Chemistry 103, Dr. Hamers
Help Sheet #8; Chapter 5 and Chapter 6
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Nuggets: *Light Equations; Electromagnetic Spectrum; Quantized System; Energy Level Diagram; Electron Transitions/calculating $\Delta E_{transition}$; Wavefunction ψ and Quantum Numbers n, l, m_l, and m_s; Orbital Shapes*

CHAPTER 5 – WORK (revisited)

Work and the 1st Law of Thermodynamics: energy is conserved: $\mathbf{\Delta E = q + w}$ (q = heat; w =work)

Work is defined as PV-work which is: $w = -P\Delta V$ and

Enthalpy is defined as: $\Delta H = \Delta E + P\Delta V$ and subbing $\Delta E = q + w$ and at constant P this becomes:

$\Delta H = q_p + w + (-w)$; $\mathbf{\Delta H = q_p}$

Back to $\Delta E = q + w$ and subbing $w = -P\Delta V$ yields: $\Delta E = q - P\Delta V$ and at constant V: $\mathbf{\Delta E = q_v}$

Again using $\Delta E = q - P\Delta V$ at constant P yields: $\Delta E = q_p - P\Delta V$ then subbing:

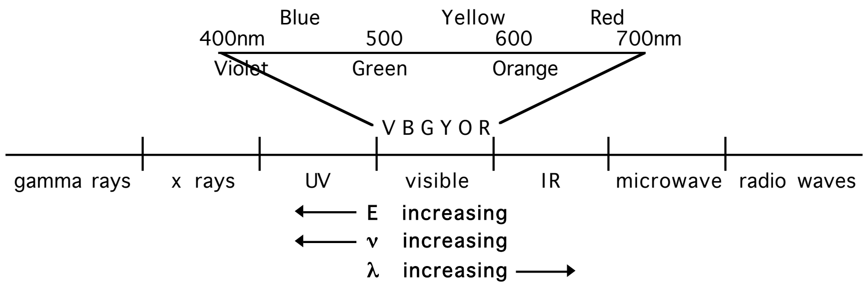
$\Delta E = q_v$ and $w = -P\Delta V$ yields: $q_v = q_p + w$ and rearranging yields: $\mathbf{q_p = q_v - w}$

work done by the system < 0 (-); work done on the system > 0 (+)

$$\mathbf{\Delta E = q + w \ ; \ \Delta H = q_p \ ; \ \Delta E = q_v \ ; \ q_p = q_v - w}$$

CHAPTER 6

Electromagnetic Spectrum:



visible spectrum,: violet – highest energy; red – lowest energy; ROYGBV

$\boldsymbol{\nu = \frac{c}{\lambda}}$ where ν is frequency (in s^{-1}), c is speed of light (3×10^8 m/s), and λ is wavelength (in m)

Quantized: something that is found in "packets" or units; there are specific values in a quantized system (i.e., 1 or 2 or 3, etc. but not other values like 1.33 or 1.766, etc.)

$\mathbf{E = h\nu}$; $\mathbf{E = \frac{hc}{\lambda}}$ where h is Planck's constant = 6.626×10^{-34} Js

Absorption** of light* - an electron absorbs energy and jumps to a higher energy level; ***endothermic process
Emission** of light* - an electron drops to a lower energy level (n) and emits light energy; ***exothermic process
Blackbody radiation – when a metal is heated, light is emitted as a continuous spectrum; as T increases, the λ decreases/ν increases, and the intensity increases ("red hot" cooler than "blue hot" cooler than "white hot")
UV Castastrophe – the power emitted by hot substances should increase as the square of the frequency; what this implies is that the power emitted goes to infinity as the frequency increases; hence, the power emitted from a substance as it gets hotter approaches infinity which isn't possible; this approach is based on classical physics which is incorrect because light does not behave classically (Planck)
Photoelectric effect – when light of a minimum (threshold) frequency impacts a metal, electrons are ejected; if the intensity of the light is increased, more electrons are ejected; if the light is not at the minimum frequency no electrons are ejected; conclusion: light can be treated as particles rather than waves (Einstein)
Atomic emissions - quantized and appear as a line spectrum

Bohr Model: based on classical physics; had quantized energy levels; explained H emission spectra;

Problems with Bohr model: assumed circular orbits for electrons (they're not) and only worked with 1 e^- systems (i.e., H only); electrons are treated as particles

