SUPPORTING INFORMATION

Combined ab initio Molecular Dynamics and Experimental Studies of Carbon Atom Addition to Benzene

Michael L. McKee,[a]* Hans Peter Reisenauer,[b] and Peter R. Schreiner[b]*

[a]Department of Chemistry and Biochemistry, Auburn University, Auburn, Alabama 36849, USA 36849, USA, mckee@chem.auburn.edu and [b]Institute of Organic Chemistry, Justus-Liebig University, Heinrich-Buff-Ring 58, 35392 Giessen, Germany, prs@uni-giessen.de

Table of Contents

Figure S1: Additional FTIR Spectra S2

Figure S2: EPR Spectra S3

Table S1: Total and relative energies of all computed species S4

Table S2: Cartesian coordinates of all computed species S5

Full Gaussian03 reference S14

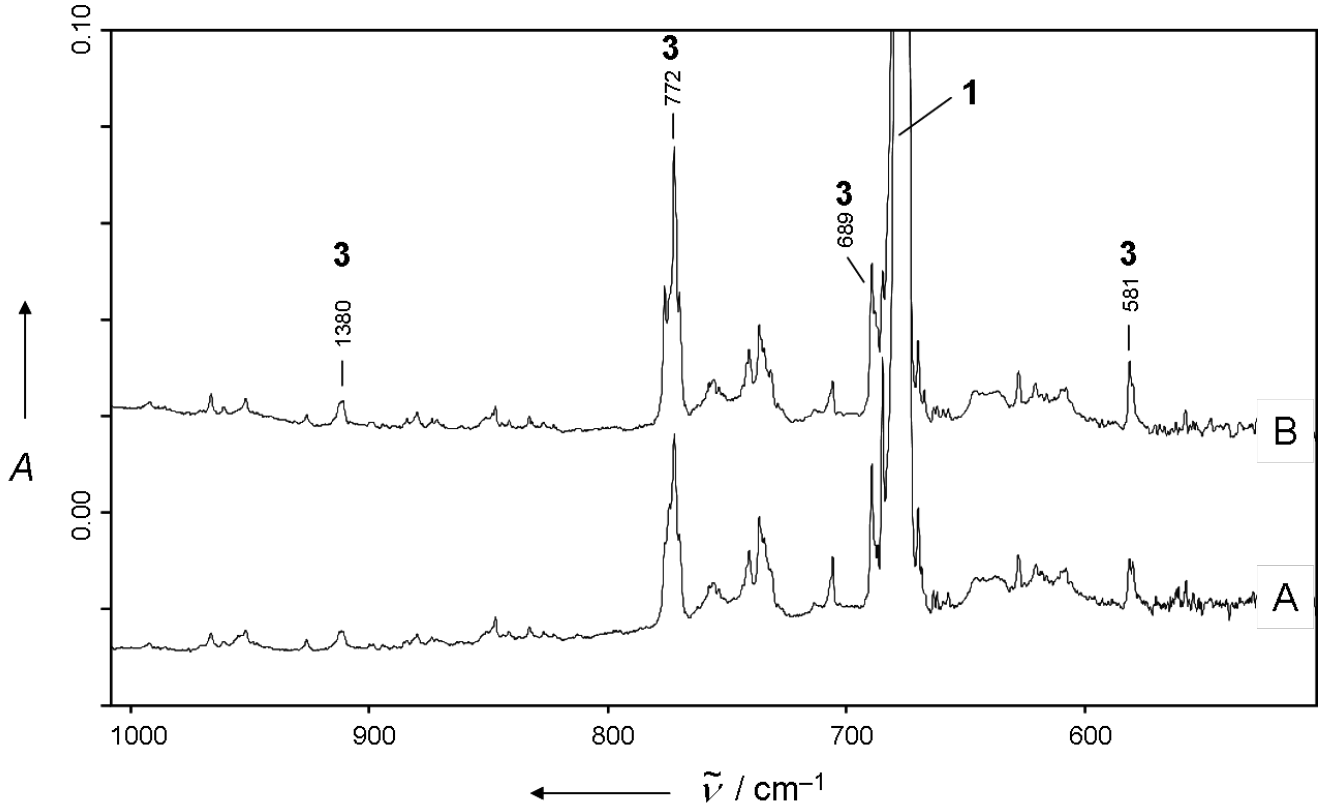


Figure S1. Part of the FTIR-spectra of the matrix isolated (Ar, 10 K) reaction products of atomic carbon generated by laser ablation of graphite and co-condensation with benzene (**1**) (4/1000 in Argon). (A) recorded directly after condensation; (B) recorded after warming the matrix for 10 min to 27 K and recooling to 10 K showing the growth of the cycloheptatetraene (**3**) bands by ca. 30%.

