Supporting Information

Symmetric C···H···C Hydrogen Bonds Predicted by Quantum Chemical Calculations

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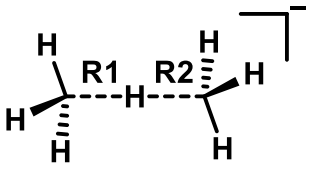
S1. Potential Energy Surface Scans on $[H_3C\cdots H\cdots CH_3]^-$

Potential energy surface scans on $[H_3C\cdots H\cdots CH_3]^-$ were performed by using the C···H distances (R1 and R2) as variables in steps of 0.05 Å at the CCSD(T)/aug-cc-pVTZ//MP2/aug-cc-pVTZ level (Table S1 and Figure 2).[1,2] C_{3v} symmetry was applied while the remaining geometry parameters were allowed to relax.

Table S1. Potential Energy Surface Scans on $[H_3C\cdots H\cdots CH_3]^-$



R1 + R2 (Å)	R1 − R2 (Å)	SPE[a] (a.u.)	SPE[b] (a.u.)
2.50	0.00	−80.159804	−80.206212
2.50	0.10	−80.159628	−80.206094
2.50	0.20	−80.158955	−80.205616
2.50	0.30	−80.157349	−80.204249
2.50	0.40	−80.154072	−80.201298
2.50	0.50	−80.148079	−80.195677
2.50	0.60	−80.137966	−80.185970
2.50	0.70	−80.121910	−80.170309
2.50	0.80	−80.097565	−80.146323
2.60	0.00	−80.168188	−80.215942
2.60	0.10	−80.168243	−80.216010
2.60	0.20	−80.168291	−80.216158
2.60	0.30	−80.167991	−80.216065
2.60	0.40	−80.166766	−80.215094
2.60	0.50	−80.163791	−80.212367
2.60	0.60	−80.157976	−80.206854
2.60	0.70	−80.147903	−80.197062
2.60	0.80	−80.131759	−80.181181
2.70	0.00	−80.173370	−80.221957
2.70	0.10	−80.173587	−80.222205
2.70	0.20	−80.174147	−80.222865
2.70	0.30	−80.174783	−80.223678
2.70	0.40	−80.175037	−80.224119
2.70	0.50	−80.174262	−80.223575
2.70	0.60	−80.171601	−80.221114
2.70	0.70	−80.165951	−80.215679
2.70	0.80	−80.155903	−80.205824
2.80	0.00	−80.175798	−80.224969
2.80	0.10	−80.176131	−80.225356
2.80	0.20	−80.177054	−80.226366
2.80	0.30	−80.178355	−80.227783
2.80	0.40	−80.179677	−80.229299
2.80	0.50	−80.180502	−80.230300

2.80	0.60	−80.180155	−80.230121
2.80	0.70	−80.177770	−80.227905
2.80	0.80	−80.172250	−80.222525
2.90	0.00	−80.175933	−80.225537
2.90	0.10	−80.176342	−80.225988
2.90	0.20	−80.177515	−80.227248
2.90	0.30	−80.179282	−80.229138
2.90	0.40	−80.181359	−80.231373
2.90	0.50	−80.183339	−80.233504
2.90	0.60	−80.184681	−80.234989
2.90	0.70	−80.184702	−80.235134
2.90	0.80	−80.182542	−80.233078

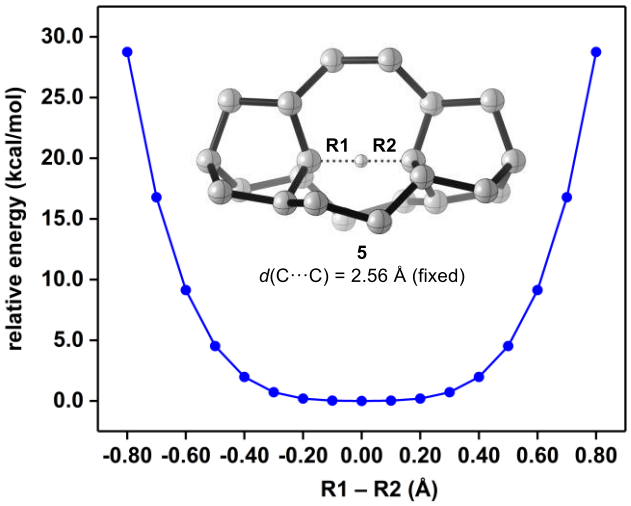
[a]Computed at the MP2/aug-cc-pVTZ level.

[b]Computed at the CCSD(T)/aug-cc-pVTZ//MP2/aug-cc-pVTZ level.

S2. Potential Energy Surface Scans on Carbanions 5–8

Based on the optimized structures, potential energy surface scans on carbanions **5**–**8** were performed by using the C···H distances (R1 and R2) as variables in steps of 0.05 Å at the ωB97XD/6-311+G(d,p) level (Tables S2–S5 and Figure 4).[3,4] C_3 symmetry was applied while the remaining geometry parameters were allowed to relax. The potential energy surface scans together with the lack of imaginary frequencies supported the presence of single-well C···H···C hydrogen bonds in carbanions **5**–**8**.

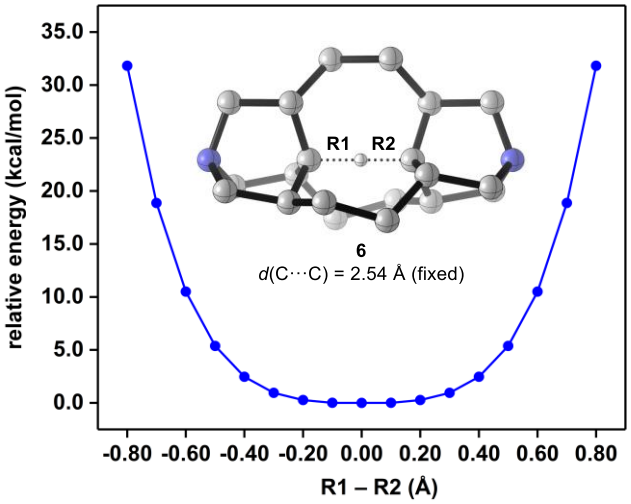
Table S2. Potential Energy Surface Scan on Carbanion 5[a]



R1 + R2 (Å)	R1 − R2 (Å)	SPE (a.u.)
2.56	0.00	−858.103422
2.56	0.10	−858.103378
2.56	0.20	−858.103106
2.56	0.30	−858.102274
2.56	0.40	−858.100272
2.56	0.50	−858.096210
2.56	0.60	−858.088869
2.56	0.70	−858.076669
2.56	0.80	−858.057599

[a]Computed at the ωB97XD/6-311+G(d,p) level. The relative energy of the minimum (R1 = R2) was set to 0.0 kcal/mol. Hydrogens are not fully shown for clarity.

