.048051	-0.094324
H	0.111191	0.038108	1.839128
C	1.492977	-0.071880	1.583651
C	3.642745	0.289454	1.711379
C	3.439777	-1.027432	2.199825
C	4.942288	0.816546	1.666000
C	4.494152	-1.831928	2.643233
C	5.996192	0.020774	2.107337
H	5.109096	1.827439	1.303094
C	5.775737	-1.285762	2.589751
H	4.328727	-2.839599	3.015525
H	7.010400	0.411699	2.084941
H	6.622066	-1.878314	2.927754
N	2.433942	0.852987	1.345992
O	-1.081336	-0.053270	1.620512
C	-1.843981	1.048543	2.048321
H	-2.329613	0.858950	3.020465
H	-1.233471	1.962266	2.160805
H	-2.643222	1.277065	1.324711
H	-2.774490	-1.430666	-0.206767
C	-2.493409	-1.313902	-1.250498
C	-3.350414	-1.693473	-2.301392
C	-2.920357	-1.546707	-3.609259
H	-4.325339	-2.114512	-2.076827
C	-0.871300	-0.621239	-2.739425
C	-1.644414	-0.996040	-3.865064
H	-3.551654	-1.849797	-4.440760
C	0.425214	-0.017244	-2.922850
C	-1.091688	-0.811014	-5.178311
C	0.947455	0.142713	-4.228195
C	0.153381	-0.279081	-5.349914
H	-1.684706	-1.110321	-6.038621
C	2.222583	0.739900	-4.343282
C	2.278853	0.965755	-1.943062
H	0.562061	-0.151254	-6.348935
C	2.886756	1.145306	-3.198569
H	2.664768	0.880815	-5.326223
H	2.749498	1.283404	-1.014913
H	3.863354	1.615238	-3.254962
N	-1.285364	-0.805686	-1.461943
N	1.078235	0.402736	-1.804332
N	2.079520	-1.227765	2.109826
C	1.356088	-2.404006	2.546095
H	1.628263	-3.285219	1.950636
H	1.565535	-2.621967	3.600644
H	0.287242	-2.207664	2.431166

3 for N-benzimidazole (Table 1 entry 11)

E_{gas} = -2630.677930 a.u.

E_{sol} = -2630.691932 a.u.

Cu	-0.079148	-0.006409	-0.051602
C	-0.106372	-0.013819	1.827558
C	0.654775	-0.019986	3.875436
C	-0.759713	-0.024963	3.988073
C	1.436437	-0.022338	5.038156
C	-1.412739	-0.032174	5.222774
C	0.792163	-0.029537	6.274634
H	2.520981	-0.018568	4.965484
C	-0.613005	-0.034407	6.366925
H	-2.497426	-0.035889	5.298184
H	1.382770	-0.031460	7.187689
H	-1.084050	-0.039999	7.346812
N	1.022354	-0.013245	2.540685
H	3.133216	-0.003675	1.124371
C	3.268598	0.001102	0.043030
C	4.537927	0.007177	-0.578021
C	4.613460	0.013041	-1.958139
H	5.437009	0.007166	0.030402
C	2.203942	0.006774	-2.002199
C	3.423566	0.012991	-2.723533
H	5.575566	0.017740	-2.464749
C	0.945468	0.006640	-2.714345
C	3.389239	0.018846	-4.158184
C	0.947884	0.012546	-4.131882
C	2.203102	0.018574	-4.831690
H	4.329923	0.023539	-4.703014
C	-0.301841	0.012236	-4.789184
C	-1.370838	0.000812	-2.638476
H	2.185892	0.023001	-5.918225
C	-1.462297	0.006355	-4.039007
H	-0.338148	0.016635	-5.875408
H	-2.266156	-0.003838	-2.025825

H	-2.439184	0.005954	-4.511040
N	2.144320	0.000888	-0.656256
N	-0.208808	0.000880	-1.980496
N	-1.212354	-0.020914	2.683495
C	-2.587823	-0.023302	2.252687
H	-2.573049	-0.018640	1.158158
H	-3.121782	-0.917340	2.601220
H	-3.127207	0.864545	2.608638

TS$_{(3-4)}$ for N-benzimidazole (Table 1 entry 11)

E_{gas} = -2873.680274 a.u.

E_{sol} = -2873.692290 a.u.

Cu	-0.133348	0.079385	-0.008028
C	-0.176353	0.024431	1.929752
C	0.597093	0.052128	3.975893
C	-0.798537	-0.165271	4.090648
C	1.382749	0.117747	5.133195
C	-1.433268	-0.315938	5.325482
C	0.756895	-0.032358	6.370442
H	2.454560	0.281311	5.057219
C	-0.631371	-0.246177	6.466331
H	-2.504946	-0.481450	5.403818
H	1.349495	0.015554	7.280819
H	-1.087801	-0.360040	7.446464
N	0.944150	0.164185	2.637793
C	-0.505299	-2.027605	-0.415186
C	-1.601764	-2.244497	-1.269407
C	-0.374085	-2.827705	0.738921
C	-2.636086	-3.102481	-0.880654
H	-1.641211	-1.763539	-2.239092
C	-1.404028	-3.683879	1.108841
H	0.504323	-2.729695	1.365967
C	-2.550611	-3.817846	0.312108
H	-3.491497	-3.233632	-1.539310
H	-1.306893	-4.258311	2.026479
H	-3.345044	-4.498632	0.603977
I	1.457047	-1.617155	-1.567137
H	-2.706422	0.097494	-1.952009
C	-2.118246	0.932925	-2.318541
C	-2.581300	1.704553	-3.398041
C	-1.808818	2.757155	-3.848879
H	-3.532394	1.462738	-3.861146
C	-0.219456	2.219337	-2.105399
C	-0.593887	3.049898	-3.193824
H	-2.129140	3.368187	-4.688807
C	0.977277	2.531851	-1.361119
C	0.250667	4.151504	-3.563607
C	1.774410	3.642643	-1.733181
C	1.386902	4.434976	-2.865278
H	-0.044361	4.765903	-4.410046
C	2.911763	3.908765	-0.937268
C	2.316510	2.033422	0.455257
H	2.011657	5.277805	-3.149446
C	3.178057	3.110151	0.158606
H	3.557721	4.746343	-1.189024
H	2.445094	1.392528	1.327023
H	4.037129	3.300086	0.794077
N	-0.962009	1.152559	-1.696995
N	1.259196	1.751715	-0.296744
N	-1.260697	-0.174375	2.786783
C	-2.633749	-0.367319	2.385416
H	-2.670911	-0.352054	1.293784
H	-3.019540	-1.333654	2.732681
H	-3.280806	0.429170	2.776054

For N-methylpyrazole (Table 1 entry 12)

N-methylpyrazole

E_{gas} = -265.507698 a.u.

E_{sol} = -265.514338 a.u.

C	0.051710	-0.057548	-0.042900
C	-0.033265	0.047848	2.158179
H	0.187572	0.088856	3.217109
N	-1.232037	-0.016456	0.405477
C	-2.452703	0.016567	-0.376226
H	-2.216421	-0.225539	-1.414842
H	-3.157291	-0.720376	0.017073
H	-2.914933	1.008328	-0.332106
H	0.278617	-0.112314	-1.098439
N	-1.303956	0.052381	1.752841
C	0.867098	-0.019788	1.072959
H	1.946841	-0.044901	1.096674

2 for N-methylpyrazole (Table 1 entry 12)

E_{gas} = -2592.743022 a.u.

E_{sol} = -2592.755190 a.u.

Cu	-0.150378	0.372566	0.138350
H	0.471732	0.863549	2.783023
C	1.485980	0.480916	2.795007
C	3.646607	0.005319	2.805073
O	-1.247607	0.399809	1.588364
C	-2.586407	0.705305	1.389985
H	-3.144041	0.653207	2.343648
H	-2.758547	1.729181	0.992095
H	-3.108303	0.015822	0.691659
H	-3.212035	1.627384	-1.570195
C	-2.453048	1.572067	-2.347611
C	-2.752571	1.953558	-3.671369
C	-1.757882	1.863759	-4.624226
H	-3.747046	2.307644	-3.924274
C	-0.280513	1.041946	-2.889981
C	-0.476875	1.397851	-4.252994
H	-1.944398	2.145955	-5.657521
C	1.019063	0.559612	-2.463428
C	0.604530	1.275056	-5.186412
C	2.064203	0.448763	-3.417910
C	1.822400	0.818665	-4.784005
H	0.432036	1.552964	-6.222978
C	3.318473	-0.028921	-2.980848
C	2.406589	-0.231515	-0.769401
H	2.640345	0.724899	-5.493346
C	3.484829	-0.370560	-1.653763
H	4.134007	-0.122806	-3.693000
H	2.522955	-0.500768	0.274022
H	4.431002	-0.744252	-1.277243
N	-1.263909	1.132170	-1.966556
N	1.202242	0.222234	-1.148784
N	1.707162	-0.853332	2.647647
C	0.696234	-1.895060	2.556050
H	-0.250746	-1.416853	2.286138
H	0.997217	-2.616138	1.791008
H	0.601121	-2.420780	3.512503
H	4.728997	0.032925	2.837435
C	2.733057	1.076267	2.901309
H	2.945770	2.128247	3.027342
N	3.025527	-1.168632	2.648897

TS$_{(2-3)}$ for N-methylpyrazole (Table 1 entry 12)

E_{gas} = -2592.700950 a.u.

E_{sol} = -2592.718321 a.u.

Cu	0.103378	-0.126279	-0.028939
H	-0.038550	-0.040931	1.904366
C	1.296291	0.016986	1.672418
C	3.460637	0.519536	2.056190
O	-1.280888	-0.174501	1.663148
C	-2.033416	0.930586	2.074781
H	-2.548801	0.755563	3.036680

H	-1.415339	1.841158	2.208422
H	-2.816231	1.185731	1.337618
H	-2.801422	-1.208397	-0.136023
C	-2.530997	-1.120174	-1.185243
C	-3.426175	-1.416388	-2.230355
C	-2.995416	-1.314360	-3.542851
H	-4.434204	-1.744393	-1.997365
C	-0.862535	-0.582928	-2.693197
C	-1.674740	-0.889245	-3.810632
H	-3.659005	-1.560793	-4.367840
C	0.487773	-0.117531	-2.883515
C	-1.109249	-0.776457	-5.126892
C	1.026425	-0.046656	-4.190472
C	0.187690	-0.390554	-5.306441
H	-1.733110	-1.019957	-5.982960
C	2.365938	0.385738	-4.310372
C	2.439254	0.645096	-1.915679
H	0.606625	-0.325005	-6.307224
C	3.074295	0.720094	-3.169004
H	2.825167	0.453950	-5.293232
H	2.955363	0.920281	-0.998176
H	4.103615	1.059305	-3.227819
N	-1.280838	-0.728597	-1.411597
N	1.176572	0.251410	-1.769967
N	2.053591	-1.064274	2.064350
C	1.574981	-2.420392	2.250826
H	0.482921	-2.401079	2.237650
H	1.940394	-3.081851	1.455831
H	1.926032	-2.805652	3.212288
H	4.420995	1.006003	2.181659
C	2.223432	1.075260	1.679324
H	2.010560	2.114834	1.465158
N	3.355792	-0.793207	2.290996

3 for N-methylpyrazole (Table 1 entry 12)

E_{gas} = -2477.006128 a.u.

E_{sol} = -2477.023764 a.u.

Cu	0.125057	0.077313	0.082439
C	0.049001	-0.054874	1.954825
C	0.477978	-0.148619	4.167678
H	3.212276	1.707527	0.988441
C	3.223547	1.695257	-0.099617
C	4.307374	2.238955	-0.820959
C	4.271746	2.202792	-2.201143
H	5.148678	2.674158	-0.290837
C	2.121928	1.112462	-2.031104
C	3.156783	1.629809	-2.854143
H	5.087863	2.610069	-2.792813
C	0.951638	0.521713	-2.644798
C	3.032104	1.552336	-4.281306
C	0.860524	0.464814	-4.059559
C	1.931695	0.992595	-4.857938
H	3.834767	1.950310	-4.896768
C	-0.297008	-0.113537	-4.623857
C	-1.117790	-0.496957	-2.402101
H	1.842635	0.937050	-5.939523
C	-1.288207	-0.595026	-3.790431
H	-0.395709	-0.172531	-5.704489
H	-1.879198	-0.867662	-1.724219
H	-2.191472	-1.045497	-4.188204
N	2.169900	1.146877	-0.682317
N	-0.036273	0.043200	-1.830692
H	0.941863	-0.189857	5.147188
N	-1.080312	-0.108493	2.735159
C	-2.450338	-0.096768	2.277545
H	-2.429500	-0.094829	1.185043
H	-2.988098	-0.982839	2.634127
H	-2.979917	0.795844	2.632119
C	1.085422	-0.080606	2.897075
H	2.147307	-0.078282	2.682289
N	-0.852283	-0.163463	4.074683

TS$_{(3-4)}$ for N-methylpyrazole (Table 1 entry 12)

E_{gas} = -2720.007709 a.u.

E_{sol} = -2720.022754 a.u.

Cu	0.012057	-0.331532	0.018160
C	0.274238	0.083402	1.904021
C	1.129258	0.398014	3.969303
C	-0.568654	-2.375483	0.088420
C	-1.586531	-2.710629	-0.822034
C	-0.635690	-2.881467	1.402103
C	-2.736613	-3.373272	-0.377802
H	-1.480252	-2.462837	-1.871523
C	-1.780945	-3.543037	1.828747
H	0.172059	-2.689056	2.096777
C	-2.846091	-3.783003	0.948955
H	-3.527175	-3.598237	-1.090180
H	-1.840270	-3.877543	2.861205
H	-3.731335	-4.311645	1.290696
I	1.527771	-2.441982	-0.961133
H	-2.813005	-0.579099	-1.437679
C	-2.315528	0.185323	-2.026428
C	-2.983785	0.805824	-3.095174
C	-2.317674	1.759355	-3.840706
H	-4.007481	0.525905	-3.321349
C	-0.413703	1.436944	-2.381950
C	-0.997525	2.109050	-3.487746
H	-2.798389	2.250267	-4.682904
C	0.904836	1.823756	-1.940974
C	-0.244810	3.120320	-4.176805
C	1.609731	2.847842	-2.623600
C	1.005342	3.474096	-3.764715
H	-0.702716	3.610554	-5.031782
C	2.879399	3.201099	-2.115456
C	2.575432	1.569114	-0.374427
H	1.559616	4.248914	-4.287875
C	3.360606	2.565805	-0.985974
H	3.458913	3.976230	-2.610519
H	2.901457	1.065705	0.532107
H	4.327286	2.823623	-0.565520
N	-1.058823	0.462112	-1.681439
N	1.393087	1.200861	-0.847572
H	1.751207	0.414870	4.857585
N	-0.547697	0.796883	2.736070
C	-1.887533	1.262789	2.455303
H	-2.024776	2.262598	2.877198
H	-2.025092	1.300282	1.371960
H	-2.645057	0.595814	2.887358
C	1.392740	-0.180751	2.708339
H	2.276651	-0.735147	2.415419
N	-0.060308	0.995804	3.995056

For 1-methyl-1,2,4-triazole (Table 1 entry 13)

1-methyl-1,2,4-triazole

E_{gas} = -281.559001 a.u.

E_{sol} = -281.567805 a.u.

C	-0.014323	-0.047977	0.066887
C	-0.007831	0.023690	2.155530
H	0.342230	0.050242	3.178763
N	-1.291724	-0.001541	0.508573
C	-2.533150	0.003116	-0.241036
H	-2.299501	-0.039428	-1.307164
H	-3.139669	-0.864074	0.033892
H	-3.095909	0.915905	-0.027522
H	0.244470	-0.090393	-0.982883
N	-1.301990	0.045413	1.865655
N	0.830992	-0.033686	1.084001

2 for 1-methyl-1,2,4-triazole (Table 1 entry 13)

E_{gas} = -2608.795297 a.u.

E_{sol} = -2608.809592 a.u.

Cu	0.049679	-0.076071	-0.051513
H	0.034146	0.103312	2.666460
C	1.099715	0.029634	2.853363
C	3.132002	0.327052	3.273090
O	-1.152960	-0.784441	1.115326
C	-2.481482	-0.851751	0.715777
H	-3.106406	-1.290742	1.515096
H	-2.929697	0.138131	0.485076
H	-2.648402	-1.481047	-0.184852
H	-2.990367	0.395232	-2.139155
C	-2.179152	0.845204	-2.707362
C	-2.432228	1.475647	-3.942800
C	-1.370690	2.027722	-4.630984
H	-3.443388	1.518090	-4.335220
C	0.073088	1.299746	-2.828373
C	-0.070224	1.951366	-4.084100
H	-1.518870	2.520807	-5.588548
C	1.388969	1.202795	-2.226707
C	1.081602	2.496228	-4.741739
C	2.506663	1.747555	-2.911850
C	2.317238	2.395341	-4.179097
H	0.948687	2.990582	-5.700576
C	3.778698	1.629910	-2.311432
C	2.742043	0.486215	-0.474536
H	3.189167	2.806599	-4.680553
C	3.893120	0.993498	-1.091823
H	4.649576	2.039544	-2.816084
H	2.815986	-0.014573	0.483782
H	4.852272	0.880356	-0.598058
N	-0.973876	0.757650	-2.166518
N	1.517313	0.584918	-1.011699
N	1.765894	-1.132844	2.665609
C	1.227170	-2.422298	2.262011
H	0.219293	-2.246200	1.870417
H	1.870821	-2.851159	1.489059
H	1.201630	-3.105537	3.116958
H	4.062509	0.803769	3.554424
N	3.089617	-0.956420	2.930845
N	1.940824	0.983223	3.239909

TS$_{(2-3)}$ for 1-methyl-1,2,4-triazole (Table 1 entry 13)

E_{gas} = -2608.757259 a.u.

E_{sol} = -2608.776089 a.u.

Cu	0.013885	0.064578	-0.033441
H	0.123236	0.068206	1.918865
C	1.484803	-0.137055	1.578498
C	3.625976	-0.040980	1.570177
O	-1.067673	0.088433	1.745984
C	-1.703405	1.245064	2.236226
H	-2.149700	1.074936	3.229871
H	-1.007108	2.097218	2.330317
H	-2.516009	1.557915	1.561674
H	-3.060975	-1.098674	-0.050688
C	-2.819607	-0.953410	-1.100888
C	-3.755256	-1.213980	-2.120803
C	-3.378220	-1.037939	-3.440954
H	-4.749048	-1.567374	-1.864495
C	-1.219710	-0.321926	-2.638541
C	-2.075264	-0.578832	-3.737916
H	-4.071278	-1.248957	-4.251462
C	0.112689	0.183362	-2.864801
C	-1.576312	-0.375534	-5.069541
C	0.578678	0.364914	-4.188767
C	-0.302187	0.063153	-5.283892
H	-2.234380	-0.584786	-5.908907
C	1.890457	0.863876	-4.349516
C	2.091459	0.967995	-1.949243
H	0.065690	0.206852	-6.296488
C	2.644463	1.159967	-3.227570
H	2.289952	1.016568	-5.348808
H	2.635660	1.201923	-1.036239
H	3.651590	1.554112	-3.317845
N	-1.586372	-0.532331	-1.351106
N	0.857503	0.494128	-1.767042
N	2.040185	-1.307134	2.018052
C	1.347064	-2.490902	2.482868
H	0.277626	-2.269123	2.502922
H	1.536884	-3.339532	1.816267
H	1.687066	-2.754268	3.489071
H	4.635593	0.332819	1.446304
N	3.399091	-1.269112	2.017355
N	2.518385	0.695160	1.294724

3 for 1-methyl-1,2,4-triazole (Table 1 entry 13)

E_{gas} = -2493.068391 a.u.

E_{sol} = -2493.084279 a.u.

Cu	-0.156809	0.166157	-0.101072
C	-0.070884	0.320506	1.768232
C	0.723363	0.677050	3.726286
H	3.026154	1.106082	0.796677
C	3.082880	1.049268	-0.290068
C	4.262212	1.329052	-1.016437
C	4.243402	1.232078	-2.395095
H	5.166771	1.615675	-0.489017
C	1.923769	0.598006	-2.231167
C	3.048771	0.856268	-3.053408
H	5.134691	1.440849	-2.981929
C	0.666750	0.209284	-2.831928
C	2.921568	0.726683	-4.476977
C	0.576211	0.090496	-4.241625
C	1.737012	0.359890	-5.044954
H	3.790221	0.927068	-5.099084
C	-0.668081	-0.291709	-4.788949
C	-1.556048	-0.389730	-2.559913
H	1.649127	0.264081	-6.123836
C	-1.735109	-0.532157	-3.944615
H	-0.773412	-0.392588	-5.865957
H	-2.376677	-0.571646	-1.874079
H	-2.704967	-0.827534	-4.330904
N	1.955824	0.695874	-0.887833
N	-0.395900	-0.030208	-2.004647
H	1.415836	0.923937	4.522978
N	-1.017330	0.127762	2.732538
C	-2.393682	-0.264340	2.547318
H	-2.551488	-0.381742	1.471875
H	-2.602863	-1.212445	3.055169
H	-3.074635	0.500147	2.937664
N	-0.532972	0.349568	3.989621
N	1.064824	0.678533	2.410902

TS$_{(3-4)}$ for 1-methyl-1,2,4-triazole (Table 1 entry 13)

E_{gas} = -2736.070885 a.u.

E_{sol} = -2736.085227 a.u.

Cu	-0.162759	0.192702	-0.023427
C	-0.194946	0.137949	1.914915
C	0.483077	0.311093	3.942778
C	-0.183991	-1.933823	-0.451802
C	-1.229401	-2.316314	-1.311092
C	0.071490	-2.710640	0.697161
C	-2.114908	-3.330889	-0.931300
H	-1.341119	-1.838388	-2.276550
C	-0.809655	-3.722324	1.058263

H	0.920993	-2.478425	1.328617
C	-1.918439	-4.031716	0.256887
H	-2.937545	-3.591604	-1.593119
H	-0.625364	-4.279418	1.973163
H	-2.595518	-4.831494	0.542581
I	1.682025	-1.193500	-1.594665
H	-2.735081	-0.201319	-1.936976
C	-2.299140	0.723283	-2.302496
C	-2.900099	1.415634	-3.367900
C	-2.319243	2.584584	-3.819338
H	-3.804998	1.023053	-3.820195
C	-0.637356	2.305579	-2.101853
C	-1.159684	3.069824	-3.177973
H	-2.748127	3.140513	-4.649092
C	0.500688	2.808949	-1.369503
C	-0.514233	4.298035	-3.550140
C	1.097923	4.038443	-1.743549
C	0.569464	4.761531	-2.864921
H	-0.919068	4.859408	-4.387980
C	2.185681	4.486048	-0.959620
C	1.925390	2.533647	0.429236
H	1.042817	5.697349	-3.150703
C	2.593461	3.738883	0.128869
H	2.680799	5.419905	-1.214373
H	2.168568	1.923694	1.298449
H	3.416574	4.066386	0.755917
N	-1.186369	1.126997	-1.694565
N	0.921632	2.082099	-0.313224
H	1.122527	0.504385	4.796318
N	-1.168204	-0.227783	2.797391
C	-2.507171	-0.691854	2.515708
H	-3.250934	-0.009474	2.941843
H	-2.630353	-0.736457	1.431700
H	-2.664269	-1.690504	2.935455
N	-0.754853	-0.128084	4.097857
N	0.879591	0.492623	2.653594

For pyridazine (Table 1 entry 14)

pyridazine

E_{gas} = -264.281538 a.u.

E_{sol} = -264.291284 a.u.

C	-0.088640	-0.002798	-0.001232
C	0.011453	-0.013626	1.379651
C	1.302015	0.012112	1.919236
H	-1.046338	-0.020861	-0.513134
H	1.463973	0.007021	2.994625
N	2.415938	0.045677	1.181981
H	-0.862211	-0.041237	2.024376
C	1.110991	0.032903	-0.720241
H	1.117856	0.043947	-1.807652
N	2.319349	0.055749	-0.150162

2 for pyridazine (Table 1 entry 14)

E_{gas} = -2591.516470 a.u.

E_{sol} = -2591.530728 a.u.

Cu	0.004306	0.035404	-0.000700
H	-0.005873	-0.056658	5.075928
O	1.234544	0.027786	1.334168
C	2.184672	-0.981938	1.289575
H	2.944857	-0.839320	2.082340
H	1.772450	-2.004905	1.441871
H	2.749797	-1.029617	0.333587
H	3.069102	-0.364027	-2.135794
C	2.234006	-0.345895	-2.833336
C	2.457835	-0.460557	-4.220582
C	1.368285	-0.434732	-5.067775
H	3.468358	-0.567640	-4.602512
C	-0.042818	-0.181733	-3.115473
C	0.070111	-0.291512	-4.529564
H	1.493184	-0.521739	-6.144416
C	-1.356854	-0.026909	-2.520141
C	-1.108068	-0.253455	-5.345862
C	-2.499512	0.009621	-3.361898
C	-2.339719	-0.109726	-4.783748
H	-0.997909	-0.340941	-6.423763
C	-3.766356	0.166970	-2.759088
C	-2.680313	0.229394	-0.616790
H	-3.231404	-0.080562	-5.404444
C	-3.852173	0.276926	-1.385737
H	-4.655456	0.198213	-3.383634
H	-2.715176	0.295802	0.469851
H	-4.807157	0.396524	-0.884861
N	1.031730	-0.214053	-2.295568
N	-1.461524	0.084404	-1.160445
C	-3.357734	0.270841	4.769619
C	-2.133699	0.147017	5.438208
C	-1.000898	0.041034	4.651905
C	-1.170929	0.065370	3.260917
H	-0.315657	-0.010503	2.579017
H	-4.294276	0.359010	5.316001
H	-2.091789	0.137347	6.523856
N	-2.375009	0.187855	2.687928
N	-3.476037	0.291535	3.441051

TS$_{(2-3)}$ for pyridazine (Table 1 entry 14)

E_{gas} = -2591.470600 a.u.

E_{sol} = -2591.492746 a.u.

Cu	-0.027235	0.004944	-0.010392
H	-0.006019	0.015174	1.943424
O	1.183586	0.028874	1.750306
C	1.799870	-1.150042	2.203672
H	2.260108	-1.020423	3.197294
H	1.088974	-1.994161	2.284835
H	2.600024	-1.466201	1.514567
H	2.981422	0.958133	-0.051128
C	2.723974	0.867951	-1.103291
C	3.650076	1.132505	-2.130856
C	3.243894	1.026959	-3.449480
H	4.662273	1.432491	-1.879277
C	1.069183	0.374109	-2.639678
C	1.916194	0.639935	-3.742031
H	3.932085	1.241727	-4.263042
C	-0.295291	-0.042174	-2.857266
C	1.383742	0.522615	-5.070815
C	-0.795080	-0.128621	-4.178419
C	0.082775	0.166619	-5.277542
H	2.036787	0.733721	-5.913467
C	-2.143373	-0.522423	-4.333538
C	-2.304920	-0.717353	-1.937888
H	-0.311826	0.091636	-6.287378
C	-2.897707	-0.809132	-3.211135
H	-2.571114	-0.599701	-5.329768
H	-2.868984	-0.963774	-1.041972
H	-3.934055	-1.119803	-3.293402
N	1.470727	0.507224	-1.352441
N	-1.037428	-0.349807	-1.757636
C	-3.591778	1.037694	1.699795
C	-2.199451	1.148875	1.720839
C	-1.403968	-0.001507	1.596960
C	-2.192392	-1.179597	1.528361
H	-1.751277	2.136638	1.829134
H	-4.233714	1.914542	1.782852
H	-1.713223	-2.158551	1.472443
N	-3.527642	-1.252776	1.496306
N	-4.246862	-0.121593	1.572837

3 for pyridazine (Table 1 entry 14)

E_{gas} = -2475.779318 a.u.