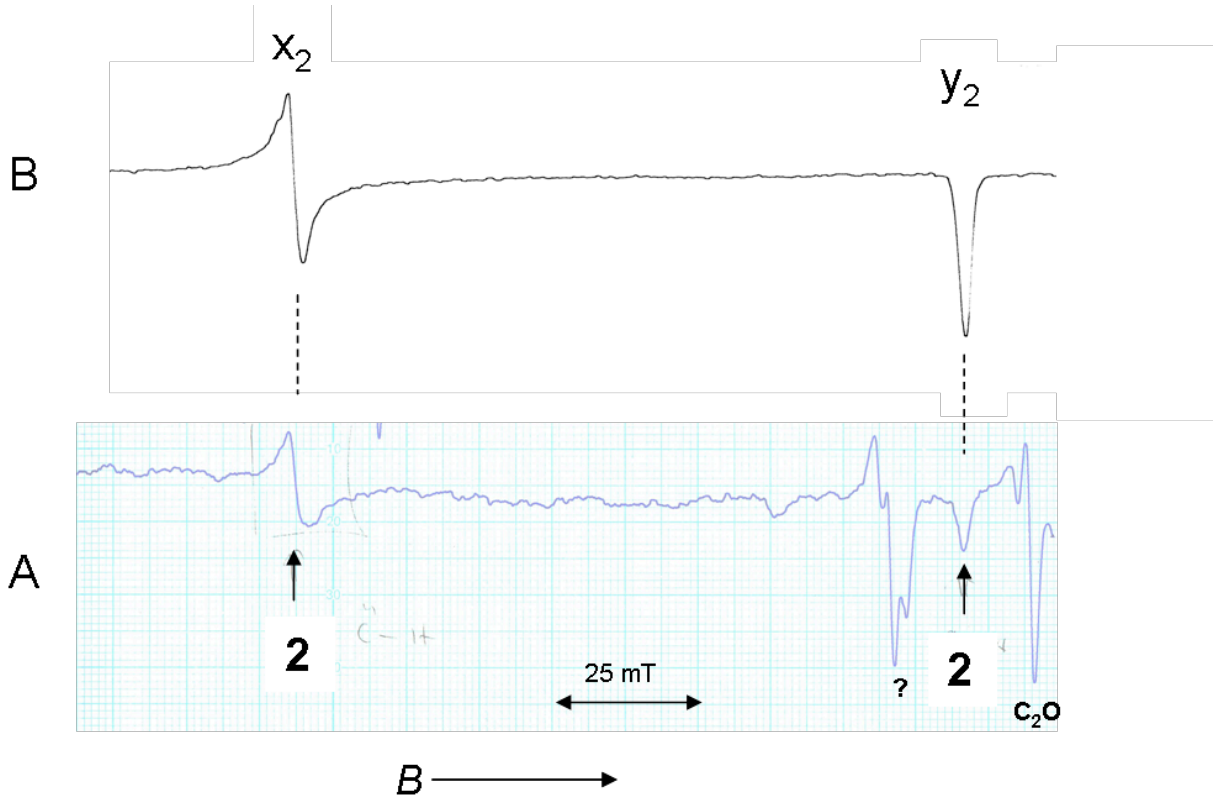


Figure S2. (A): High field part of the ESR x-band spectrum (microwave frequency 9.38 GHz) of the reaction products of laser ablated C-atoms with benzene (**1**) in an argon matrix after annealing at 34 K and recooling to 18 K; lines assigned to **2** are marked. (B): High field part of the ESR x-band spectrum (microwave frequency 9.38 GHz) of phenylcarbene (**2**) in an argon matrix at 18 K (recorded after photolysis of matrix isolated phenyldiazomethane with 254 nm) showing x_2 and y_2 lines of **2** at 495.2 and 598.0 mT.

Table S1. Total Energies (Hartrees) and Relative Energies (kcal mol^{-1}) of Triplet and Singlet Species in Tables 4 and 5

	PG	State	G3B3 Enthalpy(298K)	Relative
C(^{3}P)	K	^{3}P	-37.826091	
C_6H_6	D_{6h}	$^1A_{1g}$	-232.051702	0.0
^{3}1,3-(^{3}6)	C_s	$^3A''$	-269.921227	-27.2
^{3}TS(1,3-/1,2-)	C_1	^3A	-269.897087	-12.1
^{3}TS(3/1,2-)	C_1	^3A	-269.899131	-13.4
^{3}1,2-(^{3}7)	C_s	$^3A''$	-269.903233	-16.0
^{3}TS(1,2-/2)	C_s	$^3A''$	-269.889136	-7.1
^{3}3	C_{2v}	$^3A_2$	-269.987615	-68.9
^{3}TS1(3/4)	C_1	^3A	-269.926670	-30.7
