

Practice Problems for Exam 1

CHE371, Fall 2008

1. Explain, in words, what g_j , β , $q(V, T)$, and ϵ_j are in the following equation:

$$q(V, T) = \sum_{\text{levels}, j} g_j e^{-\beta \epsilon_j}$$

2. How many total, translational, vibrational, and rotational degrees of freedom does acetylene (C_2H_2) have?
3. At the Boyle temperature, circle the following statement that is true:
- $B_{2V} > 0$
 - $B_{2V} < 0$
 - $\bar{V} > \bar{V}_{ideal}$
 - $\bar{V} < \bar{V}_{ideal}$
 - None of the above are true. (If you choose e, give a reason.)
4. The following plot shows the second virial coefficient, B_{2V} , as a function of T for 4 different gases. At 300 K, which gas has the smallest molar volume, \bar{V} ?

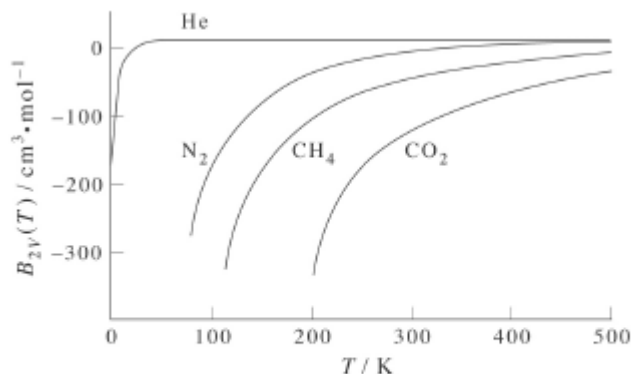
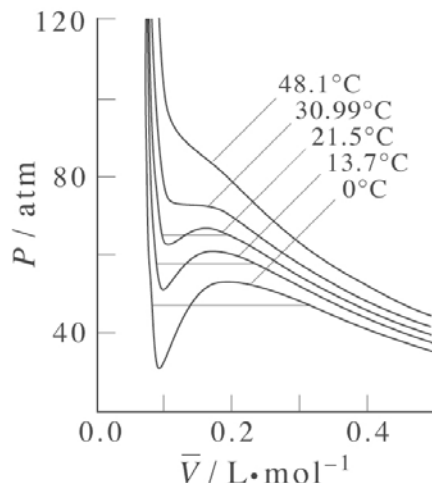


Figure 1: This is Figure 16.12 from Simon and McQuarrie.

5. The partition function for a van der Waals equation of state is given below. Derive an expression for (a) the energy, $\langle E \rangle$ and (b) the constant volume heat capacity, C_V . Give answers in terms of N , k_B , T , V and the constants a and b . Show all work.

$$Q(N, V, \beta) = \frac{1}{N!} \left(\frac{2\pi m}{\beta h^2} \right)^{3N/2} (V - Nb)^N e^{\beta a N^2 / V}$$

6. In the plot below, mark the critical point and the places on the graph that describe gases, liquids, and supercritical fluids. Also describe the meaning of the horizontal lines and the “van der Waals” loops.



7. Which of the following is true about typical energy spacings between adjacent translational, electronic, rotational, and vibrational energy levels in molecules:
- Translational < electronic < rotational < vibrational
 - Translational > electronic < rotational < vibrational
 - Electronic > rotational > translational \approx vibrational
 - Rotational \approx electronic \gg vibrational > translational
 - Electronic > vibrational > rotational > translational
 - None of the above; If you choose (f) write out the correct answer.
8. The electronic energy of the first excited electronic state for helium (He) is $159,850 \text{ cm}^{-1}$ higher than the ground state. The electronic energy of the first excited electronic state for atomic fluorine (F) is 404 cm^{-1} higher than the ground state. Which statement is true about the fraction of F atoms in the first excited electronic state [$f_2(\text{F})$] and the fraction of He atoms in the first excited electronic state [$f_2(\text{He})$] at 404K?
- $f_2(\text{F}) = 1$
 - $f_2(\text{F}) > f_2(\text{He})$
 - $f_2(\text{He}) > f_2(\text{F})$
 - $f_2(\text{F}) = 0$
 - $f_2(\text{F}) = f_2(\text{He})$
9. What two assumptions does the ideal gas equation of state make about gases? How does the van der Waals equation overcome these assumptions?
10. The frequency of vibration for an unknown diatomic gas is $5.3 \times 10^{13} \text{ Hz}$. If an IR spectrum for this gas was collected, at what cm^{-1} would a peak appear?