

NATIONAL UNIVERSITY OF SCIENCE AND TECHNOLOGY

DEPARTMENT OF APPLIED CHEMISTRY
SUPPLEMENTARY EXAMINATIONS - MARCH 2003
PHYSICAL CHEMISTRY FOR TEXTILE TECHNOLOGY - SCH1122
TIME: 3 HOURS

INSTRUCTIONS TO CANDIDATES

Answer **ALL** questions from Section A and **ANY THREE** from Section B.

$$\text{Gas Constant } R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1} = 0.0821 \text{ L atm K}^{-1} \text{ mol}^{-1}$$

$$\text{Avogadro's Number } N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$$

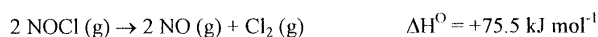
Graph Paper and Periodic Tables Required

SECTION A

1. In the ground state of argon, Ar,
 - (i) How many electrons have $n = 3$ as one of their quantum numbers?
 - (ii) How many electrons have $l = 1$?
 - (iii) How many electrons have $m_l = 0$?
 - (iv) How many electrons have $m_s = +\frac{1}{2}$? (4 marks)
2. (a) The terms (i) first ionisation energy, (ii) electron affinity, refer to the enthalpies of which processes? (4 marks)

(b) The Mulliken definition relates the electronegativity of an element to both its first ionisation energy and electron affinity. Define electronegativity, state Mulliken's formula, and explain its significance. (8 marks)
3. Calculate the standard enthalpy of formation of NOCl (g) from the following data:-

$$\Delta H^{\circ}(\text{formation}) \text{ of NO} = +90.25 \text{ kJ mol}^{-1}$$



(6 marks)

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4. The heat capacity of chloroform, CHCl_3 , is given in the range 240 K to 330 K by

$$C_p (\text{J K}^{-1} \text{mol}^{-1}) = 91.47 + 0.075 (T/\text{K}).$$

Calculate the change in molar enthalpy, and in molar entropy, in heating a sample of chloroform from 273 K to 300 K. (10 marks)

5. At 400 K the mole fraction of trans-2-butene in equilibrium with its isomer cis-2-butene is 0.674. Calculate the equilibrium constant and standard Gibbs energy for the isomerisation reaction. (8 marks)
6. At 300 K the partial pressure of HCl gas in equilibrium with its solution in liquid GeCl_4 are as follows:

$x(\text{HCl})$	0.005	0.012	0.019
$p(\text{HCl})$ (kPa)	32.0	76.9	121.8

(a) Show graphically that the solution obeys Henry's Law in this range, and calculate the Henry's Law constant at 300 K. (7 marks)

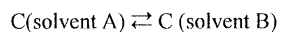
(b) Predict the partial pressure of HCl above a solution in GeCl_4 of molality 0.10 mol kg^{-1} . (8 marks)

SECTION B

7. (a) Describe in detail the bonding in ethene (ethylene, C_2H_4). Include explanations of the terms hybrid orbital, σ -bond and π -bond. (10 marks)
- (b) The lowest energy unoccupied molecular orbital (LUMO) in ethene is π^* in character. Describe, with the aid of a sketch, how this orbital is formed from atomic orbitals. (5 marks)
8. (a) Describe the geometry of a trigonal bipyramid. (3 marks)
- (b) Describe the geometry of the following species in detail, including a sketch and an estimate of the bond angles in each case: (i) ClF_3 (ii) SeOF_4 (iii) IF_5 (12 marks)

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9. The partition coefficient for the process



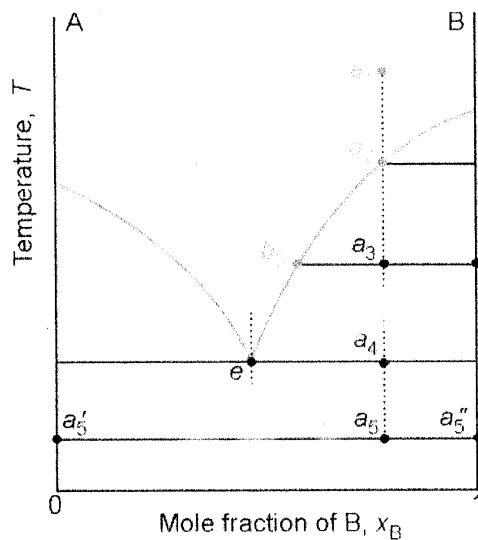
has a value of 100. Initially there is 1.00 L of a 1.00 molar solution of C in A, and 50.0 mL of B available. Show by a calculation, whether, to extract C into solvent B, it is better to use all 50.0 mL in one step, or in five steps using 10.0 mL each time. (15 marks)

10. The diagram below shows a binary solid/liquid phase diagram.

(a) Sketch the diagram, labelling all the regions present. (4 marks)

(b) State the Phase Rule, and explain how it applies to the eutectic point. (3 marks)

(c) Describe what happens on cooling a mixture of composition $x_B = 0.75$ from the melt, i.e. along the line a_1 to a_5 . How much of each phase is present when the overall system is at a_3 ? (8 marks)



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11. The following table gives the volume of nitrogen (reduced to 1 atm) adsorbed per gram of active carbon at 0 °C at various pressures.

p (Pa)	524	1731	3058	4534	7497
v (cm ³ /g)	0.987	3.04	5.08	7.04	10.31

- (a) Plot the data according to the Langmuir isotherm, and determine the constants.
(10 marks)
- (b) Estimate the pressure of nitrogen which would result in a fractional coverage of 0.5.
(5 marks)

END OF QUESTION PAPER!!!!