

**M.Sc. DEGREE I SEMESTER EXAMINATION IN APPLIED CHEMISTRY,
DECEMBER 2006**

CHE 2101 THEORETICAL CHEMISTRY

Time: 3 Hours

Maximum marks : 50

PART - A

(Answer **ALL** questions)

(All questions carry **EQUAL** marks)

(5 x 2 = 10)

- I. (1) How are molecules classified based on symmetry ?
(2) Explain (i) eigen function (ii) expectation values.
(3) What is the gross selection rule for Raman spectra ?
(4) Explain the concept of degeneracy in the case of particle in a three dimensional box with quantum numbers (1,2,3).
(5) What are the bonding and antibonding orbitals ?

PART - B

(Answer **ALL** questions)

(All questions carry **EQUAL** marks)

(8 x 5 = 40)

- II. A. What is a character table ? State the general rules on the nomenclature for labeling of the irreducible representation.
OR
B. Construct the C_4 character table.
- III. A. State and explain great orthogonality theorem.
OR
B. The molecule of formaldehyde is planar with angle $HCH = \text{angle } HCO = 120^\circ$. (a) list the symmetry operation for this molecule and (b) use the valence atomic orbitals to form the symmetry adopted molecular orbitals, grouping them by symmetry types.
- IV. A. Describe projection operators.
OR
B. Discuss the application of projection operators to pi-bonding in Benzene.
- V. A. State the postulates of quantum mechanics and give their importance.
OR
B. What are operators in quantum mechanics ? Give their application.

- VI. A. Describe the application of Schrodinger wave equation to a particle in one dimensional box.
- OR**
- B. Explain the energy separation from a particle in the dimensional box for different values of n (quantum number) with a sketch. Also sketch nodes for the wave function.
- VII. A. Explain angular momentum and show by the application of de Broglie relationship that the angular momentum for a particle in a ring is quantified in units of $h/2\pi$.
- OR**
- B. Discuss the Schrodinger wave equation for a rigid rotator.
- VIII. A. Describe the concepts of directed valences with examples.
- OR**
- B. Explain Huckel molecular orbital methods in pi-bonds and delocalization of bonds.
- IX. A. Compare and contrast M.O. and U.B. methods for hydrogen molecule.
- OR**
- B. Give a sketch of d-orbitals of hydrogen like atoms.
