Name: ____ Date: ______________________ CHEM 1A

Wednesday/Thursday, November 13 & 14, 2019 - Quantum Mechanics & Atomic Theory (All Chapter 12)

I. A Brief History of Quantum Theory: The Quantization of Light & Matter

(a) 1845 – Faraday, Maxwell, & Hertz – Light as Electromagnetic Radiation

Faraday's work and Maxwell's theories led to the conclusion that light was a form of electromagnetic radiation. Hertz's experiments confirmed Maxwell's theory using radio waves and showed that light behaves the same way when it came to reflection, refraction, diffraction, and constructive & destructive interference.

Light as a wave: (Draw a wave a talk about wavelength, amplitude, and frequency)

1. Which of the following frequencies corresponds to light with the longest wavelength?

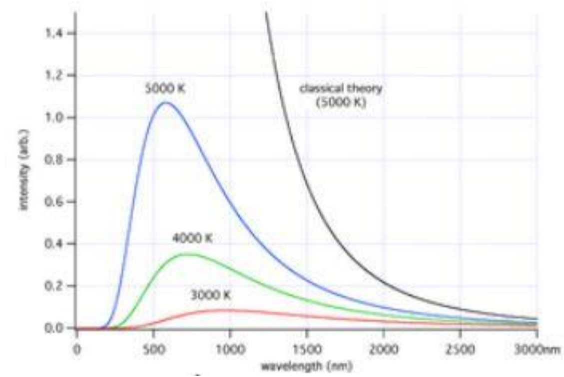
(A) 3.00×10^{13} s^{-1} (B) 4.12×10^{5} s^{-1} (C) 8.50×10^{20} s^{-1} (D) 9.12×10^{12} s^{-1} (E) 3.20×10^{9} s^{-1}

(b) 1900 - Black Body Radiation & the Problem with Classical Mechanics

From physics, Stefan-Boltzmann law: $I_{tot} = 5.67 \times 10^{-8} \frac{W}{m^2K^4} T^4$

and Wien's displacement law: $T\lambda_{max} = 2.9\ Kmm$

put them together and get: $Energy\ Density\ \alpha\ \frac{T}{\lambda^4}$



(c) 1900 - Planck's Quantization Hypothesis

Planck proposed that individual things (particles) oscillate with a given frequency and that each wave of each frequency had a discrete energy level and could only exchange energy in discrete packets (quanta or photons). He determined the following relationship between frequency and energy: $E_{photon} = h\nu,\quad h = 6.626 \times 10^{-34} Js,$

(d) 1905 – Einstein & the Photoelectric Effect

Hit metal with laser, if wavelength is short enough, electron pops off

$KE = \frac{1}{2}mv^2 = E_{photon} - \Phi$

Φ – Work Function – energy to take electron off the metal

2. It takes 208.4 kJ of energy to remove 1 mol of electrons from the atoms on the surface of rubidium metal. If rubidium metal is irradiated with 254-nm light, what is the maximum kinetic energy (kJ/mol) the released electrons can have? $KEe\text{-} = E_{photon} - E_{binding}$ $KEe\text{-} = \frac{hc}{\lambda} - E_{binding}$

$KEe\text{-} = \frac{(6.626\ x\ 10^{-34} Js)(3\ x\ 10^{8}\ ms^{-1})}{(2.54\ x\ 10^{-7} m)}\ x\ \frac{kJ}{10^3 J}\ x\ \frac{6.022\ x\ 10^{23}}{mol} - 208.4\ KJ/mol = 262.9 kJ/mol$

(e) Putting it all together: Wave-Particle Duality

Phenomenon	Reflection	Refraction	Interference	Diffraction	Polarization	Photoelectric Effect
Can be explained with **waves**	X	x	x	x	x	
Can be explained with **particles**	X	x	x			x

3. Calculate the energy of 2.9 moles of yellow photons with a wavelength of 580 nm.

for one photon ⇒ $E = \frac{hc}{\lambda}$ ⇒ $E = \frac{(6.626x10^{-34} Js)(3x10^{8} m/s)}{(580\ nm)(\frac{1\ m}{10^{9} nm})}$ = $3.43x10^{-19}$ J/photon

($3.43x10^{-19}$ J/photon)($6.022x10^{23}$ photons/mol)(2.9 mol) = 5.99x105 J

(f) 1924 - De Broglie's Hypothesis: Wavelength of Matter $\lambda_{matter} = \frac{h}{p} = \frac{h}{mv}$

