

Supplementary Material

Computational Study of Hydrido Boronium Dications and Comparison with the Isoelectronic Carbon Analogs

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<p>S1. CCSD(T)/cc-PVTZ coordinates of 1 B 0.0000 0.0000 0.2045 H 0.0000 0.0000 1.4141 H 0.0000 0.4445 -1.2184 H 0.0000 -0.4445 -1.2184</p> <p>S3. CCSD(T)/cc-PVTZ coordinates of 3 B 0.0000 0.0000 0.0000 H 0.0000 0.5212 1.2126 H 0.0000 -0.5212 1.2126 H 0.0000 -0.5212 -1.2126 H 0.0000 0.5212 -1.2126</p> <p>S5. CCSD(T)/cc-PVTZ coordinates of 5 B 0.0000 0.1980 0.0000 H -1.0026 -0.6328 0.4121 H 1.0026 -0.6329 0.4122 H 1.0026 -0.6327 -0.4124 H 0.0001 0.7708 -1.0302 H -1.0026 -0.6328 -0.4125 H -0.0000 0.7702 1.0306</p> <p>S7. CCSD(T)/cc-PVTZ coordinates of 7 B 0.0000 -0.0000 0.0704 H -1.0585 -0.3944 -0.6940 H 0.8708 -0.7194 -0.6941 H 1.0412 -0.8601 0.1505 H 0.1876 1.1137 -0.6941 H 0.2244 1.3317 0.1505 H -1.2655 -0.4716 0.1506 H 0.0001 0.0001 1.2784</p> <p>S9. CCSD(T)/cc-PVTZ coordinates of 9 B -0.0848 1.0693 0.0000 B -0.0848 -0.6827 0.0000 H -0.1663 2.2450 0.0000 H 1.2564 -1.0381 0.0000 H 0.7950 -1.7580 0.0000 H -1.0375 -1.3821 0.0000</p> <p>S11. CCSD(T)/cc-PVTZ coordinates of 11 B 0.9985 -0.0563 0.0004 B -0.6561 0.1435 -0.0002 H 0.1710 -0.0043 -1.0545 H -1.2427 -1.0955 -0.0003 H 2.1754 -0.0683 -0.0024 H -1.1246 1.2364 0.0004 H 0.1711 -0.0045 1.0549 H -1.8626 -0.4997 0.0004</p>	<p>S2. CCSD(T)/cc-PVTZ coordinates of 2 B 0.0000 0.0000 0.2168 H 0.0000 1.1043 0.6039 H 0.0000 -1.1043 0.6039 H 0.0000 0.4078 -1.1459 H 0.0000 -0.4078 -1.1459</p> <p>S4. CCSD(T)/cc-PVTZ coordinates of 4 B -0.0000 0.1578 0.0000 H 1.3835 -0.1615 0.0000 H -0.0000 1.3417 0.0000 H -1.3834 -0.1616 0.0000 H -0.9288 -0.9040 -0.0000 H 0.9288 -0.9039 0.0000</p> <p>S6. CCSD(T)/cc-PVTZ coordinates of 6 B -0.0000 0.0000 -0.0000 H 0.1122 -1.2523 -0.4542 H 1.0285 0.7233 -0.4542 H -1.1406 0.5289 -0.4542 H -1.1406 0.5289 0.4542 H 1.0284 0.7233 0.4542 H 0.1122 -1.2522 0.4542</p> <p>S8. CCSD(T)/cc-PVTZ coordinates of 8 B 0.0000 0.0000 0.2614 H 0.0000 0.0000 -1.5421 H 0.0000 1.2842 -0.0211 H 0.0000 1.1615 0.8865 H -1.1121 -0.6421 -0.0211 H -1.0059 -0.5808 0.8865 H 1.1121 -0.6421 -0.0211 H 1.0059 -0.5808 0.8865 H 0.0000 0.0000 -2.3611</p> <p>S10. CCSD(T)/cc-PVTZ coordinates of 10 B 0.0000 0.0000 0.8656 B 0.0000 0.0000 -0.8656 H 0.0000 1.0765 0.0000 H 0.0000 -1.0765 0.0000 H 0.0000 0.0000 2.0483 H 0.0000 0.0000 -2.0483</p> <p>S12. CCSD(T)/cc-PVTZ coordinates of 12 B -0.0045 -0.9139 0.0000 B -0.0045 0.5960 0.0000 H 0.0261 -2.0898 0.0000 H 1.1288 -0.0015 0.0000 H -0.5445 -0.0548 0.9805 H -0.5445 -0.0548 -0.9805 H 0.4249 1.8971 0.0000 H -0.4461 1.8930 0.0000</p>
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S13. CCSD(T)/cc-PVTZ coordinates of 13

