Problem Sheet 3 (2005)

Answers to questions 1 - 4 should be handed in by Wednesday 30 November, 2005.

1. (a) Describe briefly the interactions that take place when two Ne atoms approach each other from large separations.

(b) Sketch the Lennard-Jones form of the interaction potential energy, U(r), and the force, F(r) between two Ne atoms. Mark the binding energy ε , contact separation σ , and equilibrium spacing r_0 on your diagram. Show that in the Lennard-Jones function $r_0 = 2^{1/6} \sigma$.

(c) The Lennard-Jones parameters for neon are $\varepsilon = 0.492 \times 10^{-21}$ J and $\sigma = 2.75 \times 10^{-10}$ m. Estimate the critical temperature for neon. Explain briefly why your estimate differs from the experimental value of 44 K.

(d) Estimate the equilibrium distance between nuclei of neon molecule from the value of excluded volume in "real" neon gas (b = 0.0158 L/mol) and compare it with the value found from Lennard-Jones potential energy function. [10]

2. Krypton has Lennard-Jones parameters $\varepsilon = 2.3 \times 10^{-21}$ J and $\sigma = 3.68 \times 10^{-10}$ m, and forms a crystal structure with 12 atoms surrounding each atom. Estimate the amount of energy required for melting 1 mol of krypton, assuming that the number of nearest neighbours in a liquid phase drops to 10. Explain why your calculated value differs from the experimental data: $L_{melt} = 1.64$ kJmol⁻¹.

3. For carbon dioxide gas (CO₂), the constants in the van der Waals equations are $a = 0.364 \text{ J} \text{ m}^3/\text{mol}^2$ and $b = 4.27 \times 10^{-5} \text{ m}^3/\text{mol}$

i) If 1.00 mol of CO_2 gas at 350 K is confined to a volume of 400 cm³, find the pressure of the gas using both the ideal gas equation and the van der Waals equation. [2]

ii) Give physical reasons for the influence on the pressure of the non-zero a and b parameters in van der Waals equation. [5]

4. (a) The density of mercury at 0 °C is 13600 kg/m³. Calculate the density of mercury at 50 °C. The volume expansion coefficient of liquid mercury is 1.82×10^{-4} K⁻¹.

(b) A thermometer contains 15 mm³ of liquid mercury and has a capillary radius of 0.05mm. Calculate how far will the mercury rise in the capillary if the temperature of the mercury increases from 25 °C to 27 °C, if the expansion of the glass is neglected.

(c) Assume that Δl_1 is expansion of mercury in the thermometer in problem (b) and let Δl_2 be the actual expansion which allows for the expansion of the glass. Calculate the numerical value of $(\Delta l_1 - \Delta l_2)/\Delta l_1$. Assume that only the thermometer bulb is immersed in the object whose temperature is being measured and that the initial volume of mercury is equal to the volume of the bulb. The coefficient of linear expansion of glass is $\alpha = 8.3 \times 10^{-6} \text{ K}^{-1}$.



[10]

[5]