CHE-371 Fall 2007

Homework #1

As the first part of this class is "review", the homework problems from the QM section are taken from various chapters of M&S (i.e., 1-13).

QM

1. The anti-symmetric stretch of CO_2 appears in an IR spectrum at 2349.16 cm^{-1}. Translate this value into frequency (in Hz), wavelength (in nm), and energy (in J).
2. Problem 1-22 from McQuarrie and Simon
3. Problem 5-14 from McQuarrie and Simon; The following definitions will be useful:

$$\upsilon = \frac{1}{2\pi}\left(\frac{k}{\mu}\right)^{1/2} \quad \text{and} \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

   where υ is the frequency, k is the force constant, and μ is the reduced mass.

4. Given that $\tilde{\upsilon}$ = 2330 cm^{-1} and D_0 = 78715 cm^{-1} for N_2, calculate D_e.
5. Problem 13-33 from McQuarrie and Simon
6. The energy difference between the J=0 and J=1 rotational levels for carbon monoxide ($^{12}C^{16}O$) is $\upsilon = 1.153 \times 10^5$ MHz.
   a. Calculate the energy difference between the J=0 and J=2 rotational levels. Give your answers in Hz, kJ, nm, and cm^{-1}.
   b. Calculate the degeneracy of the first 4 rotational levels.

Gas Laws

1. McQuarrie and Simon: 6, 7 (use virial expansion to B_{2V}), 16, 31-34 (hint: make one spreadsheet for all 3 problems!), 44, 57, 58**;
2. Imagine you have a small sealed glass vial containing CO_2. You can clearly see a meniscus about half way up the vial, showing that the liquid and vapor phases are in coexistence. The vial has a volume of 9 mL, contains 4.9 grams of CO_2, and is at a temperature of 300 K. Using the van der Waals EOS and the critical values for CO_2, T_C = 304 K, $\overline{V}_C$ = 0.095 $dm^3 \cdot mol^{-1}$, P_C = 73.84 bar, find the pressure in the vial. Although you will use the van der Waals EOS, do not use the specific values of the van der Waals coefficients, *a* and *b*, for CO_2.

   Hint: Write the van der Waals EOS in terms of reduced variables using the following definitions,

$$T_C = \frac{8a}{27bR} \qquad P_C = \frac{a}{27b^2} \qquad \overline{V}_C = 3b$$

<u>For Review on 9/14</u>

Group A= M&S, 5-14

Group B= M&S, 16-7

Group C= Gas Laws, #2

** The key to the problem is understanding partial differential notation. If you don't know how to do this problem, ask!! This type of problem will reoccur often in CHE371!