^{3}4	C_1	^3A	-269.930381	-33.0
^{3}TS2(4/2)	C_1	^3A	-269.914145	-22.8
^{3}2	C_s	$^3A''$	-270.007458	-81.4
H_2	D_{ih}	$^1\Sigma_g$	-1.164170	
C_7H_4	C_{2v}	$^1A_1$	-268.776416	-39.4
1,2-	C_1	^1A	-269.945788	-42.7
TS(1,2-/3)	C_1	^1A	-269.942904	-40.8
1,4-(8)	C_s	$^1A'$	-269.967652	-56.4
TS(1,4-/3)	C_1	^1A	-269.946433	-43.1
3	C_2	^1A	-270.030069	-95.6
TS1(3/4)	C_1	^1A	-270.003868	-79.1
4	C_1	^1A	-270.007740	-81.5
TS2(4/2)	C_1	^1A	-269.981989	-65.4
2	C_s	$^1A'$	-270.002497	-78.2
TS(2/5)	C_1	^1A	-269.946446	-43.1
5	C_{2v}	$^1A_1$	-270.038082	-100.6

Table S2. Cartesian Coordinates of Triplet and Singlet Species Optimized at the B3LYP/6-31(2df,p) Level in Tables 4 and 5

C_6H_6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.396819	0.000000
2	6	0	1.209681	0.698410	0.000000
3	6	0	-1.209681	0.698410	0.000000
4	6	0	1.209681	-0.698410	0.000000
5	6	0	-1.209681	-0.698410	0.000000
6	6	0	0.000000	-1.396819	0.000000
7	1	0	0.000000	2.483625	0.000000
8	1	0	2.150882	1.241813	0.000000
9	1	0	-2.150882	1.241813	0.000000
10	1	0	2.150882	-1.241813	0.000000
11	1	0	-2.150882	-1.241813	0.000000
12	1	0	0.000000	-2.483625	0.000000