B -0.8399 -0.1356 -0.0908
 B 0.8399 0.1356 -0.0908
 H -1.3436 0.8039 0.7827
 H -2.0037 0.3916 0.4332
 H -1.4535 -0.8911 -0.7620
 H 2.0037 -0.3915 0.4332
 H 1.3436 -0.8039 0.7827
 H 1.4535 0.8912 -0.7619

S15. CCSD(T)/cc-PVTZ computed frequencies of 1

Frequency (cm ⁻¹)	Intensity (km/mol)
570	1993
639	2250
882	573
1475	216
2505	1288
2959	713

S17. CCSD(T)/cc-PVTZ computed frequencies of 3

Frequency (cm ⁻¹)	Intensity (km/mol)
82	799
194	431
497	262
952	0
1665	0
1705	0
1805	813
2065	0
2225	973

S19. CCSD(T)/cc-PVTZ computed frequencies of 5

Frequency (cm ⁻¹)	Intensity (km/mol)
485	65
662	0
841	65
901	57
1064	2
1080	0
1094	0
1320	16
1340	22
1815	0
1845	120
2670	21
2788	54
3360	48
3423	1

S14. CCSD(T)/cc-PVTZ coordinates of 14

B 0.0000 0.8502 0.0000
 B 0.0000 -0.8502 0.0000
 H -0.8679 1.6459 0.0000
 H 0.8679 -1.6459 0.0000
 H 1.0001 1.8135 0.0000
 H -1.0001 -1.8135 0.0000
 H 1.3802 1.0712 0.0000
 H -1.3802 -1.0712 0.0000
 H 0.0000 0.0000 -1.0318
 H 0.0000 0.0000 1.0318

S16. CCSD(T)/cc-PVTZ computed frequencies of 2

Frequency (cm ⁻¹)	Intensity (km/mol)
839	0
938	0
975	362
977	555
1258	280
1621	56
2714	34
2916	247
3507	32

S18. CCSD(T)/cc-PVTZ computed frequencies of 4

Frequency (cm ⁻¹)	Intensity (km/mol)
521	122
602	0
714	251
819	61
953	1
1289	6
1364	161
1426	249
1585	276
2679	294
3023	47
3040	451

S20. CCSD(T)/cc-PVTZ computed frequencies of 6

Frequency (cm ⁻¹)	Intensity (km/mol)
457	522
767	0
767	0
834	0
842	111
842	111
1507	417
1507	417
1702	0
1754	0
1754	0
1822	748
2621	165
2621	165
2807	0

S21. CCSD(T)/cc-PVTZ computed frequencies of 7		S22. CCSD(T)/cc-PVTZ computed frequencies of 8	
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
681	565	296	11
741	1	296	11
741	1	373	1062
764	0	673	3407
850	92	673	3407
850	92	677	1985
1025	3	832	89
1025	3	832	89
1419	66	883	73
1592	155	883	73
1592	155	922	0
1721	143	1444	141
1721	143	1444	141
1745	407	1640	481
2488	328	1891	6
2942	213	1891	6
2942	213	1937	272
3012	1	2588	61
		2588	61
		2699	564
		2988	8355
S23. CCSD(T)/cc-PVTZ computed frequencies of 9		S24. CCSD(T)/cc-PVTZ computed frequencies of 10	
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
461	32	436	13
522	6	496	0
710	19	641	0
737	39	731	0
783	104	877	0
890	4	1084	20
1032	36	1284	178
1392	24	1514	0
1615	84	1904	0
2701	118	1949	171
2757	198	2692	411
3124	122	2729	0
S25. CCSD(T)/cc-PVTZ computed frequencies of 11		S26. CCSD(T)/cc-PVTZ computed frequencies of 12	
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
311	33	128	10
522	3	435	2
700	24	480	21
705	41	682	3045
723	0	695	3097
833	93	1052	214
860	95	1144	134
1039	0	1191	86
1062	16	1322	201
1445	142	1368	39
1575	107	1375	103
1665	52	1596	167
1685	2	1785	0
2028	10	2160	8
2054	155	2189	22
2627	171	2198	37
2759	205	2771	2482
3089	169	3019	245

S27. CCSD(T)/cc-PVTZ computed frequencies of 13		S28. CCSD(T)/cc-PVTZ computed frequencies of 14	
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
289	82	335	793
433	157	456	0
451	67	501	1
709	83	607	193
711	54	671	0
755	94	778	0
916	9	846	0
931	10	859	1859
1006	21	890	260
1069	54	1040	1605
1345	88	1063	0
1396	80	1081	0
1679	176	1363	36
1690	19	1417	0
2699	211	1560	423
2702	75	1594	0
3122	190	1630	96
3127	20	1722	0
		2048	7
		2065	0
		2732	1032
		2737	0
		3332	402
		3370	0