E_{sol} = -2475.799860 a.u.

Cu	-0.006578	-0.048356	-0.066159
H	-0.023164	-0.218445	2.755173
C	1.038315	-0.125705	2.551343
C	1.970068	-0.111003	3.599218
C	3.312596	0.007101	3.297804
H	1.625355	-0.192658	4.624591
C	2.704772	0.089763	0.950633
C	3.714311	0.110339	1.948384
H	4.063755	0.021108	4.083057
C	3.081542	0.191857	-0.444891
C	5.091563	0.231527	1.560378
C	4.455328	0.306006	-0.786960
C	5.447718	0.324293	0.248836
H	5.847044	0.245844	2.341231
C	4.772510	0.397486	-2.161430
C	2.425349	0.251867	-2.646641
H	6.493360	0.414197	-0.033812
C	3.757410	0.369506	-3.096461
H	5.812210	0.487906	-2.465927
H	1.601042	0.223830	-3.356375
H	3.967297	0.436711	-4.159227
N	1.380901	-0.029432	1.263155
N	2.095438	0.169368	-1.367504
C	-3.788751	-0.721446	-1.835942
C	-2.756501	-0.769230	-0.893627
C	-1.557701	-0.089556	-1.137027
C	-1.588424	0.588063	-2.380470
H	-0.727140	1.175679	-2.703785
H	-4.730724	-1.244189	-1.668240
H	-2.913093	-1.345141	0.018216
N	-2.590681	0.613277	-3.264633
N	-3.717681	-0.056665	-2.992055

TS$_{(3-4)}$ for pyridazine (Table 1 entry 14)

E_{gas} = -2718.781294 a.u.

E_{sol} = -2718.800233 a.u.

Cu	-0.118520	-0.036566	0.008765
C	-0.079241	-0.165860	2.149479
C	1.122900	0.360317	2.657479
C	-0.549869	-1.397638	2.647529
C	1.928223	-0.419089	3.494516
H	1.427774	1.367705	2.398762
C	0.259076	-2.160472	3.480381
H	-1.515733	-1.777193	2.336448
C	1.508920	-1.684639	3.900884
H	2.869887	-0.010864	3.854410
H	-0.094518	-3.133311	3.811305
H	2.127249	-2.281812	4.564655
I	-1.667027	1.461555	1.795256
H	2.926882	0.407932	0.842497
C	2.840510	0.998807	-0.064323
C	3.976070	1.600800	-0.630538
C	3.833166	2.357225	-1.778234
H	4.944604	1.466788	-0.159853
C	1.471742	1.827647	-1.722575
C	2.556344	2.482244	-2.364106
H	4.687601	2.846314	-2.238739
C	0.160978	1.882910	-2.323383
C	2.320644	3.217434	-3.575357
C	-0.034318	2.601733	-3.531233
C	1.079459	3.276405	-4.134818
H	3.161774	3.720592	-4.044780
C	-1.335322	2.600660	-4.079329
C	-2.043454	1.218061	-2.245646
H	0.915374	3.828965	-5.056193
C	-2.342743	1.905702	-3.436038
H	-1.529701	3.140956	-5.002237
H	-2.810208	0.656366	-1.718846
H	-3.352559	1.882792	-3.832611
N	1.612954	1.115458	-0.569853
N	-0.832887	1.208281	-1.701897
C	-0.637486	-1.839185	-0.510504
C	-1.986628	-2.262868	-0.511201
C	0.218585	-2.836415	-0.985916
C	-0.303044	-4.072935	-1.380235
H	-2.775543	-1.594733	-0.157729
H	1.296147	-2.683670	-1.058140
H	0.344724	-4.868942	-1.748288
N	-2.457915	-3.453428	-0.902563
N	-1.602254	-4.380421	-1.345662

For pyrimidine (Table 1 entry 15)

pyrimidine

E_{gas} = -264.317897 a.u.

E_{sol} = -264.324166 a.u.

C	-0.012127	0.008540	-0.010527
C	0.043608	-0.015422	1.381981
C	1.315171	0.011309	1.952336
H	-0.965293	-0.009547	-0.537145
H	1.448937	-0.004271	3.033089
C	2.250911	0.077103	-0.110683
H	3.152005	0.115439	-0.720119
N	2.431510	0.057953	1.214570
N	1.088290	0.055114	-0.771839
H	-0.854797	-0.052732	1.989590

2 for pyrimidine (Table 1 entry 15)

E_{gas} = -2591.550397 a.u.

E_{sol} = -2591.563859 a.u.

Cu	-0.019851	0.102639	-0.016853
H	-0.039354	-0.144354	4.988256
O	1.158743	0.300706	1.345683
C	2.295824	-0.492559	1.298317
H	2.988524	-0.231012	2.121576
H	2.097656	-1.583214	1.400218
H	2.884810	-0.384474	0.361629
H	3.099269	0.284156	-2.087010
C	2.285974	0.175673	-2.801727
C	2.550037	0.141137	-4.186305
C	1.487802	-0.001044	-5.056317
H	3.570073	0.223566	-4.548410
C	0.021297	-0.054961	-3.129599
C	0.175742	-0.103378	-4.542861
H	1.644382	-0.034925	-6.131733
C	-1.309022	-0.151369	-2.559099
C	-0.976826	-0.251214	-5.382992
C	-2.425885	-0.296192	-3.423694
C	-2.223714	-0.344775	-4.844365
H	-0.834940	-0.287049	-6.460100
C	-3.709782	-0.384418	-2.843847
C	-2.687390	-0.186830	-0.678561
H	-3.095666	-0.456673	-5.483333
C	-3.835797	-0.329918	-1.470033
H	-4.580242	-0.495051	-3.485221
H	-2.754814	-0.155534	0.407619
H	-4.805995	-0.397211	-0.988848
N	1.070189	0.079258	-2.287168
N	-1.453579	-0.095823	-1.199427
C	-2.157746	-0.329985	5.422139
C	-1.047093	-0.215064	4.592110
C	-1.277410	-0.190744	3.215950
H	-0.448643	-0.099402	2.505871
H	-2.055065	-0.355691	6.506398
N	-2.525381	-0.273452	2.718394
C	-3.515627	-0.379761	3.612274
H	-4.525910	-0.445864	3.210008
N	-3.407710	-0.414532	4.942533

TS$_{(2-3)}$ for pyrimidine (Table 1 entry 15)

E_{gas} = −2591.504394 a.u.

E_{sol} = −2591.523021 a.u.

Cu	−0.075789	0.066837	−0.034494
H	0.062586	−0.002151	1.897659
O	1.265135	0.035685	1.639161
C	1.919781	−1.149303	2.005970
H	2.441258	−1.054878	2.973900
H	1.225500	−2.007434	2.099419
H	2.679493	−1.432658	1.257818
H	2.870584	1.128290	−0.201212
C	2.559582	1.069067	−1.241100
C	3.419462	1.396193	−2.306874
C	2.943650	1.329715	−3.605365
H	4.435032	1.717687	−2.099235
C	0.838697	0.576908	−2.704314
C	1.614011	0.912340	−3.839780
H	3.578773	1.598036	−4.445749
C	−0.518536	0.116947	−2.862269
C	1.007937	0.833243	−5.139791
C	−1.095003	0.074451	−4.154244
C	−0.292884	0.447982	−5.287259
H	1.603910	1.100308	−6.008507
C	−2.435816	−0.360252	−4.248258
C	−2.440061	−0.682181	−1.861092
H	−0.744011	0.405933	−6.275125
C	−3.109266	−0.729040	−3.097311
H	−2.921820	−0.405189	−5.219375
H	−2.936730	−0.995254	−0.946170
H	−4.137397	−1.074231	−3.134327
N	1.303289	0.683104	−1.435392
N	−1.176231	−0.279250	−1.736922
C	−2.112267	1.114066	1.923316
C	−1.329248	−0.031100	1.665233
C	−2.102937	−1.211019	1.672729
H	−1.639778	2.095912	1.993711
H	−1.626320	−2.183315	1.529544
C	−4.031484	−0.080192	2.039223
H	−5.112860	−0.099103	2.174287
N	−3.435371	−1.262193	1.837144
N	−3.442468	1.118653	2.102098

3 for pyrimidine (Table 1 entry 15)

E_{gas} = −2475.813995 a.u.

E_{sol} = −2475.830759 a.u.

Cu	0.008936	−0.049813	−0.154881
H	−0.064868	−0.271855	2.647697
C	1.000678	−0.169368	2.471809
C	1.906006	−0.164487	3.542377
C	3.254711	−0.031217	3.276582
H	1.536472	−0.264616	4.557432
C	2.704503	0.080037	0.916096
C	3.688650	0.094665	1.939147
H	3.986073	−0.022874	4.080379
C	3.115041	0.201413	−0.468217
C	5.074075	0.232413	1.587545
C	4.496331	0.331454	−0.773776
C	5.462208	0.345511	0.286819
H	5.809601	0.242715	2.387315
C	4.848409	0.441679	−2.138097
C	2.516452	0.280263	−2.685025
H	6.513738	0.448011	0.031564
C	3.858112	0.415322	−3.099387
H	5.894858	0.544651	−2.414173
H	1.712200	0.252207	−3.417451
H	4.094612	0.496231	−4.155622
N	1.374191	−0.051300	1.193595
N	2.152873	0.180089	−1.416285
C	−2.788144	−0.642529	−0.849702
C	−1.552523	−0.074218	−1.211840
C	−1.596846	0.480652	−2.504304
H	−0.713171	0.969732	−2.922018
H	−2.914232	−1.112658	0.128100
N	−2.664218	0.480131	−3.320191
C	−3.758354	−0.103216	−2.822840
H	−4.638760	−0.116853	−3.466175
N	−3.888360	−0.670727	−1.620678

TS$_{(3-4)}$ for pyrimidine (Table 1 entry 15)

E_{gas} = −2718.816169 a.u.

E_{sol} = −2718.831130 a.u.

Cu	−0.531662	−0.024061	0.073102
C	−0.468065	−0.288527	2.076782
C	0.469369	0.676538	2.487748
C	−0.421734	−1.585994	2.622777
C	1.530752	0.297838	3.319170
H	0.378134	1.705902	2.160715
C	0.632601	−1.941547	3.453790
H	−1.178291	−2.313862	2.354205
C	1.619058	−1.005858	3.802870
H	2.265149	1.044030	3.613062
H	0.685680	−2.957641	3.835786
H	2.428430	−1.289908	4.469337
I	−2.615773	0.663704	1.843586
H	2.830044	−0.100591	0.812927
C	2.785816	0.477016	−0.106903
C	3.964069	0.829182	−0.791223
C	3.867351	1.588703	−1.941949
H	4.927210	0.507392	−0.408256
C	1.467078	1.559877	−1.652299
C	2.593841	1.979316	−2.408414
H	4.755741	1.885978	−2.493299
C	0.139214	1.900841	−2.105268
C	2.396105	2.761403	−3.595517
C	−0.019903	2.672360	−3.285914
C	1.143298	3.096749	−4.013250
H	3.269394	3.078519	−4.159408
C	−1.335353	2.978907	−3.693557
C	−2.145687	1.748631	−1.797331
H	1.001636	3.686908	−4.914717
C	−2.400880	2.516479	−2.944218
H	−1.495969	3.570154	−4.591270
H	−2.962783	1.367880	−1.191222
H	−3.425728	2.731636	−3.228269
N	1.572473	0.832236	−0.514386
N	−0.917198	1.447905	−1.377056
C	−0.717463	−1.835478	−0.636307
C	−1.947951	−2.493552	−0.796053
C	0.362894	−2.616045	−1.078742
H	−2.879162	−2.012425	−0.487878
H	1.385675	−2.236705	−1.015278
N	−2.105236	−3.726204	−1.312129
N	0.264390	−3.851717	−1.599348
C	−0.977647	−4.336263	−1.685730
H	−1.081568	−5.337371	−2.105221

For pentafluorobenzene (Table 1 entry 16)

pentafluorobenzene

E_{gas} = −728.372837 a.u.

E_{sol} = −728.376111 a.u.

C	−0.001480	0.000108	0.001710
C	0.012043	0.000572	1.395387
C	1.207909	−0.000001	2.103809
C	2.403891	−0.000994	1.395502
C	2.417550	−0.001454	0.001870
C	1.208056	−0.000919	−0.691636
H	1.207892	0.000317	3.187054
F	3.573812	−0.001592	2.048283
F	3.573186	−0.002471	−0.671001
F	1.208188	−0.001387	−2.026784

F	-1.157094	0.000595	-0.671191
F	-1.157993	0.001455	2.047964

2 for pentafluorobenzene (Table 1 entry 16)

E_{gas} = -3055.602197 a.u.

E_{sol} = -3055.616259 a.u.

Cu	-0.041192	0.011353	-0.019073
H	-0.028483	-0.010685	2.645270
O	1.240517	0.011446	1.260243
C	2.042953	-1.126113	1.323914
H	2.871054	-0.975362	2.040047
H	1.498623	-2.034111	1.657713
H	2.516673	-1.389063	0.355853
H	2.496624	-1.820100	-2.104458
C	1.603983	-1.759309	-2.723607
C	1.588573	-2.330949	-4.012462
C	0.435033	-2.232526	-4.763989
H	2.470433	-2.835630	-4.394289
C	-0.566290	-1.026476	-2.918206
C	-0.689484	-1.566231	-4.228229
H	0.377798	-2.659282	-5.762276
C	-1.696324	-0.332449	-2.331946
C	-1.920957	-1.421007	-4.948410
C	-2.898435	-0.204112	-3.077429
C	-2.979730	-0.767749	-4.395460
H	-1.992245	-1.843531	-5.947297
C	-3.980086	0.483600	-2.486977
C	-2.621421	0.834223	-0.544140
H	-3.911263	-0.659077	-4.944260
C	-3.837428	1.005411	-1.215641
H	-4.909961	0.594274	-3.038138
H	-2.482696	1.225628	0.457706
H	-4.646221	1.539962	-0.728808
N	0.568121	-1.130629	-2.190036
N	-1.571657	0.187861	-1.072568
C	-2.326307	0.546344	5.151151
C	-1.280400	0.777257	4.257952
C	-2.971576	-0.688418	5.138558
C	-0.865425	-0.186967	3.347557
C	-2.574846	-1.675421	4.238340
C	-1.526973	-1.409128	3.359093
F	-0.679828	1.978395	4.293676
F	-2.715828	1.492813	6.017830
F	-3.202952	-2.860688	4.228246
F	-1.167132	-2.378942	2.496969
F	-3.979111	-0.925609	5.988562

TS$_{(2-3)}$ for pentafluorobenzene (Table 1 entry 16)

E_{gas} = -3055.577308 a.u.

E_{sol} = -3055.595064 a.u.

Cu	0.013112	-0.002417	-0.008101
H	-0.008254	-0.007170	2.066168
O	1.023939	-0.009117	1.686128
C	1.670088	-1.218592	2.066794
H	2.179154	-1.098972	3.032612
H	0.950499	-2.045016	2.149249
H	2.422277	-1.481767	1.313181
H	3.418891	0.459813	-0.641063
C	2.948208	0.413859	-1.620703
C	3.715876	0.529969	-2.797318
C	3.072174	0.476930	-4.018089
H	4.791218	0.662028	-2.732480
C	0.992667	0.200723	-2.817470
C	1.669103	0.310466	-4.059856
H	3.628779	0.564736	-4.947704
C	-0.446543	0.035173	-2.802475
C	0.918405	0.255841	-5.281674
C	-1.156656	-0.007418	-4.027871
C	-0.435970	0.105225	-5.265018
H	1.452543	0.340785	-6.224319
C	-2.559717	-0.162309	-3.967735
C	-2.396511	-0.217156	-1.571095
H	-0.998381	0.067850	-6.194041
C	-3.177905	-0.264862	-2.737255
H	-3.135657	-0.198260	-4.888617
H	-2.850720	-0.299435	-0.589126
H	-4.252901	-0.384118	-2.653248
N	1.633603	0.251458	-1.626650
N	-1.069812	-0.073046	-1.593974
C	-3.782262	0.963890	2.079405
C	-2.393814	1.019377	1.962937
C	-4.395679	-0.285164	2.170253
C	-1.568668	-0.095221	1.901292
C	-3.616927	-1.441102	2.131085
C	-2.234514	-1.306742	2.012594
F	-1.852563	2.265934	1.877555
F	-4.541094	2.076742	2.118720
F	-4.215051	-2.645399	2.221071
F	-1.523548	-2.475736	1.982571
F	-5.732252	-0.375739	2.280713

3 for pentafluorobenzene (Table 1 entry 16)

E_{gas} = -2939.891088 a.u.

E_{sol} = -2939.901827 a.u.

Cu	0.028801	-0.014110	-0.179804
H	-0.098694	-0.018394	3.296985
C	0.964060	-0.013107	3.071050
C	1.935116	-0.009533	4.094937
C	3.273236	-0.002977	3.751063
H	1.622849	-0.012005	5.134468
C	2.585133	-0.003805	1.439308
C	3.639982	0.000123	2.385510
H	4.046706	-0.000146	4.515015
C	2.894159	-0.000655	0.027876
C	4.998963	0.006976	1.921800
C	4.244412	0.006237	-0.398739
C	5.288225	0.009885	0.588795
H	5.799053	0.009839	2.657470
C	4.486313	0.009185	-1.790754
C	2.109628	-0.001507	-2.153032
H	6.320492	0.015090	0.249303
C	3.416737	0.005337	-2.666968
H	5.509019	0.014459	-2.158522
H	1.243248	-0.004725	-2.807371
H	3.569256	0.007482	-3.741103
N	1.278509	-0.010361	1.784419
N	1.848683	-0.004460	-0.844438
C	-1.853531	-0.022673	-0.224689
C	-2.692075	-0.028828	0.881685
C	-2.518753	-0.023173	-1.445378
C	-4.083557	-0.035100	0.813722
C	-3.903969	-0.029250	-1.585733
C	-4.693197	-0.035278	-0.438106
F	-1.801437	-0.017452	-2.606906
F	-4.493243	-0.029413	-2.796364
F	-4.844089	-0.040980	1.924988
F	-2.165247	-0.029143	2.143557
F	-6.033055	-0.041229	-0.538768

TS$_{(3-4)}$ for pentafluorobenzene (Table 1 entry 16)

E_{gas} = -3182.893530 a.u.

E_{sol} = -3182.903987 a.u.

Cu	-0.003454	0.000415	0.000191
C	-0.001576	0.000381	2.154930
C	1.317138	0.006470	2.639403
C	-0.919049	-0.948947	2.643930
C	1.756102	-1.035183	3.459943
H	1.993128	0.811047	2.374364

C	-0.468099	-1.975653	3.464970
H	-1.953904	-0.919433	2.322601
C	0.872037	-2.033422	3.868471
H	2.788992	-1.045673	3.798713
H	-1.170431	-2.736625	3.794441
H	1.213385	-2.835427	4.516241
I	-0.845687	2.050332	1.677879
H	3.145333	0.236696	0.532004
C	3.005797	0.897254	-0.318345
C	4.108282	1.536864	-0.911915
C	3.896539	2.363222	-1.998084
H	5.103770	1.374194	-0.511916
C	1.543302	1.823121	-1.838890
C	2.587312	2.519076	-2.502310
H	4.722665	2.882290	-2.477236
C	0.199134	1.896605	-2.366516
C	2.281520	3.323583	-3.652092
C	-0.063524	2.681407	-3.518746
C	1.010762	3.404453	-4.138033
H	3.092503	3.860940	-4.136501
C	-1.390233	2.690200	-4.003904
C	-1.989569	1.179941	-2.232158
H	0.792809	4.009361	-5.014292
C	-2.354333	1.935904	-3.362740
H	-1.636006	3.282607	-4.881639
H	-2.710744	0.555392	-1.712431
H	-3.379901	1.915242	-3.717052
N	1.754636	1.050586	-0.740700
N	-0.755889	1.169434	-1.743981
C	-0.451164	-1.857349	-0.419342
C	-1.762319	-2.287259	-0.538138
C	0.496653	-2.840485	-0.657878
C	-2.144941	-3.586117	-0.861362
C	0.189277	-4.160405	-0.983566
C	-1.148663	-4.533528	-1.087101
F	1.824473	-2.538804	-0.576517
F	1.151112	-5.077369	-1.203077
F	-3.440355	-3.942559	-0.962536
F	-2.786805	-1.397804	-0.313115
F	-1.476322	-5.798402	-1.402602

For 1,2,4,5-tetrafluorobenzene (Table 1 entry 17)

1,2,4,5-tetrafluorobenzene

E_{gas} = -629.155949 a.u.

E_{sol} = -629.159420 a.u.

C	0.010401	0.000084	0.002806
C	0.010326	0.000563	1.397209
C	1.207908	0.000000	2.102852
C	2.405595	-0.001001	1.397319
C	2.405663	-0.001459	0.002953
C	1.208055	-0.000938	-0.702659
H	1.207893	0.000337	3.186593
F	3.575508	-0.001574	2.054029
F	3.575678	-0.002480	-0.653648
F	-1.159580	0.000580	-0.653846
F	-1.159692	0.001486	2.053728
H	1.208156	-0.001324	-1.786369

2 for 1,2,4,5-tetrafluorobenzene (Table 1 entry 17)

E_{gas} = -2956.384310 a.u.

E_{sol} = -2956.398950 a.u.

Cu	0.036790	-0.031036	0.024524
H	0.040711	-0.013982	2.670542
O	1.339510	-0.032613	1.282049
C	2.119775	-1.184500	1.353799
H	2.958673	-1.039990	2.058841
H	1.561529	-2.076575	1.706865
H	2.578292	-1.471812	0.384824
H	2.537224	-1.870101	-2.096871
C	1.634816	-1.809625	-2.701729
C	1.597013	-2.385846	-3.988108
C	0.431631	-2.287076	-4.721152
H	2.471276	-2.894132	-4.382455
C	-0.536791	-1.072493	-2.863490
C	-0.682424	-1.616188	-4.169596
H	0.357190	-2.717099	-5.716918
C	-1.655507	-0.374212	-2.260911
C	-1.925076	-1.469991	-4.870115
C	-2.869131	-0.244801	-2.987221
C	-2.973026	-0.812175	-4.302083
H	-2.013721	-1.895408	-5.866406
C	-3.939245	0.447496	-2.381355
C	-2.548548	0.799412	-0.461240
H	-3.913012	-0.702758	-4.836182
C	-3.774600	0.972181	-1.113829
H	-4.877578	0.559260	-2.917776
H	-2.393235	1.192020	0.537706
H	-4.574004	1.510127	-0.615343
N	0.609180	-1.176743	-2.153679
N	-1.509058	0.148960	-1.005000
C	-2.332220	0.573937	5.087608
C	-1.253195	0.801047	4.233254
C	-2.999963	-0.645034	5.074108
C	-0.819203	-0.176182	3.345154
C	-2.571325	-1.628863	4.190308
H	-3.836862	-0.824855	5.738641
C	-1.493305	-1.392196	3.339232
F	-0.638586	1.996474	4.279410
F	-2.726003	1.546534	5.930103
F	-3.199896	-2.818428	4.151108
F	-1.112749	-2.370855	2.493730

TS$_{(2-3)}$ for 1,2,4,5-tetrafluorobenzene (Table 1 entry 17)

E_{gas} = -2956.357926 a.u.

E_{sol} = -2956.375972 a.u.

Cu	0.020990	0.197841	-0.019459
H	-0.037479	0.112347	2.039723
O	1.009835	0.219055	1.696394
C	1.751236	-0.941463	2.050504
H	2.230393	-0.813202	3.030809
H	1.105901	-1.830295	2.090197
H	2.538573	-1.114296	1.306044
H	3.378847	0.967602	-0.511278
C	2.946890	0.921791	-1.508520
C	3.739410	1.149360	-2.651920
C	3.142440	1.093193	-3.896181
H	4.796968	1.368291	-2.543862
C	1.056576	0.594499	-2.782282
C	1.760623	0.812249	-3.994595
H	3.719553	1.265726	-4.801121
C	-0.362863	0.308540	-2.823627
C	1.055822	0.747026	-5.242967
C	-1.028315	0.259759	-4.073431
C	-0.281133	0.484676	-5.279273
H	1.610089	0.915617	-6.162469
C	-2.414587	-0.013224	-4.067028
C	-2.320526	-0.157573	-1.669599
H	-0.808885	0.440739	-6.228173
C	-3.058921	-0.219280	-2.863147
H	-2.957210	-0.057433	-5.007619
H	-2.795554	-0.318672	-0.707368
H	-4.122109	-0.430802	-2.820701
N	1.651692	0.650705	-1.568286
N	-1.010624	0.096086	-1.642283
C	-3.872314	0.723325	1.946575
C	-2.493852	0.925219	1.885010

C	-4.390427	-0.568824	1.964924
C	-1.566073	-0.106949	1.816600
C	-3.490957	-1.630036	1.914202
H	-5.458697	-0.742679	2.018963
C	-2.121213	-1.379060	1.852084
F	-2.067234	2.219540	1.866154
F	-4.716513	1.778471	1.998049
F	-3.955722	-2.899928	1.934484
F	-1.302746	-2.476188	1.802716

3 for 1,2,4,5-tetrafluorobenzene (Table 1 entry 17)

E_{gas} = -2840.671919 a.u.

E_{sol} = -2840.682868 a.u.

Cu	0.027148	-0.014003	-0.194895
H	-0.100490	-0.018342	3.295163
C	0.962552	-0.013102	3.070466
C	1.933253	-0.009620	4.094898
C	3.271470	-0.003119	3.751552
H	1.620591	-0.012116	5.134344
C	2.584165	-0.003824	1.439433
C	3.638758	0.000015	2.386125
H	4.044760	-0.000356	4.515728
C	2.894038	-0.000644	0.027922
C	4.997980	0.006817	1.923292
C	4.244795	0.006204	-0.397663
C	5.288012	0.009764	0.590496
H	5.797654	0.009611	2.659466
C	4.488238	0.009197	-1.789346
C	2.112128	-0.001386	-2.154355
H	6.320482	0.014932	0.251560
C	3.419707	0.005428	-2.666814
H	5.511415	0.014440	-2.155868
H	1.246281	-0.004557	-2.809391
H	3.573507	0.007610	-3.740777
N	1.277731	-0.010320	1.784179
N	1.849669	-0.004378	-0.845869
C	-1.855129	-0.022563	-0.231335
C	-2.687557	-0.028553	0.880657
C	-2.525321	-0.023173	-1.450103
C	-4.078404	-0.034744	0.805093
C	-3.912486	-0.029249	-1.569334
C	-4.712328	-0.035152	-0.431920
H	-5.793247	-0.039922	-0.507258
F	-1.810901	-0.017585	-2.615624
F	-4.488880	-0.029422	-2.791648
F	-4.817071	-0.040409	1.936944
F	-2.152405	-0.028744	2.141156

TS$_{(3-4)}$ for 1,2,4,5-tetrafluorobenzene (Table 1 entry 17)

E_{gas} = -3083.674449 a.u.

E_{sol} = -3083.684641 a.u.

