
بسم الله الرحمن الرحيم

Title

The B–C and C–C bonds as preferred electron source for H-bond and Li-bond interactions in complex pairing of C4B2H6 with HF and LiH molecules

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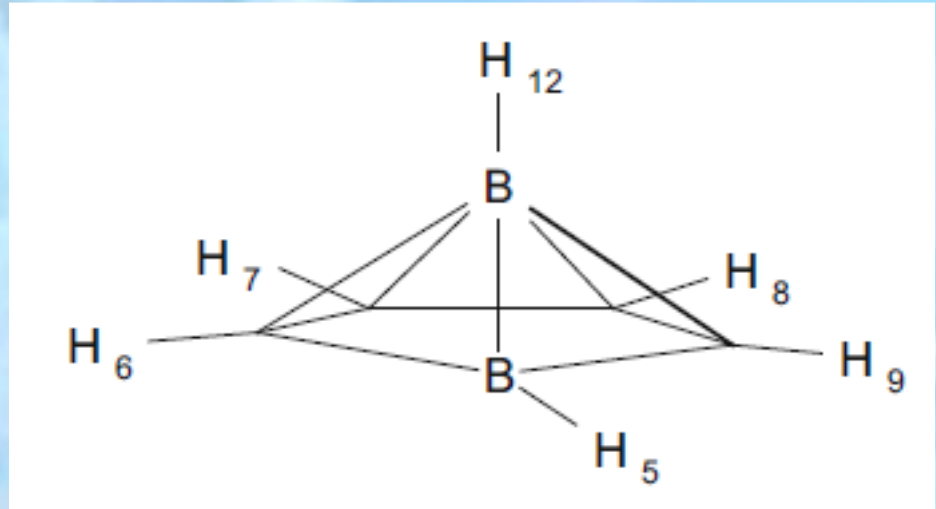
Introduction

- ✓ C4B2H6 and its derivatives have been subject of heoretical studies, molecular and electronic structure calculations, dipole moment, and ionization potential
- ✓ An interesting overview of activities of C4B2H6 could be pictured through its intermolecular interactions such as H-bonding, DHB-bonding and Li-bonding. The traditional idea that the hydrogen atoms involved in the HB should be electron-deficient has been overcome with those cases where both interacting atoms were hydrogen, one positively charged and another negatively charged, and this special kind of hydrogen bond has designated as dihydrogen bond.

