3.11: Chapter Summary

This Chapter has shown how the solution of the Schrödinger equation governing the motions and interparticle potential energies of the nuclei and electrons of an atom or molecule (or ion) can be decomposed into two distinct problems:

i. solution of the **electronic** Schrödinger equation for the electronic wavefunctions and energies, both of which depend on the nuclear geometry and
ii. solution of the **vibration/rotation** Schrödinger equation for the motion of the nuclei on any one of the electronic energy surfaces.

This decomposition into approximately separable electronic and nuclearmotion problems remains an important point of view in chemistry. It forms the basis of many of our models of molecular structure and our interpretation of molecular spectroscopy. It also establishes how we approach the computational simulation of the energy levels of atoms and molecules; we first compute electronic energy levels at a 'grid' of different positions of the nuclei, and we then solve for the motion of the nuclei on a particular energy surface using this grid of data.

The treatment of electronic motion is treated in detail in Sections 2, 3, and 6 where molecular orbitals and configurations and their computer evaluation is covered. The vibration/rotation motion of molecules on BO surfaces is introduced above, but should be treated in more detail in a subsequent course in molecular spectroscopy.