Supporting Information

for

Conformational analysis and intramolecular interactions in monosubstituted phenylboranes and phenylboronic acids

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^{1}H and ^{11}B NMR spectra for 2-fluorophenylboronic acid.

Potential energy surfaces for compounds **3–9**.

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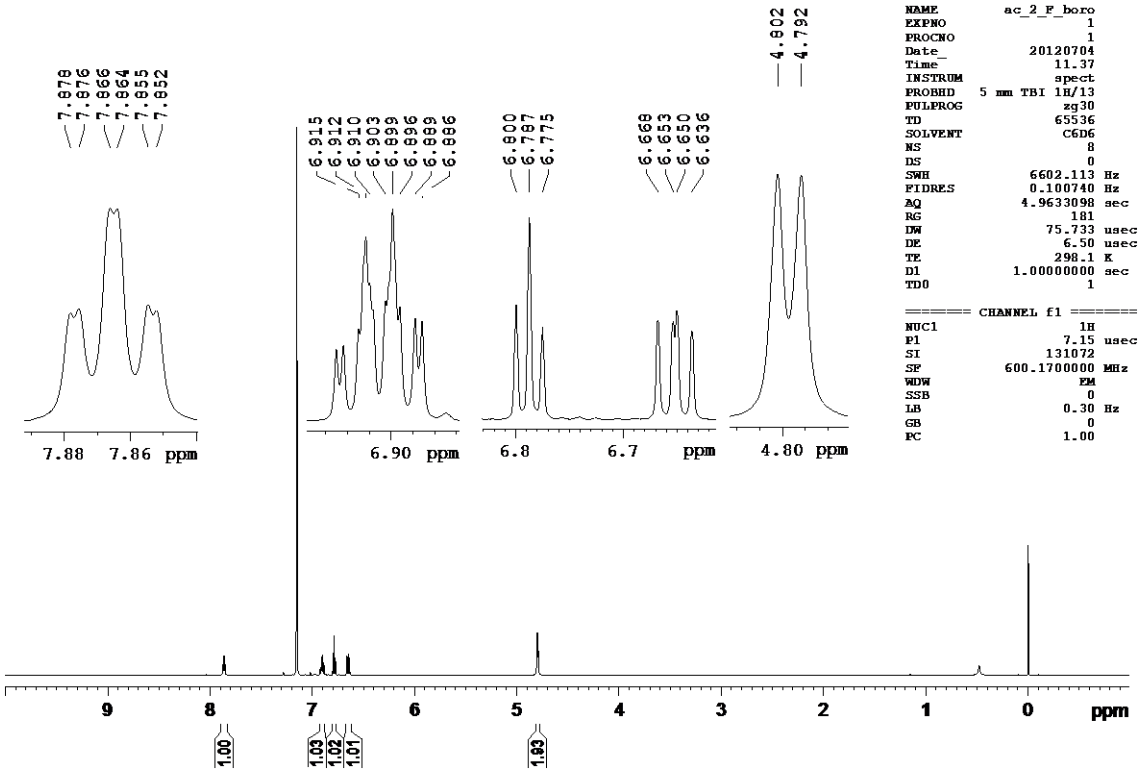


Figure S1: ^{1}H NMR spectrum for **1** in C_6D_6 solution (2 mg mL^{-1}).

