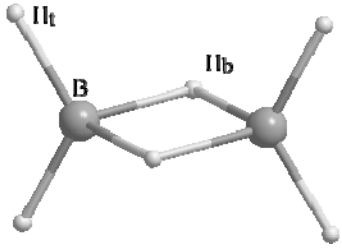
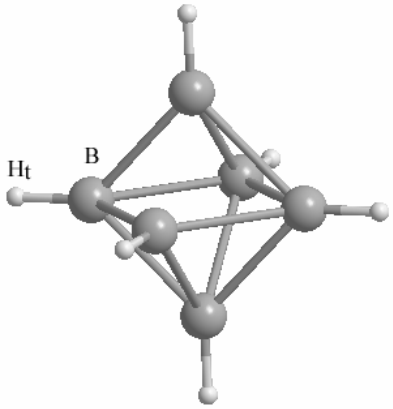
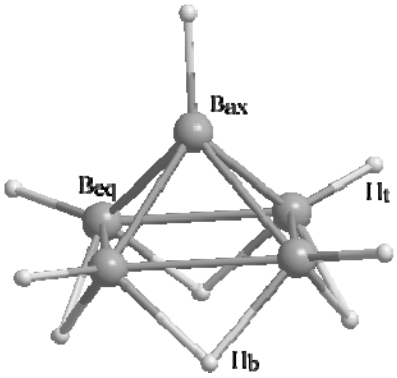
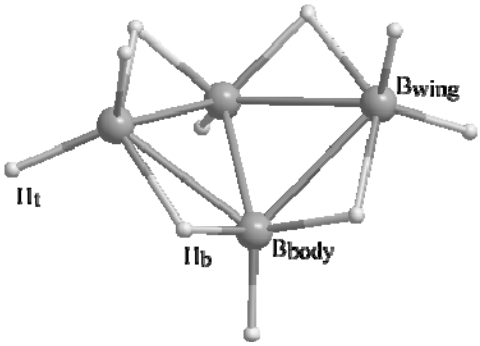
Supplementary Information

Table 1. Borane structures.

Compound	Structure	Bond lengths (Å)	Reference
B_2H_6		B-H_t: 1.20 (1.19) B-H_b: 1.32 (1.32) B-B: 1.77 (1.78)	1
$B_6H_6^{2-}$		B-H_t: 1.74 (1.69)	2
B_5H_9		B_{ax} - B_{eq}: 1.69 (1.69) B_{eq}-B_{eq}: 1.80 (1.80)	3
B_4H_{10}		B_{wing} – B_{body}: 1.86 (1.87) B_{body} – B_{body}: 1.72 (1.74) B_{body} – H_t: 1.19 (1.21) B_{body} – H_b: 1.27 (1.24) B_{wing} – H_t: 1.20 (1.23) B_{wing} - H_b: 1.42 (1.43)	4

