NORTH CAROLINA STATE UNIVERSITY
Department of Chemistry Name_____

Physical Chemistry CH437 Problem Set #3
Due Date: September 15, 2015

1. What is the concentration of a dye molecule that has ε(540 nm) = 65,000 $M^{-1}cm^{-1}$ if it has a transmittance of 50% at 540 nm in a 1 cm pathlength cell? What is the absorbance of the sample?

   Concentration of dye = _____.

   Absorbance = _____.

2. The atmosphere is made up of 79% N_2 and 20% O_2. To apply rotational or vibrational spectroscopy formulae to these diatomic molecules, you will need to use the reduced mass, given by:

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

   A. Calculate the reduced mass for both N_2 and O_2 in kilograms.

   Reduced mass for oxygen = _____.

   Reduced mass for nitrogen = _____.

   B. Given the rotational constant $\widetilde{B}$ = 1.99 cm^{-1} for N_2 and 1.45 cm^{-1} for O_2 determine the bond length of each molecule.

Bond length for oxygen = _____.

Bond length for nitrogen = _____.

C. Calculate the intensity of the J=0 → J=1 transition in the rotational spectra of N_2.

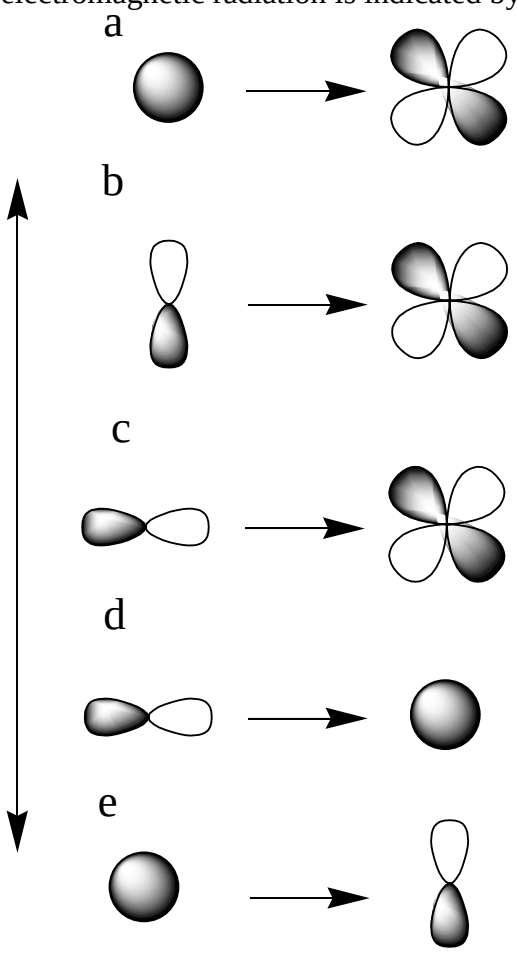
Microwave absorption intensity for nitrogen = _____.

D. Given the force constants for N_2 and O_2 are 2287 and 1133 N/m, respectively, calculate their vibrational frequencies.

E. Calculate the infrared absorption intensity of the v=0 → v=1 transition of O_2.

Infrared absorption intensity for oxygen = _____.

3. Which of the following properly obey a selection rule? Note: the polarization of the electromagnetic radiation is indicated by the two-headed vertical arrow.



4. The particle-in-a-box or free electron model predicts that the transition energy of ethene is 109,060 cm^{-1}. Fill in the table below with the energies for butadiene and hexatriene. One easy way to do this is to determine the ratio of the transition energies of both butadiene and hexatriene relative to ethene. Use those ratios to calculate the transition energies (6 points).

Molecule	L (Å)	Ratio	ΔE (cm^{-1})
Ethene	2.89	1	109,060
Butene	5.78		
Hexene	8.67		