Schrodinger Model: treated electrons as waves

Light and electron duality – both of these have properties of particles and waves

Light: Wave properties: *diffraction*; Particle properties: *photoelectric effect*

Electrons: Wave properties: *electron diffraction*, de Broglie equation assigns λ to electron;

Particle properties: *charge-to-mass ratio*

ELECTRONS

Rydberg equation: $\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$ or the more general equation: $\frac{1}{\lambda} = R\left(\frac{1}{n_f^{\,2}} - \frac{1}{n_i^{\,2}}\right)$;

$R = 1.09 \times 10^7 m^{-1}$; λ in m; n_f = final energy level; n_i = initial energy level;

Balmer emission (**$n_f = 2$**) in H: n_i = 5, 4, 3, 2; Lyman emission (**$n_f = 1$**) in H: n_i = 6, 5, 4, 3, 2

Energy of electron in the n^{th} energy level $= - -\frac{Rhc}{n^2} = -\frac{2.18 \times 10^{-18}}{n^2}$

where n = energy level; $R = 1.09 \times 10^7 m^{-1}$, $c = 3 \times 10^8$ m/s, $h = 6.626 \times 10^{-34}$ Js

ELECTRON TRANSITION

And we can get an energy difference equation for *1 electron* going from $n_{initial}$ to n_{final}:

$$\Delta E_e = -Rhc\left(\frac{1}{n_f^{\,2}} - \frac{1}{n_i^{\,2}}\right) = h\nu = \frac{hc}{\lambda} \rightarrow \Delta E_e = -2.178 \times 10^{-18}\left(\frac{1}{n_f^{\,2}} - \frac{1}{n_i^{\,2}}\right) = h\nu = \frac{hc}{\lambda}$$

- ΔE for **1 atom/ion**; For E of 1 mol of atoms/ions, multiply by 6.022×10^{23}; ΔE = J/atom
- To **ionize** an atom means electron is removed → $n_{final} = \infty \rightarrow {}^1/(\infty)^2 = 0$
- When setting the above ΔE equal to hν and hc/λ assumes the energy going in/coming out is light energy
- Sometimes ΔE_e is presented in terms of Rhc (e.g., ${}^5/_{36}$Rhc for a $n_i = 2$, $n_f = 3$, in H atom)

de BROGLIE WAVELENGTH: $\lambda = \frac{h}{mv}$ where mass (m) is in **kg**; velocity (v) is in m/s; λ is in m;

describes the wave properties of an electron or other moving object

Heisenberg Uncertainty Principle: There is a limit to how well the position (Δx) and momentum (Δ(mv)) of anything can be measured. (If the position is known accurately then the momentum will not be known that well, and vice versa.) $\Delta x \bullet \Delta(mv) \geq \frac{h}{4\pi}$

Schrodinger's Equation $E\Psi = \hat{H}\Psi$

- Wave functions, Ψ (psi, pronounced "sigh") are equations that describe the electron as a wave. The solution to Ψ are 3 variables: n, l, and m_l.
- Ψ^2 - the probability of finding an electron at position (x, y, z); units = ${}^1/_{volume}$
- Orbital – a surface containing a region in space in which the electron is found 90% of the time

QUANTUM NUMBERS (qn): a set of 3 qn (n, l, m_l) that are a solution to the Schrodinger wave equation;

n = principle qn: **the energy level/shell/distance from the nucleus** of the electron (n = 1, 2, 3, 4, 5, 6, 7 …)

l = angular momentum qn = azimuthal qn: **describes orbital shape** (l = 0, 1,..., n-1); l is the subshell

$l = 0 \rightarrow$ s subshell; $l = 1 \rightarrow$ p subshell; $l = 2 \rightarrow$ d subshell; $l = 3 \rightarrow$ f subshell

m_l = magnetic qn: **describes orientation of orbital** (m_l = -l,...,0,...+l);

m_s = spin qn ($m_s = +\frac{1}{2}$ or $-\frac{1}{2}$)

- n^2 = #orbitals in the nth energy level
- $2n^2$ = #electrons in the nth energy level
- $2l + 1$ = #orbitals in the l-subshell (also, #m_l values = #orbitals in the l-subshell)
- Each orbital can hold a maximum of 2 electrons
- Pauli Exclusion Principle: No two electrons can have the same set of 4 qn; each e^- has a unique set of 4 qn

