













* Br-HC

ΔH_{B3LYP} (ΔG_{B3LYP})
 ΔH_{MP2} (ΔG_{MP2})
 $\Delta H_{\text{MP2-AUG}}$ ($\Delta G_{\text{MP2-AUG}}$)

70.9 (-6.3)

72.6 (-4.5)

78.1 (0.9)

188.9 (84.3)

212.7 (108.1)

235.5 (130.9)

2,5-A

2,5-B

3,5

Figure S3