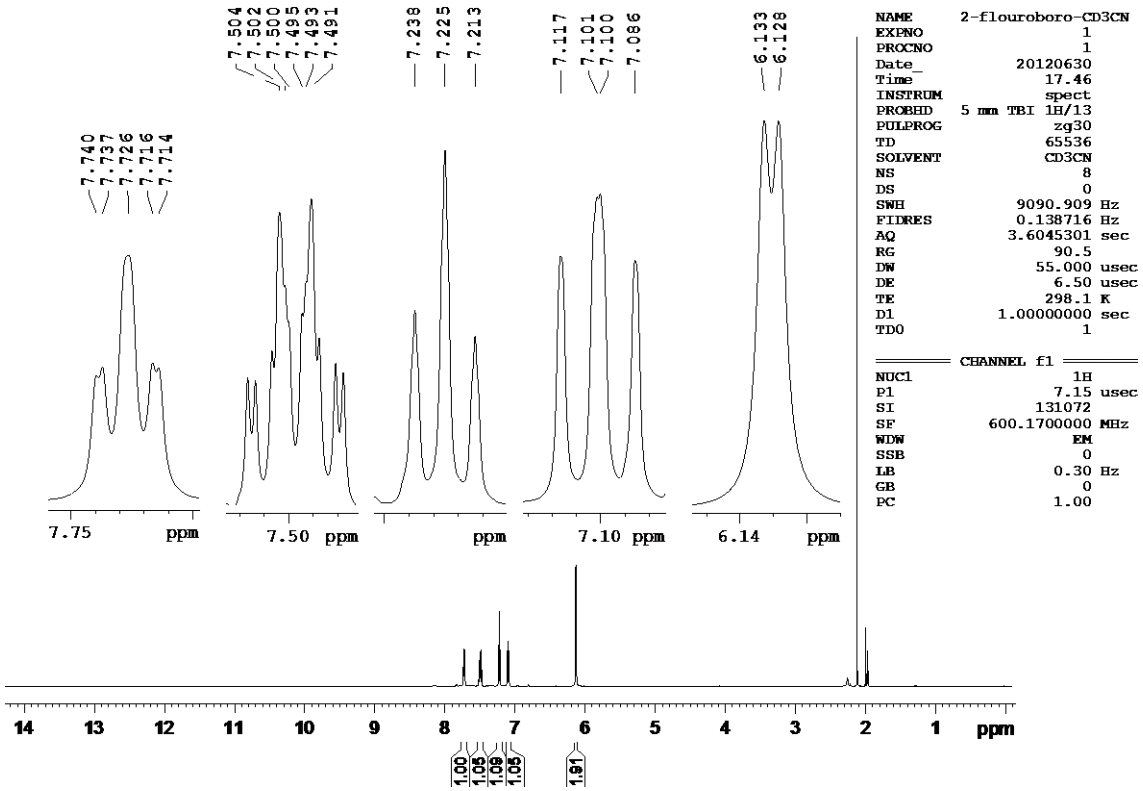
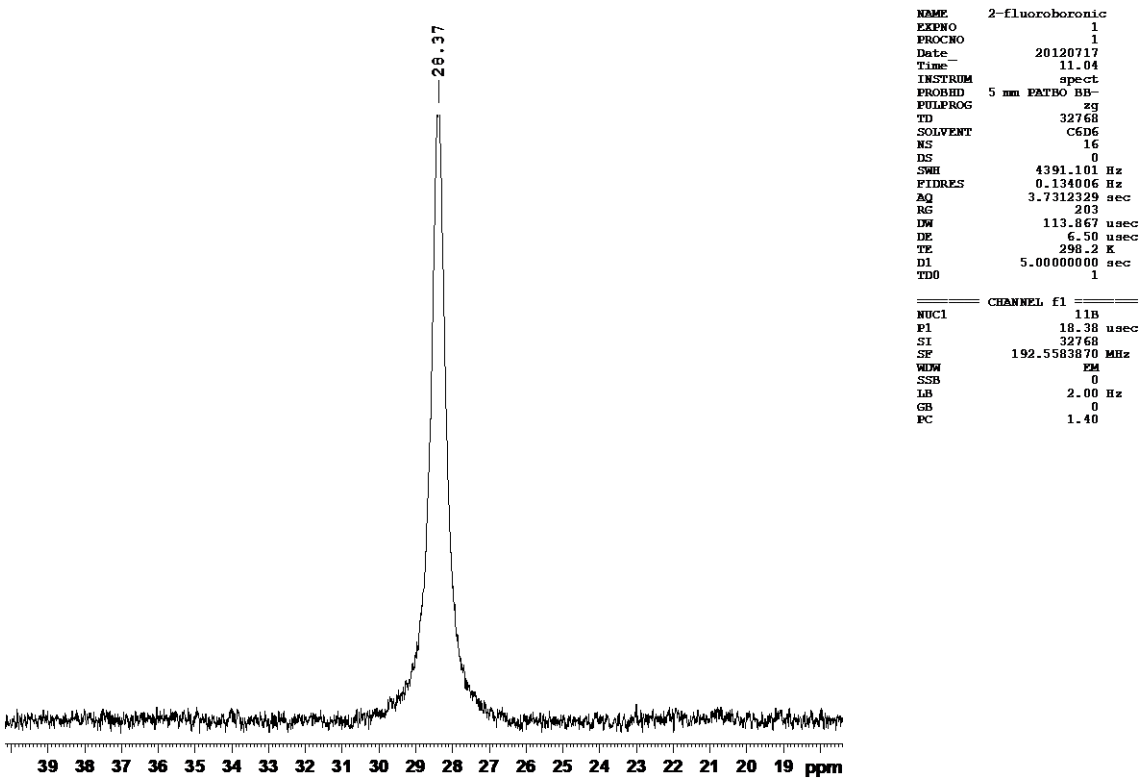


Figure S2: ^{1}H NMR spectrum for **1** in CD_3CN solution (20 mg mL^{-1}).