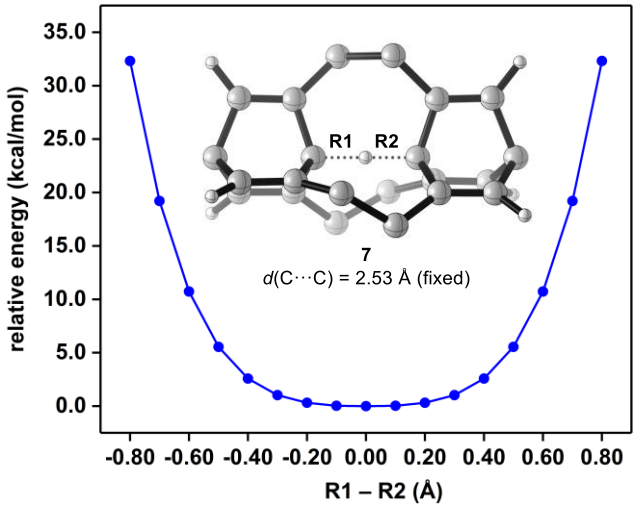
Table S3. Potential Energy Surface Scan on Carbanion 6[a]



R1 + R2 (Å)	R1 − R2 (Å)	SPE (a.u.)
2.54	0.00	−890.137148
2.54	0.10	−890.137136
2.54	0.20	−890.136717
2.54	0.30	−890.135623
2.54	0.40	−890.133221
2.54	0.50	−890.128576
2.54	0.60	−890.120413
2.54	0.70	−890.107071
2.54	0.80	−890.086434

[a]Computed at the ωB97XD/6-311+G(d,p) level. The relative energy of the minimum (R1 = R2) was set to 0.0 kcal/mol. Hydrogens are not fully shown for clarity.

Table S4. Potential Energy Surface Scan on Carbanion 7[a]



R1 + R2 (Å)	R1 − R2 (Å)	SPE (a.u.)
2.53	0.00	−850.661367
2.53	0.10	−850.661302
2.53	0.20	−850.660859
2.53	0.30	−850.659724
2.53	0.40	−850.657261
2.53	0.50	−850.652534
2.53	0.60	−850.644257
2.53	0.70	−850.630752
2.53	0.80	−850.609874

[a]Computed at the ωB97XD/6-311+G(d,p) level. The relative energy of the minimum (R1 = R2) was set to 0.0 kcal/mol. Hydrogens are not fully shown for clarity.

Table S5. Potential Energy Surface Scan on Carbanion 8[a]

R1 + R2 (Å)	R1 − R2 (Å)	SPE (a.u.)
2.49	0.00	−854.357399
2.49	0.10	−854.357232
2.49	0.20	−854.356600
2.49	0.30	−854.355075
2.49	0.40	−854.351911
2.49	0.50	−854.346015
2.49	0.60	−854.335917
2.49	0.70	−854.319720
2.49	0.80	−854.295023

[a]Computed at the ωB97XD/6-311+G(d,p) level.

S3. Natural Population Analysis

We have also performed natural population analysis on carbanions **3**–**8** (Table S6).[5] Interestingly, these carbanions possess similar charge distributions, whether it be a transition state or a minimum. The most positively charged hydrogen atoms in these carbanions are those in the C–H···C/C···H···C hydrogen bonds, whose natural atomic charges are ca. +0.3 e. For comparison, the corresponding values of hydrogens in methane and methyl anion are +0.20 and +0.13 e, respectively.

Table S6. Natural Population Analysis[a]

species	transition state/minimum	X–H···Y/X···H···Y	natural atomic charge (e)		
			X	H	Y
3	transition state	C···H···C	−0.49	+0.33	−0.49
4	minimum	C–H···C	−0.42	+0.33	−0.51
5	minimum	C···H···C	−0.37	+0.32	−0.37
6	minimum	C···H···C	−0.37	+0.31	−0.37
7	minimum	C···H···C	−0.50	+0.30	−0.50
8	minimum	C···H···C	−0.35	+0.30	−0.35

[a]Computed at the ωB97XD/6-311+G(d,p) level.

S4. Computed Energies of the Stationary Points

Table S7. Single-Point Energies (SPEs), Thermal Corrections to Enthalpies (TCHs), and Thermal Corrections to Gibbs Energies (TCGs)[a]

species	SPE (a.u.)	TCH (a.u.)	TCG (a.u.)
3	−548.468337	0.370152	0.320095
4	−548.474252	0.374719	0.323547
5	−858.103422	0.520145	0.462726
6	−890.137148	0.498031	0.441567
7	−850.661367	0.374746	0.317972
8	−854.357399	0.448603	0.392706
F−H···CO	−213.767000	0.023118	−0.008162
F−H···N_2	−209.975369	0.023528	−0.008238
F−H···OC	−213.764029	0.022721	−0.009871
[F···H···F]$^-$	−200.382201	0.013795	−0.010321
9	−858.728057	0.546766	0.489613
10	−890.756019	0.523520	0.466996
11	−851.274354	0.399354	0.344193
12	−854.978560	0.474576	0.419509
CH_3^-	−39.833263	0.032511	0.010529
CH_4	−40.515488	0.048600	0.027470
NH_2^-	−55.898155	0.022577	0.001131
NH_3	−56.560677	0.038387	0.016542
OH^-	−75.796177	0.012068	−0.007483
H_2O	−76.432257	0.025459	0.004050
F^-	−99.855502	0.002360	−0.014159
HF	−100.453724	0.012825	−0.006875
complex (B = CH_3)	−891.131396	0.431537	0.367167
complex (B = NH_2)	−907.208297	0.421509	0.359020
complex (B = OH)	−927.108612	0.410287	0.348489
TS (B = CH_3)	−891.104156	0.426645	0.366194
TS (B = NH_2)	−907.176307	0.416382	0.356295
TS (B = OH)	−927.075931	0.404582	0.345333

[a]Computed at the ωB97XD/6-311+G(d,p) level.

