

Quiz 8.2 - Multi-Electron Atoms

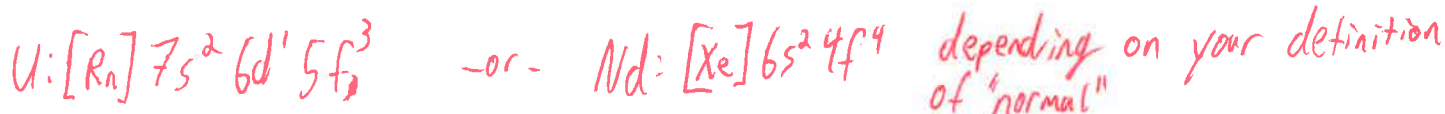
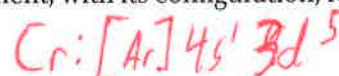
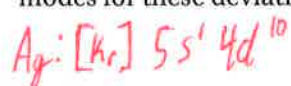
Name: Kery

Electronic Configurations

List the three principles which lead to proper electronic configurations

- 1) Aufbau principle
- 2) Pauli Exclusion Principle
- 3) Hund's Rule

Many of the elements break from the normal pattern for electronic configurations. There are three primary modes for these deviations. Give an example of an element, with its configuration, for each of these modes



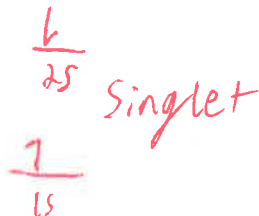
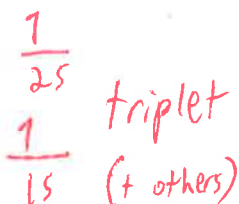
What do these exceptions to the normal pattern tell us qualitatively about the orbital energies?

The difference in orbital energies is smaller than the spin pairing energy. The energies are very close, and depend on how each subshell is affected by shielding, so the exceptions usually apply to only a single family (and not all members of that family)

Spin States of Multi-Electron Atoms

Consider the excited He electronic state with a configuration $1s^1 2p^1$. This configuration can give rise to both singlet and triplet terms

Draw energy level diagrams which illustrate the difference between these excited states



Explain one experimental difference between the singlet and triplet states of excited He

In a Stern-Gerlach experiment, Singlet He will pass straight through the magnetic field while triplet He will split into three paths

The Pauli Principle

For the singlet state of excited He, give a valid total wavefunction which obeys the Pauli Principle

$$\Psi = \frac{1}{\sqrt{2}} [1s\alpha(1) 2s\beta(2) - 1s\alpha(2) 2s\beta(1)]$$

For the triplet state of excited He, give two valid total wavefunctions which obey the Pauli Principle (A third one exists, but it involves a new paradigm to derive it so we will leave it alone for now)

$$\Psi = \frac{1}{\sqrt{2}} [1s\alpha(1) 2s\alpha(2) - 1s\alpha(2) 2s\alpha(1)]$$

$$\Psi = \frac{1}{\sqrt{2}} [1s\beta(1) 2s\beta(2) - 1s\beta(2) 2s\beta(1)]$$

True Multi-Electron Wavefunctions

True electron orbitals for multi-electron atoms are not actually identical to the hydrogenic orbitals. What theory is used to approximate the true wavefunctions for multi-electron atoms, and what factor limits its accuracy?

Hartree-Fock Self-consistent field theory

The estimate of the $\frac{e^2}{4\pi\epsilon_0 r_{12}}$ term in H-F theory doesn't account for electron correlation. Various other theories attempt to improve H-F by estimating the exchange correlation energy.