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GIET UNIVERSITY, GUNUPUR - 765022
M. Sc. (First Semester) Regular Examinations, February - 2024
22CHPC103 - Physical Chemistry-I
(Chemistry)

Time: 3 hrs

Maximum: 70 Marks

(The figures in the right hand margin indicate marks.)

PART - A**(2 x 10 = 20 Marks)**

Q.1. Answer ALL Questions

CO# Blooms
Level

a. Identify the Mulliken notation for the following irreducible representation:

CO1 K4

E	C _n	nC ₂	i	σ _h
1	1	-1	-1	-1

b. How many meta stable curves are there in the phase diagram of sulphur?

CO2 K2

c. Calculate the zero point energy of a electron of path length 10 nm.

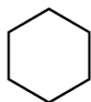
CO3 K2

d. Define Recursion of a function.

CO4 K2

e. The symmetry point group of the given structure:

CO1 K4



f. Explain Meta stable curve with suitable example.

CO2 K2

g. What is the degeneracy of SHO given that $E_{3D} = 23/2$ hU.

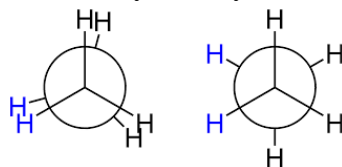
CO3 K2

h. Describe the process of program writing.

CO4 K2

i. Find the symmetry elements and point group of the given molecules:

CO1 K4



j. Calculate the Electron density and bond order of butadiene system.

CO3 K2

PART - B**(10 x 5 = 50 Marks)**Answer ANY FIVE the questionsMarks CO# Blooms
Level

2. a. Find out the matrix representation of different symmetry elements (E, i, σ-matrix)

5 CO1 K4

b. Prepare the GMT for C₄, C_{2h}, C_{2v}

5 CO1 K4

3. State the phase rule with different case studies.

10 CO2 K4

4. Derive Schrödinger wave function for hydrogen atom. Conversion of Cartesian co-ordinate into spherical co-ordinate.

10 CO3 K4

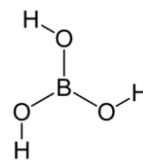
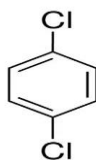
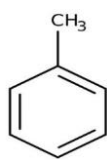
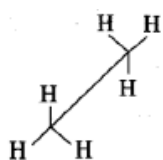
5. Programme for Computer Vander Waal's constants 'a' and 'b' for a gas by

10 CO4 K4

$$a = \frac{PV^2}{n^2}, \quad b = \frac{V}{n}$$

6. Define Point group and its types. Find the point group for the following Species:

10 CO1 K4



- 7.a Prove that momentum operator is a Hermitian Operator. 5 CO3 K4
b. Derive Schrödinger wave equation for a free particle in 1D box. 5 CO3 K3
8. Draw and discuss the phase diagram for one component system application to Sulphur. 10 CO2 K4

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