Model Questions For Semester-VI B.Sc Chemistry Honours

(Physical Chemistry)

1) Deduce Bragg's equation in connection with crystal analysis. How is the interplaner distance in a crystal determine with its help?
2) What is Miller indices of a crystal?
3) A metal has a body centred cubic lattice and the length of the unit cell is 2.9A^0. If the density of the metal is 10 g /cc, calculate the atomic weight of the metal.
4) Show that the body centered cubic lattice is less economically packed compared to the face centred cubic lattice.
5) What types of crystals would be expected to be i) the hardest, ii) the softest iii) the highest melting iv) good conductors of heat and electricity.
6) Examine the statement and indicate which are true or false:
   i) All crystalline solids are isotropic
7) Show by drawing the (100), (110) and (111) planes in a b.c.c lattice.
8) Find the number of nearest neighbours and the nearest neighbour distance in each of the following systems:
simple cube, body centred cube and face-centred cube.
9) The characteristic K_∞ lines of Cr, Fe and Ni have wavelengths of 2.2909,1.9378 and 1.6591 A^0 respectively. Which of these can be used to determine a lattice spacing of 1A^0. 3
10) The element Polonium (at wt. 210) crystallizes in the cubic system. Bragg first order reflections. Using X-ray of wavelength 0.154nm, occur at sinθ values of 0.225, 0.316 and 0.388 for reflection from (100), (110) and (111) –types planes.
i) Show whether the unit cell is simple, face centred or body centred.
ii) Calculate the value of 'a', the side of the unit cell.
iii) Calculate the density of polonium
11) What is a unit cell? Explain the uses of Miller indices in labeling crystal planes. Find the Miller indices of a plane having intercepts 2a, 3b, and 3c where a, b and c are intercept s by unit plane in the crystal axes.
12) The density if NaCl (molecular weight 58.48) being 2.17gm/ml, calculate the distance between 100 planes and hence the value of the sine of the glancing angle for the X-ray wavelength 1.54 A^0 in order to obtain the first order Bragg reflection maxima.
13) State and explain the 'law of constancy of interfacial angles.
b) Sketch a cubic unit cell and label each face with proper Miller indices.
c) Estimate the number of particles per unit-crystal of i) SC ii) BCC &iii) FCC.
14) What is the Bragg condition for constructive interference in connection with the crystal analysis? On what factors and how does the intensity of diffracted beam for constructive interference depend?
15) Calculate the glancing angle at which a simple cubic crystal will give a first order constructive interference from the (123) planes, where edge-length of the unit cell is 687 pm, (1pm= 10^{-12} m).

16) Show that the body-centre cubic lattice is less economically packed compared to face-centre cubic lattice.
17) Explain why the distance between two successive (hkl) planes for a cubic system cannot be a/√7, where 'a' is the length of the edge of the cube.
18) Deduce a relation between the wave length of radiation and spacing of lattice planes in a crystal.
19) The unit cell of a cube with edge length $4.05A^0$. If the density of the metal is 2.8 g cm^{-3}, what is the structure if the metal (at wt of metal = 27)?
20)(i) KCl has a face centre d cubic lattice and a density of $2.7g/cm^3$. Calculate the length of the unit all and the distance between the (1000 planes.
21) Explain whether X-ray of wavelength $0.1A^0$ is suitable for studying Bragg reflection of a cubic crystal with a = $0.045A^0$.
22) Calculate the Miller indices of a plane having 3a, 4b and 6c intercepts in three axes of unit cell with cell lengths a, b and c respectively.
23) What is the lowest limit to the spacing of the lattice planes to produce X-ray diffraction pattern for a given radiation?
24) Show that the body-centred cubic lattice is less economically packed compared to the face-centred cubic lattice.
25) A metal has a body-centred cubic lattice and the length of the unit cell is $2.95A^0$. If the density of the metal be 9.95 g/ cm^3, calculate the atomic weight of the metal. (Av. number = 6 x 10^{23}).
26) Calculate the Miller indices of a plane having 2a, b and 3c intercepts in three axes of unit cell with cell length a, b and c respectively. 2
27) Show that the body-centred cubic lattice is less economically packed compared to the face-centred cubic lattice.
28) Potassium crystallises with a bodycentred cubic lattice and hasa density of 0.856 gm/cm^3. What is the size of edge of the unit cell and the distance between 110 planes. (atomic weight of potassium = 39, Avogadro number = 60 x 10^{23})
29) Obtain the Boltzmann law $N_i/N = g_i e^{-\beta\varepsilon_i} / \Sigma\, g_i e^{-\beta\varepsilon_i}$
for the distribution energy among molecules of a gas at constant volume and temperature. N_i is the number of molecules in energy level ε_i which is g fold degenerate, β is a constant, and N represents the total number of molecules.
30) Write an expression for the population (fraction of molecules) of a state based on Boltzmann distribution explaining the symbols used.
31) Explain: Ensemble and partition function.
32) State and explain the Maxwell-Boltzmann distribution law and its significance.
33) Calculate the number of ways of distributing three distinguishable molecules between three levels given the condition that each level is occupied by one molecule.
b) What are phase space, phase trajectory, ensemble and partition function?
34) Explain what is meant by thermodymanic probability.

35) Calculate the number of ways of distributing three distinguishable molecules between three levels given the condition that each level is occupied by one molecule.
36) What is phase space? Explain the concept of an ensemble.
37) Considering all necessary assumption and non-degeneracy of energy levels, derive the Boltzmann distribution law for n molecules in a system, where the total energy E and total number of molecules n remain constant.
38) Define microcanonical ensemble.
37) Assume a hypothetical gaseous atom with three energy levels at ε_i = 0,1 and 2(in units of kT) Assume also that the atom has 6 electrons. Calculate the entropy of the atom at (i) very low temperature and (ii) very high temperature. Calculate also the electronic partition function of the system.
38) What are difference between canonical and grandcanonical ensemble?
39) How partition function of a system related to its Helmholtz free energy?
40) What is a grand canonical ensemble?
41) What is the physical significance of the partition function of a system?
42) Explain what is meant by thermodynamic probability. How can you apply this to explain the occurrence of residual entropy in ice ?
43) Calculate the number of ways of distributing distinguishable molecules x, y, z between 3 energy levels E_1, E_2, E_3 such that each level is occupied by one molecule
44) Define thermodynamic probability (W) of system. Show that entropy (S) of a system is logarithmic function of *W*.
45) Three identical but distinguishable particles are distributed among three energy levels, 0, ε, 2 ε. Write down the different possible distributions of the particles for total energy (i) ε & (ii) 2 ε. Also obtain the thermodynamic probability *(W)* for each distribution and hence the change in entropy for increasing the total energy from (i) to (ii).
46) Derive the Maxwell-Boltzmann distribution law for a system of *N* molecules where the energy levels $\varepsilon_1, \varepsilon_2 .... \varepsilon_n$ are non-degenerate emphasizing the condition involved. Assume $\beta = 1/kT$