

9.S: The Electronic States of the Multielectron Atoms (Summary)

In this chapter we have used the independent particle model for electrons (i.e, the idea that multi-electron wavefunctions can be approximated as products of single-electron wavefunctions) to approximate multi-electron atoms. State energies are calculated to be as accurate as possible through use of the Variational Method and Perturbation Theory. A large number of basis functions can be used with the SCF method to get the best possible one-electron functions. Although we only considered the helium atom explicitly, the method has been applied to all atoms of the Periodic Table.

We also introduced the idea of configuration interaction to account for electron correlation. Configuration interaction gives us a mathematical way to describe the electrons as they try to avoid each other. In the CI method excited state electron configurations are used to let the electrons avoid each other.

The various ideas presented here require computers to evaluate all the variational parameters and integrals. Many person-years of time and energy were required to write the computer code to do the calculations and assess the results. At this point in time, only the speed and capacity of the computers, our financial resources to pay for them, and the person-time to write the code limit the accuracy of the energies and wavefunctions. Once these demands were severe, and only dedicated experts could carry out such calculations. Today meaningful calculations can be done with desktop PC's or relatively inexpensive workstations using software that can be obtained commercially at little cost.

As we have seen, the single electron orbitals have associated energies and physically interpretable parameters such as the effective nuclear charge. It is precisely this independent particle picture that leads to an understanding of the ordering of atomic orbitals of atoms, the structure of the periodic table, the periodic trends in ionization energies and other properties of atoms, the chemical properties of the elements, and the nature of the chemical bond.

In modern quantum mechanical calculations in chemistry, the focus of research is primarily on molecules and their electronic properties and how the electronic properties determine chemical reactivity and molecular structure. Undergraduate students can do today with small computers what research scientists were doing a mere 10 years ago.

The following chapter will focus on the quantum mechanical concepts used in calculations to study molecules. We include an older method, the Hückel Molecular Orbital method, because it contains the elements found in more sophisticated computational approaches and provides the insight needed to relate the results of calculations to molecular properties.

Some Key Questions for Self Study

- What is a Slater determinant and why is it useful?
- What is the independent electron approximation?
- Why must each electron in an atom have a different set of quantum numbers (*[Math Processing Error]*)?
- How do you add angular momentum to obtain term symbols?
- How do you use term symbols to decide on the relative energies of states?
- How many states result from the carbon configuration *[Math Processing Error]*? What are the term symbols for these states?
- How many states result from the carbon configuration *[Math Processing Error]*? What is the term symbol for the ground state of carbon?
- What happens to the energies of states of an atom in a magnetic field and why? Describe an example.

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