M. Sc. DEGREE I SEMESTER EXAMINATION IN
APPLIED CHEMISTRY
DECEMBER 2003

CHE 2101/1 AC1 THEORETICAL CHEMISTRY

Time: 3 Hours | Maximum Marks: 50

PART - A

(Answer *ALL* questions)
(All questions carry *EQUAL* marks)

(5 x 2 = 10)

I. (1) Explain reducible and irreducible representations with examples.
(2) Show that conjugate elements will have identical characters.
(3) Show that $[L^2, L_z] = 0$
(4) What is one electron orbital approximation?
(5) Explain Coloumb and exchange interaction.

PART - B

(Answer *ALL* questions)
(All questions carry *EQUAL* marks)

(8 x 5 = 40)

II. A. How systematically point group of a given molecule is determined?

OR

II. B. Identify the point groups of the following and list out all the symmetry elements in each point group.
(i) Allene, (ii) Methane, (iii) CH_2Cl_2, (iv) CO_2

III. A. Construct the character table D_3 systematically.

OR

III. B. Write the character table C_{3v} and reduce the direct product $E \otimes E \otimes E$ of C_{3v}.

IV. A. Construct the hybrid orbitals for AB_3CD_{3h} system.

OR

(Turn Over)

IV. B. What is a projection operator? Explain its use in deriving Π MOS in ethylene.

V. A. Identify the symmetry types of BCl_3 molecule and predict the activity of fundamentals in IR and Raman.

OR

V. B. Using group theory identify the symmetry allowedness of electronic transitions in formaldehyde.

VI. A. Outline the postulatory basis of quantum mechanics.

OR

VI. B. Derive the operator for energy. Using this deduce the general form of Schrodinger wave equation.

VII. A. Set up the hamiltonian operator for a particle in a cubical box and solve it for energy and ψ

OR

VII. B. Deduce first four hermit polynomials and explain the nodal behaviour.

VIII. A. State and prove variation theorem.

OR

VIII. B. What are slater determinants? Using them explain Pauli exclusion principle.

IX. A. Explain the basis of Huckel approximations and obtain the Π energy levels of butadiene system.

OR

IX. B. Discuss the VB treatment of H_2 molecule.

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C_{2v}	E	C_2^z	σ_{xz}	σ_{yz}		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

D_{3h}	E	σ_{xy}	$2C_3^z$	$2S_3$	$3C_2$	$3\sigma_v$		
A_1'	1	1	1	1	1	1	—	x^2+y^2, z^2
A_2'	1	1	1	1	-1	-1	R_z	—
A_2''	1	-1	1	-1	1	-1	—	—
E'	2	2	-1	-1	0	0	(x, y)	x^2-y^2, xy
E''	2	-2	-1	1	0	0	(R_x, R_y)	xz, yz

D_{2h}	E	C_2^z	C_2^y	C_2^x	i	σ_{xy}	σ_{zx}	σ_{yz}		
A_g	1	1	1	1	1	1	1	1	—	x^2, y^2, z^2
A_u	1	1	1	1	-1	-1	-1	-1	—	—
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	—
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	—
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	—