CSO202—Atoms, Molecules & Photons
Homework – 2

1.(a) Complete the following table for electromagnetic waves in vacuum (Plank's constant, $h = 6.62 \times 10^{-34}$ Js; velocity of light, $c = 3 \times 10^{8}$ m/sec):

λ (μm)	v (Hz)	E(eV)	Wavenumber(cm^{-1})	Spectral region
0.6				
	4×10^{12}			
		13.6		
			4000	

1.(b) Now redo this table below but assume that the medium has an index of refraction n=1.5 (this is pretty close to correct for glass at visible frequencies, and for coaxial cables at radiofrequencies).

λ (μm)	v (Hz)	E(eV)	Wavenumber(cm^{-1})	Spectral region
0.6				
	4×10^{12}			
		13.6		
			4000	

1.(c) Based on your answers to a & b, which are the preferred units to use & why?

2. Consider the vibrational motion of HI. Since Iodine is very heavy, assume it is stationary and the hydrogen atom undergoes harmonic motion. With force constant $k = 317\ N.m^{-1}$. What is the fundamental vibration frequency ν_0 ? How much error has resulted because of neglecting the motion of I ? What is ν_0 if H is replaced by D?

3. The wavenumber of the j=1 ← j=0 rotational transitions for $^{1}H^{35}Cl$ and $^{2}H^{35}Cl$ are 20.8784 cm^{-1} and 10.7840 cm^{-1} respectively. Accurate atomic masses are 1.007825 and 2.0140 for ^{1}H and ^{2}H (i.e., D) respectively. The mass of ^{35}Cl is 35.96885. Based on this information alone, can you conclude that the bond lengths are the same or different in the two molecules?

4. Calculate the proportion of HI molecules in their ground, first, and second excited vibrational states at 298 K. On substituting H with D would you expect a larger proportion of DI in the first excited state as compared to the case of HI? (Fundamental Frequency of vibration of HI = 2230 cm^{-1}.)

5. Use the collision theory of gas phase reactions to calculate the theoretical value of the second-order rate constant for the reaction $H_2(g) + I_2(g) \rightarrow 2HI\ (g)$ at 650 K, assuming that it is elementary bimolecular. The collision cross section is 0.36 nm^{-1}, the reduced mass is 3.32×10^{-27} kg, and the activation energy is 171 $kJ.mol^{-1}$.