

Ex/SC/CHEM/PG/CORE/TH/XVI-P/2022

M. Sc. (CHEMISTRY) EXAMINATION, 2022

(4th Semester, CBCS)

PHYSICAL CHEMISTRY SPECIAL

PAPER – XVI-P

Time : Two hours

Full Marks : 40

(20 marks for each unit)

Use a separate answer script for each Unit.

UNIT: P-4161

1. For a molecule belonging to the C_{3v} point group symmetry, a pair of functions (xz, yz) can be considered as basis functions for the irreducible representation **E** (assuming C_3 lying along z axis) — Justify. 4
2. Consider two states ψ_1 and ψ_2 whose functions transform according to the irreducible representation **A₂**, and a transition operator which transforms according to the **E** representation of the point group symmetry D_3 . Examine if the $\psi_1 \leftrightarrow \psi_2$ transition is allowed. 2
3. Apply projection operator technique to construct symmetry adapted π -MOs for Tetramethylene Cyclobutane taking $2p_z(C)$ orbitals as basis functions. 5
4. Answer **any three** of the following. 3×3
 - a) Apply group theoretical approach and *Method of Inspection* to construct sp^3 hybrid orbitals of a AB_4 molecule which belongs to tetrahedron point group.

[Turn over

[2]

- b) Discuss how the symmetry adapted orbitals of *cis* butadiene correlate with those of cyclobutene under disrotatory mode of transformation.
- c) In an octahedral chemical environment, how many states are possible for a d^2 system when the crystal field strength is very high compared to the d-electron correlation? What are these states?
- d) Assign the types of symmetry associated with the genuine normal modes of H₂O. Which of these modes are IR and/or Raman active?

[*Character Tables will be provided*]

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Answer all the questions.

5. Consider a free electron gas in three dimensions and hence show that wave vector at the Fermi surface depends only on the particle concentration and not on the mass. 5
6. In an electric field \mathbf{E} and magnetic field \mathbf{B} , the force \mathbf{F} acting on an electron of charge $-e$ and velocity \mathbf{v} is:
$$\mathbf{F} = -e \left(\mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right)$$
. Considering the motion of the system in a uniform magnetic field \mathbf{B} derive the expressions for the components of velocity. 5

[3]

7. Assuming the two-sublattice model of antiferromagnetism, derive the expression of 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 to θ ? 5
8. Justify and draw the qualitative energy level diagrams of a p-n junction before and after equilibrium has been established, explaining all the terms involved in it. 3
9. Suggest a method to synthesize greenish-yellow colored NaCl crystal in the laboratory. 2