Triplet Species

^{3}1,3-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.712746	-1.289241	0.000000
2	6	0	-0.047056	0.912651	1.203187
3	6	0	-0.047056	-0.560486	1.153447
4	6	0	-0.043727	1.612762	0.000000
5	6	0	0.713745	-1.267269	0.000000
6	6	0	-0.047056	0.912651	-1.203187
7	6	0	-0.047056	-0.560486	-1.153447
8	1	0	-0.051112	1.423181	2.160934
9	1	0	-0.031890	-1.099770	2.098252
10	1	0	-0.033828	2.700292	0.000000
11	1	0	1.585542	-1.910604	0.000000
12	1	0	-0.051112	1.423181	-2.160934
13	1	0	-0.031890	-1.099770	-2.098252

^{3}TS(1,3-/1,2-)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.396517	-0.099914	0.851553
2	6	0	0.772477	-1.290693	-0.064393

3	6	0	-0.679791	-1.119487	0.030942
4	6	0	1.592763	-0.195800	-0.021723
5	6	0	-1.272059	0.268644	-0.519810
6	6	0	1.044899	1.120429	0.063427
7	6	0	-0.321734	1.324601	-0.095695
8	1	0	1.174170	-2.291532	-0.194306
9	1	0	-1.293010	-1.979276	-0.246747
10	1	0	2.672802	-0.322153	-0.034385
11	1	0	-1.927257	0.276171	-1.391966
12	1	0	1.678523	1.955867	0.344659
13	1	0	-0.745457	2.314245	0.056933

^{3}TS(3/1,2-)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.448782	0.627001	0.130971
2	6	0	0.334367	1.423111	-0.134071
3	6	0	-0.951150	0.868099	-0.283255
4	6	0	-1.081199	-0.664168	-0.306521
5	6	0	0.182586	-1.411397	-0.201912
6	1	0	0.135349	-2.494495	-0.291024
7	6	0	1.369039	-0.792056	0.098800
8	1	0	2.267730	-1.379283	0.262727
9	1	0	-1.820299	-1.045586	-1.023011
10	1	0	-1.747842	1.472852	-0.706209
11	1	0	0.462138	2.497246	-0.245632
12	1	0	2.412080	1.100155	0.300971
13	6	0	-1.587285	-0.075738	0.979685

^{3}1,2-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.222060	1.389559	0.708700
2	6	0	-0.222060	0.196149	1.407730
3	6	0	-0.124880	-1.057281	0.730190
4	6	0	-0.124880	-1.057281	-0.730190
5	6	0	-0.222060	0.196149	-1.407730
6	1	0	-0.268480	0.200849	-2.493680
7	6	0	-0.222060	1.389559	-0.708700
8	1	0	-0.251550	2.332979	-1.246070
9	1	0	-0.356050	-1.974341	-1.265680
10	1	0	-0.356050	-1.974341	1.265680
11	1	0	-0.268480	0.200849	2.493680
12	1	0	-0.251550	2.332979	1.246070
13	6	0	1.430030	-1.243351	0.000000

^{3}TS(1,2-/2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.168606	-0.985987	1.226048
2	6	0	0.168606	0.381088	1.263892
3	6	0	0.061183	1.203811	0.000000
4	6	0	0.168606	0.381088	-1.263892
5	6	0	0.168606	-0.985987	-1.226048
6	1	0	0.187515	-1.542449	-2.160446
7	6	0	0.160184	-1.696647	0.000000
8	1	0	0.158155	-2.781858	0.000000
9	1	0	0.168103	0.918699	-2.207045
10	1	0	0.812539	2.038653	0.000000
11	1	0	0.168103	0.918699	2.207045
12	1	0	0.187515	-1.542449	2.160446
13	6	0	-1.176114	2.034420	0.000000

^{3}3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.727650	-1.373685
2	6	0	0.000000	-0.727650	-1.373685
3	6	0	0.000000	-1.592868	-0.315096
4	6	0	0.000000	-1.285822	1.093541
5	6	0	0.000000	0.000000	1.566459
6	6	0	0.000000	1.285822	1.093541
7	6	0	0.000000	1.592868	-0.315096
8	1	0	0.000000	2.655236	-0.558553
9	1	0	0.000000	2.118013	1.793350
10	1	0	0.000000	-2.118013	1.793350
11	1	0	0.000000	-2.655236	-0.558553
12	1	0	0.000000	-1.180399	-2.362734
13	1	0	0.000000	1.180399	-2.362734

