

NORTH CAROLINA STATE UNIVERSITY

Department of Chemistry

Name _____

CH 795T

Molecular Spectroscopy

Problem Set #1

Aug. 27, 2007

Due Date: Sept. 10, 2007

1. Using formulae for the associated Legendre polynomial determine the rotational transition moment for the transition from $J = 1$ to $J = 2$. This derives from the general selection rule $\Delta J = 1$ or -1 and $\Delta M = 0$.

2. The root-mean-square motion of a harmonic oscillator is given by:

$$\sqrt{\langle Q^2 \rangle}$$

Using a general formula for the r.m.s. motion of a harmonic oscillator in quantum level v , determine the change in amplitude of motion of the diatomic CO for the transition from $v = 0$ to $v = 1$. Assume that the vibrational frequency of is 2143 cm^{-1} .

3. X-ray photoelectron spectroscopy is a method for detecting the presence of atoms on a surface. In this method a high energy X-ray ionizes the molecule by kicking out a core electron (i.e. an electron from a $1s$ orbital). Any excess energy leaves with the electron as kinetic energy. Calculate the kinetic energy of an electron ejected from a carbon atom using a 100 eV X-ray. (Hint: assume that carbon is just a hydrogen atom with a different nuclear charge)
4. A. What is the concentration of a dye molecule that has $\epsilon(400 \text{ nm}) = 105,000 \text{ M}^{-1} \text{ cm}^{-1}$ if it has an absorbance of 0.3 at 400 nm in a 0.1 cm pathlength cell?
B. What fraction of the incident light makes it through the cuvette at this concentration?
C. What flux ($F = \text{W}/\text{cm}^2$) is required for a 10 picosecond pulse at 400 nm to excite 10% of the sample? Hint: you may assume that each photon that strikes the cross section is absorbed.
5. What is the force of attraction of an electron with the proton in the nucleus of a hydrogen atom if it is in the first Bohr orbit? What is the gravitational force of the electron at that distance?