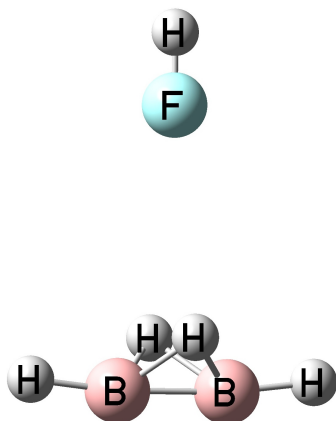


Electronic Supporting Information

Boron-boron single bond in diborane(4) as a non-classical electron donor for hydrogen bonding.

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Fig. ESI-1. Optimized geometry of the less stable minima of $B_2H_4 \cdot HF$ calculated at the MP2/aug-cc-pVTZ computational level ($E = -152.204994$ Hartree, $E_i + BSSE = -1.6$ kJ/mol).



Optimized geometries of the most stable complexes at the MP2/aug-cc-pVTZ computational level.

$B_2H_4:HF$

B,0.7342456982,0.,0.8998330084
B,-0.7342456982,0.,0.8998330084
H,1.8976824488,0.,0.7810152173
H,-1.8976824488,0.,0.7810152173
H,0.,-0.9025579357,0.2486061305
H,0.,0.9025579357,0.2486061305
H,0.,0.,2.9957439331
F,0.,0.,3.9345750969

$B_2H_4:HNC$

B,0.7338134706,0.,0.8196308041
B,-0.7338134706,0.,0.8196308041
H,1.8977927673,0.,0.7021747468
H,-1.8977927673,0.,0.7021747468
H,0.,-0.9018180327,0.1662798558
H,0.,0.9018180327,0.1662798558
H,0.,0.,3.1031618012
N,0.,0.,4.116377771
C,0.,0.,5.293517357

$B_2H_4:HCl$

B,0.7339115033,0.,0.838020501
B,-0.7339115033,0.,0.838020501
H,1.8978691042,0.,0.7194538143
H,-1.8978691042,0.,0.7194538143
H,0.,-0.9011874662,0.1816636529
H,0.,0.9011874662,0.1816636529
H,0.,0.,3.1087312163
Cl,0.,0.,4.4022205879

$B_2H_4:HCN$

B,0.7331406729,0.,0.7054667518
B,-0.7331406729,0.,0.7054667518
H,1.8971508936,0.,0.5834993449
H,-1.8971508936,0.,0.5834993449
H,0.,-0.8988249543,0.0435061043
H,0.,0.8988249543,0.0435061043
H,0.,0.,3.304693777
C,0.,0.,4.3759774328
N,0.,0.,5.5436121306

$B_2H_4:HCCH$

B,0.7329134545,0.,0.6054565512
B,-0.7329134545,0.,0.6054565512
H,1.8969522124,0.,0.4818665475

H,-1.8969522124,0.,0.4818665475
H,0.,-0.8970984281,-0.0621810162
H,0.,0.8970984281,-0.0621810162
H,0.,0.,3.3381710119
C,0.,0.,4.403978952
C,0.,0.,5.6173736586
H,0.,0.,6.6794199448

B₂H₄:H₂
B,0.7326262777,0.,0.4496956658
B,-0.7326262777,0.,0.4496956658
H,1.89636566,0.,0.3217309608
H,-1.89636566,0.,0.3217309608
H,0.,-0.8946321007,-0.2240735929
H,0.,0.8946321007,-0.2240735929
H,0.,0.,3.7484219603
H,0.,0.,4.4871608847