Name ________________________________ Section # _____ Marks _________ / 30

Chemistry 135 Semester 01-2012
Homework for Submission #5

1) a) What is an *orbital?* (3)

An orbital specifies the region of space in an atom in which an electron is likely to be found and the energy of that electron. More technically, it is a particular solution of the Shrödinger equation, which describes the electron as a wave. It is characterised by the values of 3 quantum numbers, n, ℓ, and m_ℓ .

b) State the *Pauli Exclusion Principle* and explain why it means that an orbital can hold no more than two electrons. (4)

The Pauli Exclusion Principle states that no two electrons in an atom can have the same values of the 4 quantum numbers, n, ℓ, m_ℓ and m_s.

Two electrons in one orbital in an atom must have the same values of n, m_ℓ, and m_s. Hence they must differ in their values of m_s. Since m_s can only have 2 values, an attempt to place another electron in this orbital would violate the principle. Thus an orbital can hold no more than 2 electrons.

c) State Hund's Rule of Maximum Multiplicity. (2)

Hund's rule states that when a set of degenerate orbitals is filled, each orbital is filled singly before any pairing occurs. That is, when filling orbitals of the same energy, one electron is placed in each (spins parallel) before two are placed in any one.

d) What is meant by the Aufbau principle? (3)

The Aufbau, or "building-up" principle is a principle used to determine the electronic structures of atoms in the ground state. Starting with the bare nucleus, electrons are placed in orbitals of increasing energy, lowest first until the full complement of electrons is achieved.

e) Use the above rules to construct the electronic structure of nitrogen, explaining carefully how the Aufbau Principle, the Pauli Exclusion Principle and Hund's rule are applied. (6)

Nitrogen has a total of 7 electrons. In order of increasing energy the orbitals are 1s, 2s, 2p, 3s etc. Only two electrons can be placed in any orbital (according to the Pauli Exclusion Principle) and so 2 electrons are placed in the 1s orbital and then two in the 2s orbital (following the Aufbau Principle). This leaves 3 electrons to place. There are three 2p-orbitals of equal energy, so 1 electron is placed in each, spins parallel, according to Hund's Rule. This accounts for all seven electrons. Thus the electronic structure of nitrogen is $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$.

2) Write out the electronic structures of each of the following atoms and ions. You may use symbols such as [Ar] or [Kr] to show the core electrons, but if *p*-orbitals are shown then the occupation of each orbital must be indicated. (12)

Examples: $1s^2 2s^2 2p_x^1 2p_y^1$ and $[Ar]4s^2 3d^2$ or

a) He $1s^2$ (1)

b) Be $1s^2 2s^2$ (1)

c) N $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$ (1)

d) Ti $[Ar]4s^2 3d^2$ (1)

e) Cr $[Ar]4s^1 3d^5$ (1)

f) Mn $[Ar]4s^2 3d^5$ (1)

g) Cu $[Ar]4s^1 3d^{10}$ (1)

h) Ca^{2+} $[Ar]4s^0$ (1)

i) F^- $1s^2 2s^2 2p_x^2 2p_y^2 2p_z^2$ (1)

j) Cu^{++} $[Ar]4s^0 3d^9$ (1)

k) Fe^{3+} $[Ar]4s^0 3d^5$ (1)

l) Fe^{2+} $[Ar]4s^0 3d^4$ (1)

m) Explain, on the basis of their electronic structures why Fe^{3+} is much more stable than Mn^{3+}. (3)

Mn^{3+} has electronic structure $[Ar]4s^0 3d^4$, whereas Fe^{3+} has structure $[Ar]4s^0 3d^5$. Thus Fe^{3+} has a ½-filled d subshell, wherease Mn^{3+} does not. A ½-filled d sub-shell has a lower energy and so an extra stablility.