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 CO₂ 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:
   \[ \nu = \frac{1}{2\pi} \left( \frac{k}{\mu} \right)^{1/2} \quad \text{and} \quad \mu = \frac{m_1 m_2}{m_1 + m_2} \]
   where \( \nu \) is the frequency, \( k \) is the force constant, and \( \mu \) is the reduced mass.
4. Given that \( \nu = 2330 \text{ cm}^{-1} \) and \( D_0 = 78715 \text{ cm}^{-1} \) for N₂, 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 (¹²C¹⁶O) is \( \nu = 1.153 \times 10^5 \text{ MHz} \).
   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 CO₂. 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 CO₂, and is at a temperature of 300 K. Using the van der Waals EOS and the critical values for CO₂, \( T_C = 304 \text{ K}, V_C = 0.095 \text{ dm}^3\cdot\text{mol}^{-1}, P_C = 73.84 \text{ bar} \), 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 CO₂.

Hint: Write the van der Waals EOS in terms of reduced variables using the following definitions,
\[ T_c = \frac{8a}{27bR} \quad P_c = \frac{a}{27b^2} \quad V_c = 3b \]

For Review on 9/14
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!