Cu	-0.059621	0.151870	0.105198
C	-0.103720	0.230714	2.261477
C	1.174889	-0.034161	2.779973
C	-1.215416	-0.481509	2.750463
C	1.360805	-1.121445	3.636682
H	2.014389	0.596152	2.511083
C	-1.014440	-1.556526	3.607981
H	-2.212294	-0.240181	2.399805
C	0.272877	-1.891816	4.046613
H	2.359971	-1.346171	4.001233
H	-1.871660	-2.137460	3.937576
H	0.418884	-2.729643	4.721974
I	-0.473603	2.400048	1.715928
H	3.071905	-0.195325	0.692384
C	3.070387	0.456018	-0.176333
C	4.281323	0.860968	-0.765025
C	4.243493	1.681302	-1.875539
H	5.222981	0.525637	-0.342741
C	1.828794	1.597912	-1.745721
C	2.993903	2.066179	-2.407392
H	5.158890	2.022127	-2.352396
C	0.529782	1.908663	-2.299253
C	2.860392	2.880438	-3.582963
C	0.434757	2.695557	-3.475789
C	1.634171	3.185129	-4.093930
H	3.764456	3.241237	-4.066309
C	-0.860196	2.940588	-3.984272
C	-1.756883	1.621851	-2.185195
H	1.545842	3.794570	-4.989515
C	-1.957671	2.400682	-3.340960
H	-0.978610	3.543304	-4.881242
H	-2.589245	1.160495	-1.660881
H	-2.964107	2.564552	-3.712467
N	1.876219	0.829375	-0.625511
N	-0.553208	1.392244	-1.676243
C	-0.860924	-1.592131	-0.258307
C	-2.231273	-1.762252	-0.376419
C	-0.119441	-2.748053	-0.452412
C	-2.844133	-2.979736	-0.657711
C	-0.688951	-3.988834	-0.733550
C	-2.069055	-4.119866	-0.842151
F	1.242893	-2.703783	-0.367291
F	0.099504	-5.073284	-0.905683
F	-4.190405	-3.060069	-0.755929
F	-3.064034	-0.680548	-0.193583
H	-2.525108	-5.077834	-1.061975

For 1,2,3,5-tetrafluorobenzene (Table 1 entry 18)

1,2,3,5-tetrafluorobenzene

E_{gas} = -629.156596 a.u.

E_{sol} = -629.159898 a.u.

C	0.000332	-0.000029	-0.001077
C	0.002800	-0.000048	1.392840
C	1.188807	-0.000005	2.118137
C	2.384134	0.000048	1.406692
C	2.429596	0.000065	0.016543
C	1.222041	0.000031	-0.672293
H	1.174961	-0.000013	3.201092
F	3.541986	0.000091	2.090220
F	1.213910	0.000044	-2.011995
F	-1.153376	-0.000063	-0.681152
F	-1.174631	-0.000090	2.032132
H	3.371634	0.000109	-0.518027

2 for 1,2,3,5-tetrafluorobenzene (Table 1 entry 18)

E_{gas} = -2956.384491 a.u.

E_{sol} = -2956.398880 a.u.

Cu	-0.006809	-0.014983	-0.000511
H	-0.003614	-0.007145	2.644023
O	1.306683	-0.016292	1.245729
C	2.089272	-1.166567	1.307732
H	2.935404	-1.022188	2.004309
H	1.536372	-2.060488	1.665812
H	2.537908	-1.453630	0.333841
H	2.555627	-1.661861	-2.200159
C	1.649017	-1.613663	-2.799821
C	1.629384	-2.137143	-4.108966
C	0.457879	-2.055838	-4.834421
H	2.521958	-2.592515	-4.526296
C	-0.551493	-0.959815	-2.925630
C	-0.680278	-1.454308	-4.252865
H	0.396873	-2.447004	-5.846977
C	-1.694905	-0.332719	-2.291846
C	-1.930773	-1.329856	-4.943566

C	-2.915827	-0.222886	-3.009058
C	-3.002142	-0.739287	-4.346049
H	-2.006388	-1.716959	-5.956417
C	-4.010370	0.399988	-2.372264
C	-2.626554	0.729323	-0.443077
H	-3.948042	-0.646281	-4.872773
C	-3.861507	0.878518	-1.084678
H	-4.954889	0.495278	-2.900948
H	-2.482720	1.086054	0.570987
H	-4.680065	1.362226	-0.562261
N	0.600565	-1.046803	-2.223506
N	-1.564124	0.144338	-1.016011
C	-2.375041	0.565133	5.096078
C	-1.302582	0.773668	4.232286
C	-3.026906	-0.660635	5.033710
C	-0.862812	-0.175523	3.315052
C	-2.626975	-1.647643	4.135877
C	-1.547290	-1.385183	3.293334
F	-0.669564	1.961881	4.290012
F	-3.270077	-2.825638	4.085082
F	-1.178054	-2.350665	2.431417
F	-4.068419	-0.913414	5.844379
H	-2.691709	1.325293	5.800033

TS$_{(2-3)}$ for 1,2,3,5-tetrafluorobenzene (Table 1 entry 18)

E_{gas} = -2956.356731 a.u.

E_{sol} = -2956.374096 a.u.

Cu	-0.000310	0.000262	-0.000286
H	-0.000092	-0.000128	2.050589
O	1.058012	0.000288	1.683581
C	1.698250	-1.208948	2.063586
H	2.218237	-1.091684	3.024788
H	0.975075	-2.032193	2.158368
H	2.443208	-1.486598	1.306492
H	3.366061	0.561032	-0.590157
C	2.911642	0.495205	-1.576229
C	3.691307	0.618941	-2.744208
C	3.064866	0.545085	-3.973239
H	4.762415	0.776425	-2.666757
C	0.978046	0.226666	-2.797911
C	1.666596	0.346388	-4.032241
H	3.631576	0.641330	-4.895910
C	-0.455605	0.022680	-2.797329
C	0.929793	0.271868	-5.261658
C	-1.152743	-0.035921	-4.029183
C	-0.421529	0.093074	-5.258780
H	1.471558	0.366182	-6.199089
C	-2.551894	-0.226569	-3.980813
C	-2.406156	-0.287050	-1.582060
H	-0.972888	0.042517	-6.193847
C	-3.176754	-0.348473	-2.755052
H	-3.119510	-0.275813	-4.906279
H	-2.865116	-0.388617	-0.603815
H	-4.248860	-0.497041	-2.680413
N	1.600980	0.304284	-1.599119
N	-1.083486	-0.110034	-1.593950
C	-3.750824	1.007269	2.055061
C	-2.362289	1.030080	1.927408
C	-4.354830	-0.240805	2.166433
C	-1.525786	-0.081969	1.875659
C	-3.592053	-1.406391	2.139037
C	-2.207758	-1.283521	2.009977
F	-1.796061	2.267761	1.817095
F	-4.190894	-2.609581	2.252375
F	-1.510796	-2.459086	1.997690
F	-5.693623	-0.342398	2.292577
H	-4.344275	1.914467	2.085581

3 for 1,2,3,5-tetrafluorobenzene (Table 1 entry 18)

E_{gas} = -2840.670674 a.u.

E_{sol} = -2840.681403 a.u.

Cu	0.000000	0.000000	0.000000
H	0.000000	0.000000	3.503649
C	1.054062	0.000000	3.239954
C	2.060776	0.000000	4.228901
C	3.385712	0.000000	3.837457
H	1.785754	0.000000	5.278939
C	2.615234	0.000000	1.551399
C	3.703411	0.000000	2.459679
H	4.186135	0.000000	4.573185
C	2.874330	0.000000	0.129730
C	5.045180	0.000000	1.948406
C	4.209151	0.000000	-0.343915
C	5.287161	0.000000	0.606121
H	5.870737	0.000000	2.655448
C	4.403547	0.000000	-1.743211
C	2.016108	0.000000	-2.023643
H	6.306748	0.000000	0.230119
C	3.304469	0.000000	-2.582195
H	5.413233	0.000000	-2.145349
H	1.127765	0.000000	-2.647785
H	3.419960	0.000000	-3.660975
N	1.322148	0.000000	1.943069
N	1.799367	0.000000	-0.706564
C	-1.882366	-0.000084	0.031051
C	-2.671605	0.000065	1.173166
C	-2.625455	-0.000340	-1.147260
C	-4.066140	0.000000	1.176267
C	-4.014989	-0.000423	-1.239053
C	-4.728938	-0.000233	-0.046921
F	-1.949433	-0.000531	-2.338512
F	-4.764494	0.000155	2.329714
F	-2.088168	0.000294	2.409459
F	-6.077186	-0.000299	-0.058798
H	-4.530172	-0.000626	-2.192953

TS$_{(3-4)}$ for 1,2,3,5-tetrafluorobenzene (Table 1 entry 18)

E_{gas} = -3083.672808 a.u.

E_{sol} = -3083.682826 a.u.

Cu	0.018031	-0.015909	-0.009731
C	0.012716	-0.009861	2.148276
C	1.327727	0.005851	2.642768
C	-0.903138	-0.960501	2.638336
C	1.766246	-1.027977	3.473674
H	2.001229	0.812891	2.378959
C	-0.453113	-1.979034	3.469545
H	-1.935631	-0.938277	2.309093
C	0.884560	-2.027723	3.883064
H	2.796629	-1.030102	3.820411
H	-1.154167	-2.741219	3.799008
H	1.224986	-2.823238	4.539353
I	-0.838848	2.039738	1.670482
H	3.149125	0.240230	0.545134
C	3.013334	0.899792	-0.306535
C	4.117665	1.542754	-0.892494
C	3.910985	2.368628	-1.980139
H	5.110850	1.383246	-0.485480
C	1.557982	1.822275	-1.836176
C	2.604716	2.520922	-2.492660
H	4.738749	2.890307	-2.453624
C	0.216954	1.894161	-2.371611
C	2.304383	3.324946	-3.644281
C	-0.040320	2.678945	-3.525154
C	1.036531	3.403496	-4.138134
H	3.117354	3.864079	-4.123406
C	-1.364638	2.686896	-4.016694
C	-1.971658	1.176763	-2.247167

H	0.822914	4.008327	-5.015554
C	-2.331460	1.932461	-3.379637
H	-1.606598	3.279225	-4.895570
H	-2.695022	0.552936	-1.729591
H	-3.355524	1.911905	-3.738362
N	1.764108	1.049153	-0.736952
N	-0.740254	1.166568	-1.753653
C	-0.456802	-1.864373	-0.424373
C	-1.773255	-2.279137	-0.538866
C	0.459834	-2.879153	-0.671851
C	-2.181885	-3.571708	-0.862394
C	0.148086	-4.197863	-0.998707
C	-1.198027	-4.529403	-1.092152
F	1.793856	-2.584003	-0.591836
F	-3.487274	-3.897959	-0.956097
F	-2.784809	-1.376766	-0.308884
F	-1.572119	-5.786409	-1.407518
H	0.914703	-4.943446	-1.177426

For 1,4-difluorobenzene (Table 2 entry 19)

1,4-difluorobenzene

E_{gas} = -430.707719 a.u.

E_{sol} = -430.711349 a.u.

C	0.021247	-0.000026	0.011578
C	-0.016342	-0.000042	1.402249
C	1.185607	-0.000002	2.111545
C	2.384924	0.000048	1.406532
C	2.422208	0.000065	0.015915
C	1.220492	0.000030	-0.693545
H	1.200599	-0.000011	3.196266
F	3.547671	0.000089	2.092709
F	-1.141610	-0.000058	-0.674310
H	3.379485	0.000109	-0.494773
H	-0.973302	-0.000082	1.913321
H	1.205436	0.000043	-1.778327

2 for 1,4-difluorobenzene (Table 2 entry 19)

E_{gas} = -2757.938313 a.u.

E_{sol} = -2757.951710 a.u.

Cu	-0.378958	-0.637469	-0.034239
H	0.699915	0.020622	3.635504
O	0.984696	-0.678069	1.163048
C	1.726755	-1.850140	1.191645
H	2.615548	-1.733119	1.841430
H	1.173501	-2.730068	1.590430
H	2.117646	-2.171777	0.200335
H	2.526128	-1.107613	-2.131904
C	1.675569	-1.143812	-2.808937
C	1.858234	-1.370931	-4.188627
C	0.746693	-1.400026	-5.007480
H	2.856837	-1.517897	-4.587903
C	-0.608091	-0.987095	-3.046372
C	-0.536159	-1.202102	-4.449230
H	0.843548	-1.571172	-6.076759
C	-1.898997	-0.776252	-2.422765
C	-1.739164	-1.209276	-5.229593
C	-3.066580	-0.781919	-3.229017
C	-2.951503	-1.007156	-4.642797
H	-1.664720	-1.378063	-6.300762
C	-4.309720	-0.559270	-2.598782
C	-3.147630	-0.359227	-0.506173
H	-3.861137	-1.010969	-5.237296
C	-4.345296	-0.345761	-1.235080
H	-5.219998	-0.558185	-3.192401
H	-3.165160	-0.205734	0.566967
H	-5.280196	-0.170870	-0.713280
N	0.487018	-0.962715	-2.255184
N	-1.949086	-0.568202	-1.069388
C	-1.831477	0.700885	5.843170
C	-0.542088	0.530393	5.345865
C	-2.919749	0.482551	4.995355
C	-0.301738	0.145013	4.031872
C	-2.671179	0.097894	3.683059
C	-1.388269	-0.078610	3.187179
F	0.504316	0.749969	6.173849
F	-3.733827	-0.106350	2.849745
H	-1.973059	1.002267	6.875821
H	-1.193862	-0.380979	2.161389
H	-3.940786	0.607742	5.340516

TS$_{(2-3)}$ for 1,4-difluorobenzene (Table 2 entry 19)

E_{gas} = -2757.895551 a.u.

E_{sol} = -2757.911546 a.u.

Cu	-0.085876	-0.126980	-0.031910
H	0.037959	-0.134269	1.906703
O	1.222466	-0.225484	1.612692
C	1.795867	-1.439078	2.024430
H	2.323842	-1.340143	2.987820
H	1.047190	-2.244565	2.148741
H	2.533245	-1.796779	1.286792
H	2.979586	0.698637	-0.328433
C	2.624051	0.625749	-1.353063
C	3.470632	0.837153	-2.457942
C	2.943583	0.769040	-3.736849
H	4.516824	1.076616	-2.296316
C	0.816004	0.236906	-2.737168
C	1.575019	0.464399	-3.910319
H	3.568380	0.952645	-4.607264
C	-0.580832	-0.102869	-2.833010
C	0.914528	0.400923	-5.184639
C	-1.210487	-0.127958	-4.100342
C	-0.421217	0.135481	-5.272931
H	1.498543	0.584893	-6.082619
C	-2.588007	-0.437452	-4.130671
C	-2.528492	-0.690275	-1.735436
H	-0.911874	0.106883	-6.242308
C	-3.247059	-0.707006	-2.943011
H	-3.114422	-0.465249	-5.081113
H	-3.009601	-0.925845	-0.789571
H	-4.303584	-0.954762	-2.931842
N	1.332566	0.346951	-1.488565
N	-1.226702	-0.409215	-1.672306
C	-3.416375	1.261978	2.011406
C	-2.054794	1.126791	1.764537
C	-4.177632	0.108853	2.221347
C	-1.361376	-0.086286	1.696125
C	-3.528728	-1.121361	2.175325
C	-2.163380	-1.227506	1.929057
F	-1.354421	2.282099	1.562383
F	-4.255283	-2.249013	2.390584
H	-3.868448	2.248931	2.045758
H	-1.725550	-2.223586	1.933868
H	-5.242513	0.155181	2.424710

3 for 1,4-difluorobenzene (Table 2 entry 19)

E_{gas} = -2642.206635 a.u.

E_{sol} = -2642.218528 a.u.

Cu	-0.065647	-0.000112	0.117406
H	0.204831	-0.000001	3.786046
C	1.234943	0.000014	3.435590
C	2.302474	0.000067	4.357419
C	3.596342	0.000084	3.875038
H	2.098377	0.000092	5.423482
C	2.669630	-0.000003	1.642854
C	3.816895	0.000049	2.479316
H	4.446611	0.000124	4.552548

C	2.843544	-0.000040	0.206378
C	5.125090	0.000064	1.888082
C	4.149454	-0.000023	-0.345996
C	5.284192	0.000029	0.534511
H	5.991459	0.000104	2.544493
C	4.265242	-0.000060	-1.753564
C	1.867783	-0.000122	-1.900139
H	6.278355	0.000041	0.095629
C	3.121502	-0.000110	-2.530094
H	5.251414	-0.000049	-2.210362
H	0.943530	-0.000160	-2.469814
H	3.176177	-0.000139	-3.613659
N	1.405119	-0.000020	2.122605
N	1.726771	-0.000089	-0.571147
C	-1.947915	-0.000151	0.096218
C	-2.855087	-0.000145	1.172454
C	-2.555091	-0.000192	-1.160094
C	-4.231961	-0.000178	0.966940
C	-3.924165	-0.000226	-1.399414
C	-4.791949	-0.000218	-0.304422
F	-1.747061	-0.000202	-2.279521
F	-5.061532	-0.000170	2.045783
H	-4.302988	-0.000257	-2.417312
H	-2.502656	-0.000115	2.201621
H	-5.870126	-0.000243	-0.426479

TS$_{(3-4)}$ for 1,4-difluorobenzene (Table 2 entry 19)

E_{gas} = -2885.208888 a.u.

E_{sol} = -2885.218980 a.u.

Cu	-0.511941	0.014469	0.094163
C	-0.378917	-0.208652	2.101365
C	0.627410	0.685198	2.505980
C	-0.437834	-1.497476	2.661081
C	1.651037	0.236173	3.348353
H	0.620171	1.712777	2.160784
C	0.581625	-1.924626	3.502636
H	-1.245236	-2.168080	2.392137
C	1.634272	-1.064666	3.847901
H	2.441707	0.925416	3.635160
H	0.554617	-2.937961	3.894541
H	2.417210	-1.403540	4.520400
I	-2.459843	0.909331	1.863630
H	2.775727	-0.302959	0.711190
C	2.759085	0.324257	-0.174330
C	3.947635	0.647315	-0.855568
C	3.881393	1.448924	-1.979644
H	4.896786	0.267257	-0.491443
C	1.485949	1.518607	-1.675324
C	2.624342	1.907448	-2.429029
H	4.780291	1.723494	-2.525935
C	0.169956	1.915631	-2.115620
C	2.450479	2.723958	-3.596668
C	0.033209	2.712848	-3.281557
C	1.208978	3.113031	-4.002703
H	3.332552	3.021490	-4.157744
C	-1.274054	3.063286	-3.681124
C	-2.115987	1.825119	-1.803038
H	1.086098	3.726550	-4.891287
C	-2.351134	2.617500	-2.938484
H	-1.419514	3.674618	-4.568007
H	-2.942445	1.463667	-1.197699
H	-3.369844	2.865974	-3.217618
N	1.564762	0.758735	-0.557792
N	-0.896605	1.482073	-1.392096
C	-0.804986	-1.808065	-0.569059
C	-1.993061	-2.249686	-1.177182
C	0.199754	-2.770721	-0.504504
C	-2.124209	-3.548212	-1.664983
C	0.100799	-4.072967	-0.982327
C	-1.094763	-4.477000	-1.581923
F	1.396371	-2.432857	0.085725
F	-3.296808	-3.921990	-2.243182
H	0.941283	-4.754719	-0.887138
H	-2.853524	-1.589894	-1.278995
H	-1.230884	-5.480368	-1.972004

For phenylacetylene (Table 1 entry 20)

phenylacetylene

E_{gas} = -308.386936 a.u.

E_{sol} = -308.391198 a.u.

C	0.007242	-0.001437	0.029383
C	-0.035213	0.003790	1.421640
C	1.234739	-0.000874	-0.638005
C	1.158347	0.009729	2.168836
C	2.424021	0.004986	0.095287
C	2.390834	0.010249	1.487818
H	-0.920525	-0.005955	-0.536364
H	3.312566	0.014783	2.061260
H	1.264546	-0.004919	-1.724174
C	1.118889	0.015151	3.598411
C	1.085142	0.019810	4.808134
H	1.055359	0.023979	5.873756
H	-0.986700	0.003367	1.944245
H	3.381137	0.005471	-0.419347

2 for phenylacetylene (Table 1 entry 20)

E_{gas} = -2635.618546 a.u.

E_{sol} = -2635.632572 a.u.

Cu	0.487029	-0.405592	0.320870
O	0.644409	-0.243045	2.123433
C	1.859913	0.193950	2.631084
H	1.796914	0.335553	3.725816
H	2.703152	-0.510143	2.457554
H	2.191293	1.169532	2.215478
H	2.539056	2.718012	0.307395
C	2.362162	2.485683	-0.740779
C	2.883530	3.314576	-1.755118
C	2.637454	2.980203	-3.071632
H	3.465326	4.193150	-1.494492
C	1.394565	1.063890	-2.267627
C	1.874085	1.828815	-3.366614
H	3.021723	3.589550	-3.885993
C	0.602797	-0.123473	-2.524359
C	1.574777	1.417944	-4.707510
C	0.324720	-0.497373	-3.865539
C	0.832181	0.301730	-4.945111
H	1.953061	2.016769	-5.532024
C	-0.452947	-1.654324	-4.087122
C	-0.595450	-1.945698	-1.709425
H	0.606673	-0.006787	-5.962435
C	-0.912718	-2.377510	-3.003983
H	-0.678907	-1.960978	-5.104949
H	-0.931481	-2.498488	-0.838002
H	-1.510984	-3.273331	-3.132838
N	1.645209	1.398982	-0.981747
N	0.139616	-0.851471	-1.462501
C	-3.650086	-6.316905	0.303352
C	-3.070842	-5.145872	0.787353
C	-2.856827	-7.431570	0.018619
C	-1.678735	-5.068252	0.995410
C	-1.475903	-7.367308	0.223150
C	-0.889279	-6.199748	0.706205
H	-4.725416	-6.360890	0.150757
H	0.183064	-6.147942	0.868397
H	-3.311663	-8.344393	-0.356644
C	-1.079483	-3.867439	1.488130
C	-0.559246	-2.840557	1.878322
H	-0.102229	-1.932135	2.278600

H	-3.685831	-4.280168	1.014378
H	-0.853036	-8.231582	0.007310

$TS_{(2-3)}$ for phenylacetylene (Table 1 entry 20)

E_{gas} = -2635.598754 a.u.

E_{sol} = -2635.615492 a.u

Cu	-0.169590	-0.023660	-0.110514
H	-0.188872	-0.069549	1.876358
O	1.042388	-0.098873	1.556177
C	1.587622	-1.353669	1.866798
H	2.147574	-1.335060	2.816993
H	0.809797	-2.136562	1.964494
H	2.290567	-1.690415	1.085382
H	2.975083	0.756991	-0.342508
C	2.650013	0.647740	-1.374021
C	3.543557	0.767240	-2.456389
C	3.058443	0.655668	-3.748123
H	4.593604	0.967903	-2.268607
C	0.876665	0.266672	-2.800476
C	1.683894	0.400763	-3.955756
H	3.720348	0.765301	-4.603447
C	-0.530268	-0.021128	-2.932998
C	1.068066	0.291413	-5.249178
C	-1.112569	-0.100842	-4.220466
C	-0.272144	0.066656	-5.374661
H	1.691452	0.401779	-6.132659
C	-2.498331	-0.366849	-4.286279
C	-2.540987	-0.465242	-1.879769
H	-0.727216	-0.002867	-6.359190
C	-3.211709	-0.540838	-3.113374
H	-2.988578	-0.435471	-5.253973
H	-3.062101	-0.608275	-0.936590
H	-4.276192	-0.751055	-3.129372
N	1.353798	0.415324	-1.541516
N	-1.235129	-0.224363	-1.785535
C	-6.291384	0.911376	1.862082
C	-4.903626	0.967799	1.764790
C	-6.944635	-0.319689	1.973707
C	-4.128490	-0.214078	1.775601
C	-6.192313	-1.497986	1.989159
C	-4.804178	-1.450319	1.890960
H	-6.867662	1.833401	1.853793
H	-4.219555	-2.365483	1.908224
H	-8.027839	-0.360147	2.051675
C	-2.708718	-0.160072	1.676968
C	-1.481317	-0.110164	1.569585
H	-4.395833	1.924245	1.683221
H	-6.691034	-2.459864	2.080781

3 for phenylacetylene (Table 1 entry 20)

E_{gas} = -2519.905844 a.u.

E_{sol} = -2519.921286 a.u.

Cu	0.013922	0.046193	-0.159487
H	-0.086712	0.102824	2.701841
C	0.980099	0.056899	2.510285
C	1.899394	0.045898	3.569306
C	3.250850	-0.011476	3.286192
H	1.537852	0.083200	4.591516
C	2.676914	-0.045089	0.932127
C	3.674240	-0.058888	1.940236
H	3.990122	-0.020698	4.082682
C	3.070508	-0.094356	-0.459241
C	5.058566	-0.119185	1.560731
C	4.448081	-0.153191	-0.795484
C	5.430567	-0.163903	0.250265
H	5.807782	-0.128071	2.347777
C	4.770881	-0.199289	-2.170932
C	2.419451	-0.125547	-2.663313
H	6.481723	-0.209116	-0.022683
C	3.756844	-0.185625	-3.109081
H	5.813588	-0.245205	-2.475375
H	1.591305	-0.112771	-3.369213
H	3.973821	-0.220327	-4.172091
N	1.343468	0.013443	1.224086
N	2.087402	-0.081567	-1.383821
C	-1.472682	0.105984	-1.226699
C	-2.363648	0.145832	-2.071273
C	-3.429576	0.193572	-3.014918
C	-4.777270	0.244230	-2.594349
C	-3.175910	0.192377	-4.404442
C	-5.816880	0.291118	-3.519938
H	-4.988928	0.246024	-1.529162
C	-4.219011	0.239442	-5.326229
H	-2.144993	0.153962	-4.744739
C	-5.546281	0.289107	-4.891398
H	-6.845918	0.329649	-3.169648
H	-3.995803	0.237379	-6.390837
H	-6.359462	0.325747	-5.611817

$TS_{(3-4)}$ for phenylacetylene (Table 1 entry 20)

E_{gas} = -2762.908482 a.u.

E_{sol} = -2762.920516 a.u.

Cu	0.248115	-0.551445	-0.099966
C	0.338966	-0.368700	1.990995
C	1.512605	-0.867698	2.577853
C	-0.904920	-0.649020	2.586698
C	1.430444	-1.774505	3.640865
H	2.482238	-0.546351	2.216738
C	-0.971394	-1.546743	3.645655
H	-1.810212	-0.226463	2.169977
C	0.191698	-2.124008	4.173429
H	2.346244	-2.175931	4.068501
H	-1.943112	-1.799577	4.061346
H	0.128428	-2.816873	5.007629
I	0.658429	1.811158	1.179357
H	2.692762	-2.444282	0.895639
C	3.062998	-2.071920	-0.054870
C	4.314305	-2.488380	-0.543548
C	4.763434	-1.987228	-1.749521
H	4.907599	-3.191852	0.031514
C	2.689882	-0.751328	-1.902820
C	3.941412	-1.098546	-2.474918
H	5.730303	-2.277294	-2.152808
C	1.785823	0.091405	-2.649825
C	4.304984	-0.562674	-3.757384
C	2.160515	0.577443	-3.928084
C	3.453233	0.242111	-4.453973
H	5.275291	-0.826266	-4.169827
C	1.210049	1.361057	-4.619954
C	-0.302565	1.057915	-2.774827
H	3.735381	0.631038	-5.428841
C	-0.025574	1.596262	-4.046445
H	1.455663	1.760099	-5.600883
H	-1.268473	1.195330	-2.295874
H	-0.780287	2.183356	-4.559725
N	2.274740	-1.211012	-0.691934
N	0.582263	0.343582	-2.095272
C	-1.490922	-1.271375	-0.408656
C	-2.618653	-1.691194	-0.657814
C	-3.933493	-2.167443	-0.934738
C	-5.059817	-1.328341	-0.786697
C	-4.154703	-3.493493	-1.366963
C	-6.343889	-1.794945	-1.058028
H	-4.907015	-0.305626	-0.453733
C	-5.440922	-3.955378	-1.636475
H	-3.299019	-4.151843	-1.485342
C	-6.544080	-3.110765	-1.484554
H	-7.194404	-1.128229	-0.934850

H	-5.584113	-4.981599	-1.967249
H	-7.546882	-3.473373	-1.695273

For N-benzimidazole (Table 2 entry 1)

N-methylimidazole

E_{gas} = -265.521836 a.u.

