

NATIONAL UNIVERSITY OF SCIENCE AND TECHNOLOGY

**DEPARTMENT OF APPLIED CHEMISTRY**  
**END OF SEMESTER EXAMINATIONS - DECEMBER 2002**  
**PHYSICAL CHEMISTRY FOR TEXTILE TECHNOLOGY - SCH1122**  
**TIME: 3 HOURS**

**INSTRUCTIONS TO CANDIDATES**

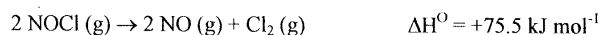
Answer **ALL** questions from Section A and **ANY THREE** from Section B.

Gas Constant  $R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1} = 0.0821 \text{ L atm K}^{-1} \text{ mol}^{-1}$   
Avogadro's Number  $N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$   
Graph Paper and Periodic Tables Required

**SECTION A**

1. List all the possible combinations of quantum numbers corresponding to the  $5d$ -subshell in an atom. How many electrons in total can be accommodated in this subshell?  
(5 marks)
2. (a) Give electronic configurations for the following species and identify each as paramagnetic or diamagnetic: (a) Mg (b) Fe (c)  $\text{Fe}^{2+}$  (d)  $\text{Pb}^{2+}$  (8 marks)  
(b) Identify the atom or ion with the larger radius in each of these pairs: (i)  $\text{Cl}^-$  or  $\text{S}^{2-}$   
(ii) Cl or  $\text{Cl}^-$  (d)  $\text{Li}^+$  or  $\text{Na}^+$ . (3 marks)
3. Calculate the standard enthalpy of formation of  $\text{NOCl (g)}$  from the following data:-

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



(6 marks)

4. The heat capacity of chloroform,  $\text{CHCl}_3$ , 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  $\text{GeCl}_4$  are as follows:

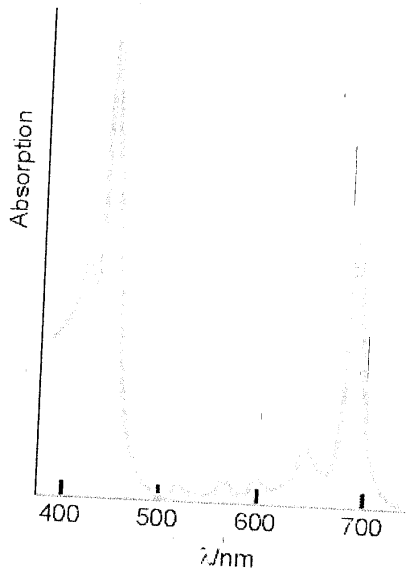
$x(\text{HCl})$	0.005	0.012	0.019
$p(\text{HCl})$ (kPa)	32.0	76.9	121.8

- (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  $\text{GeCl}_4$  of molality  $0.10 \text{ mol kg}^{-1}$ . (8 marks)

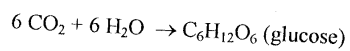
### **SECTION B**

7. (a) Describe in detail the bonding in ethene (ethylene,  $\text{C}_2\text{H}_4$ ). Include explanations of the terms hybrid orbital,  $\sigma$ -bond and  $\pi$ -bond. (10 marks)
- (b) The lowest energy unoccupied molecular orbital (LUMO) in ethene is  $\pi^*$  in character. Describe, with the aid of a sketch, how this orbital is formed from atomic orbitals. (5 marks)

8. The figure below shows the visible absorption spectrum for the photosynthetic pigment chlorophyll. The maxima are at 690 nm (red) and 440 nm (blue).



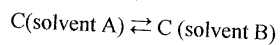
- (a) The standard enthalpy of the photosynthesis reaction



is  $-2808 \text{ kJ mol}^{-1}$ . If one carbon dioxide molecule reacts for each 4 photons (quanta of light energy) absorbed, what is the efficiency of conversion of (i) red light, (ii) blue light, in photosynthesis? (12 marks)

- (b) Explain why chlorophyll is green. (3 marks)

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)

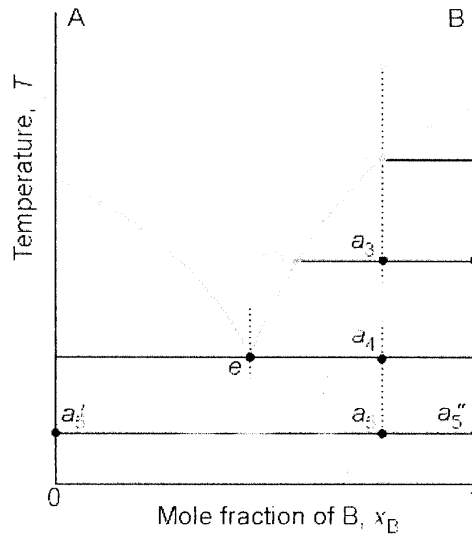
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10. The diagram below shows a binary solid/liquid phase diagram.

(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)



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 <sup>3</sup> /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!!!!**