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Table I. Structural parameters of conformers of cyclohexene (distances in Å, bond angles in degrees). Results for RHF, BP86, and BLYP are presented as differences.

Param[a]	RHF – B3LYP	BP86 – B3LYP	BLYP – B3LYP	B3LYP
		Twist Cyclohexene		
C1-C2	-0.017	0.009	0.010	1.364
C2-C3	-0.005	0.001	0.008	1.525
C3-C4	-0.010	0.003	0.011	1.548
C4-C5	-0.011	0.003	0.011	1.547
C5-C6	-0.010	0.003	0.011	1.548
C6-C1	-0.005	0.001	0.028	1.525
C1-H	-0.014	0.008	0.007	1.108
C6-H	-0.013	0.008	0.008	1.112
C2-C1-C6	0.10	-0.06	0.01	123.27
C1-C6-C5	-0.18	0.05	0.11	111.93
C6-C5-C4	0.06	0.01	0.02	110.91
C6-C1-H	-0.10	0.13	0.00	117.54
C1-C6-H	-0.11	0.10	0.08	109.51
		Boat Cyclohexene		
C1-C2	-0.018	0.009	0.010	1.363
C2-C3	-0.003	0.001	0.008	1.522
C3-C4	-0.013	0.004	0.012	1.560
C4-C5	-0.010	0.002	0.012	1.568
C5-C6	-0.013	0.004	0.012	1.560
C6-C1	-0.003	0.001	0.008	1.522
C1-H	-0.013	0.008	0.007	1.107
C6-H	-0.014	0.008	0.008	1.115

C2-C1-C6	0.32	-0.17	0.09	118.37
C1-C6-C5	0.03	-0.03	0.09	110.97
C6-C5-C4	0.31	-0.07	0.00	113.44
C6-C1-H	-0.28	0.15	-0.05	120.28
C1-C6-H	-0.07	0.04	0.05	109.07

[a] For the definition of structural parameters, see Figs. 1-2.

Table II. Structural parameters of conformers of cyclohexenyl bromonium ion(distances in Å, bond angles in degrees). Results for RHF, BP86, and BLYP are presented as differences.

Param[a]	RHF – B3LYP	BP86 – B3LYP	BLYP – B3LYP	B3LYP
		Twist Cyclohexenyl bromonium ion		
C1-C2	-0.021	0.012	0.012	1.477
C1-Br	-0.025	-0.006	0.036	2.127
C2-C3	0.004	-0.002	0.005	1.523
C3-C4	-0.012	0.003	0.012	1.556
C4-C5	-0.010	0.003	0.011	1.546
C5-C6	-0.008	0.002	0.011	1.545
C6-C1	0.004	-0.001	0.006	1.511
C1-H	-0.015	0.009	0.007	1.104
C6-H	-0.014	0.008	0.007	1.108
C2-C1-C6	0.41	-0.30	-0.10	120.73
C1-C6-C5	-0.38	0.11	0.24	113.78
C6-C5-C4	0.04	0.10	0.08	110.61
C6-C1-H	-0.33	0.14	0.11	118.40
C1-C6-H	-0.52	0.23	0.16	109.99
C6-C1-Br	-0.51	0.05	0.15	114.55
C2-C1-Br	0.28	-0.23	0.35	70.18
		Boat-down Cyclohexenyl bromonium ion		
C1-C2	-0.021	0.011	0.011	1.473
C1-Br	-0.023	-0.004	0.039	2.129
C2-C3	0.003	-0.001	0.005	1.507
C3-C4	-0.009	0.002	0.011	1.552
C4-C5	-0.010	0.002	0.011	1.567

C5-C6	-0.010	0.002	0.011	1.552
C6-C1	0.003	-0.001	0.005	1.507
C1-H	-0.015	0.009	0.007	1.104
C6-H	-0.017	0.009	0.009	1.120
C2-C1-C6	0.14	-0.11	0.13	118.51
C1-C6-C5	-0.41	0.19	0.34	115.61
C6-C5-C4	0.13	0.04	0.03	115.64
C6-C1-H	-0.01	0.07	0.05	118.86
C1-C6-H	0.63	-0.29	-0.36	101.20
C6-C1-Br	-0.57	0.18	0.20	116.29
C2-C1-Br	0.09	-0.22	0.22	69.78
	Boat-up Cyclohexenyl bromonium ion			
C1-C2	-0.021	0.012	0.012	1.475
C1-Br	-0.021	-0.008	0.037	2.120
C2-C3	0.004	-0.001	0.005	1.514
C3-C4	-0.018	0.004	0.016	1.573
C4-C5	-0.009	0.002	0.010	1.569
C5-C6	-0.018	0.004	0.016	1.572
C6-C1	0.004	-0.001	0.005	1.515
C1-H	-0.015	0.009	0.007	1.104
C6-H	-0.013	0.009	0.008	1.105
C2-C1-C6	0.06	-0.16	0.21	116.21
C1-C6-C5	0.81	-0.58	-0.26	105.74
C6-C5-C4	0.15	-0.03	0.05	113.30
C6-C1-H	0.16	-0.16	-0.03	120.13
C1-C6-H	-0.61	0.35	0.29	110.91
C6-C1-Br	-1.24	0.58	0.43	117.29

C2-C1-Br	0.22	-0.17	0.26	69.61

[a] For the definition of structural parameters, see Fig. 3-5.