E_{sol} = -265.530539 a.u.

C	0.002468	0.102034	0.060277
C	-0.014333	-0.025728	2.190905
C	1.307690	-0.079851	1.822399
N	-0.824187	0.087870	1.083636
H	-0.428640	-0.062011	3.189804
H	2.223110	-0.166429	2.389412
N	1.312573	0.003292	0.443318
C	2.475856	-0.012201	-0.424997
H	2.143932	0.072729	-1.462398
H	3.141090	0.828444	-0.200986
H	3.034694	-0.947317	-0.312192
H	-0.278988	0.181111	-0.982357

2 for N-benzimidazole (Table 2 entry 1)

E_{gas} = -2592.761400 a.u.

E_{sol} = -2592.773938 a.u.

Cu	0.307596	-0.366451	-0.374683
H	0.658770	-0.120420	1.875044
C	1.341641	-0.035462	2.710791
C	2.842156	0.594945	4.100131
C	2.443562	-0.655983	4.506862
N	2.149642	0.977936	2.971779
O	-0.456233	-1.709604	0.593074
C	-1.827884	-1.868444	0.440144
H	-2.180446	-2.769481	0.977780
H	-2.430502	-1.021480	0.836115
H	-2.153811	-1.998231	-0.614472
H	-1.372453	-2.194101	-3.033896
C	-0.951517	-1.312037	-3.511609
C	-1.161639	-1.068371	-4.884175
C	-0.601001	0.060397	-5.447965
H	-1.752279	-1.761076	-5.475453
C	0.307116	0.599625	-3.270066
C	0.163126	0.935426	-4.643965
H	-0.736586	0.285903	-6.502898
C	1.084053	1.464261	-2.403640
C	0.785234	2.121383	-5.156258
C	1.694109	2.622828	-2.949997
C	1.520068	2.928624	-4.342114
H	0.660443	2.362333	-6.208789
C	2.461205	3.437270	-2.088906
C	1.956605	1.919262	-0.293077
H	1.993347	3.825299	-4.733327
C	2.592796	3.078832	-0.763023
H	2.938319	4.331704	-2.481031
H	2.055899	1.638166	0.753907
H	3.175687	3.674802	-0.068818
N	-0.247435	-0.508743	-2.729384
N	1.214557	1.127725	-1.082635
N	1.480667	-1.053987	3.601398
C	0.750511	-2.315103	3.547829
H	0.227405	-2.351813	2.584010
H	1.450686	-3.153690	3.620400
H	0.031079	-2.381515	4.372022
H	3.585905	1.237413	4.553444
H	2.744235	-1.284221	5.332589

TS$_{(2-3)}$ for N-benzimidazole (Table 2 entry 1)

E_{gas} = -2592.716438 a.u.

E_{sol} = -2592.732779 a.u.

Cu	0.213503	-0.118833	-0.089335
H	0.148941	0.049542	1.812856
C	1.483015	-0.119342	1.558548
C	3.634573	0.144053	1.817225
C	3.349361	-1.106679	2.319119
N	2.494663	0.751461	1.363414
O	-1.096887	-0.066484	1.647508
C	-1.861287	1.029275	2.070831
H	-2.324126	0.859382	3.059798
H	-1.263331	1.956494	2.152542
H	-2.684162	1.240895	1.365663
H	-2.656454	-1.421614	-0.139792
C	-2.403657	-1.304650	-1.190488
C	-3.292086	-1.657474	-2.222779
C	-2.893111	-1.510763	-3.541816
H	-4.268242	-2.063199	-1.976441
C	-0.810583	-0.620652	-2.718586
C	-1.616527	-0.977080	-3.826118
H	-3.550175	-1.799779	-4.358185
C	0.483318	-0.024478	-2.927392
C	-1.088913	-0.791675	-5.150334
C	0.983501	0.131871	-4.241835
C	0.160381	-0.277705	-5.347448
H	-1.704693	-1.077927	-5.999087
C	2.261550	0.717872	-4.375788
C	2.356880	0.941356	-1.975018
H	0.548226	-0.152274	-6.355144
C	2.948315	1.114224	-3.239647
H	2.689219	0.859100	-5.365164
H	2.843934	1.253400	-1.053127
H	3.927245	1.577472	-3.312377
N	-1.189044	-0.819006	-1.430000
N	1.152109	0.394047	-1.819092
N	1.996270	-1.263943	2.154576
C	1.198914	-2.402820	2.575347
H	0.145490	-2.137304	2.455281
H	1.421703	-3.291633	1.971992
H	1.389965	-2.639279	3.628081
H	4.600346	0.633559	1.769622
H	3.970832	-1.869138	2.767910

3 for N-benzimidazole (Table 2 entry 1)

E_{gas} = -2477.024427 a.u.

E_{sol} = -2477.037852 a.u.

Cu	0.014240	0.005210	0.013333
C	0.030954	0.011785	1.891613
C	0.836036	0.017358	3.925670
C	-0.528358	0.018394	4.072463
N	1.176684	0.013304	2.592886
H	3.243412	0.004853	1.144231
C	3.366662	0.000564	0.060979
C	4.626832	-0.003546	-0.578672
C	4.682318	-0.008988	-1.960039
H	5.535024	-0.002429	0.016225
C	2.272560	-0.005738	-1.969038
C	3.481711	-0.010267	-2.708283
H	5.637050	-0.012310	-2.480608
C	1.003355	-0.006588	-2.661390
C	3.425573	-0.015821	-4.142140
C	0.984201	-0.012167	-4.078858
C	2.229072	-0.016746	-4.797245
H	4.357772	-0.019307	-4.701520
C	-0.274995	-0.012881	-4.717716
C	-1.311675	-0.002717	-2.550682
H	2.195337	-0.020974	-5.883468
C	-1.423890	-0.008160	-3.949279
H	-0.327763	-0.017106	-5.803268
H	-2.197589	0.001153	-1.924533
H	-2.407945	-0.008541	-4.406378
N	2.232945	-0.000548	-0.622657
N	-0.139724	-0.001878	-1.908764

H	1.586593	0.019131	4.708108
H	-1.170513	0.021828	4.942298
N	-1.028238	0.014878	2.784188
C	-2.420717	0.014492	2.402279
H	-2.444104	0.011299	1.307867
H	-2.945369	-0.875196	2.774042
H	-2.944380	0.906974	2.768739

TS$_{(3-4)}$ for N-benzimidazole (Table 2 entry 1)

E_{gas} = -2720.026887 a.u.

E_{sol} = -2720.038251 a.u.

Cu	-0.000278	0.000452	0.000374
C	-0.000155	0.000180	1.936163
C	0.811434	0.000258	3.969779
C	-0.548883	-0.068646	4.117685
N	1.143641	0.042747	2.632441
C	-0.581558	-2.077672	-0.345268
C	-1.682338	-2.205950	-1.212246
C	-0.560345	-2.841078	0.841186
C	-2.814341	-2.923771	-0.811047
H	-1.650641	-1.763043	-2.200174
C	-1.685953	-3.560430	1.222036
H	0.312781	-2.814473	1.482335
C	-2.829247	-3.595962	0.409194
H	-3.668790	-2.983515	-1.481389
H	-1.668361	-4.105614	2.162395
H	-3.700233	-4.170470	0.711276
I	1.424886	-1.942251	-1.477722
H	-2.550675	0.203604	-1.930735
C	-1.879817	0.956093	-2.333243
C	-2.266812	1.730050	-3.440275
C	-1.388984	2.673239	-3.938699
H	-3.243218	1.574994	-3.887688
C	0.149968	2.036122	-2.183223
C	-0.142991	2.857574	-3.303141
H	-1.649062	3.281209	-4.801387
C	1.380544	2.247703	-1.458958
C	0.813306	3.843988	-3.723414
C	2.291309	3.247449	-1.882216
C	1.981102	4.029861	-3.044578
H	0.578373	4.451472	-4.593405
C	3.459242	3.417725	-1.104496
C	2.673654	1.679480	0.370362
H	2.691496	4.786343	-3.368121
C	3.646507	2.640233	0.022827
H	4.191715	4.166775	-1.395558
H	2.736461	1.063486	1.267650
H	4.528648	2.759348	0.643912
N	-0.700060	1.072605	-1.727252
N	1.585043	1.486707	-0.364243
H	1.566502	0.018818	4.747121
H	-1.188873	-0.112992	4.987987
N	-1.054769	-0.064069	2.829003
C	-2.455618	-0.124440	2.475305
H	-3.007437	0.735331	2.876170
H	-2.526728	-0.112789	1.385168
H	-2.923520	-1.045540	2.842633

For N-methylpyrrole (Table 2 entry 2)

N-methylpyrrole

E_{gas} = -249.472927 a.u.

E_{sol} = -249.477323 a.u.

C	0.000149	-0.015106	-0.000473
C	0.001910	0.012210	2.255698
C	1.308761	-0.025603	1.817180
H	-0.221833	-0.021536	-1.058643
C	-0.830112	0.018889	1.100044
H	-1.911604	0.031608	1.077036
N	1.304303	-0.049284	0.440360
C	2.480300	0.012920	-0.405886
H	2.778143	1.047859	-0.617050
H	3.313065	-0.498041	0.085451
H	2.277837	-0.493795	-1.353660
H	2.241824	-0.041408	2.363252
H	-0.319348	0.018807	3.288691

2 for N-methylpyrrole (Table 2 entry 2)

E_{gas} = -2576.707183 a.u.

E_{sol} = -2576.717612 a.u.

Cu	0.077932	-0.537258	0.037984
H	0.103990	0.376519	2.604589
C	1.146419	0.262099	2.873048
C	3.338789	0.434651	3.413357
C	2.986189	-0.901725	3.418228
O	-1.263019	-0.718051	1.251322
C	-2.533024	-1.023334	0.784872
H	-3.246140	-1.116077	1.625572
H	-2.960317	-0.253013	0.106953
H	-2.591865	-1.984355	0.227539
H	-2.665395	-1.390487	-2.352276
C	-1.762472	-1.345078	-2.957467
C	-1.809282	-1.626472	-4.338219
C	-0.638696	-1.551673	-5.065930
H	-2.750773	-1.893259	-4.808116
C	0.502173	-0.942134	-3.018171
C	0.565394	-1.201080	-4.415468
H	-0.628079	-1.758334	-6.133355
C	1.714911	-0.583563	-2.308102
C	1.818813	-1.101437	-5.104482
C	2.936472	-0.491822	-3.025787
C	2.954758	-0.759984	-4.436145
H	1.843907	-1.303931	-6.172151
C	4.103104	-0.137416	-2.314384
C	2.775565	-0.000381	-0.317787
H	3.903627	-0.684257	-4.960583
C	4.017111	0.109784	-0.958959
H	5.050183	-0.062100	-2.842190
H	2.684492	0.206488	0.743638
H	4.888473	0.387463	-0.375434
N	-0.651619	-1.015406	-2.317143
N	1.648214	-0.339068	-0.962211
C	2.169121	1.173513	3.069786
H	2.083235	2.248502	2.977833
N	1.654973	-0.999199	3.088541
C	0.869979	-2.225284	3.029376
H	1.454286	-3.014487	2.543814
H	0.594843	-2.563661	4.035828
H	-0.035130	-2.019008	2.446749
H	3.566873	-1.788700	3.631921
H	4.321097	0.832011	3.634686

TS$_{(2-3)}$ for N-methylpyrrole (Table 2 entry 2)

E_{gas} = -2576.666105 a.u.

E_{sol} = -2576.679916 a.u.

Cu	0.249013	-0.013739	-0.179846
H	0.045898	0.206101	1.740105
C	1.278171	0.121872	1.496466
C	3.512052	0.449212	1.910660
C	3.169737	-0.839353	2.299042
O	-1.333642	-0.122360	1.780358
C	-2.101690	0.466498	2.774244
H	-2.836631	-0.235019	3.223603
H	-1.492226	0.845839	3.621319
H	-2.696725	1.338388	2.420675
H	-2.518481	-0.520104	0.017648
C	-2.405718	-0.524780	-1.069910
C	-3.455475	-0.749663	-1.980008
C	-3.195130	-0.736026	-3.337662
H	-4.457051	-0.932599	-1.604325

C	-0.883610	-0.277183	-2.811339
C	-1.878370	-0.496047	-3.794003
H	-3.988729	-0.908350	-4.060593
C	0.484009	-0.025493	-3.211009
C	-1.506472	-0.469236	-5.181372
C	0.814478	-0.011390	-4.590003
C	-0.217066	-0.239539	-5.563021
H	-2.278504	-0.639625	-5.927199
C	2.166584	0.233667	-4.922248
C	2.650512	0.413920	-2.573840
H	0.050459	-0.224820	-6.616448
C	3.087962	0.445367	-3.914402
H	2.467356	0.253339	-5.966892
H	3.343926	0.580318	-1.751487
H	4.132644	0.636667	-4.138900
N	-1.157975	-0.296088	-1.482412
N	1.391923	0.187359	-2.230584
C	2.329238	1.051952	1.426067
H	2.230675	2.072399	1.075864
N	1.844860	-1.029206	2.053261
C	1.071237	-2.223900	2.361499
H	1.286403	-3.033475	1.652274
H	1.303541	-2.575023	3.372763
H	0.013504	-1.946012	2.300670
H	4.497082	0.891959	1.989544
H	3.774037	-1.623101	2.738050

3 for N-methylpyrrole (Table 2 entry 2)

E_{gas} = -2460.964996 a.u.

E_{sol} = -2460.977778 a.u.

Cu	0.036454	0.022308	-0.012951
C	-0.191794	0.077382	1.848315
C	0.136789	0.273837	4.123542
C	-1.169566	-0.113820	3.908830
H	3.408654	-0.499068	1.126017
C	3.497329	-0.435389	0.043341
C	4.753342	-0.537044	-0.590990
C	4.810388	-0.455981	-1.968986
H	5.651771	-0.675060	0.002378
C	2.408673	-0.187273	-1.966630
C	3.617990	-0.278197	-2.706013
H	5.759116	-0.528921	-2.495036
C	1.154990	-0.015524	-2.666857
C	3.579681	-0.188060	-4.137170
C	1.153568	0.063941	-4.083695
C	2.398237	-0.022648	-4.795834
H	4.513855	-0.255076	-4.688969
C	-0.088004	0.221800	-4.735954
C	-1.153231	0.199918	-2.585091
H	2.375370	0.044118	-5.880298
C	-1.244116	0.288306	-3.980338
H	-0.121508	0.287112	-5.820161
H	-2.044822	0.251195	-1.969415
H	-2.216684	0.408000	-4.446252
N	2.365104	-0.260804	-0.618727
N	0.004641	0.052118	-1.929344
C	0.740851	0.390564	2.840419
H	1.760400	0.710012	2.651249
N	-1.359159	-0.225038	2.547536
C	-2.595805	-0.646113	1.930671
H	-2.472343	-0.530755	0.850326
H	-2.830397	-1.698268	2.145949
H	-3.441714	-0.029271	2.261714
H	-1.974575	-0.317683	4.603480
H	0.591591	0.458077	5.089850

$TS_{(3-4)}$ for N-methylpyrrole (Table 2 entry 2)

E_{gas} = -2703.966312 a.u.

E_{sol} = -2703.976699 a.u.

Cu	0.119199	-0.263330	-0.036820
C	0.122505	-0.118421	2.093046
C	1.405646	0.003257	2.656409
C	-0.806679	-0.988360	2.701119
C	1.811239	-0.863351	3.678694
H	2.082885	0.772445	2.303810
C	-0.393247	-1.836806	3.720671
H	-1.818301	-1.043944	2.319475
C	0.921400	-1.794128	4.208967
H	2.818154	-0.773716	4.080539
H	-1.108624	-2.538676	4.141885
H	1.230054	-2.455256	5.013810
I	-0.683716	1.987362	1.439808
H	3.032077	-0.954049	0.981133
C	3.232559	-0.398357	0.070545
C	4.552818	-0.203652	-0.366932
C	4.779222	0.531824	-1.514829
H	5.373157	-0.627898	0.202810
C	2.379800	0.771567	-1.722462
C	3.676911	1.035773	-2.235872
H	5.788358	0.714807	-1.874855
C	1.225687	1.194581	-2.478074
C	3.813547	1.769004	-3.463885
C	1.393930	1.886707	-3.704595
C	2.720535	2.179016	-4.167684
H	4.815326	1.978177	-3.829606
C	0.220643	2.234487	-4.409870
C	-1.069214	1.169384	-2.679759
H	2.838403	2.722219	-5.101751
C	-1.012022	1.869780	-3.900881
H	0.300022	2.773703	-5.350523
H	-2.012936	0.831710	-2.258618
H	-1.930185	2.113013	-4.425970
N	2.165563	0.089846	-0.561628
N	0.015639	0.859134	-1.984378
C	-1.343170	-1.510597	-0.330633
C	-2.710730	-1.234346	-0.407399
C	-2.487444	-3.438666	-0.787277
C	-3.426154	-2.436407	-0.691085
H	-3.155532	-0.256118	-0.255696
N	-1.242219	-2.874346	-0.578499
C	-0.020799	-3.642059	-0.476215
H	0.825240	-3.006194	-0.752971
H	0.149030	-4.017203	0.543188
H	-0.051989	-4.498104	-1.159409
H	-2.592449	-4.497219	-0.988396
H	-4.495019	-2.553141	-0.825888

For oxazole (Table 3 entry 2)

2A for oxazole (Table 3 entry 2)

E_{gas} = -2116.832862 a.u.

E_{sol} = -2116.906969 a.u.

Cu	0.074904	0.107231	0.042076
H	0.003508	0.083586	3.370496
C	0.356069	0.026246	4.421294
C	0.910865	0.282424	6.467598
C	1.280278	-0.973227	6.114020
N	0.321136	0.910917	5.376886
O	0.931945	-1.155402	4.804962
O	-0.642888	-0.039570	1.707974
C	-1.976898	-0.385779	1.779050
H	-2.307901	-0.470666	2.838655
H	-2.669564	0.349953	1.309454
H	-2.225376	-1.365577	1.310182
O	0.855234	0.220092	-1.585312
C	0.396983	1.219246	-2.402452
H	0.933974	1.216427	-3.382239
H	-0.689132	1.159880	-2.674956
H	0.526880	2.261177	-2.010930
H	1.759209	-1.802713	6.610720

H	1.024078	0.782162	7.420788

TS$_{(2-3)A}$ for oxazole (Table 3 entry 2)

E_{gas} = −2116.787921 a.u.

E_{sol} = −2116.867816 a.u.

Cu	0.059055	−0.006764	−0.009476
H	0.081658	0.005102	2.011719
C	1.565975	0.012718	1.710447
C	3.671500	0.536187	1.901841
C	3.618491	−0.818413	1.864646
N	2.385090	1.046004	1.816691
O	2.309725	−1.183641	1.755543
O	−1.011469	0.104973	1.798891
C	−1.394600	1.430326	2.074129
H	−1.871409	1.524359	3.067134
H	−0.533691	2.119708	2.052578
H	−2.122850	1.778963	1.325706
O	0.195425	−0.099469	−1.823677
C	1.489368	−0.190394	−2.278497
H	2.052333	−1.092054	−1.932017
H	1.519296	−0.243317	−3.393960
H	2.147947	0.672043	−2.012127
H	4.541765	1.177595	1.983071
H	4.355386	−1.608537	1.889061

3A for oxazole (Table 3 entry 2)

E_{gas} = −2001.111109 a.u.

E_{sol} = −2001.188131 a.u.

Cu	−0.004542	−0.003897	0.002930
C	−0.009456	−0.000981	1.857279
C	0.409382	−0.002231	3.995637
C	−0.940127	0.014076	3.879103
N	0.981368	−0.011157	2.731081
O	−1.243715	0.015681	2.548644
O	−0.032232	−0.004484	−1.822958
C	1.173862	−0.045695	−2.467364
H	1.044790	−0.040805	−3.577976
H	1.861154	0.815988	−2.260822
H	1.800292	−0.952853	−2.261638
H	−1.765332	0.025473	4.577449
H	1.011172	−0.008004	4.898094

TS$_{(3-4)A}$ for oxazole (Table 3 entry 2)

E_{gas} = −2244.128902 a.u.

E_{sol} = −2244.194678 a.u.

Cu	0.024771	−0.046494	−0.030524
C	−0.022571	0.068690	2.021780
C	1.252563	0.062784	2.619849
C	−1.031575	−0.760267	2.548578
C	1.538329	−0.846730	3.636346
H	2.016939	0.739060	2.257325
C	−0.728327	−1.659319	3.570863
H	−2.021866	−0.716865	2.114685
C	0.555368	−1.716257	4.121144
H	2.541628	−0.865742	4.058520
H	−1.512659	−2.317735	3.940544
H	0.783360	−2.415956	4.921883
I	−0.812246	2.361590	1.661454
C	1.848437	0.243837	−0.560899
N	2.590928	−0.500471	−1.354367
O	2.587012	1.347893	−0.113151
C	3.833338	0.115608	−1.437389
C	3.824591	1.237723	−0.678683
O	−1.720739	−0.571598	−0.336750
C	−1.936500	−1.929653	−0.429580
H	−2.996246	−2.149762	−0.681258
H	−1.327952	−2.447108	−1.205031
H	−1.741002	−2.476998	0.524612
H	4.542755	2.011156	−0.448959
H	4.639110	−0.294528	−2.034661

For benzothiazole (Table 3 entry 3)

2A for benzothiazole (Table 3 entry 3)

E_{gas} = −2593.462290 a.u.

E_{sol} = −2593.531191 a.u.

Cu	0.066867	0.145727	0.774461
H	−0.684555	2.098404	3.823008
C	−0.160896	1.583804	4.620997
C	0.826283	1.100755	6.527727
C	1.029137	−0.137331	5.864608
C	1.303578	1.280251	7.835261
C	1.703945	−1.184486	6.502735
C	1.972209	0.234834	8.462946
H	1.142302	2.233096	8.331984
C	2.171581	−0.990470	7.800458
H	1.862727	−2.132338	5.994629
H	2.346658	0.364038	9.475932
H	2.698443	−1.796017	8.307097
O	−1.035200	0.803732	2.071374
C	−2.325013	0.297495	2.074535
H	−2.917007	0.721421	2.915082
H	−2.898802	0.531824	1.151629
H	−2.385088	−0.807018	2.192102
O	1.189344	−0.523386	−0.473201
C	1.311886	0.211528	−1.623222
H	2.018486	−0.275090	−2.338082
H	0.366463	0.350839	−2.209432
H	1.711860	1.249900	−1.491375
S	0.326117	−0.066409	4.252100
N	0.144593	2.059738	5.787939

TS$_{(2-3)A}$ for benzothiazole (Table 3 entry 3)

E_{gas} = −2593.421364 a.u.

E_{sol} = −2593.494279 a.u.

Cu	−0.111787	0.018433	−0.010429
H	−0.150806	0.044256	2.039512
C	1.399776	−0.173501	1.709252
C	3.623155	0.277616	1.896879
C	3.780304	−1.131140	1.757458
C	4.762604	1.082675	2.060465
C	5.053411	−1.709688	1.774532
C	6.026260	0.497674	2.082452
H	4.633006	2.156440	2.166920
C	6.172811	−0.891684	1.939227
H	5.172204	−2.784659	1.662199
H	6.908647	1.121997	2.209208
H	7.165938	−1.336369	1.956115
N	2.321586	0.741017	1.872263
O	−1.153785	0.304758	1.761560
C	−1.334805	1.684671	2.016289
H	−1.789157	1.856544	3.006163
H	−0.380035	2.230473	1.978623
H	−2.006030	2.109866	1.258360
O	0.097208	−0.115623	−1.806901
C	1.402023	−0.192721	−2.241672
H	1.986772	−1.046013	−1.826576
H	1.441916	−0.319179	−3.348695
H	2.022734	0.711568	−2.029822
S	2.208617	−1.866332	1.590100

3A for benzothiazole (Table 3 entry 3)

E_{gas} = −2477.746118 a.u.

E_{sol} = −2477.814718 a.u.

Cu	0.004293	−0.024555	−0.157968
C	−0.177680	−0.010777	1.672449
C	0.157690	−0.007160	3.920259
C	−1.263146	0.019833	4.003299

C	0.912877	-0.016368	5.104156
C	-1.904176	0.037045	5.245975
C	0.267506	0.000838	6.338530
H	1.997014	-0.037004	5.031081
C	-1.134592	0.027480	6.410961
H	-2.989764	0.057549	5.306471
H	0.854201	-0.006401	7.255159
H	-1.627327	0.040740	7.381244
N	0.691399	-0.022731	2.645138
O	0.145261	-0.039706	-1.971081
C	1.408832	-0.041019	-2.503745
H	1.377702	-0.051593	-3.619113
H	2.038079	0.848636	-2.245353
H	2.043322	-0.921862	-2.228659
S	-1.922938	0.025247	2.388039

$TS_{(3-4)A}$ for benzothiazole (Table 3 entry 3)

E_{gas} = -2720.760529 a.u.

E_{sol} = -2720.819691 a.u.

Cu	0.016284	-0.317438	-0.029842
C	-0.068813	0.035874	1.952806
C	1.184600	0.016874	2.580470
C	-1.178170	-0.558016	2.580499
C	1.341883	-0.688681	3.775496
H	2.035635	0.493136	2.105976
C	-1.002562	-1.247349	3.780497
H	-2.147604	-0.504749	2.102129
C	0.255265	-1.320445	4.386480
H	2.328565	-0.732720	4.233329
H	-1.863589	-1.726329	4.243508
H	0.384089	-1.853693	5.325724
I	-0.685371	2.378533	1.166724
C	1.821956	0.001095	-0.633627
N	2.932913	0.308375	-0.035810
C	4.030763	0.454459	-0.867844
C	3.784108	0.241605	-2.249879
C	5.325117	0.788774	-0.441619
C	4.815052	0.360351	-3.187654
C	6.347748	0.905647	-1.378725
H	5.503263	0.952465	0.617502
C	6.095123	0.692486	-2.744380
H	4.623591	0.198243	-4.245325
H	7.352222	1.165716	-1.052112
H	6.904515	0.788316	-3.464966
O	-1.666247	-0.993233	-0.347531
C	-1.866470	-2.340002	-0.132988
H	-2.892710	-2.642463	-0.428207
H	-1.178221	-3.008979	-0.697809
H	-1.766340	-2.632781	0.938625
S	2.096396	-0.153132	-2.460910

For thiazole (Table 3 entry 4)

2A for thiazole (Table 3 entry 4)

E_{gas} = -2439.810033 a.u.

E_{sol} = -2439.881166 a.u.

Cu	0.171221	0.490970	0.585070
H	-0.525636	1.713334	4.035235
C	0.035933	1.027342	4.657452
C	1.107049	0.099282	6.340193
C	1.293428	-0.895413	5.421657
O	-0.932855	0.878465	1.983832
C	-2.206279	0.342861	1.907218
H	-2.803812	0.603981	2.808604
H	-2.797563	0.708306	1.038228
H	-2.237048	-0.768319	1.841153
O	1.317003	0.104001	-0.758992
C	0.982692	0.602632	-1.989925
H	1.738828	0.315476	-2.760532
H	0.004742	0.244939	-2.406318
H	0.919767	1.719845	-2.057617
S	0.542476	-0.464531	3.910921
N	0.390144	1.194411	5.902466
H	1.473706	0.088918	7.362925
H	1.824041	-1.829597	5.554744

$TS_{(2-3)A}$ for thiazole (Table 3 entry 4)

E_{gas} = -2439.765085 a.u.

