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Ab Initio Structural Studies of Cyclobutylmethyl Cations: Effect of Fluoroalkyl Groups on the Relative Stability of the Carbocations

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Supplementary Material

Ab initio structural studies of cyclobutylmethyl cations: effect of fluoroalkyl groups on the relative stability of the carbocations

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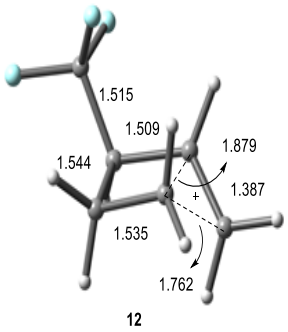
Cartesian coordinates:

The Cartesian coordinates for the MP2/cc-pVTZ optimized structures of the carbocations **7** and **12**-**17**, along with selected bond lengths in Å for each of the structures, are as follows.



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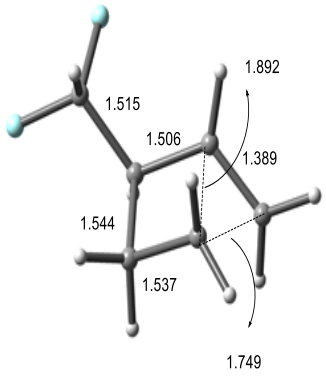
Cartesian coordinates:

Center Number	Atomic Number	Atom	Coordinates (Angstroms) X	Y	Z
1	6	C	-1.915147	0.621420	0.604587
2	6	C	-0.906736	1.283929	-0.343728
3	6	C	-1.092727	-0.941376	-0.038140
4	6	C	-2.444084	-0.787100	-0.311524
5	1	H	-1.547335	0.439271	1.612691
6	1	H	-2.938520	0.993755	0.673177
7	1	H	-0.310470	2.046936	0.147362
8	1	H	-1.396293	1.718421	-1.210011
9	1	H	-0.782479	-1.609079	0.759117
10	1	H	-3.163541	-1.380462	0.235325
11	1	H	-2.770993	-0.331204	-1.236538
12	6	C	-0.116555	0.005001	-0.694820
13	1	H	0.019638	-0.192414	-1.756159
14	6	C	1.235989	-0.063684	-0.015625
15	9	F	1.100086	0.165347	1.303444
16	9	F	2.057640	0.844433	-0.517662
17	9	F	1.767335	-1.275819	-0.166833



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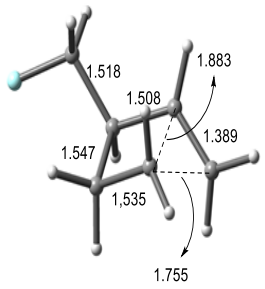
Cartesian coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.886433	0.565295	0.645034
2	6	-0.777535	1.314766	-0.109897
3	6	-0.935358	-0.931220	-0.015095
4	6	-2.255260	-0.773033	-0.419122
5	1	-1.654200	0.307244	1.677001
6	1	-2.915019	0.928385	0.614731
7	1	-0.258104	2.034902	0.516672
8	1	-1.167521	1.830692	-0.982055
9	1	-0.701442	-1.659209	0.756099
10	1	-3.015935	-1.422268	-0.008670
11	1	-2.484156	-0.259224	-1.343477
12	6	0.077492	0.082986	-0.476768
13	1	0.316161	-0.023704	-1.534727
14	6	1.373102	-0.020013	0.301835
15	9	2.233514	0.892241	-0.183046
16	9	1.882741	-1.260458	0.113387
17	1	1.257880	0.144450	1.375434



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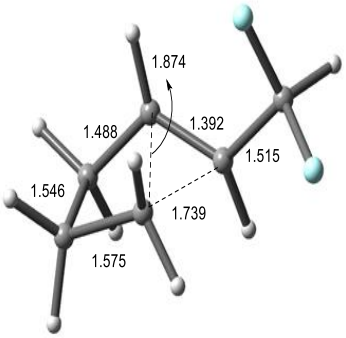
Cartesian coordinates

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.440955	0.770395	0.603218
2	6	-0.208589	1.159758	-0.224885
3	6	-0.909575	-0.955288	0.067453
4	6	-2.160230	-0.516767	-0.348144
5	1	-1.247643	0.545693	1.650837
6	1	-2.354225	1.365792	0.553211
7	1	0.491194	1.782340	0.325098
8	1	-0.492835	1.674360	-1.138156
9	1	-0.854645	-1.647807	0.902735
10	1	-3.047295	-0.921754	0.118350
11	1	-2.276925	-0.035065	-1.309840
12	6	0.319296	-0.271986	-0.478608
13	1	0.484535	-0.506407	-1.529233
14	6	1.563654	-0.594137	0.328188
15	9	2.560192	0.249128	-0.091585
16	1	1.393809	-0.426080	1.394562
17	1	1.880703	-1.625073	0.173364