S5. Cartesian Coordinates of the Stationary Points

3

C	0.000000	0.000000	1.378056
C	0.000000	0.000000	−1.378056
C	1.377346	0.515506	1.724117
C	1.955483	1.514411	0.696224
C	2.289260	0.936293	−0.696224
C	1.135114	0.935063	−1.724117
C	−0.242231	−1.450569	1.724117
C	0.333777	−2.450704	0.696224
C	−0.333777	−2.450704	−0.696224
C	0.242231	−1.450569	−1.724117
C	−1.135114	0.935063	1.724117
C	−2.289260	0.936293	0.696224
C	−1.955483	1.514411	−0.696224
C	−1.377346	0.515506	−1.724117
H	0.000000	0.000000	0.000000
H	1.413005	1.003406	2.724082
H	2.082427	−0.327134	1.790752
H	1.247910	2.346554	0.572208
H	2.868755	1.956846	1.121569
H	3.129056	1.505992	−1.121569
H	2.656130	−0.092555	−0.572208
H	0.757907	1.967002	−1.790752
H	1.575478	0.721995	−2.724082
H	0.162473	−1.725402	2.724082
H	−1.324520	−1.639868	1.790752
H	1.408220	−2.253999	0.572208
H	0.260300	−3.462838	1.121569
H	−0.260300	−3.462838	−1.121569
H	−1.408220	−2.253999	−0.572208
H	1.324520	−1.639868	−1.790752
H	−0.162473	−1.725402	−2.724082
H	−1.575478	0.721995	2.724082
H	−0.757907	1.967002	1.790752
H	−2.656130	−0.092555	0.572208
H	−3.129056	1.505992	1.121569
H	−2.868755	1.956846	−1.121569
H	−1.247910	2.346554	−0.572208
H	−2.082427	−0.327134	−1.790752
H	−1.413005	1.003406	−2.724082

4

C	0.000000	0.000000	−1.404024
C	0.000000	0.000000	1.525657
C	1.020705	1.076695	−1.764119
C	2.115524	1.221399	−0.689467
C	1.652119	1.809134	0.664445
C	1.239040	0.796680	1.769599
C	−1.442797	0.345609	−1.764119
C	−2.115524	1.221399	−0.689467
C	−2.392815	0.526210	0.664445
C	−1.309465	0.674700	1.769599
C	0.422093	−1.422303	−1.764119
C	0.000000	−2.442797	−0.689467
C	0.740696	−2.335344	0.664445
C	0.070425	−1.471380	1.769599
H	0.000000	0.000000	−0.282874
H	1.488393	0.873086	−2.741504
H	0.517491	2.048540	−1.866285
H	2.571331	0.237479	−0.510479
H	2.915391	1.855727	−1.095543
H	2.463026	2.437506	1.066990
H	0.807593	2.489408	0.486488
H	2.093172	0.114270	1.911247
H	1.198364	1.400104	2.717362
H	−1.500311	0.852443	−2.741504
H	−2.032833	−0.576110	−1.866285
H	−1.491329	2.108099	−0.510479
H	−3.064802	1.596939	−1.095543
H	−3.342455	0.914290	1.066990
H	−2.559688	−0.545308	0.486488
H	−1.145547	1.755605	1.911247
H	−1.811708	0.337762	2.717362
H	0.011918	−1.725529	−2.741504
H	1.515342	−1.472430	−1.866285
H	−1.080003	−2.345578	−0.510479
H	0.149411	−3.452666	−1.095543
H	0.879429	−3.351796	1.066990
H	1.752094	−1.944100	0.486488
H	−0.947625	−1.869875	1.911247
H	0.613344	−1.737866	2.717362

5

C	0.000000	0.000000	1.278669
C	0.000000	0.000000	−1.278669
C	0.000000	0.000000	3.727915
C	0.000000	0.000000	−3.727915
C	0.016190	1.470263	3.206151
C	0.362537	1.396855	1.688267
C	−0.256723	2.459696	0.739712
C	0.256723	2.459696	−0.739712
C	−0.362537	1.396855	−1.688267
C	−0.016190	1.470263	−3.206151
C	1.265190	−0.749152	3.206151
C	1.028444	−1.012394	1.688267
C	2.258521	−1.007519	0.739712
C	2.001798	−1.452177	−0.739712
C	1.390981	−0.384461	−1.688267
C	1.281380	−0.721110	−3.206151
C	−1.281380	−0.721110	3.206151
C	−1.390981	−0.384461	1.688267
C	−2.001798	−1.452177	0.739712
C	−2.258521	−1.007519	−0.739712
C	−1.028444	−1.012394	−1.688267
C	−1.265190	−0.749152	−3.206151
H	0.000000	0.000000	0.000000
H	0.000000	0.000000	4.825476
H	0.000000	0.000000	−4.825476
H	−0.972678	1.923369	3.369351
H	0.740472	2.067819	3.780909

H	1.451572	1.520537	1.596565
H	−1.349083	2.337860	0.729470
H	−0.072586	3.460363	1.158582
H	0.072586	3.460363	−1.158582
H	1.349083	2.337860	−0.729470
H	−1.451572	1.520537	−1.596565
H	−0.740472	2.067819	−3.780909
H	0.972678	1.923369	−3.369351
H	2.152026	−0.119321	3.369351
H	1.420548	−1.675177	3.780909
H	0.591038	−2.017367	1.596565
H	2.699187	−0.000590	0.729470
H	3.033055	−1.667320	1.158582
H	2.960469	−1.793043	−1.158582
H	1.350105	−2.337270	−0.729470
H	2.042610	0.496830	−1.596565
H	2.161020	−0.392642	−3.780909
H	1.179348	−1.804048	−3.369351
H	−1.179348	−1.804048	3.369351
H	−2.161020	−0.392642	3.780909
H	−2.042610	0.496830	1.596565
H	−1.350105	−2.337270	0.729470
H	−2.960469	−1.793043	1.158582
H	−3.033055	−1.667320	−1.158582
H	−2.699187	−0.000590	−0.729470
H	−0.591038	−2.017367	−1.596565
H	−1.420548	−1.675177	−3.780909
H	−2.152026	−0.119321	−3.369351