E_{sol} = -2439.840743 a.u.

Cu	-0.032606	-0.017723	-0.018214
H	-0.063439	-0.015468	2.019761
C	1.458214	-0.116987	1.730309
C	3.628935	0.492070	1.981158
C	3.886401	-0.844598	1.865069
N	2.309112	0.874672	1.918729
O	-1.111728	0.175281	1.765334
C	-1.383935	1.534303	2.028376
H	-1.854728	1.673010	3.017593
H	-0.467136	2.144329	2.002650
H	-2.077479	1.928365	1.271588
O	0.137250	-0.111881	-1.827077
C	1.435522	-0.177203	-2.276009
H	2.029627	-1.037021	-1.884335
H	1.468170	-0.282297	-3.387005
H	2.058962	0.723742	-2.053067
S	2.391650	-1.699309	1.656240
H	4.852733	-1.332646	1.872810
H	4.393469	1.254751	2.117796

3A for thiazole (Table 3 entry 4)

E_{gas} = -2324.089003 a.u.

E_{sol} = -2324.162043 a.u.

Cu	-0.013248	-0.017881	-0.106562
C	-0.095537	-0.007017	1.737887
C	0.382194	-0.011999	3.953706
C	-0.970439	0.026940	4.128717
N	0.846061	-0.030136	2.656850
O	0.030213	-0.028856	-1.929061
C	1.263394	-0.043657	-2.524362
H	1.177933	-0.048340	-3.638174
H	1.918509	0.836368	-2.295176
H	1.901459	-0.933826	-2.286413
H	-1.516896	0.046034	5.063187
H	1.105425	-0.029412	4.767146
S	-1.742450	0.042895	2.571712

$TS_{(3-4)A}$ for thiazole (Table 3 entry 4)

E_{gas} = -2567.106288 a.u.

E_{sol} = -2567.167534 a.u.

Cu	-0.009162	0.006768	0.006295
C	0.000292	-0.000967	2.044142
C	1.293122	0.021519	2.591188
C	-0.968412	-0.873963	2.573579
C	1.635878	-0.903239	3.578816
H	2.034465	0.706766	2.193790
C	-0.608241	-1.781972	3.569005
H	-1.970764	-0.858034	2.165904
C	0.693178	-1.806270	4.079726
H	2.653903	-0.905710	3.964895
H	-1.359809	-2.472382	3.948314
H	0.965367	-2.511182	4.862225
I	-0.933902	2.295121	1.799396
C	1.722013	0.607181	-0.590690
N	2.791641	1.036336	0.031698
C	3.837103	1.384159	-0.795073
C	3.627455	1.235219	-2.134389
O	-1.662476	-0.742480	-0.335662
C	-1.727436	-2.115829	-0.412510
H	-2.747846	-2.454531	-0.692144

H	-1.042137	-2.575312	-1.161748
H	-1.502303	-2.624524	0.555614
H	4.313613	1.450074	-2.943452
H	4.757779	1.753227	-0.349989
S	2.022678	0.623145	-2.386585

For pentafluorobenzene (Table 3 entry 5)

2A for pentafluorobenzene (Table 3 entry 5)

E_{gas} = -2599.147185 a.u.

E_{sol} = -2599.212181 a.u.

Cu	-0.244776	-0.216265	-0.100795
O	-0.205658	0.207616	1.669608
C	1.019498	0.575962	2.195616
H	0.922880	0.842497	3.269829
H	1.795365	-0.220929	2.147230
H	1.474180	1.465446	1.706835
O	-0.355407	-0.602766	-1.861753
C	0.477372	-1.592943	-2.313282
H	0.338160	-1.766762	-3.407534
H	1.573924	-1.391454	-2.195355
H	0.328706	-2.599563	-1.844452
C	-1.986496	1.132222	4.789172
C	-2.075092	0.162344	3.798959
C	-3.074650	-0.792457	3.937587
H	-1.369207	0.153910	2.919858
C	-3.844544	0.194517	5.990613
C	-3.960299	-0.792080	5.015457
C	-2.851888	1.164311	5.882199
F	-3.221688	-1.764481	3.020250
F	-4.921784	-1.728024	5.127921
F	-4.689389	0.209620	7.037849
F	-2.743178	2.114439	6.830809
F	-1.037895	2.086668	4.727011

$TS_{(2-3)A}$ for pentafluorobenzene (Table 3 entry 5)

E_{gas} = -2599.116355 a.u.

E_{sol} = -2599.184508 a.u.

Cu	0.121515	-0.030934	-0.080075
H	0.090380	0.017692	2.001290
O	1.100723	-0.050012	1.742824
C	1.558016	-1.353940	2.064747
H	1.984369	-1.388917	3.080274
H	0.744346	-2.088855	2.001976
H	2.343640	-1.638370	1.354492
O	-0.072200	-0.037694	-1.886465
C	-1.383840	-0.017743	-2.302300
H	-1.972982	0.870951	-1.969478
H	-1.447865	-0.008427	-3.415431
H	-1.994827	-0.897878	-1.983792
C	-2.297620	-1.160405	1.699885
C	-1.541123	-0.003678	1.588052
C	-2.298563	1.159563	1.622279
C	-4.390410	-0.001677	1.761124
C	-3.687384	-1.203739	1.766194
C	-3.689132	1.199523	1.685678
F	-1.673846	-2.384828	1.741479
F	-4.371457	-2.369850	1.862463
F	-5.741072	-0.000797	1.821491
F	-4.377211	2.366756	1.704443
F	-1.677908	2.376691	1.583275

3A for pentafluorobenzene (Table 3 entry 5)

E_{gas} = -2483.434812 a.u.

E_{sol} = -2483.497932 a.u.

Cu	0.010663	0.005845	0.003159
O	-0.001585	-0.004350	1.825554
C	1.214867	-0.009157	2.456281
H	1.096579	-0.015256	3.566561
H	1.866670	-0.893684	2.236312
H	1.868518	0.876460	2.246274
C	-0.024894	0.014960	-1.866413
C	-1.202889	0.040752	-2.612641
C	1.126275	-0.005049	-2.653606
C	-0.074739	0.026093	-4.732067
C	1.135938	-0.000298	-4.047058
C	-1.260729	0.046941	-4.004959
F	2.356215	-0.031724	-2.067293
F	2.293906	-0.021038	-4.749426
F	-0.098647	0.031179	-6.084343
F	-2.442124	0.072615	-4.666969
F	-2.411501	0.061856	-1.984036

$TS_{(3-4)A}$ for pentafluorobenzene (Table 3 entry 5)

E_{gas} = -2726.449774 a.u.

E_{sol} = -2726.506010 a.u.

Cu	0.007307	-0.002458	0.001579
C	-0.003212	0.001229	1.985252
C	1.279418	-0.006741	2.556308
C	-1.034890	-0.745798	2.576502
C	1.546949	-0.845037	3.639916
H	2.055611	0.627878	2.148200
C	-0.751843	-1.570015	3.665999
H	-2.028516	-0.693885	2.150750
C	0.538166	-1.632602	4.201270
H	2.553211	-0.866235	4.054200
H	-1.553196	-2.167181	4.097426
H	0.750738	-2.273932	5.053467
I	-0.721855	2.418078	1.531367
O	-1.761273	-0.497745	-0.277180
C	-1.973747	-1.854905	-0.426956
H	-3.020651	-2.057784	-0.733905
H	-1.325162	-2.339636	-1.185347
H	-1.827741	-2.426904	0.520553
C	1.803965	0.024363	-0.808246
C	2.856714	0.904366	-0.588310
C	2.086384	-0.958493	-1.751265
C	4.308671	-0.165429	-2.171553
C	4.091242	0.838755	-1.233603
C	3.294482	-1.079749	-2.435345
F	2.737314	1.903755	0.328365
F	5.077237	1.724700	-0.971188
F	5.491529	-0.253814	-2.814166
F	3.503919	-2.058846	-3.343317
F	1.145112	-1.892790	-2.066294

For 1,2,4,5-tetrafluorobenzene (Table 3 entry 6)

2A for 1,2,4,5-tetrafluorobenzene (Table 3 entry 6)

E_{gas} = -2499.927357 a.u.

E_{sol} = -2499.994614 a.u.

Cu	-0.203017	-0.168754	-0.111999
O	-0.181391	0.254516	1.658400
C	1.036170	0.637198	2.190495
H	0.930951	0.902813	3.264129
H	1.822780	-0.150075	2.146801
H	1.484136	1.532085	1.704352
O	-0.291658	-0.552085	-1.875435
C	0.439784	-1.632571	-2.293434
H	0.321245	-1.797639	-3.391712
H	1.547320	-1.555022	-2.136580
H	0.162267	-2.612872	-1.827371
C	-1.976998	1.119505	4.807265
C	-2.065792	0.168176	3.797990
C	-3.066319	-0.789854	3.913351

H	-1.360134	0.175923	2.922622
C	-3.849553	0.157932	5.997098
C	-3.947788	-0.799018	4.994125
C	-2.851451	1.119202	5.893059
F	-3.210067	-1.743137	2.973914
F	-4.906571	-1.748616	5.067587
F	-2.727377	2.062452	6.853760
F	-1.025550	2.074401	4.764046
H	-4.532517	0.153638	6.838463

$TS_{(2-3)A}$ for 1,2,4,5-tetrafluorobenzene (Table 3 entry 6)

E_{gas} = -2499.894477 a.u.

E_{sol} = -2499.964649 a.u.

Cu	0.111852	-0.029881	-0.073412
H	0.085366	0.017143	1.996754
O	1.105015	-0.047451	1.744049
C	1.563050	-1.350246	2.064508
H	1.998005	-1.384702	3.076821
H	0.747821	-2.084602	2.010780
H	2.342967	-1.640025	1.349393
O	-0.089514	-0.036235	-1.879376
C	-1.402730	-0.022201	-2.290181
H	-1.994816	0.863050	-1.953812
H	-1.471170	-0.011881	-3.403321
H	-2.008068	-0.905586	-1.970237
C	-2.289487	-1.162584	1.700823
C	-1.530009	-0.004567	1.600755
C	-2.288860	1.159720	1.631684
C	-4.402847	-0.002040	1.750776
C	-3.679476	-1.190653	1.757008
C	-3.679657	1.185398	1.686069
F	-1.665639	-2.388544	1.739109
F	-4.346403	-2.373680	1.842845
F	-4.348872	2.369811	1.702101
F	-1.666724	2.377818	1.598219
H	-5.485909	-0.000996	1.788664

3A for 1,2,4,5-tetrafluorobenzene (Table 3 entry 6)

E_{gas} = -2384.213391 a.u.

E_{sol} = -2384.278879 a.u.

Cu	0.009803	0.015414	0.003011
O	-0.000912	0.012719	1.826354
C	1.215574	-0.010991	2.455872
H	1.098898	-0.009554	3.566635
H	1.851333	-0.908248	2.239750
H	1.885225	0.861529	2.240975
C	-0.026382	0.018174	-1.865327
C	-1.205406	0.038651	-2.612468
C	1.126792	-0.000722	-2.651879
C	-0.074701	0.021135	-4.750471
C	1.122829	0.000391	-4.044227
C	-1.247804	0.040448	-4.004282
F	2.357445	-0.021867	-2.062425
F	2.297390	-0.019075	-4.729873
F	-2.444484	0.061107	-4.650536
F	-2.415375	0.058619	-1.982352
H	-0.093084	0.022234	-5.833932

$TS_{(3-4)A}$ for 1,2,4,5-tetrafluorobenzene (Table 3 entry 6)

E_{gas} = -2627.228667 a.u.

E_{sol} = -2627.286862 a.u.

Cu	-0.004521	-0.003436	-0.008027
C	0.000581	0.005503	1.979454
C	1.284850	0.008035	2.547529
C	-1.020826	-0.757411	2.568757
C	1.564677	-0.834632	3.624287
H	2.052489	0.653894	2.140891
C	-0.725273	-1.586534	3.651333
H	-2.016547	-0.712600	2.147232
C	0.566712	-1.638383	4.182665
H	2.572365	-0.847348	4.035593
H	-1.518756	-2.195780	4.080563
H	0.789145	-2.283654	5.029413
I	-0.746162	2.416814	1.552948
O	-1.778884	-0.479342	-0.278696
C	-2.000745	-1.833725	-0.440218
H	-3.049154	-2.027137	-0.748656
H	-1.355497	-2.316640	-1.202619
H	-1.858302	-2.415300	0.502192
C	1.795340	0.022127	-0.801651
C	2.843067	0.910915	-0.587018
C	2.086823	-0.974035	-1.729445
C	4.325683	-0.178462	-2.154348
C	4.077066	0.829260	-1.230334
C	3.304547	-1.088846	-2.396128
F	2.711623	1.923626	0.315685
F	5.047769	1.737155	-0.959036
F	3.504125	-2.092180	-3.287576
F	1.148647	-1.916850	-2.036072
H	5.279638	-0.252849	-2.663002

For 1,2,3,5-tetrafluorobenzene (Table 3 entry 7)

2A for 1,2,3,5-tetrafluorobenzene (Table 3 entry 7)

E_{gas} = -2499.927523 a.u.

E_{sol} = -2499.994579 a.u.

Cu	-0.309840	-0.217772	-0.068445
O	-0.207035	-0.322303	1.745515
C	1.057352	-0.314359	2.303216
H	0.998770	-0.341442	3.412516
H	1.693016	-1.181460	2.011167
H	1.659139	0.589483	2.058691
O	-0.485948	-0.073410	-1.861357
C	0.283271	-0.923958	-2.610642
H	0.107362	-0.769121	-3.702764
H	1.391588	-0.810705	-2.483555
H	0.096462	-2.016523	-2.445412
C	-1.840134	-0.056041	5.112876
C	-2.115597	-0.598808	3.864872
C	-3.325947	-1.274489	3.745555
H	-1.404105	-0.492954	3.004512
C	-3.911643	-0.857608	6.015834
C	-4.238725	-1.421123	4.789208
C	-2.714738	-0.172560	6.195007
F	-3.651986	-1.826410	2.559173
F	-2.410563	0.366549	7.393273
F	-0.689758	0.610847	5.326598
H	-5.172289	-1.954413	4.654181
F	-4.757811	-0.969843	7.062540

$TS_{(2-3)A}$ for 1,2,3,5-tetrafluorobenzene (Table 3 entry 7)

E_{gas} = -2499.892841 a.u.

E_{sol} = -2499.962528 a.u.

Cu	0.114209	-0.019671	-0.080535
H	0.063935	0.003217	1.987043
O	1.092341	-0.050458	1.749150
C	1.554601	-1.353245	2.058492
H	1.986574	-1.396570	3.072083
H	0.742747	-2.091247	1.996575
H	2.337903	-1.635372	1.343606
O	-0.058055	-0.009350	-1.890594
C	-1.365084	0.008990	-2.318880
H	-1.961253	0.893206	-1.985662

H	-1.419286	0.025936	-3.433016
H	-1.976806	-0.875158	-2.012625
C	-2.302473	-1.170745	1.728832
C	-1.538343	-0.021470	1.594679
C	-2.315609	1.133680	1.610838
C	-4.389606	-0.008560	1.780228
C	-3.694421	-1.212873	1.803644
C	-3.706711	1.198337	1.683066
F	-1.685585	-2.396812	1.789118
F	-4.371571	-2.382353	1.922577
F	-1.679674	2.346162	1.541407
H	-4.244060	2.141017	1.675036
F	-5.744644	-0.027908	1.854643

3A for 1,2,3,5-tetrafluorobenzene (Table 3 entry 7)

E_{gas} = -2384.211848 a.u.

E_{sol} = -2384.277093 a.u.

Cu	0.010335	0.010322	0.008073
O	-0.003351	0.004114	1.832165
C	1.211743	-0.010172	2.463399
H	1.093745	-0.012287	3.574264
H	1.856429	-0.901234	2.246592
H	1.874517	0.868807	2.251882
C	-0.021060	0.016011	-1.862369
C	-1.195992	0.040754	-2.612241
C	1.118836	-0.004890	-2.670401
C	-0.072549	0.022772	-4.728379
C	1.147292	-0.002694	-4.065125
C	-1.259430	0.044900	-4.007009
F	2.347974	-0.030313	-2.070345
F	-2.448238	0.069825	-4.659208
F	-2.405692	0.063356	-1.985980
H	2.080425	-0.020231	-4.617760
F	-0.120804	0.026329	-6.085681

TS$_{(3-4)A}$ for 1,2,3,5-tetrafluorobenzene (Table 3 entry 7)

E_{gas} = -2627.228055 a.u.

E_{sol} = -2627.285508 a.u.

Cu	0.060432	0.095740	0.139543
C	0.010648	-0.088106	2.140747
C	1.278101	-0.290107	2.713250
C	-1.088331	-0.818386	2.627905
C	1.458457	-1.286234	3.672758
H	2.117742	0.312901	2.390575
C	-0.892447	-1.806311	3.592689
H	-2.069592	-0.626794	2.213220
C	0.378839	-2.052841	4.119534
H	2.454924	-1.454777	4.076372
H	-1.748964	-2.384171	3.935572
H	0.524123	-2.822140	4.874320
I	-0.517545	2.379778	2.040539
O	-1.692799	-0.351846	-0.229765
C	-1.950582	-1.690567	-0.438245
H	-3.004350	-1.846721	-0.749571
H	-1.326440	-2.167320	-1.227488
H	-1.816111	-2.312197	0.478054
C	1.884811	0.393804	-0.491264
C	2.281134	1.539524	-1.180312
C	2.903290	-0.544739	-0.371966
C	4.514350	0.799440	-1.523083
C	3.553078	1.785936	-1.697980
C	4.201902	-0.379644	-0.857366
F	1.365161	2.524670	-1.389521
F	5.143025	-1.339519	-0.697514
F	2.666502	-1.723226	0.265078
H	3.789138	2.706136	-2.220745
F	5.770029	0.971336	-2.001726

For phenylacetylene (Table 3 entry 8)

2A for phenylacetylene (Table 3 entry 8)

E_{gas} = -2179.157618 a.u.

E_{sol} = -2179.227974 a.u.

Cu	0.071915	0.051502	-0.043645
O	-0.110070	-0.164000	1.755982
C	1.049425	-0.378407	2.477284
H	0.822548	-0.489364	3.560408
H	1.602438	-1.300384	2.188898
H	1.791234	0.448454	2.408055
O	0.212705	0.322795	-1.824803
C	0.350768	-0.800670	-2.596754
H	0.428437	-0.537225	-3.679426
H	1.262586	-1.419296	-2.389566
H	-0.497282	-1.530892	-2.542440
C	-4.762085	1.049930	5.836942
C	-3.992400	-0.104051	5.578470
C	-5.949347	-0.088103	7.615706
C	-5.194750	-1.238866	7.371257
C	-5.726517	1.054593	6.842359
H	-5.359848	-2.134143	7.966726
H	-6.702826	-0.081984	8.399685
H	-6.308256	1.955758	7.023447
H	-4.588639	1.937052	5.235285
C	-4.228979	-1.249863	6.367172
H	-3.642530	-2.143582	6.176182
C	-3.004032	-0.111953	4.549673
C	-2.158257	-0.118896	3.675346
H	-1.390368	-0.122427	2.863530

TS$_{(2-3)A}$ for phenylacetylene (Table 3 entry 8)

E_{gas} = -2179.128384 a.u.

E_{sol} = -2179.201375 a.u.

Cu	-0.086188	-0.028601	0.058921
H	-0.005598	0.085273	2.084097
O	1.086822	0.083153	1.745782
C	1.628057	-1.177529	2.047575
H	2.200241	-1.164370	2.992763
H	0.842117	-1.948174	2.147184
H	2.314831	-1.502195	1.250847
C	-6.256610	0.862332	2.372784
C	-4.877231	0.952372	2.211180
C	-6.882506	-0.383634	2.490393
C	-4.064049	-0.207526	2.159801
C	-6.098352	-1.541489	2.441502
C	-4.718403	-1.459122	2.280466
H	-6.851902	1.773454	2.405675
H	-4.115063	-2.361591	2.241018
H	-7.960889	-0.451106	2.615648
C	-2.657027	-0.118909	2.015672
C	-1.432270	-0.044427	1.861029
H	-4.396981	1.922222	2.117898
H	-6.569382	-2.519348	2.528509
O	-0.505510	-0.080037	-1.706936
C	-1.743280	-0.616884	-1.978856
H	-2.003093	-0.493283	-3.056611
H	-1.832641	-1.716292	-1.785617
H	-2.588262	-0.161355	-1.414188

3A for phenylacetylene (Table 3 entry 8)

E_{gas} = -2063.451757 a.u.

E_{sol} = -2063.521780 a.u.

Cu	-0.017856	0.041595	-0.113918
O	-0.003994	0.074627	1.711445
C	1.213611	-0.012622	2.331577
H	1.108422	0.021670	3.443046
H	1.788963	-0.953863	2.131924
H	1.936227	0.810004	2.091290

C	-0.064647	0.018480	-1.925802
C	-0.067529	0.010365	-3.159473
C	-0.076873	0.001503	-4.575840
C	-1.288241	0.039772	-5.312075
C	1.125329	-0.045142	-5.326520
C	-1.293470	0.031919	-6.704238
H	-2.223260	0.076089	-4.759981
C	1.113574	-0.052741	-6.718614
H	2.067117	-0.075117	-4.785647
C	-0.094341	-0.014317	-7.423611
H	-2.243527	0.062470	-7.235824
H	2.057056	-0.089074	-7.261422
H	-0.101045	-0.020216	-8.511398

$TS_{(3-4)A}$ for phenylacetylene (Table 3 entry 8)

E_{gas} = -2306.467814 a.u.

E_{sol} = -2306.528485 a.u.

Cu	0.122025	0.096112	0.079443
C	0.019123	-0.027391	2.089987
C	1.291109	-0.190325	2.667479
C	-1.067215	-0.765670	2.590892
C	1.484643	-1.155468	3.655790
H	2.121566	0.406576	2.311569
C	-0.856212	-1.721887	3.584816
H	-2.049938	-0.607711	2.165467
C	0.416999	-1.927837	4.123530
H	2.482874	-1.295043	4.066720
H	-1.702892	-2.306236	3.941072
H	0.573608	-2.671095	4.901911
I	-0.571040	2.413335	1.897031
O	-1.612548	-0.410842	-0.300972
C	-1.828758	-1.762981	-0.463284
H	-2.875518	-1.960607	-0.775371
H	-1.185408	-2.248163	-1.231627
H	-1.683451	-2.348749	0.474981
C	1.911088	0.405936	-0.449635
C	3.064729	0.532865	-0.857964
C	4.397110	0.716018	-1.317465
C	4.868136	1.989979	-1.713453
C	5.304354	-0.366177	-1.399147
C	6.173423	2.168225	-2.164654
H	4.185218	2.832518	-1.656265
C	6.608966	-0.181884	-1.850762
H	4.960722	-1.352221	-1.099800
C	7.055388	1.085385	-2.237729
H	6.506719	3.160891	-2.461712
H	7.284016	-1.034273	-1.901864
H	8.074490	1.227049	-2.590371

For benzothiophene (Table 4 entry 1)

2A for benzothiophene (Table 4 entry 1)

E_{gas} = -2577.412587 a.u.

E_{sol} = -2577.480844 a.u.

Cu	-0.093113	0.015593	-0.175002
H	0.002656	-0.369241	3.123021
C	0.380829	-0.409487	4.167679
C	1.069823	0.179849	6.336703
C	1.289748	-1.223568	6.377163
C	1.368110	0.940009	7.483842
C	1.791211	-1.851454	7.522166
C	1.865777	0.315327	8.621168
H	1.207234	2.015843	7.472911
C	2.077471	-1.075573	8.642386
H	1.955013	-2.926137	7.537152
H	2.095139	0.906409	9.504909
H	2.468151	-1.549441	9.539792
O	-0.734422	-0.359023	1.486492
C	-2.102016	-0.507754	1.601603
H	-2.392090	-0.696494	2.659438
H	-2.692703	0.382730	1.285269
H	-2.521728	-1.360421	1.020307
O	0.602997	0.344740	-1.810331
C	0.358777	1.589447	-2.327595
H	0.828575	1.706180	-3.334283
H	-0.721851	1.841725	-2.488529
H	0.756687	2.448362	-1.727706
S	0.850829	-1.960946	4.845445
C	0.551750	0.602846	5.060483
H	0.317349	1.636285	4.824842

$TS_{(2-3)A}$ for benzothiophene (Table 4 entry 1)

E_{gas} = -2577.368685 a.u.

E_{sol} = -2577.439844 a.u.

Cu	-0.068400	0.079613	-0.014131
H	-0.052535	0.104890	2.009073
C	1.409182	-0.005367	1.683309
C	3.768943	0.419983	1.841919
C	3.797175	-1.003072	1.863970
C	4.995163	1.112985	1.918938
C	5.001086	-1.707087	1.951349
C	6.191496	0.409989	2.013363
H	4.998988	2.201543	1.902648
C	6.199395	-0.996628	2.028963
H	5.004199	-2.794960	1.960656
H	7.133229	0.952831	2.072762
H	7.143025	-1.533462	2.102028
O	-1.153122	0.188920	1.776776
C	-1.602893	1.491852	2.039725
H	-2.076632	1.574934	3.034738
H	-0.784024	2.233667	2.004412
H	-2.351452	1.794684	1.291798
O	0.095341	0.087809	-1.825944
C	1.382681	-0.106151	-2.271872
H	1.829391	-1.095262	-2.008467
H	1.431082	-0.052495	-3.385159
H	2.125909	0.645343	-1.911014
S	2.155413	-1.621226	1.774911
C	2.426656	0.925275	1.751193
H	2.229329	1.995697	1.722903

3A for benzothiophene (Table 4 entry 1)

E_{gas} = -2461.694145 a.u.

E_{sol} = -2461.760316 a.u.

Cu	-0.033258	-0.021115	-0.225837
C	-0.186635	-0.010513	1.615487
C	0.245895	-0.007977	3.976971
C	-1.176656	0.016371	4.018015
C	0.945668	-0.014910	5.201131
C	-1.872045	0.033053	5.229674
C	0.251700	0.001670	6.407058
H	2.034432	-0.033430	5.197013
C	-1.154386	0.025679	6.426563
H	-2.960024	0.051486	5.240333
H	0.802072	-0.003954	7.346448
H	-1.684953	0.038486	7.376578
O	0.120309	-0.030849	-2.042562
C	1.388524	-0.044105	-2.558909
H	1.373861	-0.049224	-3.675371
H	2.026933	0.837190	-2.289278
H	2.011839	-0.933583	-2.280956
S	-1.805172	0.020237	2.376090
C	0.746238	-0.022067	2.628723
H	1.815408	-0.041283	2.426613

$TS_{(3-4)A}$ for benzothiophene (Table 4 entry 1)

E_{gas} = -2704.708457 a.u.

E_{sol} = -2704.766757 a.u.

Cu	-0.095561	0.134261	0.145537

C	-0.162493	-0.022216	2.180929
C	1.109259	-0.065130	2.783982
C	-1.153285	-0.928312	2.603035
C	1.412610	-1.076711	3.693628
H	1.861562	0.664661	2.509773
C	-0.833551	-1.929899	3.519803
H	-2.141374	-0.861164	2.166964
C	0.448542	-2.018145	4.069352
H	2.413953	-1.119205	4.118075
H	-1.603405	-2.643971	3.807123
H	0.689863	-2.798321	4.787437
I	-1.013796	2.287551	2.075500
C	1.717801	0.528159	-0.360371
C	3.943287	0.237575	-1.195177
C	3.949641	1.648006	-1.017579
C	5.108766	-0.380282	-1.690998
C	5.077476	2.416216	-1.323184
C	6.229614	0.384848	-1.994733
H	5.126133	-1.459163	-1.834891
C	6.217319	1.779951	-1.812399
H	5.066173	3.494535	-1.180692
H	7.126279	-0.098789	-2.377551
H	7.101712	2.365863	-2.053737
O	-1.806763	-0.452722	-0.244895
C	-1.926749	-1.801070	-0.503691
H	-2.961981	-2.058448	-0.812353
H	-1.267061	-2.181159	-1.317353
H	-1.714987	-2.443637	0.385079
S	2.393477	2.172059	-0.393377
C	2.680070	-0.340284	-0.817366
H	2.509292	-1.413168	-0.882033

For thiophene (Table 4 entry 2)

2A for thiophene (Table 4 entry 2)

E_{gas} = -2423.761834 a.u.