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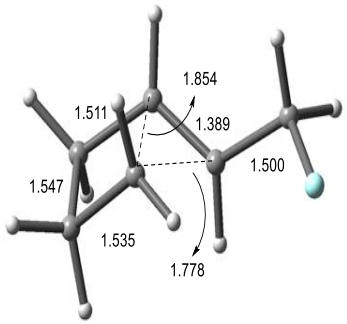
Cartesian coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.189187	0.691482	0.437002
2	6	2.290738	-0.581531	-0.433642
3	6	0.858780	-0.863436	-0.141111
4	6	0.628300	0.897359	0.456101
5	1	2.539884	0.514451	1.447566
6	1	2.696222	1.550846	0.013337
7	1	2.975811	-1.335334	-0.068280
8	1	2.470813	-0.364540	-1.482207
9	1	0.597629	-1.474917	0.717790
10	1	0.125928	0.801852	1.409733
11	1	0.317409	1.802725	-0.061181
12	6	-0.154140	-0.108443	-0.726743
13	1	0.018347	0.345771	-1.694719
14	6	-1.606951	-0.295086	-0.339588
15	9	-2.195558	0.915877	-0.309913
16	9	-1.676019	-0.843464	0.893431
17	1	-2.133339	-0.934636	-1.045812



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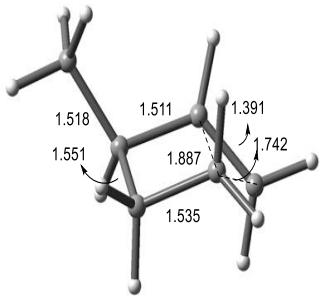
Cartesian coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.828859	0.912739	-0.183770
2	6	2.073538	-0.614553	-0.200709
3	6	0.680270	-0.959247	0.270075
4	6	0.462219	0.865248	0.514300
5	1	2.562688	1.475533	0.383564
6	1	1.748481	1.341087	-1.178375
7	1	2.816834	-0.932742	0.521968
8	1	2.312081	-1.041419	-1.171448
9	1	0.503940	-1.511084	1.187852
10	1	0.484690	0.773677	1.599456
11	1	-0.329674	1.570715	0.251924
12	6	-0.408623	-0.398056	-0.384599
13	1	-0.278492	-0.029605	-1.396739
14	6	-1.822260	-0.584783	0.080354
15	9	-2.506228	0.581758	-0.158558
16	1	-2.281453	-1.392641	-0.489111
17	1	-1.867054	-0.817439	1.144017



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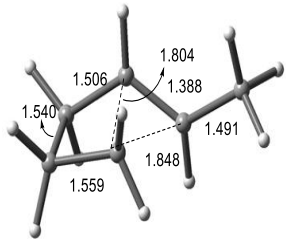
Cartesian coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.094826	0.688637	0.600332
2	6	0.046453	1.220348	-0.278585
3	6	-0.337212	-0.961420	0.085211
4	6	-1.652205	-0.703362	-0.286142
5	1	-0.828784	0.517262	1.642264
6	1	-2.076822	1.163514	0.581226
7	1	0.660324	1.951169	0.240215
8	1	-0.336984	1.665202	-1.192649
9	1	-0.153249	-1.614495	0.933783
10	1	-2.458143	-1.215138	0.220703
11	1	-1.867615	-0.274501	-1.255788
12	6	0.773099	-0.129145	-0.512753
13	1	0.902584	-0.369358	-1.567696
14	6	2.082650	-0.269692	0.242634
15	1	2.475467	-1.281843	0.166431
16	1	1.953630	-0.026360	1.297684
17	1	2.821837	0.412359	-0.170356



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Cartesian coordinates:

C	1.712048	0.627473	-0.033469
C	1.482523	-0.893633	-0.106256
C	0.076263	-0.720686	0.404534
C	0.215173	1.048720	0.079019
H	2.235979	0.915441	0.872051
H	2.204174	1.064073	-0.895370
H	2.115566	-1.490869	0.538056
H	1.503076	-1.285978	-1.119061
H	-0.122343	-0.804629	1.468002
H	-0.132815	1.531947	0.983909
H	-0.162707	1.568818	-0.799301
C	-0.953317	-0.292056	-0.421894
H	-0.799797	-0.376458	-1.492476
C	-2.329424	0.009976	0.065027
H	-2.968098	-0.833430	-0.199362
H	-2.356332	0.139509	1.144198
H	-2.736294	0.892814	-0.422414

