# Learning Objectives and Worksheet III

## Chemistry 1B-AL Fall 2016

### ~~Lectures~~ (5-6) Many Electron Atoms and the Aufbau Principle

Read pp. 557-569 (*you will not be responsible for the material on pp-569-571; however the CHEM1B-AL staff would be more than happy to discuss these concepts with you)*

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Atomic orbital **APPROXIMATION**

To describe the electronic structure of atoms we will be using a model that is an approximation to the actual (exact) solutions to the Schrödinger equation. In this model the many-electron wavefunction is 'built' up by placing electrons into 'hydrogen-like' atomic orbitals.

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I. Pauli Exclusion Principle (PEP)

1. What did the Stern-Gerlach experiment indicate?


2. What is Pauli Exclusion Principle as related to allowed orbital occupancy?

HW#2: 19

Addition information on Stern-Gerlach and electron 'spin' (University of Toronto): http://www.upscale.utoronto.ca/GeneralInterest/Harrison/SternGerlach/SternGerlach.html

II. Energies of orbitals In many-electron atoms

1. In the hydrogen atom, and for all 1-electron ions, the energy of an electron in an orbital with quantum numbers n, $\ell$, $m_\ell$ , $m_s$ is given by $E_n = -\frac{m_e e^4}{8h^2\varepsilon_0{}^2}\frac{Z^2}{n^2} = -\left(2.18\times10^{-18}\ J\right)\frac{Z^2}{n^2}$ . For the energy of an electron in a many electron atom the nuclear charge Z is replaced by ________________________________ which takes into account both Z, the _______________ of the nucleus, and the repulsion ($\sigma$=shielding of nuclear charge ) of the _________________.

2. In a helium atom $Z_{eff}$ for an electron will be ______________ the +2 charge on the nucleus.

3. In the ground state of the Li atom has configuration ________. The electron in the 2s orbital has the higher (less negative) energy both because $n_{2s}$ ________ $n_{1s}$ and $(Z_{eff})_{2s}$ ________ $(Z_{eff})_{1s}$ .
4. In a hydrogen atom the 2s and 2p orbitals have the ___________ energy. However in many-electron atoms (e.g. boron) $E_{2s}$ ______ $E_{2p}$ since $(Z_{eff})_{2s}$ ________ $(Z_{eff})_{2p}$ .
5. Why is $(Z_{eff})_{2s}$ > $(Z_{eff})_{2p}$ in boron ?

6. What is the energy ordering of the n=3 orbitals in a many-electron atom:

   $E_{3s}$ ____________ $E_{3p}$ _____________ $E_{3d}$

7. The relative values of E3d and $E_{4s}$ result from a balance of (competition between) two factors.

   i. In applying the relationship $E_n = = -(2.18 \times 10^{-18}\ J)\dfrac{Z_{eff}^2}{n^2}$ to compare $E_{4s}$ vs $E_{3d}$:

   the lower value of ____________ favors the 3d orbital to be of lower energy and

   the higher value of _____________ (due to greater penetration) favors the 4s orbital.

**HW#2: S5**

   ii. In the ground state of neutral species which orbital is filled first (circle correct answer): 3d or 4s ? (i.e. ___________ wins the energy competition)
   iii. In the ground state of transition metal cations which orbital is filled first (circle correct answer): 3d or 4s ? (i.e. ___________ wins the energy competition)

8. Know the usual ordering of the energies of many-electron orbitals (pneumonic) for neutral and positive ions.

III. Writing electronic configurations for many-electron atoms

1. When filling a level with degenerate orbitals Hund's Rule state that the state of lowest energy has the electrons in _____________ orbitals with ____________ spins.
2. Which arrangement of the $2p^3$ configuration would have the lowest energy (circle one):

| ↓↑ | ___ | ↑ | or | ↓↑ | ___ | ↓ | or | ↑ | ↑ | ↑ |
|---|---|---|---|---|---|---|---|---|---|---|
| $2p_x$ | $2p_y$ | $2p_z$ | | $2p_x$ | $2p_y$ | $2p_z$ | | $2p_x$ | $2p_y$ | $2p_z$ |

3. Know why the configurations $np^2$, $np^3$, $np^4$, $nd^2$, $nd^3$, $nd^4$, $nd^5$, $nd^6$, $nd^7$, and $nd^8$ are ambiguous (i.e. each could correspond to one of several allowed energy states depending on how the electrons are distributed among degenerate orbitals and how the electrons'

spins are assigned) and **thus one must give the spin assignment to specify the ground or particular excited state.**


**HW#2:** 16,17 20,21,22,

4. Be able to write the ground state configuration of neutral atoms and of ions.
5. Be able to identify a given configuration as
   i. **ground state** (lowest energy configuration)
   or
   ii. **excited state** (allowed but not the lowest energy)
   or
   iii. **not allowed** (breaks one of the rules of electron assignment in many-electron atoms).
6. Know how the balance between the energy considerations associated with the balance between filling the lowest energy orbitals, satisfying Hund's Rule, and other factors lead to some apparent 'exceptions'. You will only be asked to write a ground state configuration for atoms which are NOT EXCEPTIONS (i.e. asked 'cold'); but you may be asked to why a given ground state configurations appears to be an exception due to the extra stability of ________________________________.


**HW#2: 18**

Resource on electronic configuration of atoms:
http://chemistry.about.com/od/electronicstructure/ss/aufbau.htm#step2