E_{sol} = -2423.831944 a.u.

Cu	0.141840	0.067758	0.008640
H	0.054846	0.011295	3.369000
C	0.371397	-0.001779	4.430601
C	1.145832	0.614589	6.558374
C	0.927395	-0.719530	6.773162
O	-0.613574	0.016213	1.662925
C	-1.980669	0.190525	1.721056
H	-2.336672	0.180024	2.775581
H	-2.345113	1.154231	1.294346
H	-2.569241	-0.600292	1.200252
O	0.954168	0.072676	-1.607352
C	0.691335	1.151297	-2.408881
H	1.236527	1.073660	-3.381089
H	-0.383669	1.287919	-2.697768
H	0.993915	2.147588	-1.993525
S	0.329447	-1.489020	5.333496
H	1.521409	1.288870	7.323150
H	1.083213	-1.287403	7.681415
C	0.827274	1.018669	5.222555
H	0.933935	2.035606	4.858016

TS$_{(2-3)A}$ for thiophene (Table 4 entry 2)

E_{gas} = -2423.714749 a.u.

E_{sol} = -2423.789434 a.u.

Cu	0.179883	0.004987	0.046440
H	0.165899	0.078982	2.014301
C	1.472519	-0.001641	1.712704
C	3.792818	0.495888	1.983688
C	3.867484	-0.872741	2.021899
O	-1.084767	0.145760	1.830900
C	-1.539250	1.442289	2.019721
H	-2.043772	1.589892	2.999014
H	-0.726328	2.202272	1.978057
H	-2.273106	1.738171	1.245330
O	0.138004	-0.023776	-1.784115
C	1.376905	-0.144312	-2.361361
H	1.936519	-1.076786	-2.098666
H	1.305595	-0.158062	-3.476198
H	2.092366	0.685639	-2.131352
S	2.280249	-1.565176	1.865256
C	2.457257	0.972476	1.830256
H	2.220182	2.033036	1.793903
H	4.752657	-1.491341	2.107324
H	4.663938	1.143059	2.059967

3A for thiophene (Table 4 entry 2)

E_{gas} = -2308.038216 a.u.

E_{sol} = -2308.108548 a.u.

Cu	-0.044771	-0.030510	-0.152457
C	-0.108414	-0.012617	1.699787
C	0.419987	-0.015743	4.037174
C	-0.943089	0.037198	4.148551
O	0.019553	-0.051552	-1.978554
C	1.260051	-0.039815	-2.554009
H	1.194519	-0.054386	-3.669784
H	1.891734	0.858013	-2.322177
H	1.918482	-0.912283	-2.300643
H	-1.543398	0.066512	5.050213
H	1.088096	-0.035113	4.896888
S	-1.657052	0.052882	2.555837
C	0.871729	-0.042952	2.677933
H	1.930386	-0.085553	2.427640

TS$_{(3-4)A}$ for thiophene (Table 4 entry 2)

E_{gas} = -2551.055306 a.u.

E_{sol} = -2551.115836 a.u.

Cu	-0.008538	0.010668	0.002635
C	-0.007610	0.004266	2.063980
C	1.284256	0.023341	2.628266
C	-0.950752	-0.921086	2.554801
C	1.654319	-0.947954	3.556824
H	2.001200	0.765602	2.300447
C	-0.564338	-1.881696	3.488620
H	-1.955471	-0.902121	2.153561
C	0.738376	-1.910253	3.995550
H	2.669926	-0.940452	3.948996
H	-1.298982	-2.611494	3.824851
H	1.031436	-2.659134	4.727638
I	-0.920956	2.249512	1.893116
C	1.771446	0.447266	-0.575067
C	4.104771	0.350427	-1.080603
C	3.762405	1.386045	-1.907857
O	-1.734473	-0.607170	-0.270951
C	-1.863392	-1.965202	-0.458288
H	-2.912989	-2.239284	-0.699302
H	-1.246719	-2.384207	-1.286780
H	-1.603043	-2.566706	0.447058
H	4.403628	1.962665	-2.563730
H	5.119105	-0.033390	-0.992033
S	2.058072	1.713660	-1.765236
C	2.988907	-0.166451	-0.347411
H	3.093409	-0.983104	0.364491

For benzofuran (Table 4 entry 3)

2A for benzofuran (Table 4 entry 3)

E_{gas} = -2254.434206 a.u.

E_{sol} = -2254.503529 a.u.

Cu	0.126014	0.141208	-0.058820
H	0.148924	-0.206024	3.272959
C	0.462635	-0.124165	4.331245
C	1.031237	0.412753	6.445497

C	1.201432	-0.972355	6.229765
C	1.337652	0.935232	7.711957
C	1.657394	-1.850997	7.205286
C	1.796343	0.069279	8.703979
H	1.220434	1.996826	7.916746
C	1.955200	-1.306831	8.456575
H	1.773836	-2.909637	6.993831
H	2.037102	0.463032	9.688939
H	2.315537	-1.956647	9.250290
O	-0.543391	-0.173818	1.603902
C	-1.887963	-0.473785	1.680549
H	-2.199204	-0.630389	2.738183
H	-2.561456	0.322453	1.287417
H	-2.186278	-1.402925	1.142447
O	0.865316	0.430651	-1.683021
C	0.229033	1.345440	-2.479312
H	0.753828	1.460816	-3.458681
H	-0.828940	1.094206	-2.752897
H	0.167758	2.385774	-2.066446
C	0.549936	0.928840	5.188743
H	0.300260	1.953272	4.948918
O	0.857565	-1.296409	4.951275

TS$_{(2-3)A}$ for benzofuran (Table 4 entry 3)

E_{gas} = -2254.388609 a.u.

E_{sol} = -2254.461216 a.u.

Cu	0.163312	-0.002066	0.029442
H	0.240640	0.053591	1.985361
C	1.571199	0.133606	1.609803
C	3.805629	0.645238	1.755290
C	3.619716	-0.749783	1.902681
C	5.114055	1.156410	1.813244
C	4.668678	-1.639711	2.102451
C	6.177090	0.275614	2.017454
H	5.296735	2.223180	1.700422
C	5.961262	-1.106665	2.160253
H	4.481838	-2.704660	2.208678
H	7.193070	0.663397	2.064504
H	6.808671	-1.770231	2.318311
O	-0.974780	-0.025402	1.867595
C	-1.571796	1.202399	2.138755
H	-2.042000	1.238057	3.142496
H	-0.854183	2.050286	2.101473
H	-2.368222	1.435017	1.408490
O	0.143934	-0.008499	-1.794279
C	1.394603	-0.019491	-2.364652
H	1.990495	-0.947468	-2.179723
H	1.330590	0.064418	-3.475403
H	2.067297	0.814995	-2.048569
O	2.301401	-1.060886	1.832185
C	2.483653	1.171077	1.583931
H	2.223740	2.211807	1.434817

3A for benzofuran (Table 4 entry 3)

E_{gas} = -2138.712850 a.u.

E_{sol} = -2138.780810 a.u.

Cu	-0.005152	-0.046654	-0.000822
C	-0.006709	-0.018796	1.848562
C	0.400532	-0.012793	4.114719
C	-0.993519	0.062898	3.880207
C	0.851971	-0.021944	5.445287
C	-1.934098	0.128612	4.900841
C	-0.081431	0.043497	6.482856
H	1.916101	-0.079472	5.668109
C	-1.459706	0.118053	6.218618
H	-2.995695	0.185647	4.674690
H	0.263921	0.036724	7.515504
H	-2.165954	0.167999	7.044879
O	0.009182	-0.081484	-1.824694
C	1.231324	-0.059305	-2.440335
H	1.128835	-0.083413	-3.552405
H	1.858121	0.847769	-2.235320
H	1.907301	-0.921760	-2.201562
C	0.985400	-0.062573	2.805387
H	2.044311	-0.125683	2.584158
O	-1.246340	0.060328	2.546918

TS$_{(3-4)A}$ for benzofuran (Table 4 entry 3)

E_{gas} = -2381.728831 a.u.

E_{sol} = -2381.787968 a.u.

Cu	-0.030340	-0.041453	-0.008729
C	-0.032608	0.054221	2.016072
C	1.242953	0.071530	2.608013
C	-1.042793	-0.750673	2.573129
C	1.527749	-0.793193	3.663874
H	2.007583	0.731576	2.216667
C	-0.740989	-1.604223	3.635069
H	-2.033898	-0.721966	2.139718
C	0.542796	-1.638285	4.186072
H	2.530980	-0.795675	4.086244
H	-1.526100	-2.244065	4.034397
H	0.769532	-2.301432	5.017686
I	-0.834954	2.383167	1.600585
C	1.787723	0.180670	-0.589975
C	3.868666	0.031503	-1.547090
C	3.807831	1.164208	-0.705044
C	5.068663	-0.231715	-2.227538
C	4.875823	2.033323	-0.515212
C	6.152300	0.629618	-2.047905
H	5.155022	-1.094197	-2.885549
C	6.060311	1.749899	-1.202738
H	4.783253	2.894179	0.140881
H	7.086119	0.432733	-2.571172
H	6.920496	2.404605	-1.081815
O	-1.764997	-0.601898	-0.324988
C	-1.956384	-1.964392	-0.397474
H	-3.007182	-2.208613	-0.661548
H	-1.326941	-2.485793	-1.155381
H	-1.764099	-2.490962	0.568502
C	2.564850	-0.566445	-1.443208
H	2.233606	-1.463464	-1.952613
O	2.576852	1.259096	-0.135092

For furan (Table 4 entry 4)

2A for furan (Table 4 entry 4)

E_{gas} = -2100.780314 a.u.

E_{sol} = -2100.852419 a.u.

Cu	0.142475	0.111764	-0.040616
H	0.133811	-0.189088	3.352994
C	0.417943	-0.112748	4.415150
C	0.939783	0.377077	6.551086
C	1.101744	-0.957929	6.335459
O	-0.541480	-0.161889	1.622442
C	-1.897863	-0.395545	1.697403
H	-2.218924	-0.528083	2.755441
H	-2.534029	0.428188	1.295915
H	-2.241667	-1.314061	1.166097
O	0.895488	0.357799	-1.667125
C	0.286033	1.277131	-2.478122
H	0.816853	1.366216	-3.457466
H	-0.777275	1.049609	-2.752792
H	0.249569	2.324513	-2.079890
H	1.417026	-1.782493	6.958364
H	1.114673	0.905457	7.479582
C	0.494902	0.924055	5.299858
H	0.261612	1.957484	5.082116
O	0.790173	-1.272303	5.047000

TS$_{(2-3)A}$ for furan (Table 4 entry 4)

E_{gas} = −2100.731471 a.u.

E_{sol} = −2100.808994 a.u.

Cu	−0.009713	0.021851	−0.011282
H	−0.039081	0.011194	1.923249
C	1.220946	0.005863	1.637977
C	3.451988	0.354600	2.009654
C	3.181825	−0.980610	2.086116
O	−1.366026	0.038167	1.793419
C	−1.843474	1.305846	2.049944
H	−2.361395	1.398520	3.033060
H	−1.046455	2.090453	2.063384
H	−2.578709	1.646491	1.290204
O	−0.160084	0.063746	−1.837609
C	1.044712	0.049790	−2.491535
H	1.657034	−0.877037	−2.346650
H	0.908782	0.128517	−3.597994
H	1.741667	0.886956	−2.230547
C	2.197087	0.982333	1.740279
H	2.025003	2.043619	1.613965
H	3.799775	−1.850221	2.266124
H	4.422267	0.822607	2.123336
O	1.861914	−1.216206	1.887689

3A for furan (Table 4 entry 4)

E_{gas} = −1985.051773 a.u.

E_{sol} = −1985.125323 a.u.

Cu	0.259109	0.114440	0.020534
C	0.127014	0.045637	1.872575
C	0.337329	−0.114616	4.158105
C	−0.952064	0.197802	3.851750
O	0.467010	0.133809	−1.797540
C	−0.007724	1.224622	−2.470044
H	0.181673	1.144448	−3.569748
H	−1.113259	1.399693	−2.389520
H	0.447194	2.208623	−2.179513
H	−1.836886	0.373842	4.450402
H	0.746614	−0.257472	5.152292
C	1.017236	−0.209481	2.897253
H	2.066798	−0.443430	2.757673
O	−1.107504	0.299415	2.502178

TS$_{(3\text{-}4)A}$ for furan (Table 4 entry 4)

E_{gas} = −2228.071208 a.u.

E_{sol} = −2228.133258 a.u.

Cu	0.010045	−0.077410	−0.020956
C	−0.042826	0.101516	2.044237
C	1.233702	0.091092	2.640649
C	−1.052714	−0.728950	2.569594
C	1.520641	−0.827266	3.648357
H	1.999572	0.763884	2.274848
C	−0.747510	−1.636617	3.583167
H	−2.042349	−0.684063	2.134228
C	0.537901	−1.699544	4.129661
H	2.525395	−0.851651	4.066985
H	−1.531599	−2.297251	3.949608
H	0.767010	−2.405202	4.924933
I	−0.812354	2.350841	1.634090
C	1.830442	0.172561	−0.565866
C	3.929512	0.126301	−1.491416
C	3.844938	1.174221	−0.627036
O	−1.748891	−0.599282	−0.311500
C	−1.963580	−1.956065	−0.386319
H	−3.024286	−2.185101	−0.630118
H	−1.360208	−2.485633	−1.161201
H	−1.760211	−2.496322	0.571356
H	4.539229	1.944204	−0.318070
H	4.794559	−0.154611	−2.080902
C	2.642810	−0.509424	−1.446597
H	2.347340	−1.385611	−2.012382
O	2.604930	1.224210	−0.065143

For N-methylindole (Table 4 entry 5)

2A for N-methylindole (Table 4 entry 5)

E_{gas} = −2273.900097 a.u.

E_{sol} = −2273.966562 a.u.

Cu	−0.031417	0.014406	0.009068
H	−0.005488	−0.114205	2.573913
C	0.631528	−0.098008	3.461236
C	1.506472	−0.136226	5.549030
C	2.564101	0.029585	4.601179
C	1.831868	−0.187453	6.915832
C	3.902921	0.140376	4.993519
C	3.162840	−0.077436	7.307870
H	1.048014	−0.312605	7.660608
C	4.190004	0.084842	6.355643
H	4.694435	0.265223	4.259063
H	3.417784	−0.117058	8.365033
H	5.222173	0.167888	6.689044
O	−1.505037	0.002011	1.068481
C	−2.098141	1.228190	1.298170
H	−3.020884	1.116014	1.910405
H	−1.460683	1.953990	1.857560
H	−2.418812	1.768480	0.378090
O	1.472115	0.031642	−1.004053
C	1.958152	−1.196263	−1.397102
H	2.874309	−1.082578	−2.021239
H	2.258994	−1.872286	−0.559258
H	1.257019	−1.803173	−2.017568
C	0.294270	−0.213962	4.789204
H	−0.710005	−0.339318	5.171313
N	2.003527	0.049895	3.341680
C	2.742158	0.198866	2.097991
H	3.284022	1.153194	2.085288
H	3.468647	−0.615283	1.982856
H	2.056212	0.177192	1.243050

TS$_{(2\text{-}3)A}$ for N-methylindole (Table 4 entry 5)

E_{gas} = −2273.843917 a.u.

E_{sol} = −2273.913700 a.u.

Cu	0.576395	0.016100	−0.304407
H	0.600040	0.228132	1.542999
C	1.810072	0.147397	1.272263
C	4.058027	0.482444	1.574308
C	3.725010	−0.840805	2.009780
C	5.399286	0.901137	1.659069
C	4.693317	−1.719342	2.513138
C	6.359638	0.029649	2.163447
H	5.680813	1.900360	1.331857
C	6.010338	−1.269685	2.586855
H	4.427419	−2.723931	2.832836
H	7.397316	0.350823	2.230110
H	6.781413	−1.932660	2.973915
O	−0.749560	−0.217779	1.667691
C	−1.712960	0.584384	2.229227
H	−1.816560	0.464085	3.335499
H	−1.545532	1.677806	2.071303
H	−2.729435	0.386172	1.819282
O	0.190625	−0.100129	−2.086478
C	1.051891	0.591538	−2.902413
H	2.130219	0.312642	−2.802498
H	0.810307	0.424006	−3.978530
H	1.036032	1.704898	−2.777986
C	2.837593	1.076495	1.134807
H	2.719795	2.080415	0.747405
N	2.374726	−1.007846	1.834257
C	1.601258	−2.182937	2.189511
H	1.773203	−3.007190	1.482944
H	1.876075	−2.526283	3.195369

H	0.544307	-1.892119	2.175099

3A for N-methylindole (Table 4 entry 5)

E_{gas} = -2158.164473 a.u.

E_{sol} = -2158.230352 a.u.

Cu	0.296185	-0.649696	0.005119
C	0.161132	-0.430440	1.852228
C	0.491175	-0.255274	4.136915
C	-0.888142	0.010430	3.857259
C	0.918412	-0.203644	5.475820
C	-1.806245	0.314658	4.866102
C	0.003748	0.100101	6.484554
H	1.960509	-0.400517	5.724740
C	-1.347698	0.357422	6.185904
H	-2.850935	0.513349	4.634667
H	0.338359	0.139064	7.520255
H	-2.043328	0.591940	6.989611
O	0.423634	-0.910393	-1.796182
C	0.850150	0.141785	-2.561130
H	0.906059	-0.135044	-3.641911
H	0.193350	1.050910	-2.538106
H	1.871904	0.532672	-2.317895
C	1.103177	-0.522585	2.872473
H	2.149393	-0.763553	2.720897
N	-1.052814	-0.100629	2.493572
C	-2.307074	0.094633	1.808196
H	-2.702950	1.110069	1.961039
H	-2.115598	-0.057601	0.742964
H	-3.071893	-0.622948	2.141846

TS$_{(3-4)A}$ for N-methylindole (Table 4 entry 5)

E_{gas} = -2401.181182 a.u.

E_{sol} = -2401.238322 a.u.

Cu	0.189754	0.342466	0.602213
C	0.187665	-0.195404	2.533913
C	1.400372	-0.613228	3.113308
C	-0.974190	-0.967041	2.736821
C	1.469260	-1.838619	3.773312
H	2.284533	0.003163	3.006986
C	-0.886125	-2.190082	3.403423
H	-1.917564	-0.614145	2.340561
C	0.330942	-2.639113	3.922277
H	2.423711	-2.163719	4.183461
H	-1.786660	-2.790376	3.520531
H	0.390696	-3.589903	4.446528
I	-0.199499	2.214215	2.994810
C	2.029459	0.516765	0.048689
C	4.262258	0.404006	-0.513762
C	3.646798	1.419904	-1.309975
C	5.634607	0.155744	-0.691619
C	4.367783	2.168321	-2.246336
C	6.354898	0.898391	-1.625603
H	6.132196	-0.612257	-0.101330
C	5.728557	1.896560	-2.397226
H	3.886935	2.942867	-2.839789
H	7.417924	0.707151	-1.761768
H	6.312262	2.465097	-3.118553
O	-1.579351	0.370168	0.050942
C	-2.095568	-0.777572	-0.510955
H	-3.116695	-0.608382	-0.913130
H	-1.500725	-1.189684	-1.358108
H	-2.198843	-1.617282	0.217714
C	3.224827	-0.132398	0.314631
H	3.345228	-0.930292	1.037370
N	2.314011	1.458141	-0.959431
C	1.335294	2.344786	-1.550971
H	0.339374	1.993074	-1.266695
H	1.452865	3.381784	-1.205576
H	1.411893	2.333029	-2.646339

For N-methylpyrrole (Table 4 entry 6)

2A for N-methylpyrrole (Table 4 entry 6)

E_{gas} = -2120.246562 a.u.

E_{sol} = -2120.316268 a.u.

Cu	-0.049517	-0.068898	-0.004172
H	-0.018480	-0.002321	2.580849
C	0.606762	-0.033008	3.471387
C	1.497534	-0.058358	5.554060
C	2.520142	-0.192585	4.634972
O	-1.532684	0.347071	0.953269
C	-1.792755	1.691165	1.121982
H	-2.742130	1.846503	1.683700
H	-1.016351	2.245399	1.701635
H	-1.916828	2.266553	0.174193
O	1.448522	-0.484818	-0.942260
C	1.656929	-1.822093	-1.196561
H	2.590139	-1.977398	-1.786617
H	1.779188	-2.459996	-0.286631
H	0.852803	-2.319827	-1.789189
N	1.972277	-0.176803	3.372576
C	2.723325	-0.292801	2.130624
H	3.448553	0.525917	2.042605
H	3.266861	-1.245033	2.097267
H	2.046890	-0.249652	1.269037
C	0.284778	0.042206	4.813694
H	-0.715480	0.158060	5.210880
H	1.612503	-0.035338	6.631330
H	3.588951	-0.297856	4.768305

TS$_{(2-3)A}$ for N-methylpyrrole (Table 4 entry 6)

E_{gas} = -2120.190943 a.u.

E_{sol} = -2120.266119 a.u.

Cu	-0.016463	0.025648	-0.000676
H	-0.015751	-0.005911	1.897307
C	1.141561	0.005187	1.615208
C	3.371118	0.394831	1.957879
C	3.114294	-0.949721	2.186555
O	-1.399026	-0.684196	2.003490
C	-2.407094	-0.295046	2.836524
H	-2.205012	-0.460151	3.929290
H	-2.679909	0.790351	2.765824
H	-3.370834	-0.834124	2.650665
O	-0.564266	0.137509	-1.745121
C	0.309237	0.793294	-2.573289
H	1.336502	0.350330	-2.637071
H	-0.060465	0.803093	-3.627035
H	0.487121	1.872730	-2.327097
C	2.134194	0.993993	1.621735
H	1.968675	2.039670	1.394640
N	1.782222	-1.173754	1.995595
C	1.075699	-2.434602	2.169698
H	1.261180	-3.112460	1.325625
H	1.408831	-2.925115	3.092843
H	0.003886	-2.188875	2.228973
H	3.778779	-1.756555	2.470180
H	4.340918	0.873727	2.026542

3A for N-methylpyrrole (Table 4 entry 6)

E_{gas} = -2004.503508 a.u.

E_{sol} = -2004.574609 a.u.

Cu	0.297914	-0.663769	0.069170
C	0.101479	-0.344901	1.902354
C	0.324523	-0.056771	4.189952
C	-0.980892	0.234746	3.852238
O	0.485965	-1.020730	-1.716028
C	0.914352	-0.002356	-2.520667
H	1.011553	-0.331599	-3.585334
H	0.239466	0.893821	-2.567390

H	1.920155	0.425222	-2.268209
H	-1.824486	0.547368	4.456847
H	0.743259	-0.014133	5.191012
C	0.989284	-0.414525	2.979554
H	2.032970	-0.700283	2.895888
N	-1.104243	0.060405	2.486609
C	-2.328662	0.265940	1.749939
H	-2.696696	1.299382	1.843285
H	-2.107590	0.061614	0.698878
H	-3.129775	-0.411802	2.083457

$TS_{(3-4)A}$ for N-methylpyrrole (Table 4 entry 6)

E_{gas} = -2247.523596 a.u.

E_{sol} = -2247.583429 a.u.

Cu	0.004651	-0.007347	0.001866
C	-0.054154	0.087846	2.054098
C	1.198041	0.073446	2.705186
C	-1.024015	-0.872287	2.418863
C	1.515282	-0.962157	3.580376
H	1.928876	0.838014	2.471877
C	-0.687471	-1.898872	3.299995
H	-2.002855	-0.826264	1.959842
C	0.581098	-1.959183	3.885348
H	2.503581	-0.981647	4.036539
H	-1.434552	-2.655777	3.532819
H	0.833946	-2.759801	4.576409
I	-0.919785	2.288801	1.871748
C	1.800872	0.381648	-0.560809
C	4.043751	0.617624	-1.054033
C	3.320601	1.153071	-2.099717
O	-1.749672	-0.436780	-0.468128
C	-2.020267	-1.762597	-0.715286
H	-3.054748	-1.904391	-1.098918
H	-1.354530	-2.244442	-1.469943
H	-1.954055	-2.411925	0.193146
C	3.095020	0.139479	-0.103059
H	3.333305	-0.355088	0.831904
N	1.982103	1.001632	-1.800587
C	0.898347	1.467425	-2.640129
H	-0.026847	0.992771	-2.299345
H	0.767667	2.558156	-2.584537
H	1.071939	1.193530	-3.689458
H	5.126109	0.569078	-0.992153
H	3.638796	1.621798	-3.023503

For caffeine (Table 4 entry 7)

2A for caffeine (Table 4 entry 7)

E_{gas} = -2551.151957 a.u.

E_{sol} = -2551.218891 a.u.

Cu	-0.037905	-0.047639	0.065179
H	0.049118	0.091324	2.667583
C	0.787960	0.059310	3.483916
C	1.673874	0.029836	5.413981
C	2.728447	-0.039576	4.519314
C	4.096331	-0.112511	4.920695
C	3.173011	-0.036887	7.284154
O	-1.325822	0.267134	1.306411
C	-1.801875	1.566179	1.369816
H	-2.629128	1.650105	2.106363
H	-1.042699	2.320163	1.686239
H	-2.213318	1.947709	0.410108
O	1.309837	-0.350542	-1.102617
C	1.598341	-1.670235	-1.376873
H	2.443097	-1.751732	-2.097818
H	1.911855	-2.275860	-0.491314
H	0.763576	-2.248599	-1.839015
N	2.125954	-0.019016	3.265737
C	2.811167	-0.072736	1.974512
H	3.478855	0.787260	1.874700
H	3.411392	-0.983827	1.913526
H	2.070868	-0.062365	1.166687
N	0.477978	0.090991	4.789466
N	1.884626	0.032091	6.781045
N	4.215684	-0.104519	6.348765
O	5.091859	-0.175569	4.200956
O	3.394321	-0.038186	8.493615
C	5.559357	-0.174012	6.919209
H	5.750848	0.702256	7.545091
H	5.661472	-1.066306	7.543795
H	6.257977	-0.209693	6.084901
C	0.772153	0.105373	7.721463
H	0.762561	-0.777260	8.367897
H	0.868205	0.992710	8.354193
H	-0.145441	0.155490	7.135393

$TS_{(2-3)A}$ for caffeine (Table 4 entry 7)

E_{gas} = -2551.104759 a.u.

E_{sol} = -2551.173665 a.u.

