5.3.2.1: Orbital ionization energies

To generate molecular orbital diagrams of heteronuclear diatomic molecules, we must start with a knowledge of the relative energies of electrons in different atomic orbitals. In other words, we need knowledge of the orbital potential energies (or orbital ionization energies).

Orbital Ionization Energies

There are two approaches you can use to "know" or estimate the atomic orbital energy levels.

1. Use a table of atomic orbital ionization energies, like those found in Table 5.3.2.1.1
2. When you do not have access to a table of values like the one below, use periodic trends in electronegativity and/or ionization energies as your guide to approximate relative values for different atoms.

Table 5.3.2.1.1: These are one-electron ionization energies of the valence orbitals calculated by average energies of both the ground-state and ionized-state configurations. (From Harry Gray, "Electrons and Chemical Bonding," Benjamin, 1964, Appendix) Values are expressed in eV.

Atom	1*s*	2*s*	2*p*	3*s*	3*p*	4*s*	4*p*	*Atom*	3*d*	4*s*	4*p*
H	−13.64							*Sc*	−4.71	−5.70	−3.22
He	−24.55							*Ti*	−5.58	−6.08	−3.35
Li		−5.46						*V*	−6.32	−6.32	−3.47
Be		−9.30						*Cr*	−7.19	−6.57	−3.47
B		−14.01	−8.31					*Mn*	−7.93	−6.82	−3.60
C		−19.47	−10.66					*Fe*	−8.68	−7.07	−3.72
N		−25.54	−13.14					*Ni*	−10.04	−7.56	−3.84
O		−32.36	−15.87					*Cu*	−10.66	−7.69	−3.97
F		−46.37	−18.72								
Ne		−48.48	−21.57								
Na				−5.21							
Mg				−7.69							
Al				−11.28	−5.95						
Si				−15.00	−7.81						
P				−18.72	−10.17						
S				−20.71	−11.65						
Cl				−25.29	−13.76						
Ar				−29.26	−15.87						
K						−4.34					
Ca						−6.08					
Zn						−9.42					
Ga						−12.65	−5.95				
Ge						−15.62	−7.56				
As						−17.61	−9.05				
Se						−20.83	−10.79				
Br						−24.05	−12.52				
Kr						−27.52	−14.26				