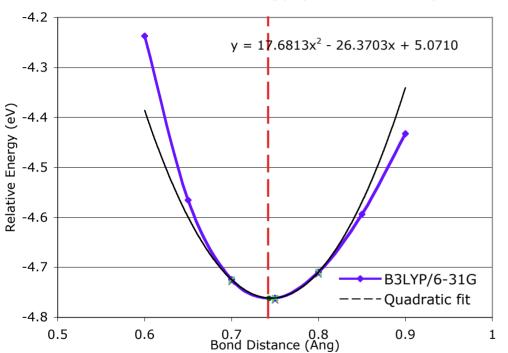
H2 - 2 H DFT Energy (B3LYP/6-31G)



Bond energy

H-H exp't:

B3LYP opt:

H-H exp't = 4.478 eV2 H: 2(-0.4969) au = -27.041 eV -1.1687 au = -31.803 eV H₂:

Bond length

0.742Å

0.743

= 4.762 eVDissociation E

ZPE corrected = 4.484 eV

Vibrational frequencies

Experiment: 4401 cm⁻¹ B3LYP harmonic: 4487 cm⁻¹

ZPE: 0.278 eV