6

N	0.000000	0.000000	3.715210
N	0.000000	0.000000	−3.715210
C	0.000000	0.000000	1.268714
C	0.000000	0.000000	−1.268714
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C	0.379238	1.386913	1.681914
C	−0.247533	2.458539	0.745348
C	0.247533	2.458539	−0.745348
C	−0.379238	1.386913	−1.681914
C	−0.051583	1.402082	−3.210281
C	1.188447	−0.745713	3.210281
C	1.011483	−1.021887	1.681914
C	2.252924	−1.014900	0.745348
C	2.005391	−1.443640	−0.745348
C	1.390721	−0.365027	−1.681914
C	1.240030	−0.656369	−3.210281
C	−1.240030	−0.656369	3.210281
C	−1.390721	−0.365027	1.681914
C	−2.005391	−1.443640	0.745348
C	−2.252924	−1.014900	−0.745348
C	−1.011483	−1.021887	−1.681914
C	−1.188447	−0.745713	−3.210281
H	0.000000	0.000000	0.000000
H	−0.924690	1.861733	3.414586
H	0.799586	1.945155	3.805483
H	1.467639	1.508844	1.579743
H	−1.340405	2.344425	0.747403
H	−0.050972	3.458663	1.159768
H	0.050972	3.458663	−1.159768
H	1.340405	2.344425	−0.747403
H	−1.467639	1.508844	−1.579743
H	−0.799586	1.945155	−3.805483
H	0.924690	1.861733	−3.414586
H	2.074653	−0.130061	3.414586
H	1.284761	−1.665039	3.805483
H	0.572878	−2.025435	1.579743
H	2.700534	−0.011388	0.747403
H	3.020776	−1.685188	1.159768
H	2.969803	−1.773475	−1.159768
H	1.360129	−2.333037	−0.747403
H	2.040517	0.516591	−1.579743
H	2.084346	−0.280116	−3.805483
H	1.149963	−1.731672	−3.414586
H	−1.149963	−1.731672	3.414586
H	−2.084346	−0.280116	3.805483
H	−2.040517	0.516591	1.579743
H	−1.360129	−2.333037	0.747403
H	−2.969803	−1.773475	1.159768
H	−3.020776	−1.685188	−1.159768
H	−2.700534	−0.011388	−0.747403
H	−0.572878	−2.025435	−1.579743
H	−1.284761	−1.665039	−3.805483
H	−2.074653	−0.130061	−3.414586

7

C	0.000000	0.000000	1.266609
C	0.000000	0.000000	−1.266609
C	0.000000	0.000000	3.646512
C	0.000000	0.000000	−3.646512
C	1.171864	0.845606	3.062293
C	1.138636	0.840615	1.728160
C	1.905452	1.608020	0.653733
C	2.345312	0.846160	−0.653733
C	1.297312	0.565780	−1.728160
C	1.318249	0.592061	−3.062293
C	0.146384	−1.437668	3.062293
C	0.158676	−1.406395	1.728160
C	0.439860	−2.454180	0.653733
C	−0.439860	−2.454180	−0.653733
C	−0.158676	−1.406395	−1.728160
C	−0.146384	−1.437668	−3.062293
C	−1.318249	0.592061	3.062293
C	−1.297312	0.565780	1.728160
C	−2.345312	0.846160	0.653733
C	−1.905452	1.608020	−0.653733
C	−1.138636	0.840615	−1.728160
C	−1.171864	0.845606	−3.062293
H	0.000000	0.000000	0.000000
H	0.000000	0.000000	4.743340
H	0.000000	0.000000	−4.743340
H	1.857986	1.372850	3.725531
H	1.256160	2.439376	0.343692
H	2.800657	2.067974	1.091229
H	3.191246	1.391453	−1.091229

H	2.740642	−0.131822	−0.343692	H	−1.409592	−1.636268	3.301416
H	2.117916	0.922638	−3.725531	H	−2.196546	−0.108848	3.722650
H	0.259930	−2.295488	3.725531	H	−1.926266	0.791845	1.548903
H	1.484482	−2.307554	0.343692	H	−3.148147	−1.466873	1.083974
H	0.390590	−3.459427	1.091229	H	−2.844423	−1.992938	−1.083974
H	−0.390590	−3.459427	−1.091229	H	−0.277375	−2.064118	−1.548903
H	−1.484482	−2.307554	−0.343692	H	−1.192539	−1.847841	−3.722650
H	−0.259930	−2.295488	−3.725531	H	−2.121846	−0.402609	−3.301416
H	−2.117916	0.922638	3.725531				
H	−2.740642	−0.131822	0.343692			F−H···CO	
H	−3.191246	1.391453	1.091229	F	0.000000	0.000000	2.157331
H	−2.800657	2.067974	−1.091229	O	0.000000	0.000000	−1.955656
H	−1.256160	2.439376	−0.343692	C	0.000000	0.000000	−0.833846
H	−1.857986	1.372850	−3.725531	H	0.000000	0.000000	1.232344
		8				$F–H···N_2$	
C	0.000000	0.000000	1.244536	F	0.000000	0.000000	2.100752
C	0.000000	0.000000	−1.244536	N	0.000000	0.000000	−0.889100
C	0.000000	0.000000	3.656392	N	0.000000	0.000000	−1.980386
C	0.000000	0.000000	−3.656392	H	0.000000	0.000000	1.179633
C	0.209944	1.463069	3.141713				
C	0.551654	1.330384	1.621302			F−H···OC	
C	0.176358	2.460799	0.654351	F	0.000000	0.000000	2.075174
C	−0.176358	2.460799	−0.654351	O	0.000000	0.000000	−0.933328
C	−0.551654	1.330384	−1.621302	C	0.000000	0.000000	−2.060975
C	−0.209944	1.463069	−3.141713	H	0.000000	0.000000	1.155907
C	1.162083	−0.913351	3.141713				
C	0.876319	−1.142938	1.621302			$[F···H···F]^-$	
C	2.042936	−1.383131	0.654351	F	0.000000	0.000000	1.142249
C	2.219294	−1.077669	−0.654351	F	0.000000	0.000000	−1.142249
C	1.427973	−0.187445	−1.621302	H	0.000000	0.000000	0.000000
C	1.372027	−0.549718	−3.141713				
C	−1.372027	−0.549718	3.141713			**9**	
C	−1.427973	−0.187445	1.621302	C	−1.317078	−0.012318	0.056997
C	−2.219294	−1.077669	0.654351	C	1.317078	0.012318	0.056997
C	−2.042936	−1.383131	−0.654351	C	−3.593246	−0.933910	−0.026454
C	−0.876319	−1.142938	−1.621302	C	3.593246	0.933910	−0.026454
C	−1.162083	−0.913351	−3.141713	C	−3.593246	0.432293	−0.762760
H	0.000000	0.000000	0.000000	C	−2.241875	1.085104	−0.418034
H	0.000000	0.000000	4.754174	C	−1.397953	1.852499	−1.473591
H	0.000000	0.000000	−4.754174	C	0.062700	2.195130	−1.001961
H	−0.712254	2.038877	3.301416	C	1.242653	1.150389	−1.000356
H	1.004008	1.956689	3.722650	C	2.611656	1.871841	−0.777257
H	1.648891	1.272273	1.548903	C	−3.126044	−0.753952	1.458508
H	0.303724	3.459812	1.083974	C	−1.585417	−0.626654	1.424816
H	−0.303724	3.459812	−1.083974	C	−0.784133	0.101600	2.534285
H	−1.648891	1.272273	−1.548903	C	0.784133	−0.101600	2.534285
H	−1.004008	1.956689	−3.722650	C	1.585417	0.626654	1.424816
H	0.712254	2.038877	−3.301416	C	3.126044	0.753952	1.458508
H	2.121846	−0.402609	3.301416	C	−2.611656	−1.871841	−0.777257
H	1.192539	−1.847841	3.722650	C	−1.242653	−1.150389	−1.000356
H	0.277375	−2.064118	1.548903	C	−0.062700	−2.195130	−1.001961
H	2.844423	−1.992938	1.083974	C	1.397953	−1.852499	−1.473591
H	3.148147	−1.466873	−1.083974	C	2.241875	−1.085104	−0.418034
H	1.926266	0.791845	−1.548903	C	3.593246	−0.432293	−0.762760
H	2.196546	−0.108848	−3.722650	H	−0.458720	0.576130	0.174820
H	1.409592	−1.636268	−3.301416	H	0.458720	−0.576130	0.174820