Cu	-0.090429	-0.270707	0.212714
H	-0.032428	0.165975	2.187766
C	1.534308	-0.193029	1.818125
C	3.627340	0.378311	1.983044
C	3.647011	-0.991757	1.762389
C	4.843183	-1.754011	1.696936
C	6.028719	0.454555	2.101565
O	-1.005293	0.487034	1.910995
C	-1.024934	1.904974	1.929827
H	-1.385052	2.287247	2.898528
H	-0.024555	2.320327	1.745978
H	-1.707514	2.265821	1.149335
O	0.116860	-0.992874	-1.442562
C	1.214530	-0.546976	-2.154248
H	2.187275	-0.660863	-1.625759
H	1.324422	-1.113166	-3.105963
H	1.168738	0.526401	-2.456929
N	2.297775	-1.330837	1.675024
C	1.770986	-2.630217	1.274231
H	2.607746	-3.311909	1.118237
H	1.116480	-3.031950	2.056813
H	1.191704	-2.505035	0.351352
N	2.378874	0.873251	2.023664
O	4.969976	-2.971128	1.516166
O	7.088146	1.068357	2.248843
N	4.804651	1.094667	2.151131
C	4.779954	2.533051	2.376330
H	5.263374	2.779916	3.326967
H	5.314797	3.055783	1.576773
H	3.732328	2.834549	2.391866
N	6.006773	-0.925969	1.878394
C	7.314993	-1.570368	1.830415
H	7.927640	-1.130882	1.037327
H	7.844364	-1.434842	2.779017
H	7.140185	-2.628009	1.638480

3A for caffeine (Table 4 entry 7)

E_{gas} = -2435.426710 a.u.

E_{sol} = -2435.493226 a.u.

Cu	0.201477	-0.489418	0.036919
C	-0.018599	-0.328200	1.874751
C	0.331045	-0.196591	4.011919
C	-1.040469	-0.056645	3.869893
C	-1.922447	0.126827	4.965598
C	0.164843	0.007904	6.407454
O	0.369823	-0.679290	-1.764261
C	1.121482	0.254688	-2.430330
H	1.159978	0.038257	-3.524075
H	0.744960	1.308089	-2.363175
H	2.193722	0.320319	-2.115764
N	-1.239266	-0.143614	2.495585

C	-2.516355	-0.057323	1.817154
H	-3.014532	0.893523	2.034716
H	-2.306502	-0.134327	0.747093
H	-3.184674	-0.869217	2.125030
N	0.958158	-0.359280	2.834550
N	0.926368	-0.163591	5.265834
N	-1.218112	0.148814	6.215580
C	2.368729	-0.313968	5.409262
H	2.603412	-1.191882	6.019512
H	2.777605	-0.428680	4.405095
H	2.797497	0.565770	5.899191
C	-2.046898	0.332053	7.403453
H	-2.623740	1.257353	7.316758
H	-2.757157	-0.495252	7.501028
H	-1.385485	0.369042	8.266864
O	0.687291	0.034529	7.524553
O	-3.150600	0.261203	4.959917

$TS_{(3-4)A}$ for caffeine (Table 4 entry 7)

E_{gas} = -2678.442395 a.u.

E_{sol} = -2678.500012 a.u.

Cu	-0.014313	0.094617	0.009041
C	0.032235	-0.110739	1.958272
C	1.295854	-0.137870	2.556043
C	-1.012894	-0.897444	2.464260
C	1.531445	-1.024256	3.609833
H	2.091371	0.488701	2.167151
C	-0.760082	-1.771818	3.523987
H	-1.997752	-0.831078	2.019793
C	0.509811	-1.842121	4.101386
H	2.525738	-1.067206	4.050578
H	-1.570379	-2.393438	3.900420
H	0.698943	-2.518077	4.932205
I	-0.852832	2.398198	1.724573
C	1.758750	0.594110	-0.630422
C	3.814921	1.199074	-0.923050
C	3.306559	1.034743	-2.200538
C	4.068304	1.234501	-3.384747
C	5.963119	1.816301	-1.801063
O	-1.619928	-0.599671	-0.566562
C	-1.751359	-1.970738	-0.674123
H	-2.717253	-2.244791	-1.143083
H	-0.960065	-2.462727	-1.281955
H	-1.738561	-2.481377	0.314837
N	1.988543	0.644194	-1.987154
C	1.007288	0.357073	-3.020459
H	0.076504	0.072993	-2.520870
H	0.833814	1.237665	-3.646797
H	1.349706	-0.458304	-3.665000
N	2.896423	0.935164	0.026883
O	7.135360	2.160968	-1.651854
O	3.700517	1.102191	-4.554807
N	5.127852	1.591816	-0.719828
N	5.411938	1.632907	-3.076181
C	5.664194	1.782870	0.622130
H	4.842396	1.638455	1.323009
H	6.463141	1.061874	0.823929
H	6.078780	2.789840	0.721297
C	6.323424	1.878074	-4.190323
H	6.691121	2.908151	-4.162089
H	7.187180	1.209067	-4.130388
H	5.761782	1.697069	-5.105575

For N-benzimidazole (Table 4 entry 8)

2A for N-benzimidazole (Table 4 entry 8)

E_{gas} = -2289.952150 a.u.

E_{sol} = -2290.022020 a.u.

Cu	0.006362	0.009857	0.070273
H	0.040434	-0.058916	2.763057
C	0.771949	-0.065014	3.581969
C	1.706206	-0.122688	5.509744
C	2.757450	-0.016730	4.561322
C	2.014282	-0.182161	6.875175
C	4.102544	0.031149	4.935590
C	3.354100	-0.134895	7.256684
H	1.216500	-0.263398	7.608724
C	4.384355	-0.029840	6.300609
H	4.897624	0.111944	4.198878
H	3.613783	-0.180010	8.312196
H	5.419469	0.004344	6.633162
O	-1.346104	0.060593	1.276455
C	-2.006428	1.269503	1.403089
H	-2.842662	1.190177	2.130471
H	-1.370691	2.109086	1.772138
H	-2.464969	1.642491	0.459626
O	1.416612	-0.030772	-1.065943
C	1.862334	-1.277716	-1.445025
H	2.728970	-1.198093	-2.141049
H	2.222136	-1.923632	-0.606129
H	1.112210	-1.902735	-1.985341
N	2.129305	0.018936	3.332455
C	2.788347	0.125381	2.040111
H	3.365769	1.056178	1.983533
H	3.469475	-0.720651	1.890056
H	2.046354	0.124254	1.232970
N	0.481805	-0.150457	4.864895

$TS_{(2-3)A}$ for N-benzimidazole (Table 4 entry 8)

E_{gas} = -2289.897264 a.u.

E_{sol} = -2289.970514 a.u.

Cu	-0.166171	-0.287184	0.191175
H	-0.029777	0.085803	2.157228
C	1.528354	-0.176857	1.796248
C	3.597780	0.468067	2.149378
C	3.680272	-0.906088	1.788316
C	4.775105	1.169317	2.444426
C	4.899809	-1.583375	1.716227
C	5.996956	0.496528	2.377251
H	4.723014	2.220212	2.720387
C	6.059888	-0.862290	2.016456
H	4.953190	-2.635025	1.441721
H	6.918461	1.028888	2.607336
H	7.025940	-1.362089	1.972891
O	-1.030777	0.403588	1.945904
C	-1.057999	1.819330	2.015790
H	-1.404295	2.163948	3.004217
H	-0.061436	2.244057	1.835069
H	-1.755757	2.208000	1.260998
O	-0.055394	-0.959746	-1.496583
C	1.063732	-0.582439	-2.210451
H	2.033700	-0.801087	-1.708025
H	1.109699	-1.115127	-3.188228
H	1.110444	0.502561	-2.469137
N	2.372302	-1.284504	1.573269
C	1.928296	-2.562894	1.056416
H	2.733416	-3.032202	0.480750
H	1.623726	-3.252812	1.856664
H	1.082338	-2.381394	0.383986
N	2.280197	0.879363	2.145612

3A for N-benzimidazole (Table 4 entry 8)

E_{gas} = -2174.219776 a.u.

E_{sol} = -2174.291844 a.u.

Cu	0.243114	-0.646021	0.062551
C	0.079352	-0.427917	1.904358
C	0.407807	-0.275865	4.063810
C	-0.974697	0.005631	3.872310
C	0.930240	-0.256893	5.364064
C	-1.832810	0.300818	4.932970

C	0.077435	0.037462	6.431093
H	1.984445	-0.470040	5.525755
C	-1.286055	0.313027	6.221108
H	-2.887911	0.513772	4.771894
H	0.472540	0.054745	7.445539
H	-1.926094	0.539016	7.072071
O	0.344526	-0.890833	-1.740695
C	0.973035	0.077426	-2.478256
H	0.980929	-0.179035	-3.565120
H	0.504353	1.095451	-2.433085
H	2.048548	0.255139	-2.222174
N	-1.156364	-0.094911	2.512136
C	-2.395007	0.102092	1.802362
H	-2.794193	1.115788	1.952874
H	-2.176844	-0.043278	0.739855
H	-3.163821	-0.620086	2.113831
N	1.016786	-0.533750	2.852750

$TS_{(3-4)A}$ for N-benzimidazole (Table 4 entry 8)

E_{gas} = -2417.238625 a.u.

E_{sol} = -2417.298450 a.u.

Cu	-0.005289	0.271505	0.121832
C	0.164291	-0.056752	2.070696
C	1.451011	-0.328061	2.555449
C	-0.932534	-0.826872	2.497540
C	1.645007	-1.430299	3.388641
H	2.291037	0.266724	2.211586
C	-0.716609	-1.921448	3.337615
H	-1.928213	-0.578544	2.151865
C	0.568691	-2.229965	3.789244
H	2.653159	-1.662648	3.727055
H	-1.567434	-2.527696	3.643711
H	0.729943	-3.077843	4.451316
I	-0.427319	2.418375	2.229110
C	1.774065	0.647019	-0.548305
C	3.888548	1.020907	-0.944034
C	3.231679	1.195945	-2.191346
C	5.276311	1.194723	-0.870421
C	3.919419	1.537196	-3.357869
C	5.971217	1.535648	-2.032097
H	5.789527	1.064830	0.079146
C	5.303394	1.704790	-3.259732
H	3.404716	1.670213	-4.306902
H	7.049772	1.675005	-1.991341
H	5.873443	1.971558	-4.147379
O	-1.727883	-0.085020	-0.457577
C	-2.086370	-1.394735	-0.698203
H	-3.105386	-1.465103	-1.132804
H	-1.416033	-1.936174	-1.404611
H	-2.109526	-2.016964	0.226391
N	1.902575	0.952801	-1.917068
C	0.813150	1.009174	-2.867291
H	-0.108382	0.735095	-2.343727
H	0.696777	2.018936	-3.283731
H	0.973883	0.308366	-3.697869
N	2.968132	0.686377	0.031330

For N-benzimidazole (Table 4 entry 9)

2A for N-benzimidazole (Table 4 entry 9)

E_{gas} = -2136.298474 a.u.

E_{sol} = -2290.022020 a.u.

Cu	-0.013690	0.034354	0.096440
H	0.082127	-0.194041	2.806965
C	0.830735	-0.210676	3.604079
C	1.833359	-0.331064	5.498293
C	2.819071	-0.123706	4.564340
O	-1.389195	-0.005619	1.275118
C	-2.027880	1.196869	1.509003
H	-2.879256	1.064451	2.212110
H	-1.384154	1.983462	1.970575
H	-2.464575	1.672817	0.600728
O	1.407360	0.080737	-1.029271
C	1.889751	-1.136657	-1.454056
H	2.755911	-1.006407	-2.143903
H	2.266050	-1.804091	-0.639346
H	1.159526	-1.762458	-2.020783
N	2.167549	-0.047405	3.349577
C	2.795780	0.167649	2.053252
H	3.315864	1.132845	2.036300
H	3.520696	-0.627360	1.844068
H	2.039817	0.166138	1.259494
N	0.597787	-0.384777	4.896583
H	3.893266	-0.025565	4.637516
H	1.945396	-0.445210	6.570478

$TS_{(2-3)A}$ for N-benzimidazole (Table 4 entry 9)

E_{gas} = -2136.238184 a.u.

E_{sol} = -2289.970514 a.u.

Cu	-0.037072	-0.264703	0.164132
H	-0.002501	0.013142	2.120228
C	1.492280	-0.126985	1.858606
C	3.536428	0.515506	2.340795
C	3.646177	-0.805998	1.984921
O	-1.078151	0.269128	1.921743
C	-1.218078	1.666098	2.037181
H	-1.637680	1.956991	3.017733
H	-0.250990	2.180154	1.924217
H	-1.904358	2.045797	1.263079
O	0.112654	-0.835743	-1.563809
C	1.250778	-0.412608	-2.214652
H	2.206725	-0.655912	-1.694514
H	1.336023	-0.884374	-3.222575
H	1.302062	0.686860	-2.407572
N	2.357121	-1.206265	1.689517
C	1.969430	-2.497838	1.154491
H	2.847320	-3.010937	0.747637
H	1.513635	-3.140435	1.921084
H	1.246333	-2.333242	0.346886
N	2.227085	0.927018	2.267875
H	4.334198	1.188557	2.641570
H	4.492018	-1.475352	1.894941

3A for N-benzimidazole (Table 4 entry 9)

E_{gas} = -2020.558779 a.u.

E_{sol} = -2174.291844 a.u.

Cu	-0.038038	-0.301166	0.008786
C	-0.016867	-0.090568	1.865512
C	0.544962	0.185608	3.967906
C	-0.824346	0.097770	3.977726
O	-0.028730	-0.528333	-1.806472
C	-1.111045	-0.070597	-2.503306
H	-0.997360	-0.244396	-3.602081
H	-2.092604	-0.552617	-2.246048
H	-1.315316	1.029466	-2.414551
H	-1.561096	0.140970	4.769755
H	1.203874	0.325731	4.820576
N	-1.173835	-0.076425	2.649924
C	-2.513027	-0.221018	2.135042
H	-3.135887	0.659153	2.353543
H	-2.422251	-0.331356	1.050019
H	-3.018500	-1.109098	2.542862
N	1.035313	0.071981	2.687613

$TS_{(3-4)A}$ for N-benzimidazole (Table 4 entry 9)

E_{gas} = -2263.581332 a.u.

E_{sol} = -2417.298450 a.u.

Cu	-0.030440	0.253856	0.107708
C	0.057187	0.063760	2.117721

C	1.350099	-0.170409	2.619160
C	-1.006506	-0.780588	2.496298
C	1.585610	-1.304156	3.394534
H	2.166211	0.475524	2.310744
C	-0.747721	-1.905778	3.280528
H	-2.007163	-0.568655	2.141156
C	0.544688	-2.176045	3.737571
H	2.599864	-1.505473	3.735251
H	-1.571996	-2.568494	3.538970
H	0.738379	-3.048856	4.357305
I	-0.605076	2.405737	2.241868
C	1.744875	0.735898	-0.481099
C	3.841847	1.286603	-0.778169
C	3.280906	1.328036	-2.029209
O	-1.736823	-0.188112	-0.483132
C	-2.041777	-1.517554	-0.666280
H	-3.053942	-1.649696	-1.106875
H	-1.346231	-2.066820	-1.344105
H	-2.051751	-2.104825	0.282964
N	1.956961	0.978006	-1.835932
C	0.938994	0.882109	-2.861072
H	0.004117	0.580241	-2.377407
H	0.779895	1.846411	-3.362637
H	1.202927	0.135159	-3.622449
H	3.681211	1.563316	-3.006719
H	4.870086	1.498804	-0.503103
N	2.902443	0.925033	0.159491

For N-methylpyrazole (Table 4 entry 10)

2A for N-methylpyrazole (Table 4 entry 10)

E_{gas} = -2136.286668 a.u.

E_{sol} = -2136.357052 a.u.

Cu	0.035208	-0.006464	0.068339
H	0.056070	-0.156258	2.635228
C	0.714540	-0.118994	3.506261
C	1.716630	-0.108836	5.480841
O	-1.428419	-0.072628	1.141276
C	-2.061169	1.131814	1.379227
H	-2.974747	0.986956	1.998735
H	-1.444224	1.877692	1.935215
H	-2.407721	1.662844	0.463200
O	1.526089	0.064685	-0.960259
C	2.039623	-1.144259	-1.375660
H	2.948112	-0.998047	-2.004441
H	2.363445	-1.825647	-0.550998
H	1.349395	-1.759052	-2.001219
N	2.056309	0.068641	3.391047
C	2.821548	0.245122	2.167617
H	3.336579	1.211468	2.189058
H	3.570498	-0.549013	2.081090
H	2.153160	0.210334	1.299661
H	1.962959	-0.141827	6.536371
C	0.456032	-0.239900	4.863649
H	-0.508138	-0.398089	5.326275
N	2.692606	0.078749	4.588001

TS$_{(2-3)A}$ for N-methylpyrazole (Table 4 entry 10)

E_{gas} = -2136.229907 a.u.

E_{sol} = -2136.304260 a.u.

Cu	-0.186877	-0.157347	0.085598
H	-0.074056	-0.186557	1.940887
C	1.125759	-0.079689	1.631637
C	3.310640	0.342156	1.908614
O	-1.358027	-0.790228	2.026951
C	-2.372643	-0.094297	2.637932
H	-2.522729	-0.361204	3.712716
H	-2.231918	1.014838	2.632979
H	-3.362302	-0.261397	2.155242
O	-0.628187	-0.044678	-1.685796
C	0.210962	0.751812	-2.423546
H	1.289197	0.452967	-2.409311
H	-0.072606	0.748003	-3.503253
H	0.216913	1.835404	-2.136769
C	2.084536	0.943159	1.576858
H	1.907225	1.976802	1.312637
N	1.845333	-1.182456	2.028498
C	1.283798	-2.497480	2.270551
H	1.497521	-3.176704	1.435065
H	1.722462	-2.914954	3.182496
H	0.201805	-2.370435	2.382411
H	4.297369	0.789416	1.962865
N	3.167475	-0.960277	2.188521

3A for N-methylpyrazole (Table 4 entry 10)

E_{gas} = -2020.550429 a.u.

E_{sol} = -2020.623411 a.u.

Cu	0.312575	-0.659063	0.047566
C	0.105167	-0.315510	1.872024
C	0.241887	0.011265	4.108126
O	0.512730	-1.040600	-1.728204
C	0.938476	-0.030702	-2.546510
H	1.040626	-0.376010	-3.604757
H	0.258662	0.860090	-2.607714
H	1.940960	0.405049	-2.296234
H	0.568716	0.090227	5.141543
N	-1.071722	0.102589	2.454264
C	-2.322575	0.331364	1.771800
H	-2.657795	1.369735	1.897154
H	-2.153746	0.125688	0.712395
H	-3.110883	-0.331592	2.153595
C	0.977960	-0.375978	2.970496
H	2.021362	-0.666441	2.937209
N	-1.023912	0.308854	3.803671

TS$_{(3-4)A}$ for N-methylpyrazole (Table 4 entry 10)

E_{gas} = -2263.568365 a.u.

E_{sol} = -2263.631498 a.u.

Cu	-0.065630	0.016431	-0.018582
C	-0.108272	-0.061331	2.040094
C	1.165674	0.028356	2.636686
C	-0.987200	-1.082101	2.456042
C	1.590968	-0.961573	3.520654
H	1.830735	0.837482	2.361844
C	-0.545176	-2.060666	3.345697
H	-1.982289	-1.118853	2.032452
C	0.744530	-2.014973	3.883360
H	2.594677	-0.898120	3.937402
H	-1.226312	-2.863414	3.622924
H	1.080491	-2.778453	4.581064
I	-1.192427	2.104566	1.947646
C	1.659399	0.706969	-0.526478
C	3.814101	1.165417	-1.021280
O	-1.723264	-0.720927	-0.395014
C	-1.752169	-2.077488	-0.628197
H	-2.769355	-2.413874	-0.923330
H	-1.073891	-2.427789	-1.440824
H	-1.488450	-2.689535	0.268711
N	1.815708	1.698600	-1.466138
C	0.762226	2.468466	-2.089776
H	-0.187690	1.960526	-1.908553
H	0.704839	3.482979	-1.674409
H	0.941797	2.541336	-3.167960
H	4.898179	1.185129	-1.079955
C	2.981468	0.344945	-0.234303
H	3.289884	-0.421452	0.465924
N	3.106415	2.005156	-1.780325

For 1-methyl-1,2,4-triazole (Table 4 entry 11)

2A for 1-methyl-1,2,4-triazole (Table 4 entry 11)

E_{gas} = -2152.341824 a.u.

E_{sol} = -2152.412818 a.u.

Cu	0.041656	0.026731	0.110697
H	0.098066	-0.130939	2.785463
C	0.866815	-0.143539	3.569408
C	1.935058	-0.222492	5.376570
O	-1.293058	0.011345	1.339879
C	-1.968104	1.205438	1.519822
H	-2.799110	1.085938	2.248070
H	-1.340481	2.037065	1.919475
H	-2.436906	1.610427	0.595118
O	1.430379	0.050432	-1.052262
C	1.882495	-1.174935	-1.490043
H	2.733693	-1.056851	-2.199456
H	2.266624	-1.849173	-0.685211
H	1.128434	-1.786748	-2.040132
N	2.192253	-0.030677	3.315305
C	2.875423	0.122269	2.041434
H	3.442073	1.058862	2.037607
H	3.568438	-0.711565	1.892821
H	2.142953	0.137008	1.225953
H	2.159280	-0.296472	6.434320
N	2.900660	-0.080191	4.478078
N	0.670547	-0.267971	4.882020

TS$_{(2-3)A}$ for 1-methyl-1,2,4-triazole (Table 4 entry 11)

E_{gas} = -2152.286914 a.u.

E_{sol} = -2152.364837 a.u.

Cu	-0.111372	-0.305258	0.189715
H	-0.118899	0.040693	2.168875
C	1.462006	-0.156184	1.910394
C	3.474757	0.431620	2.396567
O	-1.123445	0.315240	1.908100
C	-1.210958	1.726428	1.979312
H	-1.632084	2.055231	2.944349
H	-0.222467	2.192599	1.863158
H	-1.872531	2.093948	1.182138
O	0.114536	-0.924337	-1.509866
C	1.214360	-0.420750	-2.173162
H	2.181945	-0.545551	-1.635597
H	1.353913	-0.927836	-3.156307
H	1.156993	0.668249	-2.416165
N	2.355749	-1.174982	1.700941
C	2.076945	-2.470030	1.113132
H	3.001311	-2.859274	0.680221
H	1.704746	-3.185857	1.859306
H	1.325978	-2.335040	0.326614
N	2.198064	0.891836	2.368910
H	4.320435	1.033563	2.716297
N	3.646469	-0.821397	1.999086

3A for 1-methyl-1,2,4-triazole (Table 4 entry 11)

E_{gas} = -2036.609127 a.u.

E_{sol} = -2036.68502 a.u.

Cu	0.235376	-0.650740	0.080493
C	0.032309	-0.333061	1.906343
C	0.244084	-0.070063	4.026278
O	0.380062	-0.990463	-1.706769
C	1.036723	-0.066216	-2.473478
H	1.072890	-0.376556	-3.546319
H	0.576951	0.957198	-2.493361
H	2.107019	0.116842	-2.197254
H	0.688645	-0.040433	5.017085
N	-1.143531	0.072542	2.493045
C	-2.402943	0.314189	1.835439
H	-2.733141	1.351002	1.980500
H	-2.245463	0.124558	0.770243
H	-3.185508	-0.355058	2.216228
N	-1.031627	0.246429	3.846865
N	0.935446	-0.424177	2.914143

TS$_{(3-4)A}$ for 1-methyl-1,2,4-triazole (Table 4 entry 11)

E_{gas} = -2279.628733 a.u.

E_{sol} = -2279.692223 a.u.

Cu	-0.042541	0.263980	0.126701
C	0.056607	-0.008195	2.097579
C	1.343482	-0.216010	2.617810
C	-1.010765	-0.830018	2.503944
C	1.570327	-1.305528	3.458590
H	2.162096	0.419110	2.295343
C	-0.762224	-1.911129	3.352087
H	-2.008324	-0.632788	2.131947
C	0.524994	-2.156520	3.835829
H	2.580160	-1.487235	3.822209
H	-1.589896	-2.557603	3.638846
H	0.711295	-2.994564	4.503815
I	-0.640152	2.411886	2.204143
C	1.735389	0.729656	-0.478741
C	3.777744	1.239974	-0.864413
O	-1.726970	-0.195028	-0.485483
C	-2.015510	-1.526839	-0.691075
H	-3.017191	-1.660043	-1.151330
H	-1.300740	-2.059095	-1.360366
H	-2.037805	-2.120905	0.252496
N	1.949859	0.977564	-1.809666
C	0.970528	0.930614	-2.872754
H	0.016173	0.629554	-2.430165
H	0.858849	1.914045	-3.344415
H	1.265363	0.205831	-3.640753
H	4.829729	1.448748	-0.700133
N	2.922999	0.897785	0.133266
N	3.249493	1.307328	-2.078393

For pyridazine (Table 4 entry 12)

2A for pyridazine (Table 4 entry 12)

E_{gas} = -2135.054821 a.u.

E_{sol} = -2135.125278 a.u.

Cu	-0.156020	-0.051403	-0.048347
O	-0.030871	0.170355	1.753237
C	1.224921	0.037735	2.308407
H	1.184550	0.154821	3.415388
H	1.707016	-0.951838	2.133297
H	1.967484	0.791201	1.957749
O	-0.358110	-0.227887	-1.835401
C	0.280769	-1.294229	-2.411155
H	0.103082	-1.322046	-3.513322
H	1.396540	-1.303802	-2.303370
H	-0.040868	-2.304242	-2.046504
H	-1.890481	2.316507	4.652708
C	-2.356828	1.339005	4.763348
C	-2.021768	0.287041	3.899270
C	-2.683197	-0.908751	4.137434
H	-1.285835	0.383854	3.078340
C	-3.598320	-0.946829	5.193526
H	-2.494784	-1.784901	3.522479
H	-4.151035	-1.854936	5.431753
N	-3.239779	1.256701	5.765226
N	-3.871006	0.095890	5.984585

TS$_{(2-3)A}$ for pyridazine (Table 4 entry 12)

E_{gas} = −2135.004986 a.u.

E_{sol} = −2135.081034 a.u.

Cu	0.051712	−0.009383	0.000669
H	0.060681	0.007151	1.924778
O	1.277802	−0.019839	1.810091
C	1.775002	−1.286497	2.104288
H	2.236237	−1.343842	3.111116
H	0.994518	−2.076553	2.074655
H	2.554779	−1.592339	1.382899
O	0.028605	−0.031500	−1.819932
C	−1.230459	0.055013	−2.366929
H	−1.801006	0.977639	−2.097539
H	−1.183296	0.059134	−3.480681
H	−1.916837	−0.788035	−2.108551
H	−1.839827	−2.016822	1.660704
C	−2.210045	−0.992474	1.729144
C	−1.303337	0.095517	1.612556
C	−1.966759	1.326459	1.753122
H	−1.416115	2.267250	1.723730
N	−3.529551	−0.930750	1.921596
N	−4.123560	0.271348	2.022971
C	−3.349398	1.359164	1.932511
H	−3.885257	2.305411	2.028308

3A for pyridazine (Table 4 entry 12)

E_{gas} = −2019.328980 a.u.

E_{sol} = −2019.401393 a.u.

Cu	0.028941	0.011428	0.014564
O	−0.009745	0.021694	1.838371
C	1.196605	−0.002127	2.485112
H	1.065665	0.006718	3.594209
H	1.833322	−0.903105	2.284131
H	1.873332	0.866956	2.274701
C	0.031704	0.001337	−1.847350
C	−1.144431	0.015513	−2.648024
C	1.177830	−0.020949	−2.660303
H	−2.124337	0.033408	−2.167072
C	1.060134	−0.026451	−4.052048
H	2.178065	−0.034331	−2.225552
H	1.945523	−0.043603	−4.692134
N	−1.229723	0.009705	−3.982298
N	−0.101597	−0.011706	−4.712692

TS$_{(3-4)A}$ for pyridazine (Table 4 entry 12)

E_{gas} = −2262.346068 a.u.

E_{sol} = −2262.409505 a.u.