^{3}TS1(3/4)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.771237	-0.267823	0.560598
2	6	0	0.894141	-0.924477	-0.325070
3	6	0	-1.407052	0.782032	0.168471
4	6	0	-0.419730	-1.417584	-0.166760
5	6	0	1.061871	0.802236	-0.203719

6	6	0	-1.519069	-0.630556	0.104620
7	6	0	-0.217436	1.432265	-0.065421
8	1	0	-2.312482	1.372665	0.283034
9	1	0	-0.546421	-2.494936	-0.273856
10	1	0	1.760484	1.362913	-0.830752
11	1	0	-2.496860	-1.093318	0.206234
12	1	0	-0.246438	2.495305	-0.298098
13	1	0	2.857943	-0.299190	0.477115

^{3}4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.982290	-0.167546	-0.420828
2	6	0	-0.859976	-0.741310	0.200267
3	6	0	1.484480	0.694251	-0.116039
4	6	0	0.301591	-1.438821	0.047754
5	6	0	-0.949981	0.756224	0.277813
6	6	0	1.526893	-0.707438	0.054548
7	6	0	0.307328	1.425264	-0.099726
8	1	0	2.423317	1.223907	-0.266093
9	1	0	0.292989	-2.495027	-0.217423
10	1	0	-1.457267	1.241383	1.125543
11	1	0	2.479139	-1.227958	0.039282
12	1	0	0.337129	2.510565	-0.163523
13	1	0	-3.043575	-0.176619	-0.180518

^{3}TS2(4/2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.469059	0.613123	0.000000
2	6	0	1.252637	0.791721	0.000000
3	6	0	-1.719756	-0.418968	0.000000
4	6	0	0.000000	1.439532	0.000000
5	6	0	0.442596	-1.583421	0.000000
6	6	0	-1.284736	0.914670	0.000000
7	6	0	-0.901034	-1.585868	0.000000
8	1	0	-2.795289	-0.577373	0.000000
9	1	0	0.077816	2.526140	0.000000
10	1	0	1.189010	-2.368062	0.000000
11	1	0	-2.075211	1.662780	0.000000
12	1	0	-1.430470	-2.546550	0.000000
13	1	0	3.481551	0.278336	0.000000

^{3}2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.025226	2.446985	0.000000
2	6	0	0.000000	1.054238	0.000000
3	6	0	0.046067	-1.779138	0.000000
4	6	0	-1.211428	0.291647	0.000000
5	6	0	1.232419	0.332990	0.000000
6	6	0	-1.177073	-1.094377	0.000000
7	6	0	1.245388	-1.053042	0.000000
8	1	0	0.064247	-2.865160	0.000000
9	1	0	-2.162992	0.816046	0.000000
10	1	0	2.162814	0.893064	0.000000
11	1	0	-2.110078	-1.652428	0.000000
12	1	0	2.196225	-1.579785	0.000000
13	1	0	-0.811092	3.192444	0.000000

Singlet Species

C_7H_4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.221908
2	6	0	0.000000	1.465492	-0.229602
3	6	0	0.000000	0.680592	0.944001
4	6	0	0.000000	0.719283	-1.391693
5	6	0	0.000000	-0.680592	0.944001
6	6	0	0.000000	-0.719283	-1.391693
7	6	0	0.000000	-1.465492	-0.229602
8	1	0	0.000000	2.552727	-0.245764
9	1	0	0.000000	1.222330	-2.356196
10	1	0	0.000000	-1.222330	-2.356196
11	1	0	0.000000	-2.552727	-0.245764