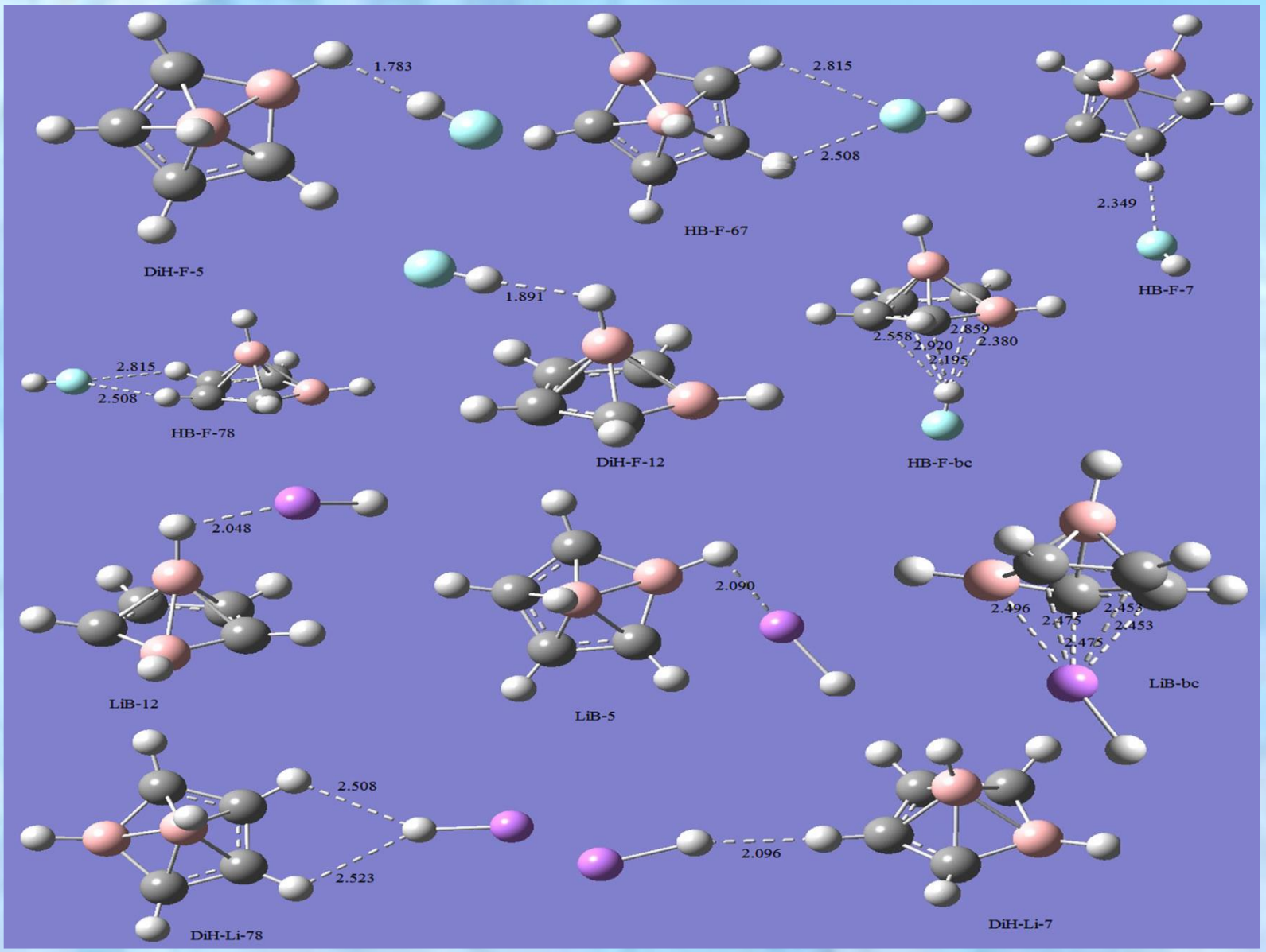
Schematic representation of C4B2H6 structure



Applications of Carboranes

- ✓ Materials Science
- ✓ Nonlinear Optics
- ✓ Medicinal Chemistry
- ✓ Boron Neutron Capture Therapy (BNCT)

C4B2H6–LiH Complexes



The SE_{uncorr} (uncorrected stabilization energies), BSSE, DZPE, and SE_{corr} (corrected with BSSE and DZPE) in kcal mol_{-1} calculated at MP2/6–311++G(2d,2p)

Complex	SE^{uncorr}	BSSE	ΔZPE	SE^{cor}
HB–F-67	−1.75	0.57	0.47	−0.71
HB–F-7	−1.74	0.53	0.42	−0.79
HB–F-78	−2.03	0.63	0.55	−0.84
DHB–F-12	−3.29	1.00	1.23	−1.06
DHB–F-5	−4.41	1.01	1.30	−2.10
HB–F-bc	−6.23	1.63	1.43	−3.17
LiB-bc	−14.73	1.83	1.47	−11.43
LiB-5	−10.45	0.97	1.26	−8.22
LiB-12	−7.46	0.91	1.13	−5.42
DHB–Li-7	−4.30	0.39	0.74	−3.17
DHB–Li-78	−4.30	0.38	0.73	−3.19

Bond length (in A °) of C4B2H6–LiH complexes at MP2/6–311++(2d, 2p)