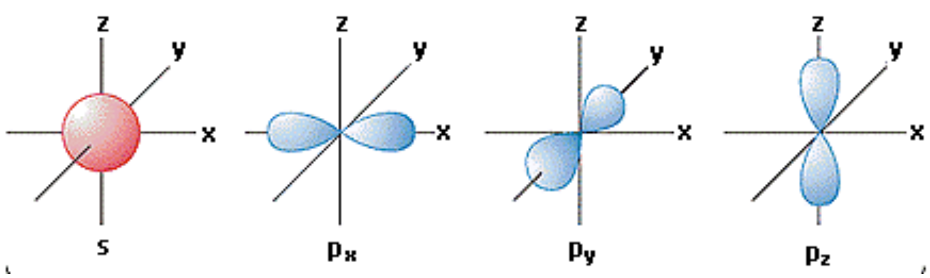
From qn, we get the Subshells: 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, 5s, 5p, 5d, 5f, 5g, 6s, 6p, 6d, 6f

There is/are: 1 s-orbital, 3 p-orbitals, 5 d-orbitals, 7 f-orbitals (from #m_l values or $2l + 1$)

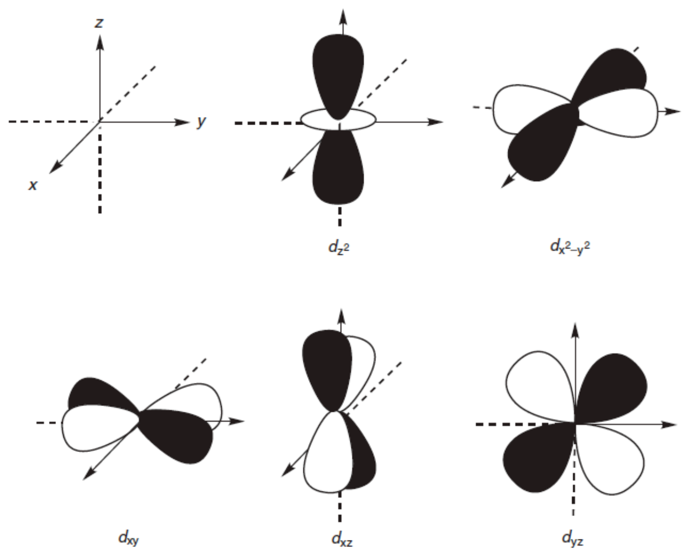
Node - zero probability of finding electron

total nodes = n - 1; #planar nodes = l (also called nodal surfaces); #spherical nodes = n - l - 1

Know the shapes of the s, p and d orbitals unless otherwise noted in lecture



Molecular Shape, The Shape of Molecules, http://www.cem.msu.edu/~reusch/VirtualText/intro3.htm



Milton Orchin,Roger S. Macomber, Allan Pinhas, and R. Marshall Wilson(2005); "Atomic Orbital Theory,"
http://media.wiley.com/product_data/excerpt/81/04716802/0471680281.pdf

Paramagnetism: An atom/molecule with an unpaired electron; attacked to a magnetic field

Ferromagnetism: A cluster of paramagnetic metallic atoms in which the magnetic behavior is enhanced

Diamagnetism: A substance with all electrons paired; repelled by a magnetic field

1. a. What color is the highest energy visible light?
b. Which region in the electromagnetic spectrum has a larger wavelength than microwave radiation?
c. Place these in order of increasing energy (highest energy on the right): UV, radio, and X-ray.

2. Microwaves transmit energy to food primarily by excitation of water molecules. The wavelength of microwave radiation whose frequency is $8.5 \times 10^9\ s^{-1}$ (cycles per second) is

a. 0.035m b. 28m c. 5.6×10^{24}m d. 1.1×10^7m e. 2.6×10^{18}m

3. Given a wavelength of 3×10^{-8} m, what is the frequency and energy of this wavelength?

4. What is the energy of **one mole** of blue photons with a wavelength of 450nm?

5. What is the frequency of ultraviolet radiation having a wavelength of 46.3nm?

6. If light has energy of 228kJ/mol, what is its wavelength?

7. When the H electron makes a transition from $n = 3 \rightarrow n = 1$, which of the following statements are true?

1. Energy is emitted. 2. Energy is absorbed. 3. The electron loses energy.
4. The electron gains energy. 5. The electron cannot make this transition.

a. 1, 4 . 1, 3 c. 2, 3 d. 2, 3 e. 5

8. a. Describe the Photoelectric Effect.
b. When electrons in the H atoms fall to first energy level, this series of emission lines is called what?
c. Describe the Pauli Exclusion principle.
d. What experiment shows electrons have particle like behavior?
e. What experiment shows electrons have wave like behavior?