1,2-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.145085	1.008956	0.159534
2	6	0	-0.120208	1.391810	-0.172902
3	6	0	-1.220569	0.444854	-0.425005
4	6	0	-0.767881	-1.007469	-0.098196
5	6	0	0.657030	-1.334403	-0.150347
6	1	0	0.940312	-2.353395	-0.395479
7	6	0	1.575233	-0.364789	0.066506
8	1	0	2.637152	-0.590924	0.085937
9	1	0	-1.454091	-1.810290	-0.386781

10	1	0	-2.012524	0.738989	-1.115761
11	1	0	-0.379224	2.446642	-0.214148
12	1	0	1.883996	1.777032	0.372828
13	6	0	-1.537959	-0.173635	0.895977

TS(1,2-/3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.324218	0.848676	0.167575
2	6	0	0.125958	1.414456	-0.157483
3	6	0	-1.143712	0.713269	-0.309176
4	6	0	-0.914103	-0.954974	-0.126191
5	6	0	0.466003	-1.385770	-0.173770
6	1	0	0.628802	-2.421267	-0.456519
7	6	0	1.514940	-0.563527	0.106678
8	1	0	2.522303	-0.967280	0.155397
9	1	0	-1.630142	-1.674875	-0.538904
10	1	0	-1.892502	1.206394	-0.936856
11	1	0	0.060032	2.489112	-0.309345
12	1	0	2.183874	1.494769	0.322331
13	6	0	-1.685365	-0.093272	0.786350

1,4-(8)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.826534	0.989719	0.000000
2	6	0	0.284689	-1.368718	0.667562
3	6	0	0.284689	0.056439	1.146875
4	6	0	0.284689	-1.368718	-0.667562
5	6	0	-0.883627	0.875879	0.686917
6	6	0	0.284689	0.056439	-1.146875
7	6	0	-0.883627	0.875879	-0.686917
8	1	0	0.202617	-2.226514	1.327298
9	1	0	0.610795	0.268371	2.164059
10	1	0	0.202617	-2.226514	-1.327298
11	1	0	-1.407526	1.607380	1.295074
12	1	0	0.610795	0.268371	-2.164059
13	1	0	-1.407526	1.607380	-1.295074

TS(1,4-/3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.988375	-0.289946	1.038826
2	6	0	1.230740	-0.910781	-0.189232
3	6	0	-0.190666	-1.205424	0.114166
4	6	0	1.530859	0.387573	-0.037820
5	6	0	-1.254226	-0.337399	-0.528575
6	6	0	0.393735	1.277799	0.204189
7	6	0	-0.845198	1.023807	-0.388167
8	1	0	1.921383	-1.672877	-0.537796
9	1	0	-0.481731	-2.245911	0.258022
10	1	0	2.519384	0.812631	-0.185071
11	1	0	-2.183140	-0.637083	-1.003375
12	1	0	0.566724	2.267762	0.618281
13	1	0	-1.603838	1.801700	-0.430382

3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.381673	-0.616330	-1.294038
2	6	0	0.381673	0.616330	-1.294038
3	6	0	0.605673	1.492876	-0.267206
4	6	0	0.000000	1.271274	1.038681
5	6	0	0.000000	0.000000	1.428880
6	6	0	0.000000	-1.271274	1.038681
7	6	0	-0.605673	-1.492876	-0.267206
8	1	0	-1.177558	-2.399717	-0.469459
9	1	0	0.475090	-2.081862	1.589653
10	1	0	-0.475090	2.081862	1.589653
11	1	0	1.177558	2.399717	-0.469459
12	1	0	0.766344	0.907653	-2.271460
13	1	0	-0.766344	-0.907653	-2.271460

TS1(3/4)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.637223	-0.518253	0.503086
2	6	0	0.624504	-1.069192	-0.078805
3	6	0	-1.123016	1.001307	0.281763
4	6	0	-0.723895	-1.369904	-0.261416
5	6	0	1.226527	0.578205	-0.406044
6	6	0	-1.572272	-0.336279	0.094725
7	6	0	0.135888	1.446459	-0.094011
8	1	0	-1.876678	1.747728	0.521334
9	1	0	-1.076840	-2.313337	-0.666679
10	1	0	1.854402	0.823278	-1.267688
11	1	0	-2.643680	-0.522833	0.134394
12	1	0	0.242921	2.506079	-0.332466