H	−4.595986	−1.369185	−0.043185	H	0.661237	0.353129	0.194051
H	4.595986	1.369185	−0.043185	H	−0.778350	−3.653497	−1.769005
H	−3.703573	0.265363	−1.840919	H	−1.609670	−4.241749	−0.330676
H	−4.438274	1.050873	−0.446067	H	−2.128678	−2.084837	0.440610
H	−2.388643	1.775511	0.423431	H	−1.499785	−1.170997	−2.410608
H	−1.351776	1.286386	−2.410559	H	−3.071836	−1.438719	−1.697925
H	−1.886337	2.800553	−1.722581	H	−2.872009	0.868364	−1.696087
H	0.414300	2.997901	−1.660886	H	−2.636045	0.418103	−0.032412
H	−0.006574	2.657878	−0.007363	H	−0.473148	1.310509	−2.003371
H	1.245930	0.703482	−1.998681	H	−1.589542	3.364317	−1.727666
H	3.045971	2.177097	−1.734447	H	−2.326125	2.879627	−0.205150
H	2.462475	2.788990	−0.194783	H	−0.605725	−3.575981	1.818963
H	−3.594479	0.141988	1.883477	H	1.152799	−3.655523	1.935389
H	−3.449623	−1.604388	2.066591	H	1.458451	−1.387278	1.403604
H	−1.191648	−1.650095	1.420728	H	−1.304100	−0.828539	2.516741
H	−0.997777	1.178717	2.493412	H	0.096284	−1.167407	3.516761
H	−1.142686	−0.240949	3.511857	H	−0.096284	1.167407	3.516761
H	1.142686	0.240949	3.511857	H	1.304100	0.828539	2.516741
H	0.997777	−1.178717	2.493412	H	−1.458451	1.387278	1.403604
H	1.191648	1.650095	1.420728	H	−1.152799	3.655523	1.935389
H	3.449623	1.604388	2.066591	H	0.605725	3.575981	1.818963
H	3.594479	−0.141988	1.883477	H	2.326125	−2.879627	−0.205150
H	−2.462475	−2.788990	−0.194783	H	1.589542	−3.364317	−1.727666
H	−3.045971	−2.177097	−1.734447	H	0.473148	−1.310509	−2.003371
H	−1.245930	−0.703482	−1.998681	H	2.636045	−0.418103	−0.032412
H	0.006574	−2.657878	−0.007363	H	2.872009	−0.868364	−1.696087
H	−0.414300	−2.997901	−1.660886	H	3.071836	1.438719	−1.697925
H	1.886337	−2.800553	−1.722581	H	1.499785	1.170997	−2.410608
H	1.351776	−1.286386	−2.410559	H	2.128678	2.084837	0.440610
H	2.388643	−1.775511	0.423431	H	1.609670	4.241749	−0.330676
H	4.438274	−1.050873	−0.446067	H	0.778350	3.653497	−1.769005
H	3.703573	−0.265363	−1.840919				

10

N	0.389944	−3.650797	−0.032684
N	−0.389944	3.650797	−0.032684
C	−0.201702	−1.284820	0.064268
C	0.201702	1.284820	0.064268
C	−0.920951	−3.476237	−0.697816
C	−1.420838	−2.045861	−0.398372
C	−2.053393	−1.109881	−1.467534
C	−2.150207	0.397138	−1.017900
C	−0.920951	1.381835	−1.008443
C	−1.391337	2.862915	−0.775909
C	0.325746	−3.196298	1.386609
C	0.392766	−1.644965	1.417104
C	−0.207773	−0.764828	2.543922
C	0.207773	0.764828	2.543922
C	−0.392766	1.644965	1.417104
C	−0.325746	3.196298	1.386609
C	1.391337	−2.862915	−0.775909
C	0.920951	−1.381835	−1.008443
C	2.150207	−0.397138	−1.017900
C	2.053393	1.109881	−1.467534
C	1.420838	2.045861	−0.398372
C	0.920951	3.476237	−0.697816
H	−0.661237	−0.353129	0.194051

