



Bond length	
H-H exp't:	0.742Å
B3LYP opt:	0.743

Bond energy	
H-H exp't	= 4.478 eV
2 H: 2(-0.4969) au = -27.041 eV	
H ₂ : -1.1687 au = <u>-31.803 eV</u>	
Dissociation E	= 4.762 eV
ZPE corrected	= 4.484 eV

Vibrational frequencies	
Experiment:	4401 cm ⁻¹
B3LYP harmonic:	4487 cm ⁻¹
ZPE:	0.278 eV