13	1	0	2.270121	-0.634967	1.375320

4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.756180	-0.376894	0.497448
2	6	0	0.742658	-0.889413	-0.135879
3	6	0	-1.233815	0.916464	0.237961
4	6	0	-0.581093	-1.425360	-0.186763
5	6	0	1.101828	0.590121	-0.456484
6	6	0	-1.543763	-0.489970	0.055259
7	6	0	-0.013640	1.460354	-0.042810
8	1	0	-2.056604	1.573396	0.510914
9	1	0	-0.800338	-2.472326	-0.372822
10	1	0	1.628301	0.862316	-1.377354
11	1	0	-2.586334	-0.794167	0.110878
12	1	0	0.090626	2.544710	-0.081357
13	1	0	2.354225	-0.425736	1.397342

TS2(4/2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.166751	0.033631	0.354448
2	6	0	-1.003111	0.411234	-0.243751
3	6	0	1.601296	-0.413415	0.213270
4	6	0	0.023930	1.403531	-0.196233
5	6	0	-0.690095	-0.995856	-0.334776
6	6	0	1.308211	0.974370	0.015452
7	6	0	0.635910	-1.378025	0.049691
8	1	0	2.624567	-0.703197	0.437079
9	1	0	-0.220709	2.459266	-0.270724
10	1	0	-1.329183	-1.703637	-0.838515
11	1	0	2.116646	1.697159	0.090389
12	1	0	0.903432	-2.431413	0.085965
13	1	0	-2.351092	0.469002	1.347201

2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.092401	2.489196	0.000000
2	6	0	0.000000	1.049118	0.000000
3	6	0	0.021116	-1.765344	0.000000

4	6	0	-1.212311	0.304479	0.000000
5	6	0	1.219959	0.322229	0.000000
6	6	0	-1.204157	-1.083747	0.000000
7	6	0	1.234116	-1.067708	0.000000
8	1	0	0.027465	-2.852721	0.000000
9	1	0	-2.154945	0.846963	0.000000
10	1	0	2.138005	0.902259	0.000000
11	1	0	-2.135249	-1.643859	0.000000
12	1	0	2.173877	-1.612587	0.000000
13	1	0	-0.955897	2.870615	0.000000

TS(2/5)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.295107	0.042634	0.069616
2	6	0	0.094985	1.417634	-0.027813
3	6	0	-0.920145	0.473761	-0.172320
4	6	0	1.393006	0.896691	0.012383
5	6	0	-0.666545	-0.874002	-0.218526
6	6	0	1.637405	-0.489161	0.063737
7	6	0	0.582105	-1.414660	0.072444
8	1	0	-0.090445	2.483034	0.070193
9	1	0	-2.564234	0.138925	1.139115
10	1	0	2.239833	1.577428	0.054577
11	1	0	-1.964479	-1.190290	-0.315688
12	1	0	2.664569	-0.845230	0.082833
13	1	0	0.760536	-2.481244	0.171846

5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.145722
2	6	0	0.000000	1.455549	-0.334785
3	6	0	0.000000	0.675886	0.803684
4	6	0	0.000000	0.702001	-1.528415
5	6	0	0.000000	-0.675886	0.803684
6	6	0	0.000000	-0.702001	-1.528415
7	6	0	0.000000	-1.455549	-0.334785
8	1	0	0.000000	2.542380	-0.350057
9	1	0	0.909629	0.000000	2.752818
10	1	0	0.000000	1.222918	-2.482829
11	1	0	-0.909629	0.000000	2.752818
12	1	0	0.000000	-1.222918	-2.482829
13	1	0	0.000000	-2.542380	-0.350057

Full Gaussian03 reference:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Revision E.1, Pittsburgh, 2003.