Ex/SC/CHEM/PG/CORE/TH/XVI-P/2023(S)

M. Sc. Chemistry (Special Supplementary) Examination, 2023

(4th Semester)

Paper: XVI-P

[Physical Chemistry Special]

Time : Two Hours Full Marks : 40

(20 marks for each Unit)

Use a separate answer script for each Unit.

UNIT – P-4161

Answer ***all*** the questions.

1. a) Using the Great Orthogonality theorem, construct the symmetry projection operator for i-th irreducible representation. 4

   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) Find the symmetries of the genuine normal modes of CH_2Cl_2 molecule using internal coordinate method. Show which of them are IR and Raman active. 5

   b) Find out which atomic orbitals of the atom A hybridize to form σ bonds with B atom for AB_4 type molecule belonging to D_{4h} point group. 4

UNIT – P-4162

Answer ***all*** the questions.

3. Consider a free electron gas in three dimension and hence find out an expression for the electron velocity at the Fermi surface and comment on which factor it depends.

OR

In an electric field $\boldsymbol{E}$ & magnetic field $\boldsymbol{B}$, the force $\boldsymbol{F}$ acting on an electron of charge $-\boldsymbol{e}$ and velocity $\boldsymbol{v}$ is: $\boldsymbol{F} = -e\left(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v} \times \boldsymbol{B}\right)$. Considering the motion of the system in a uniform magnetic field $\boldsymbol{B}$, derive the expressions for the components of velocity. 6

4. Show that the reciprocal lattice to an fcc lattice is a bcc lattice.

OR

Derive an expression for the structure factor for a I-lattice and explain which of the (hkl) reflectingS among (100), (110), (111), (200), (210), (211), (220) will be absent in the diffraction pattern of such a crystalline solid. $4\frac{1}{2}$

5. Assuming the two-sublattice model, express the Néel temperature T_N in terms of β and α, the interaction parameters for two unlike atoms and two like atoms, respectively. How is T_N related with θ?

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 such case. $5\frac{1}{2}$

6. Write a short note on (any ***one***):

   a) F-centre

   b) First Brillouin zone

   c) Density of electron states 4