9. a. If a proton is traveling with a velocity of 5×10^7 m/s, what is the wavelength of this proton in m? The mass of the proton is 1.673×10^{-24} g.
b. Which isotope will have a larger wavelength assuming both particles have the same velocity: ^{32}S or ^{56}Fe?

10. a. What energy is required to completely remove an electron in H from the n = 3 energy level? That is, to take the electron from the n = 3 level to the $n = \infty$ level. b. From the n = 1 energy level?

11. Which of the following is not a correct set of quantum numbers for an electron in an atom?

	n	l	m_l	m_s
a.	1	0	0	-1/2
b.	2	1	-1	+1/2
c.	3	2	1	-1/2
d.	4	3	-2	-1/2

e. All the above sets are correct and possible.

12. a. What does the *n* quantum number describe?
b. What subshell is described by $l = 2$?
c. How many orbitals exist in the 3rd energy level?
d. How many nodal surfaces will the 3s orbital have?
e. How many nodal surfaces will a 2p orbital have?
f. How many nodal surfaces will a 3p orbital have?
g. How many total nodes with the 4d subshell have?

13. What is the maximum number of **orbitals** that the following quantum numbers can have? (not a multiple choice question) a. $n = 5$ b. $n = 5, l = 3$ c. $n = 3, l = 3$ d. $n = 3, m_l = 2$ e. $n = 4, l = 2$

14. An electron in the 5th energy level can undergo many different transitions of which 5 are shown below. Which transition will have the longest wavelength?

a. $5 \rightarrow 4$ b. $4 \rightarrow 3$ c. $4 \rightarrow 2$ d. $3 \rightarrow 2$ e. $4 \rightarrow 1$

15. Which atomic orbitals can have an electron with the magnetic quantum number $m_l = -3$?

a. 6s b. 4f c. 4d d. 5p e. none of these

16. For the green line in the visible spectrum of an excited hydrogen atom that arises from an electron moving from energy level $n = 4$ to energy level $n = 2$

a. Calculate the energy difference between the two energy levels.
b. Calculate the wavelength in nanometers for the emitted photons.

17. Which of the following sets of quantum numbers are not allowed?

a. $n = 4, l = 2, m_l = -1$ b. $n = 5, l = 0, m_l = +1$ c. $n = 2, l = 1, m_l = 0$
d. $n = 3, l = 2, m_l = -2$ e. more than one above

18. Consider the $n = 4$ shell.

a. How many subshells are in this shell?
b. How many orbitals are in the $l = 2$ subshell?
c. Provide the number of nodal surfaces and the number of spherical nodes for the $l = 3$ subshell.
d. What are the possible values of m_l for the $l = 3$ subshell?

ANSWERS

1. a. blue/violet b. radio waves c. radio < UV < X-ray 2. a 3. frequency = 1×10^{16} s^{-1}; E = 6.6×10^{-18} J
4. 2.66×10^5 J 5. 6.48×10^{15}Hz 6. 525nm 7. b
8. a. Photoelectric effect occurs when light hits a metal surface and electrons are ejected from the surface. It was found that only light with a minimum or threshold frequency could cause electrons to be ejected and light below this frequency did not. This supported the idea of a quantized energy system for the electron.
   b. Lyman series of emission
   c. The Pauli Exclusion principle basically says that no 2 electrons can have the same 4 quantum numbers.
   d. Photelectric effect
   e. Diffraction
9. a. 7.92×10^{-15} m b. ^{32}S from de Broglie equation: as the object gets smaller, the wavelength gets larger
10. a. 2.42×10^{-19} J b. 2.178×10^{-18}J 11. e
12. a. It describes the energy level of the electron/subshell. It also describes the distance the electron is from the nucleus (as n gets bigger, the distance increases).
b. d subshell c. 9 orbitals d. 0 e. 1 f. 1 g. 3
13. a. 25 b. 7 c. 0 d. 1 e. 5 14. a 15. b 16. a. -4.09×10^{-19}J b. 486nm 17. b
18. a. 4 b. 5 c. 3 nodal surfaces; 0 spherical nodes d. –3, -2, -1, 0, 1, 2, 3