4. Calculate the wavelength of a beryllium atom traveling at 15% the speed of light.

mass of a beryllium atom = 1 atom $\frac{1\ mol}{6.022 \times 10^{23} atoms} \times \frac{9.012\ g}{mol} \times \frac{1\ kg}{1000 g}$ = 1.5×10^{-26} kg

$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} Js}{(1.5 \times 10^{-26}\ kg)(0.15 \times 3 \times 10^{8}\ ms^{-1})} = 9.84 \times 10^{-16}$ m

5. Consider an atom traveling at 1% of the speed of light. The de Broglie wavelength is found to be 3.31 □ 10–3 pm. Which element is this? Ca

$\lambda = \frac{h}{mv};\ m = \frac{h}{\lambda v} = \frac{6.626 \times 10^{-34} Js}{(3{,}31 \times 10^{-15} m)(0.15 \times 3 \times 10^{8}\ ms^{-1})} = 6.673 \times 10^{-26}\ kg\ (6.022 \times 10^{23}/mol) = 40.18\ g/mol$

(g) 1927 – Heisenberg's Uncertainty Principle $\Delta p \Delta x \geq \frac{1}{2}$(h-bar)

6. (a) The uncertainty in the momentum Δp of a 1.40 kg football traveling at 40m/s is 1×10^{-6} of its momentum p. What is its uncertainty in position Δx?

$p = mv = (0.40kg)(40m/s) = 16kgm/s;\ \Delta p = (1 \times 10^{-6})p = (1 \times 10^{-6})(16\ kgm/s) = 16 \times 10^{-6}\ kgm/s$

$\Delta p \Delta x \geq \frac{1}{2}(\text{h-bar});\ \Delta p \Delta x \geq \frac{h}{4\pi};\ \Delta x \geq \frac{(6.626 \times 10^{-34} Js)}{4\pi(16 \times 10^{-6}\ kgm/s)};\ \Delta x \geq 3.3 \times 10^{-30} m$

(b) An electron in a molecule of water on the football is traveling at the same speed and has the same relationship between Δp and p. Calculate its Δx.

$p = mv = (9.11 \times 10^{-31} kg)(40m/s) = 3.6 \times 10^{-29}\ kgm/s;\ \Delta p = (1 \times 10^{-6})p = 3.6 \times 10^{-35}\ kgm/s$

$\Delta p \Delta x \geq \frac{1}{2}(\text{h-bar});\ \Delta p \Delta x \geq \frac{h}{4\pi};\ \Delta x \geq \frac{(6.626 \times 10^{-34} Js)}{4\pi(3.6 \times 10^{-35}\ kgm/s)};\ \Delta x \geq 1.5 m$

II. The Starting Tenants of Quantum Mechanics & Some Simple Quantum Systems

Particles have wave like properties; therefore, classical mechanics are incorrect.

Classical Mechanics (large everyday objects)	Quantum Mechanics (very, very small objects)
Particles have a **defined and continuous trajectory**. Location and linear momentum can be **deterministically** specified at every moment. Follows **Newton's equations.**	Particles behave like waves, and instead have a **discrete/quantized wavefunction**. Cannot specify the precise location of a particle. QM is **probabilistic** and follows **Schrodinger's equation.**

(a) The Schrodinger Equation (we will never ask you to calculate this…)

$H\psi = E\psi$, where H = Hamilitonian operator, E = energy, and Ψ = wavefunction

Wavefunction (ψ) = A solution of the Schrödinger equation; the probability amplitude.

Probability Density (ψ^2) = A function that, when multiplied by volume of the region, gives the probability that the particle will be found in that region of space, between 0 and 1.

(b) Our First Quantum System: A Particle in a 1D Box

Wavefunction: $\psi(x) = (\frac{2}{L})^{1/2} \sin(\frac{n\pi x}{L})$, sin(0) = sin(pi) = 0

Boundary Conditions: x = 0ψ = Lψ = 0

→→ *Plug that into Schrodinger's Equation and get the energy for a particle in a 1D Box:* $E_n = \frac{h^2 n^2}{8mL^2}$

7. A carbon-carbon double bond has a length of roughly 1.34A, and the motion of an electron in the bond can be treated like a particle in a 1D box.

(a) Calculate the energy of an electron in each of its three lowest allowed states if it is confined to move in a 1D box of length 1.34A.