11

C	−0.239385	1.277470	0.111164
C	0.239385	−1.277470	0.111164
C	0.380167	3.593006	−0.006054
C	−0.380167	−3.593006	−0.006054
C	0.416157	3.048882	1.443719
C	0.139897	1.748725	1.485465
C	0.416157	0.666615	2.530169
C	−0.416157	−0.666615	2.530169
C	−0.139897	−1.748725	1.485465
C	−0.416157	−3.048882	1.443719
C	−1.022639	3.339765	−0.621714
C	−1.315904	2.047268	−0.573108
C	−2.353268	1.056651	−1.058905
C	−1.739221	−0.291662	−1.624144
C	−1.049837	−1.386208	−0.776920
C	−1.356045	−2.683513	−0.803175
C	1.356045	2.683513	−0.803175
C	1.049837	1.386208	−0.776920
C	1.739221	0.291662	−1.624144
C	2.353268	−1.056651	−1.058905
C	1.315904	−2.047268	−0.573108
C	1.022639	−3.339765	−0.621714
H	−0.698649	0.342519	0.245918
H	0.698649	−0.342519	0.245918

H	0.669170	4.641941	−0.056878
H	−0.669170	−4.641941	−0.056878
H	0.769064	3.669989	2.258784
H	1.476874	0.398925	2.425095
H	0.322934	1.106787	3.527009
H	−0.322934	−1.106787	3.527009
H	−1.476874	−0.398925	2.425095
H	−0.769064	−3.669989	2.258784
H	−1.593048	4.144887	−1.068382
H	−3.017777	0.806909	−0.221510
H	−2.982634	1.478340	−1.847175
H	−2.563145	−0.803474	−2.129608
H	−1.041050	−0.005158	−2.419092
H	−2.182054	−3.119474	−1.353142
H	2.182054	3.119474	−1.353142
H	1.041050	0.005158	−2.419092
H	2.563145	0.803474	−2.129608
H	2.982634	−1.478340	−1.847175
H	3.017777	−0.806909	−0.221510
H	1.593048	−4.144887	−1.068382

12

C	0.225626	1.238449	0.115404
C	−0.225626	−1.238449	0.115404
C	−0.403265	3.607850	−0.036869
C	0.403265	−3.607850	−0.036869
C	1.004259	3.437339	−0.674422
C	1.454037	2.017812	−0.266884
C	2.175689	1.039540	−1.195176
C	1.909297	−0.275263	−1.387846
C	0.796505	−1.317511	−1.061570
C	1.395487	−2.749684	−0.865513
C	−0.403265	3.126040	1.458394
C	−0.500480	1.583606	1.406842
C	−0.148787	0.660409	2.577792
C	0.148787	−0.660409	2.577792
C	0.500480	−1.583606	1.406842
C	0.403265	−3.126040	1.458394
C	−1.395487	2.749684	−0.865513
C	−0.796505	1.317511	−1.061570
C	−1.909297	0.275263	−1.387846
C	−2.175689	−1.039540	−1.195176
C	−1.454037	−2.017812	−0.266884
C	−1.004259	−3.437339	−0.674422
H	0.716089	0.326428	0.284453
H	−0.716089	−0.326428	0.284453
H	−0.706633	4.656964	−0.078794
H	0.706633	−4.656964	−0.078794
H	0.930874	3.557379	−1.760723
H	1.696994	4.201380	−0.310906
H	2.091309	2.105368	0.623056
H	3.057562	1.417751	−1.709837
H	2.629974	−0.759758	−2.049144
H	0.214135	−1.337988	−1.989348
H	1.577569	−3.222276	−1.835602
H	2.362773	−2.697363	−0.354190
H	0.515919	3.459184	1.953396
H	−1.243538	3.569681	2.000654
H	−1.565667	1.369485	1.243049
H	−0.271503	1.109065	3.563027
H	0.271503	−1.109065	3.563027
H	1.565667	−1.369485	1.243049
H	1.243538	−3.569681	2.000654
H	−0.515919	−3.459184	1.953396
H	−2.362773	2.697363	−0.354190
H	−1.577569	3.222276	−1.835602
H	−0.214135	1.337988	−1.989348
H	−2.629974	0.759758	−2.049144
H	−3.057562	−1.417751	−1.709837
H	−2.091309	−2.105368	0.623056
H	−1.696994	−4.201380	−0.310906
H	−0.930874	−3.557379	−1.760723

CH_3^-

C	0.000000	0.000000	0.124044
H	0.000000	1.039518	−0.248089
H	−0.900249	−0.519759	−0.248089
H	0.900249	−0.519759	−0.248089

CH_4

C	0.000000	0.000000	0.000000
H	0.629704	0.629704	0.629704
H	−0.629704	−0.629704	0.629704
H	−0.629704	0.629704	−0.629704
H	0.629704	−0.629704	−0.629704

NH_2^-

N	0.000000	0.000000	0.143101
H	0.000000	0.801555	−0.500853
H	0.000000	−0.801555	−0.500853

NH_3

N	0.000000	0.000000	0.108461
H	0.000000	0.946004	−0.253077
H	−0.819263	−0.473002	−0.253077
H	0.819263	−0.473002	−0.253077

OH^-

O	0.000000	0.000000	0.106833
H	0.000000	0.000000	−0.854665

H_2O

O	0.000000	0.000000	0.116318
H	0.000000	0.760821	−0.465274
H	0.000000	−0.760821	−0.465274

HF

F	0.000000	0.000000	0.091681
H	0.000000	0.000000	−0.825130

complex (B = CH_3)