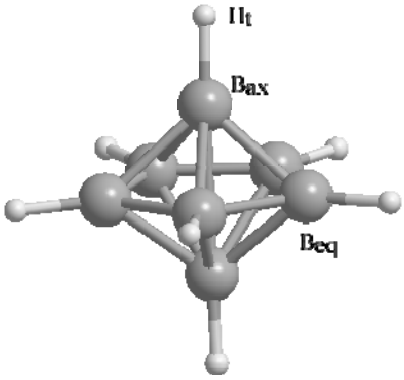
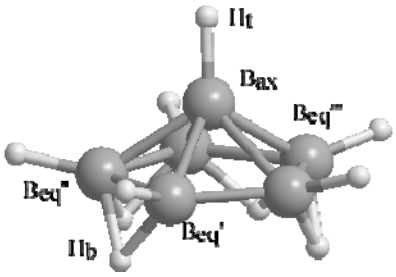
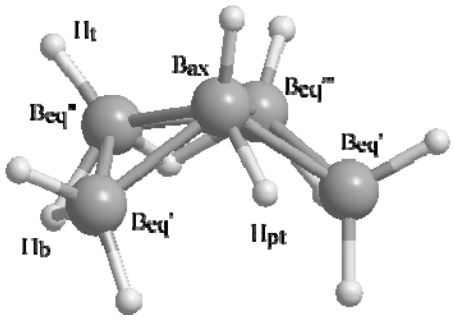
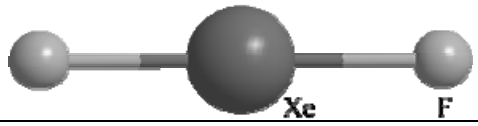
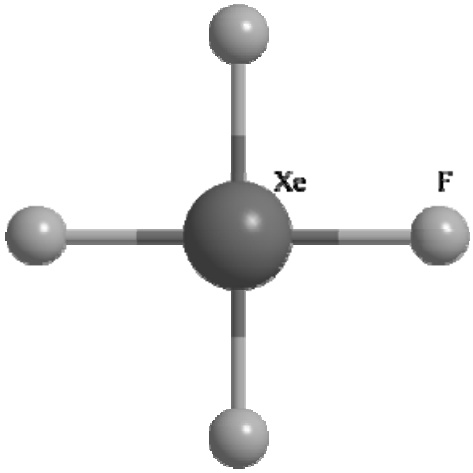
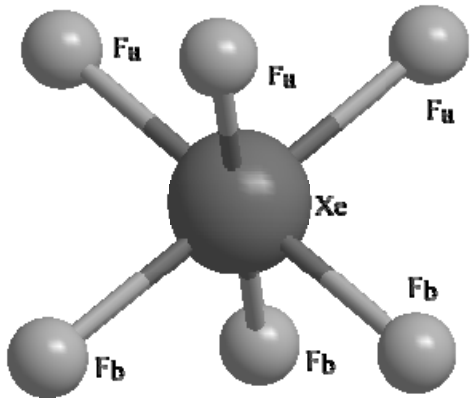
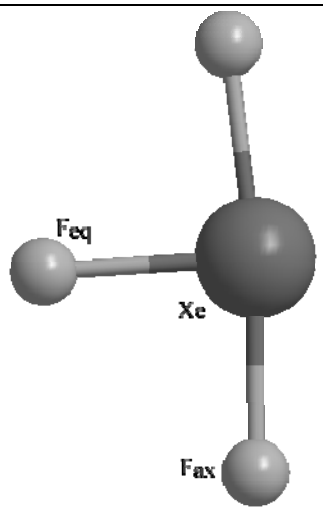
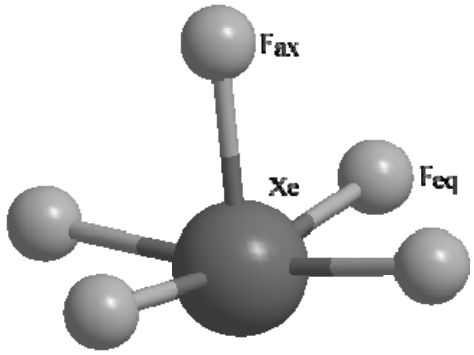
$B_7H_7^{2-}$		B_{eq}-B_{eq}: 1.66 B_{eq}-B_{ax}: 1.83	
B_6H_{10}		B_{eq}-B_{eq}: 1.64 (1.60) B_{eq}-B_{eq}': 1.74 (1.74) B_{eq}'-B_{eq}'': 1.80 (1.79) B_{eq}-B_{ax}: 1.81 (1.80) B_{eq}'-B_{ax}: 1.75 (1.75) B_{eq}''-B_{ax}: 1.75 (1.74) B_{eq}-H_t: 1.19 (1.28) B_{eq}-H_b: 1.34 (1.35) B_{eq}'-H_t: 1.19 (1.18) B_{eq}'-H_b: 1.38 (1.31) B_{eq}''-H_t: 1.19 (1.14) B_{eq}''-H_b: 1.31 (1.32) B_{ax}-H_t: 1.19 (1.25)	5
B_5H_{11}		B_{eq}-B_{eq}'': 1.74 (1.74) B_{eq}'-B_{eq}'': 1.81 (1.81) B_{eq}''-B_{eq}''': 1.80 (1.78) B_{eq}-B_{ax}: 1.88 (1.88) B_{eq}'-B_{ax}: 1.87 (1.86) B_{eq}''-B_{ax}: 1.74 (1.72) B_{eq}'''-B_{ax}: 1.75 (1.74) B_{eq}-H_t: 1.20 B_{eq}-H_b: 1.38 (1.38) B_{eq}'-H_t: 1.20 B_{eq}'-H_b: 1.40 (1.40) B_{eq}''-H_t: 1.19 B_{eq}''-H_b: 1.36 (1.35) B_{eq}'''-H_t: 1.1 B_{eq}'''-H_b: 1.33 (1.31) B_{ax}-H_t: 1.19 (1.19) B_{ax}-H_{pt}: 1.26 (1.32) B_{eq}-H_{pt}: 1.99 (1.96) B_{eq}'-H_{pt}: 1.48 (1.55)	6

Table 2. Xenon fluoride structures

Compound	Structure	Bond lengths (Å) and Angles (°)	Reference
XeF_2		Xe-F: 2.12 (2.00)	7
XeF_4		Xe-F: 2.08 (1.92)	7
XeF_6		Xe-F_a: 2.06 (1.85) Xe-F_b: 2.08 (1.94)	8
XeF_3^+		Xe-F_{eq}: 1.99 (1.84) Xe-F_{ax}: 2.01 (1.91)	9

XeF_5^+		$Xe\text{-}F_{eq}$: 1.99 (1.85) XeF_{ax}: 1.96 (1.79)	10

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