C_6H_{10} (twist conformation) BP86 optimized geometry

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.517716	.043554	.111290
2	6	.683764	1.319603	.058467
3	6	.702535	-1.201469	-.327141
4	1	2.426474	.161602	-.532793
5	1	1.910257	-.097935	1.154275
6	6	-.683773	1.319597	-.058470
7	6	-.702521	-1.201482	.327124
8	1	1.223626	2.294140	.118657
9	1	.586161	-1.191376	-1.441749
10	1	1.259166	-2.136431	-.068725
11	6	-1.517719	.043543	-.111268
12	1	-1.223644	2.294126	-.118704
13	1	-.586142	-1.191419	1.441732
14	1	-1.259147	-2.136442	.068689
15	1	-2.426453	.161582	.532852
16	1	-1.910304	-.097927	-1.154238

SCF Done: E(RB-P86) = -40.0011180913 A.U. after 18 cycles

C_6H_{10} (boat conformation) BP86 optimized geometry

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.704614	1.303854	-.189398
2	6	-.667242	1.323171	-.189928
3	6	1.406588	.071070	.364205
4	1	1.297043	2.165299	-.575244
5	6	-1.404244	.110889	.363636
6	6	.767637	-1.237815	-.205106
7	1	-1.234858	2.200980	-.576197
8	1	1.309800	.063768	1.482825
9	1	2.502008	.089869	.147586
10	6	-.802270	-1.216268	-.203973
11	1	-1.308600	.101718	1.482320
12	1	-2.498531	.160613	.146148
13	1	1.148579	-2.113186	.377401
14	1	1.134324	-1.374143	-1.252133
15	1	-1.206335	-2.079599	.380918
16	1	-1.173921	-1.344728	-1.250238

SCF Done: E(RB-P86) = -39.9930160741 A.U. after 17 cycles

$C_6H_{10}Br^+$ (twist conformation) BP86 optimized geometry

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.077634	-1.504334	.423733
2	6	-.022729	-.623938	1.050652
3	6	-1.832609	-.838126	-.750876
4	1	-.647801	-2.504401	.175101
5	1	-1.779297	-1.694181	1.285666
6	35	1.506540	.004572	-.277616
7	6	-.073099	.854149	.876539
8	6	-1.191230	1.529116	.097451
9	6	-2.337103	.570704	-.348981
10	1	.546963	-1.015293	1.922638
11	1	.500021	1.463668	1.609229
12	1	-.749721	2.092566	-.761599
13	1	-1.165592	-.785571	-1.647960
14	1	-2.693638	-1.485738	-1.036786
15	1	-1.573594	2.330672	.781456
16	1	-3.069329	.469476	.490478
17	1	-2.890487	1.043346	-1.192779

SCF Done: E(RB-P86) = -53.1413215235 A.U. after 19 cycles

$C_6H_{10}Br^+$ (boat down conformation) BP86 optimized geometry

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-.014462	-.741259	1.062918
2	6	-.014855	.743305	1.061323
3	6	-1.201716	-1.458544	.475429
4	1	.603288	-1.260404	1.828994
5	35	1.421619	.000066	-.317782
6	6	-1.202851	1.458812	.473155
7	6	-1.853093	.784002	-.766794
8	6	-1.849859	-.786534	-.766951
9	1	.602746	1.264374	1.826202
10	1	-.966690	2.533333	.291560
11	1	-1.309269	1.152272	-1.669621
12	1	-1.300709	-1.152541	-1.667496
13	1	-1.910758	-1.454159	1.353940
14	1	-.965040	-2.533396	.296497
15	1	-1.910585	1.456338	1.352729
16	1	-2.891948	1.176606	-.860207
17	1	-2.886666	-1.183422	-.864686

SCF Done: E(RB-P86) = -53.1391195423 A.U. after 22 cycles

$C_6H_{10}Br^+$ (boat up conformation) BP86 optimized geometry

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-.124253	.743547	.643267
2	6	-.123591	-.742879	.643214
3	6	-1.073041	1.408086	-.331126
4	1	.163872	1.265556	1.582739
5	35	1.704973	.000019	-.110060
6	6	-1.072355	-1.408006	-.331012
7	6	-2.487201	-.785578	-.018962
8	6	-2.487673	.784853	-.019229
9	1	.164151	-1.264557	1.582982
10	1	-.790833	-1.184280	-1.385857
11	1	-.791332	1.184282	-1.385904
12	1	-1.069251	2.513215	-.201999
13	1	-1.067932	-2.513117	-.201712
14	1	-3.186850	-1.187589	-.789525
15	1	-2.849479	-1.174338	.962612
16	1	-3.187219	1.186247	-.790211
17	1	-2.850488	1.173783	.962072

SCF Done: E(RB-P86) = -53.1342075744 A.U. after 20 cycles