C	−0.638742	4.132926	−0.020221
C	1.326938	−0.295649	0.244462
C	−1.231152	−0.437222	−0.247399

C	3.640455	−0.053914	−0.346347
C	−3.554605	−0.478858	0.352509
C	3.179515	−1.530864	−0.382298
C	1.878182	−1.639557	−0.123686
C	0.858753	−2.734182	−0.439570
C	−0.483121	−2.822998	0.374019
C	−1.622428	−1.844370	0.087565
C	−2.926421	−1.892690	0.351007
C	3.335636	0.552289	1.049766
C	2.041754	0.443415	1.322808
C	1.014970	0.905271	2.337620
C	−0.378429	1.344515	1.728735
C	−1.401498	0.406577	1.068537
C	−2.701363	0.339680	1.363603
C	2.699619	0.685273	−1.340950
C	1.398111	0.594841	−1.051591
C	0.277256	1.418699	−1.700114
C	−1.067380	0.845756	−2.309170
C	−2.030024	0.243599	−1.305223
C	−3.326541	0.195104	−1.027756
H	−0.520798	4.814895	−0.883415
H	−0.283460	4.681312	0.873023
H	−1.725569	3.965715	0.114882
H	0.394177	−0.474133	0.693728
H	−0.285544	−0.494573	−0.701425
H	4.690609	0.052532	−0.621637
H	−4.608812	−0.500658	0.631666
H	3.839902	−2.314347	−0.740302
H	0.596216	−2.609691	−1.499878
H	1.351025	−3.709713	−0.368554
H	−0.860009	−3.846287	0.274665
H	−0.234563	−2.699583	1.437855
H	−3.490698	−2.755933	0.689465
H	4.100763	1.067470	1.618872
H	0.850217	0.086722	3.054121
H	1.384822	1.760069	2.911179
H	−0.920266	1.807719	2.559926
H	−0.211106	2.185245	1.016857
H	−3.179300	0.867192	2.180707
H	3.114863	1.274363	−2.150228
H	0.004595	2.250218	−0.995268
H	0.762288	1.940509	−2.532336
H	−1.532858	1.675831	−2.847947
H	−0.825470	0.072734	−3.054147
H	−4.147930	0.636545	−1.579660

complex (B = NH_2)

N	0.037897	−3.528520	0.333918
C	1.278753	−0.045147	0.022120
C	−1.279121	0.361681	−0.251000
C	3.593546	0.546060	−0.212507
C	−3.599165	−0.070678	0.172874
C	3.051781	−0.203692	−1.455299
C	1.752733	−0.466015	−1.339718
C	0.668252	−0.827200	−2.359529
C	−0.669049	−1.507517	−1.893526
C	−1.753864	−0.693573	−1.214793
C	−3.061899	−0.881091	−1.036476
C	3.341483	−0.307865	1.063112
C	2.046813	−0.583478	1.186386
C	1.047919	−1.233595	2.103693
C	−0.300379	−0.415931	2.269909
C	−1.397316	−0.252187	1.189030
C	−2.697890	−0.477157	1.372198
C	2.684733	1.794892	−0.062907
C	1.387860	1.513980	0.080077
C	0.296872	2.546714	0.435524
C	−1.038384	2.774672	−0.386909
C	−2.035124	1.643876	−0.252156
C	−3.331983	1.439426	−0.055794
H	0.673861	−4.307629	0.140801
H	−0.841105	−3.992578	0.582063
H	0.351796	−0.523957	0.148774
H	−0.337190	0.660736	−0.606430
H	4.643666	0.821257	−0.325087
H	−4.652691	−0.276181	0.368632
H	3.675052	−0.354036	−2.330641
H	0.433410	0.109439	−2.889686
H	1.112985	−1.485811	−3.112247
H	−1.094132	−2.022387	−2.761695
H	−0.402894	−2.318547	−1.150690
H	−3.681760	−1.629193	−1.517383
H	4.151121	−0.555764	1.739847
H	0.766906	−2.216216	1.635132
H	1.449748	−1.405437	3.108139
H	−0.818929	−0.885738	3.111374
H	−0.041926	0.596659	2.611105
H	−3.134479	−0.906353	2.266922
H	3.112688	2.791989	−0.031250
H	−0.006953	2.355603	1.471574
H	0.810355	3.514055	0.448453
H	−1.459378	3.732897	−0.064776
H	−0.771083	2.882668	−1.446859
H	−4.123790	2.177110	0.020633

complex (B = OH)

O	0.171747	−3.366050	0.332104
C	1.274464	−0.047712	0.023910
C	−1.285825	0.338539	−0.253950
C	3.584969	0.554580	−0.219701
C	−3.603604	−0.095047	0.178382
C	3.047834	−0.218629	−1.450705
C	1.751005	−0.488367	−1.330773
C	0.668635	−0.885383	−2.339075
C	−0.660361	−1.565886	−1.847948
C	−1.754327	−0.740694	−1.193985
C	−3.061763	−0.928374	−1.013955
C	3.338246	−0.281769	1.069007
C	2.046400	−0.566475	1.194255
C	1.048580	−1.215664	2.116165
C	−0.299981	−0.395075	2.277027
C	−1.400605	−0.247549	1.197791
C	−2.700456	−0.471553	1.386553
C	2.669007	1.799395	−0.089064

C	1.373996	1.512218	0.057839
C	0.276363	2.543825	0.394571
C	−1.057153	2.749914	−0.436054
C	−2.048126	1.616709	−0.281685
C	−3.344147	1.410714	−0.081888
H	−0.431396	−4.087766	0.519899
H	0.350607	−0.530135	0.158587
H	−0.345686	0.635096	−0.616259
H	4.633463	0.834243	−0.336690
H	−4.656233	−0.301830	0.378090
H	3.674276	−0.384240	−2.320882
H	0.423642	0.033682	−2.895082
H	1.117558	−1.562400	−3.072402
H	−1.081293	−2.113310	−2.698233
H	−0.381954	−2.339265	−1.073187
H	−3.678091	−1.690160	−1.477976
H	4.150586	−0.520390	1.745776
H	0.776401	−2.195975	1.647634
H	1.451512	−1.377898	3.121868
H	−0.816069	−0.851545	3.127484
H	−0.038745	0.621997	2.602727
H	−3.135236	−0.886479	2.288915
H	3.090349	2.799717	−0.072895
H	−0.030006	2.367303	1.432524
H	0.783993	3.514352	0.393771
H	−1.484381	3.711808	−0.133581
H	−0.787060	2.838903	−1.497043
H	−4.139121	2.146403	−0.020162

TS ($B = CH_3$)

