#### CHEMISTRY II: INTRODUCTION TO MOLECULAR SPECTROSCOPY

Video Tutorial 1: Elementary problem solving Sessions

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 Find the wave number, frequency and wavelength of electromagnetic radiation consisting of photons each with an energy of 2 eV.

 Three energy levels are in the order A<B<C. The energy difference between A and C is 1 eV and wavelength of light required for a resonant transition from A to B is 900 nm. What is the wavelength of light required for resonant transition from level B to level C?

 The usual frequency range for vibrational spectroscopy is 400-4000 cm<sup>-1</sup> (in wave numbers). Consider a typical vibrational stretching line at 2000 cm<sup>-1</sup>. Calculate this energy in J/molecule and J/mol at room temperature.

- Calculate the relative populations  $\frac{N_1}{N_0}$  of a two level system (1- Excited, 0- Ground) subject to transitions that would occur due to electromagnetic radiation
  - with a wavelength of 500 Angstroms
  - with a wave number of 30 cm<sup>-1</sup>
  - with a frequency 10<sup>17</sup> Hz. (T=27 Celsius)

• Show that for a diatomic molecule with two atoms of mass  $m_1$  and,  $m_2$  the moment of inertia Ifor an axis passing through the centre of mass of the molecule and perpendicular to the bond axis is given by  $I = \mu r^2$  where r is the bond distance.

 Calculate the force constant in Nm<sup>-1</sup> for HBr molecule given that the fundamental transition frequency is given as 2650 cm<sup>-1</sup> wavenumbers. Calculate the same for CO given the fundamental frequency as 2170 cm<sup>-1</sup> wave numbers. Comment on the strength of the bonds based on your results.

 For HCI, calculate the maximum amplitude of the lowest vibrational level. Can the molecule be approximated as a simple harmonic oscillator? k
= 478 kg s<sup>-2</sup> = 478 N m<sup>-1</sup>. The equilibrium bond length of HCI is 127.4 pm.

 The O-H stretching vibration in a molecule was seen at 3600 cm <sup>-1</sup>. Assuming the force constant of the bond to remain the same due to isotopic substitution ( of H by D), find the expected shift in the stretching frequency.

 A certain solution in a cell absorbs 80 % of incident light. What fraction of the incident light will be absorbed in a cell 5 times longer?

Methanol absorbs at 184 nm and has an absorbance of 150 dm<sup>3</sup> mol<sup>-1</sup> cm<sup>-1</sup>.
Calculate percentage of light transmitted for a concentration of 0.01 moles dm<sup>-3</sup> through a cell of length 1 cm.

Enjoy your learning and send me problems that you may want to solve in elementary spectroscopy. Please remember learning is reinforced through problem solving and not the other way around—i.e., by solving problems you don't necessarily learn new concepts. You have to read, think about it and discuss that. Online learning through this course is by self-motivation only. All the best. Mangala Sunder