

Zero-Point-Exclusive Atomization Energies	
Species	De (kcal/mol)
H <sub>2</sub>	109.48
Li <sub>2</sub>	24.6
B <sub>2</sub>	67.14
C <sub>2</sub>	145.73
N <sub>2</sub>	228.46
O <sub>2</sub>	119.99
F <sub>2</sub>	38.20
Si <sub>2</sub>	74.97
P <sub>2</sub>	117.09
S <sub>2</sub>	101.67
Cl <sub>2</sub>	57.97

**Reference :**

1. Benjamin J. Lynch, Yan Zhao, and Donald G. Truhlar, *J. Phys. Chem. A* 2003, 107, 1384-1388
2. Curtiss, L. A.; Raghavachari, K.; Trucks, G. W.; Pople, J. A. Gaussian-2 theory for molecular energies of first-and second-row compounds. *The Journal of chemical physics* **1991**, *94* (11), 7221-7230.