Bond	$C_4B_2H_6$ *r*	LiB-bc Δ*r*	LiB-5	LiB-12	DHB–Li-7	DHB–Li-78	HB–F-67	HB–F-78 Δ*r*	HB–F-7	DHB–F-12	DHB–F-12	HB–F-bc
C1–H6	1.078	0	0.004	0.001	0.001	0.001	0	0.001	0.001	0	−0.001	0
C2–H7	1.077	−0.001	0	0.001	0.005	0	0	0	0	0.001	−0.001	0
C3–H8	1.077	−0.001	0.001	0.003	0	0	0	0	0	0.001	−0.001	0
C4–H9	1.078	0	0	0.002	0.001	0.001	0.002	0.002	0.001	0	−0.001	0
B10–H5	1.183	−0.004	0.009	−0.001	0.002	0.002	0.001	0.001	0.001	−0.001	0.006	−0.002
B11–H12	1.173	−0.001	−0.001	0.011	0.002	0.002	0.001	0.001	0.001	0.006	−0.001	0
B10–B11	1.839	−0.019	−0.022	−0.007	−0.003	−0.003	−0.001	−0.001	0	−0.004	−0.002	−0.01
C1–B10	1.533	0.006	0.004	0.002	0	0	0	0	−0.001	0.001	−0.005	0.006
C1–B11	1.717	−0.001	−0.002	−0.016	−0.003	−0.002	−0.001	−0.001	−0.002	−0.006	0.004	−0.005
C1–C2	1.442	0.004	−0.001	0.005	0.001	0.001	0	0.001	0.001	0.001	−0.001	0.004
C2–C3	1.426	0.001	−0.001	0	0	−0.002	0	−0.001	0	0.002	−0.002	−0.001
C2–B11	1.718	0.001	0.006	−0.012	0.001	−0.002	−0.001	−0.001	0	−0.004	0.002	−0.002
C3–C4	1.442	0.004	−0.003	0.004	0.002	0.002	0.001	0.001	0.001	0.001	−0.001	−0.001
C3–B11	1.718	−0.002	0.008	−0.002	−0.004	−0.002	−0.001	−0.001	−0.002	−0.003	0.002	0.004
C4–B10	1.533	0.006	−0.01	0.003	−0.001	0	0	0	0	0.001	−0.003	−0.001
C4–B11	1.717	−0.001	0.011	−0.009	−0.001	−0.002	0	−0.001	−0.001	−0.006	0.004	0.002
Li–H	1.604	0.026	0.021	0.017	0.001	0.002	0.001	0.001	0.001	0.005	0.004	0.01

Unscaled vibrational frequencies (cm−1) with corresponding intensities (values given in parenthesis, km mol−1) for C4B2H6–HLi complexes

	$C_4B_2H_6$	LiB-5		LiB-12		DHB–Li-7		DHB–Li-78		LiB-bc	
	ν	ν	$\Delta\nu$	ν	$\Delta\nu$	ν	$\Delta\nu$			ν	$\Delta\nu$
C1–H6	3246 (0)	3213 (6)	−33	3247 (0)	1	3244 (3)	−2	3242	−25	3257 (0)	−10
C2–H7	3267 (0)	3271 (1)	4	3263 (1)	−4	3197 (110)	−70	3242	−25	3283 (5)[a]	16
C3–H8	3267 (0)	3261 (1)	4	3237 (7)	−30	3260 (1)	−7	3242	−4	3274 (6)[b]	28
C4–H9	3246 (0)	3251 (1)	14	3237 (7)	−9	3242 (1)	−4	2781	−5	3257 (0)	22
B10–H5	2712 (105)	2645 (100)	−67	2722 (87)	10	2699 (126)	−13	2699	−13	2746 (66)	34
B11–H12	2786 (45)	2803 (30)	17	2698 (104)	−88	2781 (50)	−5	3242	−4	2808 (31)	11
X···Y	–	247 (37)	–	209 (165)	–	101 (78)	–	1439	21	267 (18)	–
H–Li	1418 (229)	1361 (389)	−58	1370 (318)	−49	1442 (349)	24			1343 (440)	−75

Topological parameters for the fully optimized complexes

Complex	H-bond	ρ_{BCP}	$\nabla^2_{\rho BCP}$	−Gc/Vc
LiB-5	Li···H5	0.0122	0.0649	1.2177
LiB-12	Li···H12	0.0108	0.0587	1.2641
DHB–Li-7	H14···H7	0.0113	0.0246	1.06
DHB–Li-78	H14···H7	0.0062	0.0158	1.2115
	H14···H8	0.006	0.0156	1.2168
LiB-bc	Li···B–C	0.0125	0.0665	1.218
HB–F-67	F13···H6	0.0039	0.018	1.3066
	F13···H7	0.0064	0.0284	1.2116
HB–F-7	F14···H7	0.0082	0.0343	1.1605
HB–F-78	F13···H7	0.0054	0.0241	1.2401
	F13···H8	0.0056	0.0246	1.2349
DHB–F-12	H13···H12	0.0144	0.0399	1.0536
DHB–F-5	H13···H5	0.0165	0.0453	1.0217
HB–F-bc	H···B–C	0.0184	0.049	1.0236