NAME	2-fluoroboronic
EXPNO	1
PROCNO	1
Date_	20120717
Time_	11.04
INSTRUM	spect
PROBHD	5 mm PATBO BB-
PULPROG	zg
TD	32768
SOLVENT	C6D6
NS	16
DS	0
SWH	4391.101 Hz
FIDRES	0.134006 Hz
AQ	3.7312329 sec
RG	203
DW	113.867 usec
DE	6.50 usec
TE	298.2 K
D1	5.00000000 sec
TD0	1
======	CHANNEL f1 ======
NUC1	11B
P1	18.38 usec
SI	32768
SF	192.5583870 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

Figure S3: ^{11}B NMR spectrum for **1** in C_6D_6 solution (2 mg mL^{-1}).

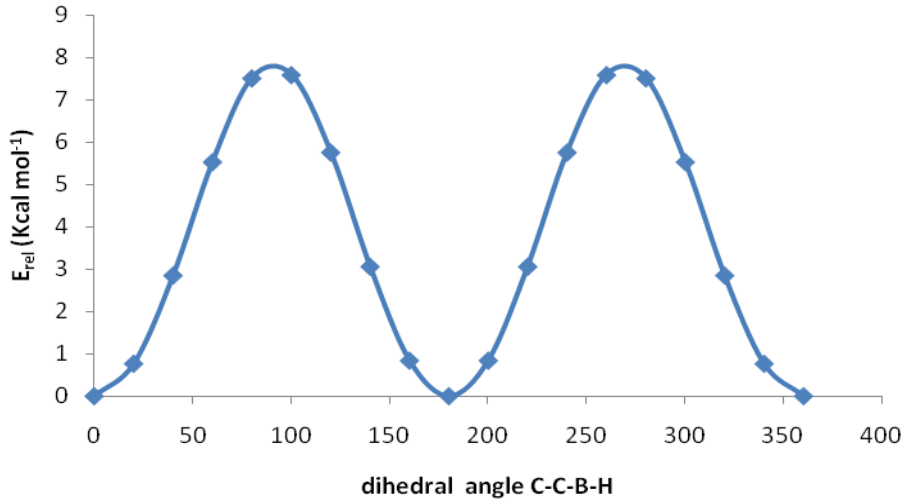


Figure S4: Potential energy surface for 2-fluorophenylborane **(3).**

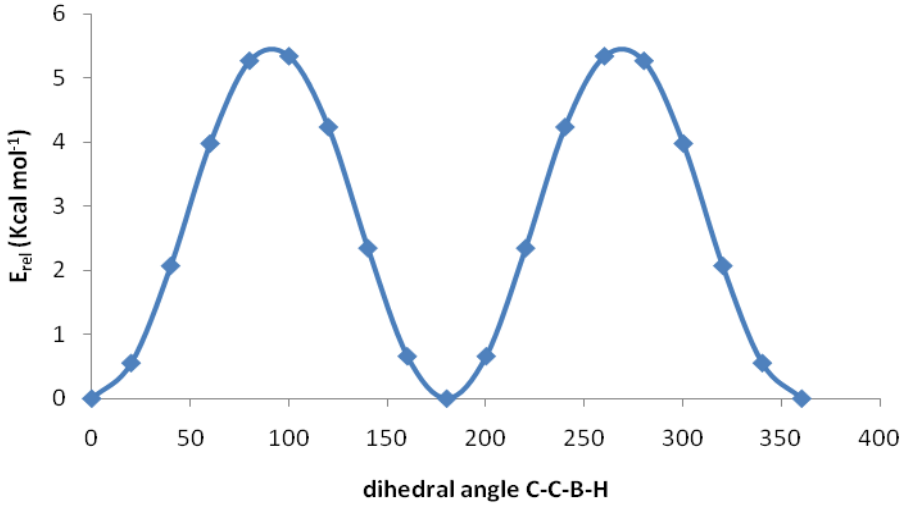


Figure S5: Potential energy surface for 2-chlorophenylborane **(4).**

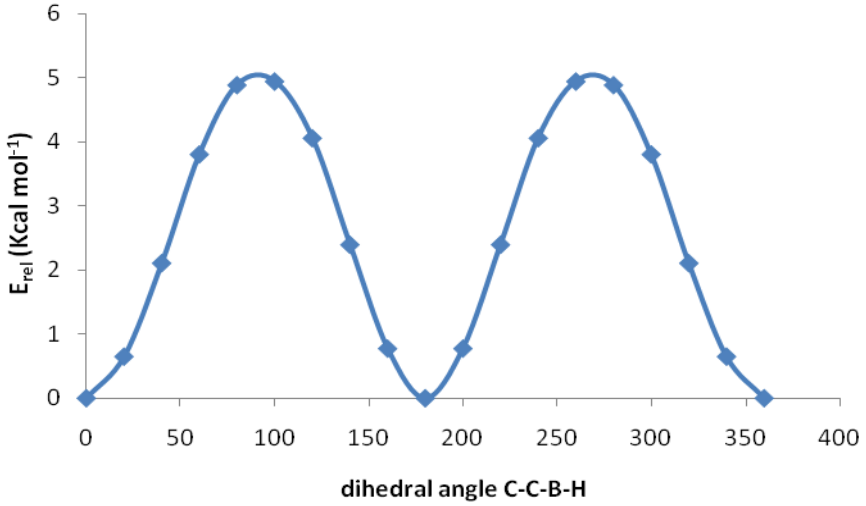


Figure S6: Potential energy surface for 2-bromophenylborane **(5).**

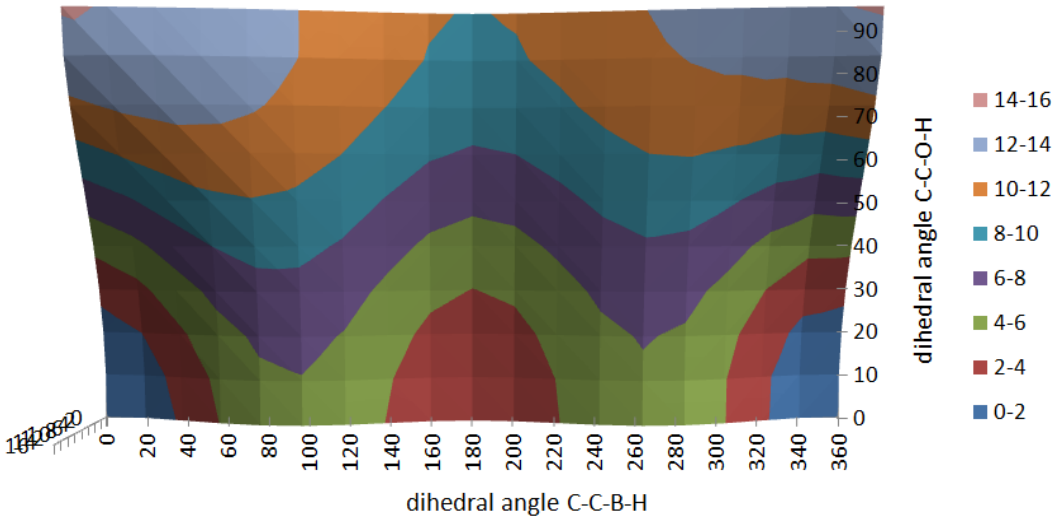


