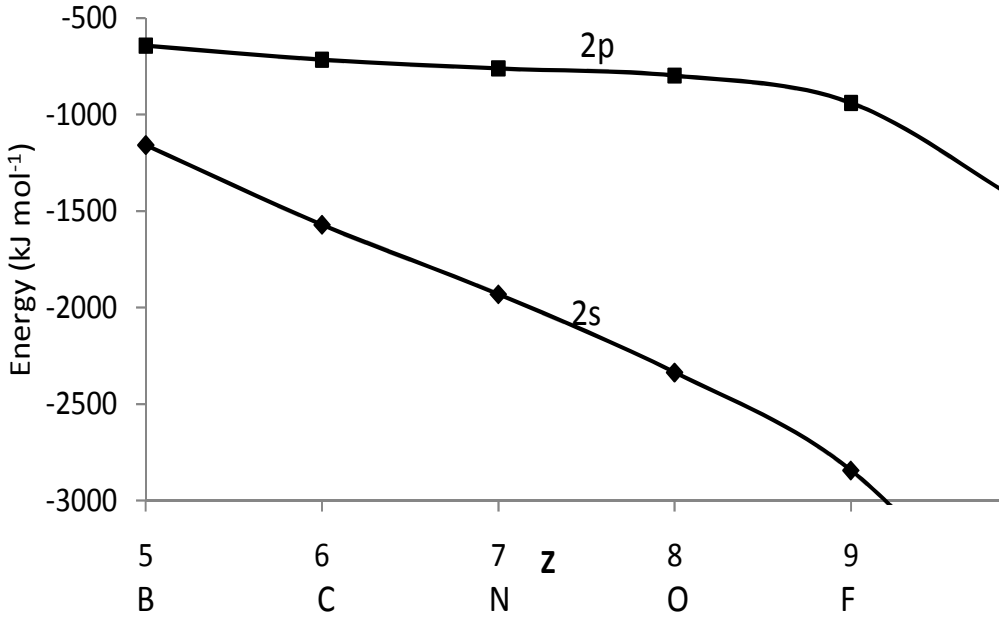
Homonuclear Diatomics

Atomic Orbital Energies[1]



Bond Order Measures[2,3]

	H_2	Li_2	LiH	B_2*	C_2	N_2	O_2*	F_2	CN	CO	NO
D_o (kJ/mol)	435	105	243	289	602	941	494	151	787	1070	632
r_o (Å)	0.76	2.68	1.61	1.59	1.24	1.10	1.21	1.44	1.18	1.13	1.15
k (N/m)	510	25	96	350	930	2240	1140	450	1580	1860	1550
Bond Order											

$D_o = D_e - \frac{1}{2} h\nu_o$ D_e = minimum in energy curve $\frac{1}{2} h\nu_o$ = zero point energy

r_o = equilibrium internuclear distance (vibrationally averaged) k = force constant

for an harmonic potential $V = \frac{1}{2} k(r-r_o)^2$ for a general potential $k = \left(\frac{\partial^2 V}{\partial r^2}\right)$

1. At B3LYP/cc-pVTZ for the neutral hydride (BH_3, CH_4, NH_3, H_2O, HF, Ne) extrapolated to long bond lengths.

2. G. C. Pimentel, R. D. Spratley, Understanding Chemistry, Holden-Day Inc., San Francisco, CA, 1971.

3. G. C. Pimentel, R. D. Spratley, Chemical Bonding Clarified Through Quantum Mechanics, Holden-Day, Inc., San Francisco, CA, 1969.