Reg. No | | | | | | | | | | |

AY 24

**GANDHI INSTITUTE OF ENGINEERING AND TECHNOLOGY, ODISHA, GUNUPUR**

# (GIET UNIVERSITY)

M. Sc. (First Semester - Regular) Examinations, February – 2025

## 24MCYPC11003 – Physical Chemistry – I

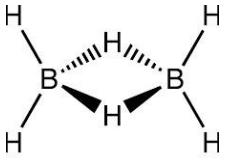
(Chemistry)

Time: 3 hrs | Maximum: 60 Marks

**Answer ALL questions**

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

**PART – A** **(2 x 5 = 10 Marks)**

| | | CO # | Blooms Level |
|---|---|---|---|
| Q.1. | Answer ***ALL*** the questions | | |
| a. | The point group symmetry of the given structure is;  | CO1 | K2 |
| b. | What is degree of freedom and find the DOF for the following system: $H_2O\ (S) \rightleftharpoons H_2O\ (l) \rightleftharpoons H_2O\ (g)$ | CO2 | K2 |
| c. | If $\psi = \sin n\pi x / l$, calculate its normalization constant. | CO3 | K2 |
| d. | What are the characteristics of Clanguage ? | CO4 | K2 |
| e. | The point group symmetry of $CH_2=C=CH_2$ is; | CO1 | K2 |

**PART – B** **(10 x 5 = 50 Marks)**

| | Answer ***ALL*** the questions | Marks | CO # | Blooms Level |
|---|---|---|---|---|
| 2.a. | Explain the "Great Orthogonality Theorem" using the example of water molecule. | 7 | CO1 | K4 |
| b. | A molecule contains the following symmetry operations: E, $2C_6$, $2C_3$, $C_2$, 3 σd, 3 σv. Calculate the number of classes and order of the symmetry point group? | 3 | CO1 | K3 |
| | (OR) | | | |
| c. | The character table of $C_{2v}$ point group is given below. In cis-butadiene molecule the vibrational modes belonging to $A_2$ irreducible representation are IR inactive. What are the remaining IR active modes? | 10 | CO1 | K4 |

| $C_{2v}$ | $E$ | $C_2$ | $\sigma_v(xz)$ | $\sigma_v'(yz)$ | | |
|---|---|---|---|---|---|---|
| $A_1$ | 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 | $y, R_x$ | $yz$ |

| | | | | |
|---|---|---|---|---|
| 3.a. | Draw and discuss the phase diagram for one component system application to $H_2O$. | 10 | CO2 | K4 |
| | (OR) | | | |
| b. | Derive all the wave function of butadiene system applying Huckel's MOT theory. | 10 | CO3 | K4 |
| 4.a. | Describe all types of looping structure with example. | 8 | CO4 | K4 |

| | | | | |
|---|---|---|---|---|
| b. | Difference between Formal argument and actual Argument. | 2 | CO4 | K3 |
| | (OR) | | | |
| c. | Derive the wave function and Energy expression for particle in 3-D box applying Schrodinger wave equation. Draw the wave probability plot for 2nd and 3rd excited state of particle in 1-D box. | 7+3 | CO3 | K4 |
| 5.a. | Explain character table of $BF_3$ molecule. | 8 | CO1 | K4 |
| b. | Write the matrix representing a two-step transformation of a general point (x,y,z) rotation through 180° (about the z-axis) followed by reflection in yz mirror plane. | 2 | CO1 | K2 |
| | (OR) | | | |
| c. | Programme for Computer Vander Waal's constants 'a' and 'b' for a gas by $a = \frac{PV^2}{n^2}$, $b = \frac{V}{n}$ | 10 | CO4 | K4 |
| 6.a. | Draw and discuss the phase diagram for one component system application to Sulphur. | 10 | CO2 | K4 |
| | (OR) | | | |
| b. | Prove that momentum operator is a Hermitian Operator. | 7 | CO3 | K4 |
| c. | If $\psi = e^{im\Phi}$ for rigid rotator ($0<x<2\pi$) calculate its normalization constant. | 3 | CO3 | K3 |

--- End of Paper ---