$E_1 = \frac{h^2(1)^2}{8mL^2} = \frac{(6.626 \times 10^{-34} Js)^2(1)^2}{8(9.11 \times 10^{-31} kg)(1.34 \times 10^{-10} m)^2} = 3.36 \times 10^{-18} J\ or\ 21.0\ eV$

$E_2 = 4E_1 = 1.34 \times 10^{-17} J\ (83.9eV)\ ;\ E_2 = 9E_1 = 3.02 \times 10^{-17} J\ (189eV)$

(b) Sketch the wave functions and the probabilities for finding the electron in the box for each of the three states. Label clearly.

(c) Calculate the wavelength of light necessary to excite the electron from its ground state to the first excited state. $\Delta E = E_2\text{-}E_1 = 1.34 \times 10^{-17} J - 3.36 \times 10^{-18} J = 1.00 \times 10^{-17} J = hc/\lambda$

$$\lambda = \frac{hc}{\Delta E} = \frac{(6.626 \times 10^{-34} Js)(3.0 \times 10^{8} m/s)}{1.00 \times 10^{-17} J} = 1.99 \times 10^{-8} m = 19.9 nm$$

(c) Next Quantum System: The Hydrogenic Atom & 1e⁻ systems

1. Consider the following transitions. Which will emit light with a longer wavelength?

a. $n = 4 \rightarrow n = 2$ <u>or</u> *$n = 3 \rightarrow n = 2$*

b. *$n = 3 \rightarrow n = 1$* <u>or</u> $n = 1 \rightarrow n = 3$

c. *$n = 5 \rightarrow n = 3$* <u>or</u> $n = 3 \rightarrow n = 1$

2. Calculate the wavelengths (nm) emitted for the following electronic transitions in a Li^{2+} ion.

a. $n = 5 \rightarrow n = 3$

$$\Delta E = -2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right) \text{ and } E\ photon = |\Delta E| = \frac{hc}{\lambda}$$

$$\frac{hc}{\lambda} = |2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right)| = \frac{(6.626 \times 10^{-34} Js)(3 \times 10^{8} ms^{-1})}{\lambda\left(\frac{10^9 nm}{m}\right)} =$$

$$|2.178 \times 10^{-18} J\left(\frac{1^2}{3^2} - \frac{1^2}{5^2}\right) \Rightarrow \lambda = 1283\ nm$$

b. $n = 3 \rightarrow n = 1$

$$\frac{(6.626 \times 10^{-34} Js)(3 \times 10^{8} ms^{-1})}{\lambda\left(\frac{10^9 nm}{m}\right)} = |2.178 \times 10^{-18} J\left(\frac{1^2}{1^2} - \frac{1^2}{3^2}\right) \Rightarrow \lambda = 103\ nm$$

The Bohr Model of the Atom:

See Figure 12.10 in the book.

The Rydberg Equation:

$$E = -2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2}\right)$$

$$\Delta E = -2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right)$$

3. An excited hydrogen atom with an electron in n = 5 state emits light having a frequency of $6.9 \times 10^{14}\ s^{-1}$. Determine the principal quantum level (n) for the final state in this electronic transition.

$$h\nu = |2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right)| = (6.626 \times 10^{-34} Js)(6.9 \times 10^{14}\ s^{-1}) = |2.178 \times 10^{-18} J\left(\frac{1^2}{x^2} - \frac{1^2}{5^2}\right) \Rightarrow n_f = 2$$

4. Consider the emission spectrum of the one-electron species X^{m+}. If the electron transitions from an initial state of n=5 to a final state of n=3, photons are emitted with a wavelength of 142.5 nm. If the electron transitions from an unknown initial state to a final state of n=3, photons are emitted with a wavelength of 111.7 nm. What is the unknown initial state responsible for this wavelength of emitted light?

X^{m+} is an one electron species $\Rightarrow \Delta E = -2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right)$ and E photon = $|\Delta E| = \frac{hc}{\lambda}$

$\frac{hc}{\lambda} = |2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right)|$ the only variables to consider is n and $\lambda \Rightarrow$ factoring out all constants

$$\lambda\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = \lambda\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right); \quad 142.5\ nm\left(\frac{1}{3^2} - \frac{1}{5^2}\right) = 111.7 nm\left(\frac{1}{3^2} - \frac{1}{n^2}\right) \Rightarrow n = 7$$

