GIET UNIVERSITY, GUNUPUR – 765022

RD19MSC026

Roll No: | | | | | | |

Total Number of Pages : 2 AR-19 M.SC

M.Sc 1ST SEMESTER REGULAR EXAMINATIONS, NOV/DEC 2019-20

CHPC103- PHYSICAL CHEMISTRY-I

Time: 3 Hours Max Marks: 80

The figures in the right hand margin indicate marks.

SECTION A

1. Answer any four of the following: [4×4=16]

a) How many σ_h, σ_v and σ_d plane are present in O_h and T_d(Tetrahedral)molecules?

b) Schematically show the C_n axis of rotation present in H_2O_2 and $XeOF_4$

c) Is the function cos(3x+5) an eigen function of the operator d^2/dx^2, the eigen value is?

d) Explain the postulates of Quantum Mechanics

e) Draw the radial distribution curves for 3s, 3p and 3d orbitals

f) List out the types operators with symbol representations in C programme

OR

2. Answer all questions from the following: [2×8=16]

a) Define a group and a class in group theory and Explain with suitable examples

b) Distinguish between symmetry elements and symmetry operations

c) Write the symmetry operations involved in D_3h point group

d**)** List out the molecules that do not have improper axis of rotation

e) Find the ground state energy for confined in a one dimensional box having a width of 0.2 nm

f) Prove that $\sigma_h \times C_2 = \sigma_v'$

g) What do you mean character constants? Mention its types.

h) Define the term an input and output data in C programme

SECTION-B

. Answer all questions: [16×4=64]

3. a) The character table for Td molecule is

Td	E	8C3	3C2	6S4	6σd	Linear function	Quadrate function	Cubic function
A1	1	1	1	1	1		x2+y2+z2	xyz
A2	1	1	1	-1	-1			
E	2	-1	2	0	0		2z2-x2-y2, x2-y2	
Γ1	3	0	-1	1	-1	Rx, Ry, Rz		[x2(z2-y2), y(z2-x2), z(x2-y2)
Γ2	3	0	-1	-1	-1	x y z	xy, yz. zx	

i. What is the order of the group?

ii. What is the number of classes in the group?

iii. What is the number of irreducible representation present in the group?

iv. Prove that irreducible representation A1 and E are Orthogonality to each other

v. Find the value of direct product for A1×E and E×E

OR

b) State great Orthogonality theorem and show how it can be useful to construct the C_3V character table

4. a)Explain the stability of the coordination compounds(any) based on LCAO theory

OR

b) Describe molecular orbital for σ-bonding in AB_6 and AB_4 type by SALC's (Symmetry Adopted Linear Combination) of AO's

5. a) i) Write down the Schrodinger equation for hydrogen atom in spherical coordinates

ii) Write down the Huckel's theory of conjugated system

OR

b) i) Discuss the quantum treatment on harmonic oscillator

ii) Write note on a rigid rotor

6. a) i)Write a 'C' programme for evaluating radioactive decay constant

ii) Explain the logical variables used in C Programme?

OR

b) Write a 'C' programme for calculating the energy (E) levels and Rate constant of the reaction