Cu	−0.019223	−0.052471	−0.005509
C	−0.030502	0.103743	2.075398
C	1.246900	0.051527	2.670502
C	−1.045703	−0.744641	2.563096
C	1.532259	−0.924688	3.622216
H	2.019470	0.740376	2.350693
C	−0.742045	−1.712000	3.519955
H	−2.037228	−0.669724	2.136399
C	0.545399	−1.817166	4.054994
H	2.538077	−0.978700	4.034362
H	−1.529806	−2.386306	3.851048
H	0.773253	−2.570827	4.804777
I	−0.777672	2.358141	1.760717
O	−1.770078	−0.562456	−0.314132
C	−2.002189	−1.916671	−0.408922
H	−3.062258	−2.126849	−0.667230
H	−1.396869	−2.443308	−1.182897
H	−1.816180	−2.469466	0.544653
C	1.806461	0.315359	−0.489299
C	2.344480	1.585969	−0.729185
C	2.765245	−0.703355	−0.721823
H	1.746343	2.486400	−0.591570
H	2.496449	−1.750989	−0.574927
N	4.036357	−0.547930	−1.110457
C	3.676354	1.716304	−1.133869
H	4.115033	2.698048	−1.321899
N	4.509378	0.689022	−1.323133

For pyrimidine (Table 4 entry 13)

2A for pyrimidine (Table 4 entry 13)

E_{gas} = −2135.088728 a.u.

E_{sol} = −2135.157136 a.u.

Cu	−0.176357	−0.080741	−0.085843
O	−0.094510	0.081620	1.724134
C	1.150121	−0.053808	2.302066
H	1.083693	0.023289	3.411417
H	1.651890	−1.029375	2.103474
H	1.889083	0.722392	1.995148
O	−0.338610	−0.200201	−1.881871
C	0.401460	−1.179882	−2.489127
H	0.241739	−1.177873	−3.594567
H	1.512160	−1.093787	−2.363102
H	0.167689	−2.228850	−2.170696
H	−1.924188	2.319476	4.267027
C	−2.396577	1.382601	4.560923
C	−2.097260	0.198570	3.886565
C	−2.766636	−0.932999	4.353528
H	−1.383694	0.158661	3.041778
H	−2.598683	−1.904034	3.888706
N	−3.260899	1.451600	5.587738
N	−3.638405	−0.907821	5.376044
C	−3.831121	0.292497	5.932188
H	−4.535758	0.330607	6.763835

TS$_{(2-3)A}$ for pyrimidine (Table 4 entry 13)

E_{gas} = −2135.037344 a.u.

E_{sol} = −2135.110791 a.u.

Cu	−0.196780	−0.047466	−0.014778
H	−0.226505	−0.070487	1.906721
O	1.019598	−0.005716	1.825140
C	1.596139	−1.240945	2.087543
H	2.049131	−1.303336	3.099631
H	0.872803	−2.084578	2.023743
H	2.404874	−1.477363	1.369821
O	−0.123824	−0.047838	−1.837939
C	−1.357465	−0.043523	−2.442746
H	−2.000558	0.840151	−2.204886
H	−1.261044	−0.037113	−3.554146
H	−2.001332	−0.929835	−2.215398
H	−1.958829	−2.212468	1.606028
C	−2.391597	−1.212954	1.682640
C	−1.561817	−0.074567	1.594062
C	−2.296060	1.118467	1.766208
H	−1.777048	2.079516	1.765456
N	−3.724006	−1.193183	1.852222
C	−4.266595	0.024642	1.959445
H	−5.348916	0.064243	2.095223
N	−3.625985	1.198955	1.934003

3A for pyrimidine (Table 4 entry 13)

E_{gas} = −2019.361052 a.u.

E_{sol} = −2019.430765 a.u.

Cu	0.009996	0.004003	−0.004064
O	−0.002323	0.002092	1.821814
C	1.212441	−0.004476	2.451362
H	1.097417	−0.005409	3.562836
H	1.862990	−0.892459	2.235814
H	1.871339	0.877891	2.238158
C	−0.024951	0.005006	−1.870349
C	−1.199986	0.027033	−2.653158
C	1.122450	−0.016493	−2.693134

H	-2.178007	0.045469	-2.166203
H	2.116433	-0.035073	-2.239499
N	-1.256692	0.028151	-3.999009
C	-0.071956	0.006673	-4.615865
H	-0.090700	0.007102	-5.708444
N	1.133234	-0.016607	-4.040062

$TS_{(3-4)A}$ for pyrimidine (Table 4 entry 13)

E_{gas} = -2262.378417 a.u.

E_{sol} = -2262.439150 a.u.

Cu	0.012525	-0.022723	0.010014
C	-0.000442	0.076784	2.089437
C	1.276051	-0.018749	2.681836
C	-1.036062	-0.751819	2.568890
C	1.538025	-1.015916	3.618507
H	2.064764	0.655922	2.371760
C	-0.756282	-1.740658	3.511017
H	-2.026740	-0.643629	2.147253
C	0.529032	-1.888470	4.041119
H	2.542640	-1.100994	4.028664
H	-1.561329	-2.397782	3.835268
H	0.738318	-2.658489	4.779703
I	-0.683590	2.358950	1.822120
O	-1.751776	-0.493498	-0.294466
C	-2.009286	-1.840495	-0.416327
H	-3.073618	-2.025749	-0.676835
H	-1.415210	-2.362805	-1.202197
H	-1.832645	-2.416070	0.525587
C	1.843713	0.304899	-0.495680
C	2.320042	1.521396	-1.021139
C	2.852136	-0.677643	-0.472708
H	1.655086	2.383878	-1.095208
H	2.637453	-1.673485	-0.077701
N	4.120971	-0.511011	-0.891299
N	3.576291	1.749393	-1.452061
C	4.405328	0.706801	-1.361628
H	5.428508	0.867119	-1.708507

For 1,4-difluorobenzene (Table 4 entry 14)

2A for 1,4-difluorobenzene (Table 4 entry 14)

E_{gas} = -2301.474694 a.u.

E_{sol} = -2301.542470 a.u.

Cu	-0.247418	-0.037969	0.082659
O	-0.081773	-0.217285	1.885952
C	1.197489	-0.099438	2.390486
H	1.202201	-0.224100	3.496876
H	1.920687	-0.855203	2.004206
H	1.680923	0.887343	2.201233
O	-0.490988	0.176331	-1.696058
C	0.248713	-0.641773	-2.508002
H	0.031683	-0.442820	-3.585657
H	1.361174	-0.532717	-2.418668
H	0.067909	-1.740608	-2.380908
C	-2.275443	0.789402	3.920012
C	-2.049940	-0.585612	4.011426
C	-2.730943	-1.305499	4.985371
H	-1.341003	-1.013396	3.298645
C	-3.847209	0.670599	5.773630
C	-3.624695	-0.705533	5.868253
C	-3.166397	1.393483	4.798660
F	-2.527089	-2.644186	5.094501
F	-3.388074	2.731479	4.715467
H	-4.133487	-1.310004	6.613040
H	-4.535565	1.180483	6.440582
H	-1.737347	1.341332	3.156459

$TS_{(2-3)A}$ for 1,4-difluorobenzene (Table 4 entry 14)

E_{gas} = -2301.425205 a.u.

E_{sol} = -2301.497558 a.u.

Cu	-0.179021	-0.029535	0.040717
H	-0.196278	-0.061398	2.005154
O	0.974711	0.019309	1.851116
C	1.603336	-1.193722	2.135366
H	2.072294	-1.204112	3.139208
H	0.909104	-2.057421	2.102799
H	2.404963	-1.405218	1.406442
O	-0.253753	-0.041917	-1.781617
C	-1.534705	-0.056359	-2.278269
H	-2.160888	0.828297	-2.003293
H	-1.533489	-0.072054	-3.394347
H	-2.150282	-0.940679	-1.978206
C	-2.333240	-1.354893	1.787409
C	-1.598509	-0.149909	1.693718
C	-2.393551	0.995992	1.813466
C	-4.465363	-0.200270	2.014329
C	-3.715938	-1.367416	1.927542
C	-3.775376	1.016031	1.958095
F	-4.370655	-2.566324	2.000287
F	-1.776549	2.219571	1.783569
H	-4.300706	1.965146	2.031010
H	-1.827279	-2.317452	1.737893
H	-5.544389	-0.247092	2.124885

3A for 1,4-difluorobenzene (Table 4 entry 14)

E_{gas} = -2185.747952 a.u.

E_{sol} = -2185.815854 a.u.

Cu	0.032145	0.019280	0.003500
O	0.006073	0.020933	1.829829
C	1.215323	-0.011885	2.470005
H	1.090139	-0.006586	3.580780
H	1.846109	-0.915205	2.262395
H	1.895698	0.853916	2.259446
C	-0.027936	0.019255	-1.864483
C	-1.227696	0.039030	-2.614431
C	1.117731	-0.000735	-2.671524
C	-0.074752	0.017895	-4.760907
C	1.137687	-0.002121	-4.062406
C	-1.239349	0.038202	-4.005878
F	2.351380	-0.021103	-2.068344
F	-2.441291	0.058106	-4.663958
H	2.088999	-0.018716	-4.589053
H	-2.192643	0.055835	-2.111324
H	-0.118569	0.017814	-5.845987

$TS_{(3-4)A}$ for 1,4-difluorobenzene (Table 4 entry 14)

E_{gas} = -2428.765830 a.u.

E_{sol} = -2428.825143 a.u.

Cu	-0.037028	0.050202	0.006347
C	0.017655	0.076204	2.059305
C	1.307207	0.100287	2.628701
C	-0.928784	-0.840462	2.563198
C	1.673673	-0.856699	3.574105
H	2.024268	0.843699	2.302427
C	-0.546827	-1.786250	3.513183
H	-1.933076	-0.824037	2.160861
C	0.754838	-1.810296	4.024159
H	2.687333	-0.842978	3.970821
H	-1.283946	-2.509062	3.858827
H	1.044059	-2.548174	4.768671
I	-0.877564	2.330981	1.865212
O	-1.771472	-0.545734	-0.259492
C	-1.922226	-1.903639	-0.430679
H	-2.975219	-2.164712	-0.670658

H	-1.310519	-2.343147	-1.252463
H	-1.672448	-2.498354	0.482286
C	1.754744	0.445357	-0.612342
C	1.964074	1.407335	-1.603904
C	2.919669	-0.258885	-0.250492
C	4.320288	0.984189	-1.807225
C	3.187864	1.703699	-2.197958
C	4.154887	0.008707	-0.832693
F	0.894513	2.136552	-2.049200
F	5.249474	-0.708577	-0.437156
H	3.248070	2.481436	-2.954891
H	2.883120	-1.024304	0.523001
H	5.299909	1.172144	-2.236180

1_L1

E_{gas} = -2024.727923 a.u.

E_{sol} = -2024.743666 a.u.

Cu	-0.008581	-0.000703	0.001629
C	0.010919	-0.004951	2.813132
C	1.551383	-0.008836	2.801751
N	-0.592540	-0.745033	1.667054
N	2.083732	0.329221	1.492934
H	-0.334907	-0.431665	3.767153
H	1.878583	0.666696	3.614819
H	1.911336	-1.009766	3.067022
H	-0.366175	1.020182	2.752780
H	3.014015	-0.058374	1.372868
C	2.082457	1.751551	1.143725
H	2.209798	1.850929	0.062664
H	2.839307	2.340377	1.688742
H	1.099857	2.179054	1.366475
H	-1.603896	-0.632896	1.754230
C	-0.311010	-2.200189	1.710254
H	-0.907167	-2.696267	0.941366
H	-0.547461	-2.633503	2.693197
H	0.742746	-2.368855	1.484785
O	0.508007	0.768100	-1.545362
C	1.235265	-0.039294	-2.404403
H	2.151452	-0.489467	-1.953820
H	1.588960	0.544622	-3.277825
H	0.665919	-0.895932	-2.831170

2_L1

E_{gas} = -2274.223166 a.u.

E_{sol} = -2274.232545 a.u.

Cu	0.000039	-0.000711	0.000150
H	0.000065	-0.000083	2.816006
C	1.069888	0.000833	2.665317
C	3.270159	-0.434558	2.371584
C	3.037593	0.901181	2.087581
O	-1.330511	0.900701	0.831722
C	-2.577664	1.074508	0.250781
H	-3.242794	1.645366	0.926803
H	-3.111405	0.126585	0.028883
H	-2.560705	1.640723	-0.705981
N	1.569163	-0.888736	-0.634020
C	2.140274	-0.266658	-1.853947
H	2.249923	-0.742176	0.120585
C	1.382482	-2.351274	-0.761119
C	1.239428	-0.376636	-3.090555
H	3.110001	-0.728467	-2.098700
H	2.330153	0.783461	-1.611743
H	1.141450	-2.750993	0.225910
H	2.289428	-2.846302	-1.139744
H	0.550431	-2.560766	-1.435527
N	-0.132755	0.052445	-2.849324
H	1.739665	0.197360	-3.895218
H	1.208492	-1.420567	-3.423650
H	-0.716407	-0.286559	-3.608634
C	-0.307102	1.499612	-2.714795
H	-1.367008	1.740799	-2.828768
H	0.269606	2.086394	-3.452297
H	-0.021721	1.809661	-1.702690
H	4.231505	-0.931168	2.341014
H	3.714585	1.692874	1.797355
N	1.700939	1.157419	2.275374
C	1.034303	2.444358	2.099738
H	1.639345	3.069097	1.436162
H	0.926523	2.959350	3.061589
H	0.048969	2.264701	1.650432
C	2.018146	-1.002742	2.751085
H	1.831936	-2.026799	3.047321

$TS_{(2-3)_L1}$

E_{gas} = -2274.179589 a.u.

E_{sol} = -2274.194600 a.u.

Cu	0.451121	0.009054	-0.320819
H	0.032968	-0.288077	1.543727
C	1.295419	-0.144755	1.446281
C	3.453944	-0.420497	2.187493
C	3.022528	0.850613	2.538504
O	-1.342043	-0.041887	1.375748
C	-2.263967	-0.544836	2.282374
H	-2.067161	-0.236982	3.331710
H	-2.313920	-1.656098	2.299350
H	-3.296179	-0.202640	2.060632
N	1.714347	0.307040	-2.191896
C	0.758012	0.579202	-3.272688
H	2.365050	1.083009	-2.107690
C	2.479912	-0.935793	-2.340888
C	-0.563201	-0.180874	-3.046541
H	1.154318	0.318850	-4.267728
H	0.559728	1.656674	-3.276685
H	3.134413	-1.047954	-1.472502
H	3.080084	-0.968797	-3.264051
H	1.796198	-1.790480	-2.347927
N	-1.054272	0.036388	-1.678054
H	-1.293711	0.130598	-3.809218
H	-0.397871	-1.256434	-3.175655
H	-1.653618	-0.729477	-1.377954
C	-1.814263	1.285415	-1.465881
H	-2.089512	1.298662	-0.407747
H	-2.705607	1.344335	-2.108716
H	-1.177725	2.149706	-1.679370
H	4.428940	-0.838833	2.404230
H	3.530845	1.640762	3.076589
N	1.742052	1.009388	2.099089
C	0.892364	2.168659	2.326475
H	1.192547	3.017582	1.697849
H	0.943395	2.479724	3.375753
H	-0.132426	1.869842	2.082662
C	2.373102	-1.044459	1.522929
H	2.355868	-2.063255	1.154348

3_L1

E_{gas} = -2158.479920 a.u.

E_{sol} = -2158.494470 a.u.

Cu	0.000554	0.010917	0.001045
C	-0.003260	0.008355	1.872709
C	0.533935	0.002941	4.115061
C	-0.818323	0.239762	3.999599
C	0.478865	1.255814	-2.533356
C	-0.634511	2.294805	-2.347326
N	0.164726	-0.071773	-1.938627
N	-1.082756	2.408305	-0.965883
H	0.674707	1.153640	-3.612177
H	-0.249042	3.246070	-2.762143
H	-1.498058	2.014700	-2.961487
H	1.403487	1.600268	-2.060316
H	-1.993669	2.858224	-0.950559

C	-0.169305	3.139831	-0.085286
H	-0.653852	3.291740	0.882216
H	0.142693	4.118074	-0.492407
H	0.719605	2.533628	0.114089
H	0.973098	-0.667413	-2.125728
C	-1.010674	-0.725495	-2.559431
H	-1.068571	-1.755624	-2.201182
H	-0.948581	-0.724209	-3.657564
H	-1.918542	-0.206315	-2.249088
H	1.092094	-0.044852	5.042709
H	-1.580903	0.401060	4.751020
N	-1.133093	0.250861	2.655712
C	-2.480357	0.361726	2.143266
H	-2.432849	0.735077	1.116209
H	-3.064050	1.064624	2.749991
H	-3.007208	-0.604221	2.137654
C	1.037062	-0.138987	2.789387
H	2.074119	-0.316777	2.526208

$TS_{(3-4)_L1}$

E_{gas} = -2401.490376 a.u.

E_{sol} = -2401.498819 a.u.

Cu	-0.001379	0.023852	0.000373
C	-0.005632	0.010000	1.928822
C	0.661684	-0.019639	4.141614
C	-0.707995	0.110377	4.105515
C	-0.851295	-1.942094	-0.525260
C	-1.013586	-2.730419	0.633290
C	-1.935992	-1.809182	-1.413496
C	-2.272671	-3.208259	0.973352
H	-0.171210	-2.895922	1.293536
C	-3.200414	-2.285757	-1.052271
H	-1.806837	-1.337396	-2.382051
C	-3.379701	-2.979440	0.143083
H	-2.389906	-3.768352	1.897301
H	-4.035540	-2.138210	-1.732869
H	-4.358080	-3.365769	0.413388
I	1.176948	-2.137373	-1.561450
C	1.286068	2.624787	-0.847049
C	0.718642	1.999817	-2.126192
N	1.869058	1.582496	-0.011142
N	-0.378637	1.050376	-1.809985
H	2.008250	3.413697	-1.119251
H	0.479729	3.110264	-0.285062
H	0.373641	2.780440	-2.820320
H	1.508422	1.433909	-2.629971
H	-0.414550	0.364346	-2.561707
H	1.744505	1.773132	0.980048
C	3.261670	1.257660	-0.304040
H	3.621598	0.540281	0.438464
H	3.926665	2.138747	-0.295268
H	3.343407	0.778405	-1.286243
C	-1.694630	1.718069	-1.740112
H	-2.464097	0.971916	-1.528173
H	-1.946058	2.244372	-2.672731
H	-1.692177	2.443418	-0.922478
H	-1.436560	0.198055	4.901507
H	1.270172	-0.084635	5.035726
N	-1.099955	0.121870	2.780248
C	-2.462227	0.355717	2.352774
H	-2.617990	-0.107969	1.375766
H	-2.695190	1.428179	2.273555
H	-3.163918	-0.093286	3.064280
C	1.097293	-0.078652	2.784481
H	2.121630	-0.235821	2.461322

1_L2

E_{gas} = -2176.196107 a.u.

E_{sol} = -2176.211220 a.u.

Cu	-0.004478	0.000784	-0.005404
N	0.006222	0.003702	2.895184
H	0.548951	0.011143	2.030983
C	0.447050	-0.880808	3.964700
H	1.475788	-1.181743	3.758201
H	-0.184436	-1.774360	4.034579
H	0.403211	-0.360938	4.925999
O	1.616904	-0.728359	-0.125206
C	1.696959	-2.118818	-0.172204
H	1.178355	-2.636579	0.664252
H	2.754323	-2.436675	-0.117978
H	1.291650	-2.565079	-1.103435
C	-1.211587	0.593089	2.955053
O	-1.966848	0.455042	3.915175
C	-1.606594	1.547889	1.787677
C	-3.055965	2.027975	1.942997
N	-1.607366	0.875148	0.434597
H	-0.878910	2.365199	1.752712
C	-3.902454	0.921419	1.259371
H	-3.177899	2.987924	1.428085
H	-3.314035	2.158733	2.993563
C	-2.887735	0.089738	0.433122
H	-4.391336	0.290209	2.005154
H	-4.682785	1.349923	0.623352
H	-2.680841	-0.872942	0.905375
H	-3.187767	-0.099045	-0.600350
H	-1.744510	1.639730	-0.233327

2_L2

E_{gas} = -2425.691555 a.u.

E_{sol} = -2425.702534 a.u.

Cu	0.002427	0.002351	0.000979
H	-0.000864	0.000940	2.890675
C	1.039928	-0.000170	2.602345
C	3.219456	-0.431718	2.186624
C	2.967426	0.903485	1.913656
O	-1.370427	1.030067	0.539054
C	-2.494644	0.407453	1.075749
H	-3.019111	-0.263136	0.365199
H	-3.237372	1.163463	1.388181
H	-2.288208	-0.209220	1.978869
H	4.178410	-0.926170	2.101574
H	3.623224	1.692866	1.573464
N	1.645545	1.159802	2.178103
C	0.973257	2.451050	2.062846
H	1.545748	3.089103	1.384310
H	0.911657	2.943034	3.040141
H	-0.029206	2.283181	1.649788
C	1.994922	-1.000320	2.643621
H	1.830249	-2.020976	2.963046
H	2.546228	0.285192	-1.969402
C	2.079034	-0.704337	-2.022413
C	1.103920	-0.669709	-3.229291
C	3.113434	-1.831269	-2.195606
N	1.458446	-0.999138	-0.688919
N	-0.185735	-0.336651	-2.983832
O	1.540059	-0.909712	-4.352378
C	2.455711	-3.063532	-1.519066
H	4.039973	-1.557277	-1.679291
H	3.338780	-1.985618	-3.251060
C	1.273785	-2.486781	-0.698730
H	2.198387	-0.811768	0.001816
H	-0.455413	-0.079526	-2.033820
C	-1.152479	-0.173963	-4.056839
H	2.093715	-3.779468	-2.262525
H	3.167637	-3.591940	-0.877935
H	0.314828	-2.699350	-1.177021
H	1.227611	-2.836916	0.334330
H	-1.178136	0.858642	-4.427558
H	-2.147810	-0.442214	-3.692153
H	-0.871717	-0.830305	-4.882448

$TS_{(2-3)_L2}$

E_{gas} = −2425.656673 a.u.

E_{sol} = −2425.671389 a.u.

Cu	−0.000569	0.000379	0.000365
H	0.001077	−0.000683	2.027841
C	1.160961	0.000221	1.556398
C	3.162296	0.918645	2.102578
C	3.384413	−0.444528	1.927840
O	−1.369674	0.291485	2.310724
C	−1.757109	0.294534	3.652707
H	−2.316002	1.210397	3.923485
H	−2.415788	−0.558176	3.913972
H	−0.892296	0.238682	4.342093
H	3.852380	1.708105	2.372822
H	4.336335	−0.947562	2.036178
N	−1.316991	0.089515	−1.380297
C	−2.641381	−0.407057	−0.841512
C	−1.191534	−0.580560	−2.715546
H	−1.469331	1.083251	−1.575421
C	−2.465993	−1.846672	−0.307549
C	−3.564441	−0.377916	−2.072376
H	−2.935940	0.262690	−0.029714
C	−2.628764	−0.644182	−3.285940
H	−0.798739	−1.582752	−2.547360
H	−0.483418	−0.019689	−3.331568
N	−2.215278	−1.929208	1.012979
O	−2.560156	−2.804697	−1.083599
H	−4.036466	0.608156	−2.153233
H	−4.354168	−1.126690	−1.993628
H	−2.816720	−1.628581	−3.718183
H	−2.778444	0.105126	−4.070559
H	−1.994182	−1.052362	1.557269
C	−1.961841	−3.210050	1.650022
H	−2.719012	−3.421281	2.414960
H	−0.978069	−3.206322	2.134981
H	−1.991701	−3.994802	0.891989
C	2.140074	−1.014277	1.606565
H	1.944975	−2.066421	1.438964
N	1.851600	1.180872	1.884616
C	1.200153	2.476990	2.001028
H	1.390030	3.101749	1.119158
H	1.563131	3.004867	2.888465
H	0.126415	2.296685	2.099507

3_L2

E_{gas} = −2309.947147 a.u.

E_{sol} = −2309.960974 a.u.

Cu	0.170787	−0.051388	0.064734
C	0.235323	−0.070194	1.924741
N	1.369534	−0.039995	2.731544
C	−0.350987	0.123969	4.144328
C	1.023063	0.066947	4.062035
C	2.727177	−0.222010	2.266488
H	−0.928147	0.222945	5.055515
H	1.782432	0.085439	4.833139
H	3.079335	−1.253480	2.408626
H	3.410959	0.452613	2.794701
H	2.761834	0.009381	1.198634
C	−0.840055	0.042357	2.809685
H	−1.884432	0.055051	2.517555
H	−1.009672	−0.709835	−4.668226
C	−1.386254	−0.058475	−3.873839
C	−0.647373	1.306253	−3.860540
C	−1.131957	−0.665948	−2.470290
H	−2.457504	0.079810	−4.039554
C	−0.352894	1.562818	−2.375746
H	0.296443	1.245813	−4.414655
H	−1.249760	2.111279	−4.281175
N	−0.072748	0.184543	−1.830221
H	−2.022182	−0.604386	−1.840505
H	−0.797363	−1.705962	−2.478726
H	0.538673	2.177885	−2.212775
C	−1.558219	2.268064	−1.687147
H	0.812114	−0.089593	−2.267220
N	−1.530632	2.340089	−0.337653
O	−2.450666	2.769507	−2.367030
H	−0.808452	1.851703	0.188928
C	−2.596735	2.987093	0.412665
H	−2.539173	4.078023	0.323975
H	−2.492877	2.703008	1.462052
H	−3.573591	2.667678	0.037959

$TS_{(3-4)_L2}$

E_{gas} = −2552.954610 a.u.

E_{sol} = −2552.963981 a.u.

Cu	0.000698	0.000716	−0.000287
C	0.000511	0.000842	1.925678
C	0.769392	−0.000006	4.076179
C	−0.584171	−0.266544	4.142746
H	1.508491	0.108257	4.859679
H	−1.151647	−0.446551	5.047229
C	0.693825	−1.669622	−0.837526
C	1.619318	−2.440023	−0.117980
C	−0.366946	−2.295873	−1.509940
I	1.653659	0.163076	−2.089214
C	1.390304	−3.802155	0.051029
H	2.482933	−1.974793	0.342528
C	−0.588916	−3.663604	−1.324440
H	−1.023269	−1.733825	−2.165489
C	0.281756	−4.418869	−0.541040
H	2.084661	−4.385241	0.649872
H	−1.434877	−4.135313	−1.817427
H	0.116511	−5.484349	−0.411939
H	−0.903732	2.822027	−1.920084
C	−1.760663	2.469362	−1.336416
C	−1.817469	3.345252	−0.062814
C	−3.086524	2.581970	−2.114536
N	−1.604091	0.996728	−1.111277
N	−1.346392	2.818345	1.086716
O	−2.273656	4.484240	−0.150896
C	−3.972881	1.462245	−1.510163
H	−2.903108	2.397915	−3.179700
H	−3.513280	3.580143	−2.008624
C	−2.980184	0.538570	−0.751946
H	−1.408660	0.631043	−2.044866
H	−0.935989	1.886180	1.114944
C	−1.349015	3.581549	2.324407
H	−4.716217	1.873987	−0.820955
H	−4.519084	0.919019	−2.287723
H	−3.089769	0.641916	0.330422
H	−3.083143	−0.522357	−0.996243
H	−0.548326	4.331650	2.339486
H	−1.209362	2.884962	3.153850
H	−2.302264	4.105740	2.434286
C	−1.057385	−0.271209	2.804103
H	−2.077299	−0.477677	2.499153
N	1.114167	0.149442	2.753540
C	2.436501	0.540098	2.307387
H	2.503560	0.374913	1.229942
H	3.206600	−0.058334	2.807593
H	2.640432	1.601156	2.503757