SECTION OVERVIEW

9.9: Chemical Applications of Atomic Structure Theory

In this section we examine how the results of the various approximation methods considered in this chapter can be used to understand and predict the physical properties of multi-electron atoms. Our results include total electronic energies, orbital energies and single-electron wavefunctions that describe the spatial distribution of electron density. Physical properties that can be used to describe multi-electron atoms include total energies, atomic sizes and electron density distributions, ionization energies and electron affinities. Trends in these properties as Z increases form the basis of the periodic table and, as we see in Chapter 10, control chemical reactivity. Spectroscopic properties are considered in a link that includes a development of term symbols for multi-electron systems.

9.9.9A: Total Electronic Energies

9.9.9B: Orbital Energies

9.9.9C: Atomic Sizes and Electron Density Distributions

9.9.9D: Ionization Potentials

9.9.9E: Electron Affinity