CHM2330
Assignment #3 - 2014

Due: March 11 **in class**.
Assignments handed in on the 11th after class will lose 25% of the total marks.
Assignments will not be accepted after the 11th (i.e., they get zero).

- Show units at least in the first step and final answer for each calculation.
- Show all work for full marks.

1. (5 marks) The vibrational-rotational absorption spectrum of $^{12}C^{16}O$ shows two branches, one on each side of the centre of the spectrum. The centre is at 2143.26cm^{-1}. The separation between the between the peak immediately to the left of centre and the peak immediately to the right of centre is 7.655 cm^{-1}. Using the rigid rotor and harmonic oscillator approximations, answer the following questions:
(a) What is the vibrational wavenumber for $^{12}C^{16}O$?

a) $\tilde{\nu}_Q = \tilde{\nu} = 2143.26\ cm^{-1}$

(b) What is the force constant, *k*, of the carbon-oxygen bond in $^{12}C^{16}O$?

c) $\tilde{\nu} = \frac{1}{2\pi c}\sqrt{\frac{k}{m_{eff}}}$

$\therefore k = (\tilde{\nu}(2\pi c))^2 \cdot m_{eff}$

$k = 1855.69\ N\ m^{-1}$

$m_{eff} = \left\{\frac{(12u)(15.9949u)}{12 + 15.9949}\right\}(1.6605 \times 10^{-27})$

$= 1.1385 \times 10^{-26}\ kg$

(c) What is the bond length of $^{12}C^{16}O$?

$$B = \frac{\hbar}{4\pi c\, m_{eff}\, r^2}$$

$$\therefore \quad r = \sqrt{\frac{\hbar}{4\pi c\, m_{eff}\, B}} = \sqrt{\frac{1.05457\times10^{-34}\ \text{Js}}{4\pi(2.998\times10^{10}\ \frac{\text{cm}}{\text{s}})(1.914\ \text{cm}^{-1})\, m_{eff}}}$$

$$= \underline{1.133\ \text{Å}}$$

2. **(4 marks)** The rotational Raman spectrum of $^{19}F_2$ has a series of Stokes lines separated by 3.5312 cm^{-1}. Calculate the bond length of the molecule. The mass of ^{19}F is 18.9984 u.

Separation = 4B

① ∴ $B = 0.88280\ cm^{-1}$

$= \hbar / 4\pi c I$

$I = \frac{\hbar}{4\pi c B} = \frac{6.626\times10^{-34}\ Js}{(2\pi)(4\pi)(2.9979\times10^{8}\ \frac{m}{s})(0.88280\ cm^{-1})}$

① $= 3.1708977\times10^{-46}\ kg\ m^2$

$I = m_{eff}\ r^2$ ①

$= \left(\frac{18.9984\ u}{2}\right)\left(1.660538\times10^{-27}\ \frac{kg}{u}\right) r^2$

$\therefore r^2 = 2.01023\times10^{-20}\ m^2$

$\therefore r = 1.4178268\times10^{-10}\ m$

The bond length is: 1.4178 Å

3. (6 marks) If the wavenumber of the $J = 1 \leftarrow 0$ rotational transition of $^{1}H^{81}Br$ is 16.933 cm^{-1}, what is (a) the moment of inertia (b) the bond length? You may treat the molecule as a rigid rotor.

$\tilde{\nu} = 16.933\ cm^{-1}$ line spacing $= 2B = 16.933\ cm^{-1}$

(a) $B = 8.4665\ cm^{-1}$

$$I = \frac{h}{4\pi c B} = \frac{6.626\times10^{-34}\ Js}{(8\pi^2)(2.9979\times10^{10}\ \frac{cm}{s})(8.4665\ cm^{-1})}$$

$$I = 3.3063\times10^{-47}\ kg\,m^2$$

b)

$$R = \sqrt{\frac{I}{m\mu}} = \sqrt{\frac{3.3063\times10^{-47}\ kg\,m^2}{\left(\frac{(1.0078u)(80.9163u)}{1.0078u + 80.9163u}\right)\left(1.66054\times10^{-27}\ \frac{kg}{u}\right)}}$$

$$R = 1.4143\ \mathring{A}$$