5. Calculate the ground state ionization energy (in kJ/mol) and the wavelength (in nm) required for B^{4+}.

B^{4+} is an one electron species $\Rightarrow \Delta E = -2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right)$

ground state $\Rightarrow n_i = 1$ and ionization $\Rightarrow n_f = \infty \Rightarrow \Rightarrow \Delta E = (2.178 \times 10^{-18} J)(Z^2)$

$\Rightarrow \Delta E = (2.178 \times 10^{-18} J)(4^2)\left(\frac{1\ kJ}{1000 J}\right)\left(\frac{6.022 \times 10^{23}}{mol}\right) = 2.1 \times 10^4$ kJ/mol

$\frac{hc}{\lambda} = 2.178 \times 10^{-18} J(Z^2) \Rightarrow \frac{(6.626 \times 10^{-34} Js)(3 \times 10^8\ ms^{-1})}{\lambda} = 2.178 \times 10^{-18} J(5^2) \Rightarrow \lambda = 3.65$ nm

6. The ground-state ionization energy of the one-electron ion X^{m+} is 1.18×10^4 kJ/mol. What is the value of "m" in X^{m+}?

X^{m+} is an one electron species $\Rightarrow \Delta E = -2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right)$

ground state $\Rightarrow n_i = 1$ and ionization $\Rightarrow n_f = \infty \Rightarrow \Rightarrow \Delta E = (2.178 \times 10^{-18} J)(Z^2)$

$\Rightarrow 1.18 \times 10^4$ kJ/mol $= (2.178 \times 10^{-18} J)(Z^2)\left(\frac{1\ kJ}{1000 J}\right)\left(\frac{6.022 \times 10^{23}}{mol}\right) \Rightarrow Z = 3 \Rightarrow Li^{2+}$

7. The wavelength of light associated with the *n* = 2 to *n* = 1 electron transition in the hydrogen spectrum is 1.216 × 10–7 m. By what coefficient should this wavelength be multiplied to obtain the wavelength associated with the same electron transition in the Li^{2+} ion?

(A) 1/9 (B) 1/7 (C) 1/4 (D) 1/3 (E) 1

1/9 The energy of the transition is proportional To Z^2. Li 2+ has one electron since Z=3 so the energy would be 9 times more than hydrogen, and wavelength being inverse to energy would be 9 times shorter.

8. Which of the following statements is(are) true?

I. An excited atom can return to its ground state by absorbing electromagnetic radiation.

II. The energy of an atom is increased when electromagnetic radiation is emitted from it.

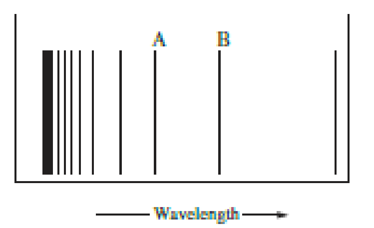
III. The energy of electromagnetic radiation increases as its frequency increases.

IV. An electron in the *n* = 4 state in the hydrogen atom can go to the *n* = 2 state by emitting electromagnetic radiation at the appropriate frequency.

V. The frequency and wavelength of electromagnetic radiation are inversely proportional to each other.

(A) II, III, IV (B) III, V (C) I, II, III (D) III, IV, V (E) I, II, IV

9. ***Line Spectra & the Bohr Model -*** The figure below represents part of the emission spectrum for a one-electron ion in the gas phase. All the lines result from electronic transitions from excited states to the *n* = 3 state.



(a) What electronic transitions correspond to lines A and B?

The largest energy jump will occur between n=∞ and n=3. The larger the ΔE the larger the frequency and the smaller the wavelength. Therefore, the lines seen at the highest wavelength are due to the smallest energy jumps. A n=6 → n=3. B n=5 → n=3.

(b) If the wavelength of line B is 142.5 nm, calculate the wavelength of line A.

$\Delta E = \frac{hc}{\lambda} = |2.178 \times 10^{-18} J\left(\frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2}\right)| = \frac{(6.626 \times 10^{-34} Js)(3 \times 10^8\ ms^{-1})}{142.5 nm\left(\frac{10^9 nm}{m}\right)} = 2.178 \times 10^{-18} J\left(\frac{Z^2}{5^2} - \frac{Z^2}{3^2}\right);\ Z=3$

$\Delta E = \frac{hc}{\lambda}| = \frac{(6.626 \times 10^{-34} Js)(3 \times 10^8\ ms^{-1})}{142.5 nm\left(\frac{10^9 nm}{m}\right)} = 1.216 \times 10^{-7} m = 121.6\ nm =$