C	−0.012314	−2.622527	0.973867
C	1.238856	−0.198368	0.104439
C	−1.260330	0.184630	−0.237171
C	3.598363	0.296279	−0.358355
C	−3.585934	−0.065600	0.289476
C	3.022247	−0.781360	−1.305840
C	1.711834	−0.928491	−1.111753
C	0.629130	−1.335005	−2.123815
C	−0.813617	−1.867990	−1.780412
C	−1.788245	−1.018900	−0.960660
C	−3.086075	−1.153039	−0.693776
C	3.361973	−0.084263	1.122169
C	2.061014	−0.256389	1.341077
C	1.142515	−0.310377	2.549252
C	−0.296987	0.324623	2.343329
C	−1.385557	0.000528	1.293115
C	−2.685452	−0.152415	1.551378
C	2.692446	1.540741	−0.591528
C	1.397378	1.336584	−0.338473
C	0.356226	2.475152	−0.324685
C	−1.001164	2.449989	−1.123262
C	−1.989382	1.437573	−0.602998
C	−3.286890	1.325304	−0.341975
H	0.224955	−2.864415	2.021380
H	0.601742	−3.296050	0.351096
H	−1.071148	−2.875096	0.824985
H	0.401634	−1.145402	0.499632
H	−0.273947	0.312846	−0.554174
H	4.649548	0.510970	−0.569854
H	−4.643184	−0.188118	0.532858
H	3.613156	−1.161061	−2.136782
H	0.484015	−0.418181	−2.718363
H	1.058947	−2.061529	−2.824029
H	−1.276594	−2.057022	−2.758683
H	−0.723789	−2.839317	−1.293011
H	−3.746767	−1.945480	−1.030488
H	4.170573	−0.044707	1.848248
H	1.018436	−1.340927	2.877349
H	1.586274	0.244704	3.386208
H	−0.797185	0.194850	3.311462
H	−0.136444	1.407554	2.257859
H	−3.127375	−0.276136	2.534425
H	3.131702	2.491723	−0.884699
H	0.095240	2.670358	0.722456
H	0.892690	3.367829	−0.666302
H	−1.411242	3.466690	−1.120997
H	−0.773991	2.199903	−2.169100
H	−4.067489	2.065932	−0.481876

TS ($B = NH_2$)

N	0.117188	−2.519956	0.928495
C	1.233883	−0.195849	0.103000
C	−1.270520	0.161255	−0.239349
C	3.586236	0.316003	−0.365561
C	−3.591889	−0.102749	0.296655
C	3.026154	−0.792366	−1.289041
C	1.714828	−0.944982	−1.099641
C	0.627572	−1.388067	−2.093505
C	−0.785224	−1.950290	−1.685628
C	−1.781417	−1.072954	−0.928323
C	−3.077911	−1.211925	−0.655596
C	3.353938	−0.031725	1.123814
C	2.053913	−0.211969	1.343362
C	1.130004	−0.255593	2.550006
C	−0.301756	0.391001	2.330071
C	−1.392432	0.031577	1.294584
C	−2.689030	−0.136371	1.559451
C	2.663895	1.542215	−0.628265
C	1.370147	1.328398	−0.374198
C	0.317656	2.458504	−0.402298
C	−1.038571	2.394269	−1.200881
C	−2.017199	1.392163	−0.644525
C	−3.312456	1.273514	−0.376258
H	0.936487	−2.879953	1.417819
H	−0.641825	−2.555129	1.608265
H	0.429268	−1.183442	0.519092
H	−0.285531	0.289355	−0.559028
H	4.634638	0.540767	−0.581095
H	−4.646926	−0.232005	0.546319
H	3.628283	−1.190274	−2.103225
H	0.460276	−0.489313	−2.710473
H	1.061890	−2.126795	−2.777820
H	−1.256185	−2.283172	−2.620159
H	−0.608087	−2.815270	−1.038470

H	−3.732694	−2.016503	−0.973818	H	0.863610	3.191703	−1.228714
H	4.161792	0.029283	1.849680	H	−1.436079	3.191153	−1.715972
H	0.983611	−1.289305	2.865754	H	−0.785718	1.758703	−2.513285
H	1.572681	0.290284	3.394025	H	−4.095865	1.895929	−0.847424
H	−0.799844	0.303377	3.304315				
H	−0.129801	1.467283	2.201066				
H	−3.129299	−0.219724	2.548013				
H	3.090799	2.490217	−0.946972				
H	0.052787	2.690748	0.636393				
H	0.847812	3.342352	−0.775060				
H	−1.457200	3.406809	−1.235429				
H	−0.808782	2.107480	−2.236565				
H	−4.103399	1.998272	−0.539345				

TS (B = OH)

O	0.114799	−2.225516	1.291845
C	1.240278	−0.186102	0.132521
C	−1.266231	0.129435	−0.252840
C	3.596441	0.247810	−0.382445
C	−3.590620	−0.057227	0.293368
C	3.041252	−0.978298	−1.146370
C	1.727741	−1.096607	−0.945890
C	0.644130	−1.672149	−1.871556
C	−0.766336	−2.172634	−1.382999
C	−1.768006	−1.194236	−0.759553
C	−3.067584	−1.293493	−0.482307
C	3.352458	0.104672	1.139118
C	2.049549	−0.038061	1.370883
C	1.115143	0.047742	2.564852
C	−0.301630	0.699736	2.263581
C	−1.400537	0.224359	1.282358
C	−2.699876	0.094282	1.557529
C	2.678750	1.426706	−0.820423
C	1.382469	1.251378	−0.548667
C	0.330807	2.367693	−0.740623
C	−1.020800	2.193509	−1.531777
C	−2.007400	1.285040	−0.843227
C	−3.305343	1.205304	−0.572470
H	−0.801851	−2.169012	1.566040
H	0.414404	−1.147764	0.705487
H	−0.271590	0.205274	−0.560631
H	4.647072	0.439756	−0.619322
H	−4.648004	−0.151024	0.548837
H	3.651728	−1.498625	−1.881884
H	0.467728	−0.867137	−2.604021
H	1.075499	−2.496989	−2.451561
H	−1.240162	−2.630474	−2.261512
H	−0.590793	−2.953690	−0.640860
H	−3.722501	−2.132731	−0.693831
H	4.159693	0.240541	1.855507
H	0.942553	−0.965093	2.933056
H	1.554893	0.650516	3.371217
H	−0.801505	0.750195	3.239581
H	−0.109299	1.745743	1.992041
H	−3.150164	0.151824	2.543458
H	3.111015	2.320758	−1.263606
H	0.059003	2.741421	0.254276

S6. References

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