The total atomization energies for hydrides H_2、LiH、BeH_2、BH_3、CH_4、NH_3、H_2O、HF		
Species	Multiplicity	Equilibrium bond energy (D_e，kcal/mol)
H_2	1	109.5
LiH	1	57.95
BeH_2	1	143.14
BH_3	1	281.08
CH_4	1	420.34
NH_3	1	298.02
H_2O	1	232.75
HF	1	141.25

Reference :

1. Yu, H. S.; Zhang, W.; Verma, P.; He, X.; Truhlar, D. G., Nonseparable exchange-correlation functional for molecules, including homogeneous catalysis involving transition metals. *Phys. Chem. Chem. Phys.* **2015,***17*, 12146-12160.

2. http://cccbdb.nist.gov/expbondlengths1x.asp

3. Barreto, P. R.; Vilela, A. F.; Gargano, R., Thermochemistry of molecules in the B/F/H/N system. *Int. J. Quantum Chem.***2005,***103*(5), 659-684.

4. Shayesteh, A.; Tereszchuk, K.; Bernath, P.; Colin, R., Infrared emission spectra of BeH 2 and BeD 2. *J.Chem.Phys.***2003,***118*(8), 3622-3627.