Figure S7: Potential energy surface for 2-hydroxyphenylborane **(6).**

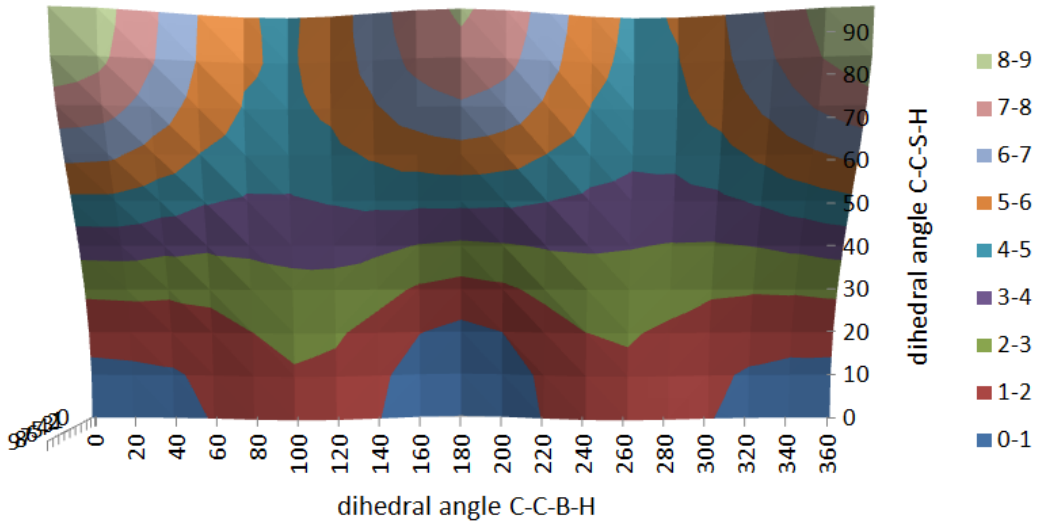


Figure S8: Potential energy surface for 2-sulfanylphenylborane **(7).**

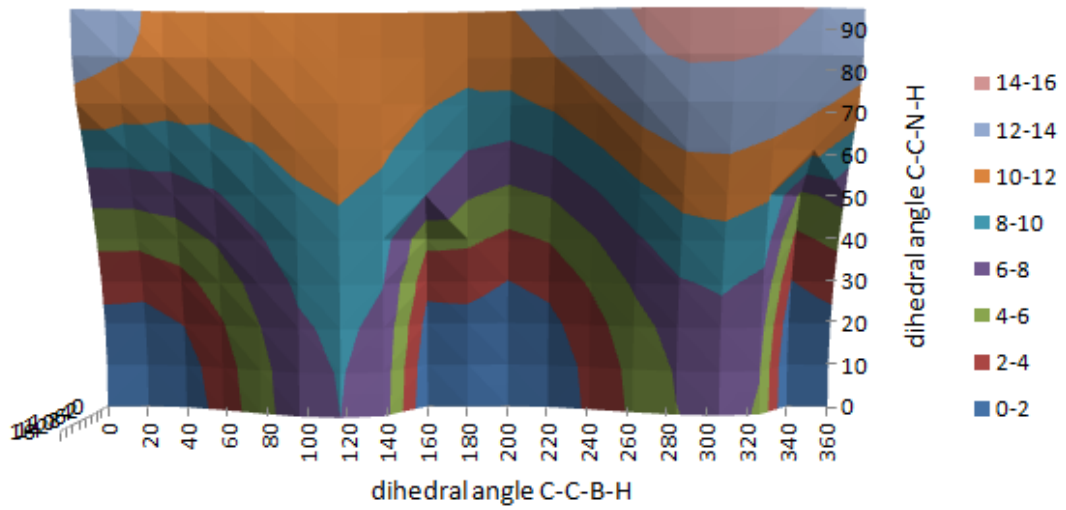


Figure S9: Potential energy surface for 2-aminophenylborane **(8).**

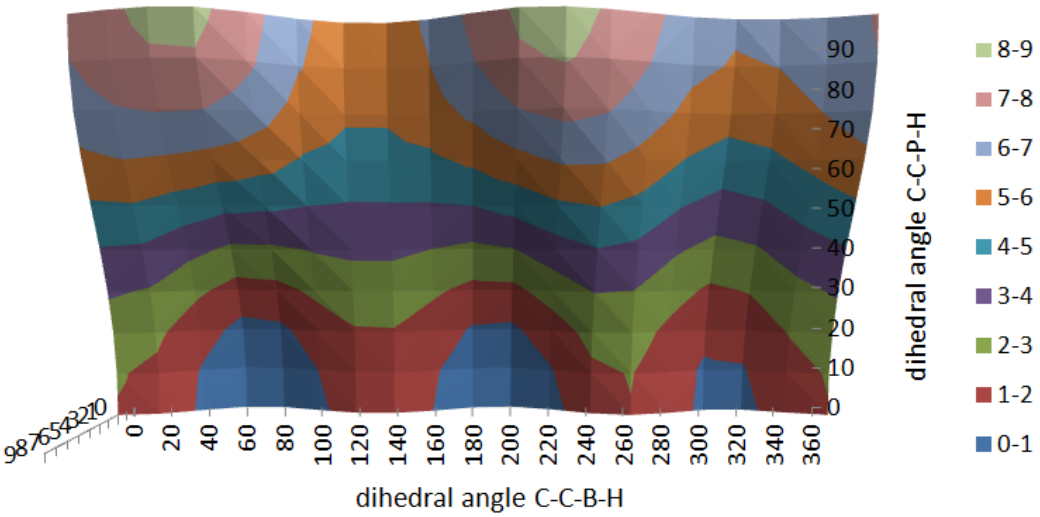


Figure S10: Potential energy surface for 2-phosphanylphenylborane **(9)**.