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EASTERN UNIVERSITY, SRI LANKA

THIRD EXAMINATION

SECOND SEMESTER 2012-2013

CH 206 X-Ray Crystallography, Symmetry & Symmetry elements  
and Phase rule  
(Proper and Repeat)

Answer all questions

Time allowed: ONE Hour

Avogadro's No. is  $6.022 \times 10^{23}$  (mol<sup>-1</sup>)

a) List the symmetry elements present in the following molecules (Marks will be deducted for wrong symmetry elements).

- i)  $\text{PCl}_5$     ii) *trans*-2-butene    iii) 2,6-dichlorobenzene    iv)  $\text{PtCl}_4$

(20 marks)

b) Write the Miller indices for the plane having following intercepts and draw a schematic diagram to show the planes in the unit cell.

- i)  $\infty a, b/2, \infty c$     ii)  $a/3, b/2, c$     iii)  $a, 2b, 3c$

(30 marks)

c) A sample of chromium (Cr) is analyzed by X-ray diffraction using copper  $K\alpha$  radiation for which  $\lambda_{K\alpha} = 1.5418 \text{ \AA}$ . Determine the Miller indices of the plane from which the angle of reflection,  $\theta$ , is  $31.4^\circ$ . The lattice constant of Cr (length of the unit cell),  $a$ , is  $2.96 \text{ \AA}$ . Report your answer in the form (hkl).

(25 marks)

d) i) A crystal of iridium (Ir) is analyzed by X-ray diffraction through exposure to molybdenum  $K\alpha$  radiation, for which  $\lambda_{K\alpha} = 0.721 \text{ \AA} = 7.21 \times 10^{-11} \text{ m}$ . The lowest-index plane present in the diffractogram is (111). The lattice constant (length of the unit cell) of Ir,  $a$ , is  $3.84 \text{ \AA}$ . Calculate  $\sin \theta$ .

(15 marks)

Contd...

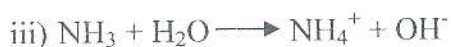
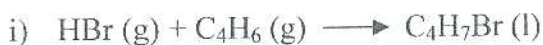
- ii) If you wanted to increase the angle at which the reflection described in part (i) is observed, would you replace the Mo target with a silver (Ag) target or a copper (Cu) target? Explain the reasoning behind your choice ( $\lambda_{\text{Cu}} = 1.54 \times 10^{-11} \text{ m}$ ,  $\lambda_{\text{Ag}} = 0.56 \times 10^{-11} \text{ m}$ ).

(10 marks)

2. a) State the phase rule and identify the terms in it.

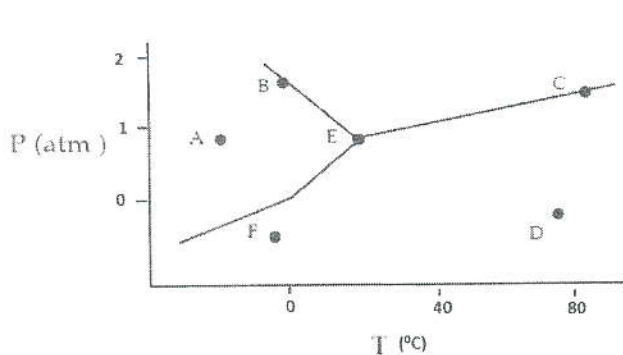
(10 marks)

b) Using phase rule, determine the number of components, phases and degrees of freedom in each of the following.

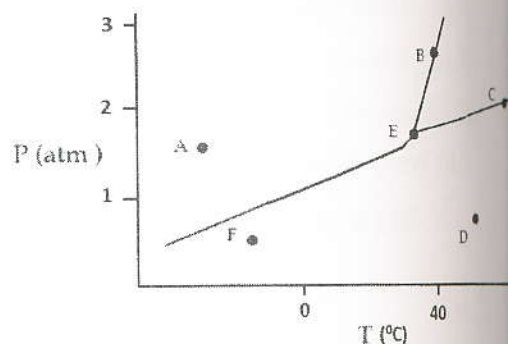


(24 marks)

- c) Phase diagram of two compounds X and Y are given below.



X



Y

- Identify the number of phases present in the points A, B, C, D, E and F.
- Which compound could be transformed from gas to solid and then to liquid at particular temperature. Explain by drawing a line in the above suitable diagram.
- Which compound melts at higher temperature than the other one? Explain.
- Which compounds can exist as liquid and gas respectively at room temperature ( $P=1 \text{ atm}$ )?
- Explain what will happen to the compounds X and Y if the pressure is increased from 1 to 2 atm at room temperature.

(45 marks)

Contd...

A

d) Benzene and toluene form an ideal solution. At 298K, what is the mole fraction of benzene in the liquid that is in equilibrium with a vapor that has equal partial pressures of benzene and toluene? At 298K, the vapor pressures of pure benzene and pure toluene are 95 and 28 torr, respectively.

(21 marks)

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