CHM201

Problem set 1

(Rotational spectroscopy)

(Will be discussed in the Tutorial session)

In all the calculations, where the speed of light, *c*, is required, assume it to be 2.9979 x 10^{10} cm s^{-1}

1. The human eye can see electromagnetic radiation over the region from about 350 nm to 750 nm. Convert these two wavelengths to wavenumbers (in cm^{-1}) and eV.

2. The microwave region extends from about 1 GHz to 100 GHz. Convert these frequencies to wavelengths.
   (These problems should help you become familiar converting from one unit to another and also to have a feel for the sort of magnitudes of numbers, one encounters in various units.)

3. What is the energy of one photon of radiation of a) frequency 4.6 GHz and b) 37,000 cm^{-1}. What is the energy of one mole of these photons?

4. Calculate the reduced mass for the following species a) $^{12}C^{1}H$; b) $^{13}C^{1}H$; c) $^{12}C^{2}H$. (These are chemically identical species, with isotopic substitution.)

5. In problem, 4, calculate the rotational constant (in cm^{-1}), for all the three species, assuming that all three of them have an internuclear distance of 1.1199 Å.

6. If you recorded a pure rotation spectrum for all the three species, what would be the spacings between the rotational lines for each of them, in units of cm^{-1}. Draw inferences on the effect of isotopic substitution.

7. Calculate the *B* value for a)$^{127}I_2$, given that *r*(I-I) = 2.6663 Å. (This is to show you what heavy atom rotational spectroscopy is likely to look like.)

8. Calculate the reduced mass for $^{202}Hg^{1}H$ b)H_2. Which is likely to show a larger spacing between rotational lines in the spectrum.

9. Which of the molecules would show pure rotational spectrum: a) H_2 b) HCl c) $^{1}H^{2}H$

10. In a certain experiment, the rotational constant *B* for $^{12}C^{16}O$ was determined to be 1.929 cm^{-1}. Using this value for *B*, calculate the bond length in CO. Another experimentalist measures the same quantity and reports a *B* value of 3.858 cm^{-1} for CO. Can you pass a judgement on who is more likely to be correct and if any of the values of *B* is clearly indicated to be incorrect?