

[4]

Or

Justify and draw the qualitative energy level diagram of a p-n junction at equilibrium explaining all the terms involved in it. What changes take place when such a junction is biased with an external voltage ? Find out the expressions for the net current in each case.

- b) Assuming the two-sublattice model, derive an expression for the susceptibility of an antiferromagnetic material when $T > T_N$. 4

Or

Derive an expression for the stabilization energy density of the superconducting state at absolute zero.

- c) Write a short note on (*any one*) : 3
- Density of electron states
 - First Brillouin zone
-

Ex/MSc/CH/4/P-4161/102/2017

M. SC. CHEMISTRY EXAMINATION, 2017

(4th Semester)

PHYSICAL CHEMISTRY SPECIAL

PAPER - XVI-P

Time : Two hours

Full Marks : 50

(25 Marks for each Unit)

Use a separate answerscript for each unit.

UNIT – P- 4161

1. a) Using the Great Orthogonality theorem, construct the symmetry projection operator for i-th irreducible representation. 5

Or

Using the projection operator techniques, construct the SALC's of cyclopropenyl group (C_3H_3) from three P_z atomic orbitals of carbon atoms.

- b) Using Huckel approximation, evaluate the energies corresponding to SALCs after constructing them for cis-butadiene. Calculate the delocalization energy of the molecule. 7
2. a) Assign the symmetry of the pure normal modes of NH_3 through internal coordinate method. Show which of them are IR and Raman active. 4

[Turn over

[2]

Or

Find the symmetries of the genuine normal modes of cis planar N_2F_2 (non linear) molecule using internal coordinate method. Show which of them are IR and Raman active.

- b) Find out which atomic orbitals of the atom A hybridize to form σ bonds with B for a molecule AB_5 type belonging to D_{3h} point group. 4

Or

Find out which atomic orbitals of the atom A hybridize to form σ bonds with B for a molecule AB_4 belonging to T_d point group.

- c) Give reasons on the basis of symmetry why thermal and photo-chemical bond breaking of cyclobutene derivatives produce different stereo isomers. 5

[Note : Character Table for required point groups will be supplied at the time of examination.]

[3]

UNIT – P- 4162

3. a) Show that the scattering amplitude of X-ray's becomes a maximum when the change in wave vector of the scattered X-rays ($\Delta\vec{k}$) becomes equal to a reciprocal lattice vector (\vec{G}) of the crystal. 5

Or

Derive a quantitative expression for the electronic heat capacity of the free electron gas valid at low temperatures ($T \ll T_F$) and hence show its linear dependence on the temperature.

- b) Consider a free electron gas in three dimensions and hence show that the wave vectors at the Fermi surface depends only on the particle concentration and not on the mass. 5
- c) What is ferroelectric effect ? Cite some examples and applications of crystals exhibiting such behavior. 3

Or

What is dc Josephson effect ?

4. a) Express the structure factor in terms of atomic form factor for an fcc lattice and hence explain why reflections from the (211) planes vanish, but those of (111) planes appear strongly in the X-ray diffraction pattern corresponding to such a lattice. 5

[Turn over