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**GIET UNIVERSITY, GUNUPUR – 765022**  
M. Sc. (First Semester) Examinations, March – 2023  
**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

- |   | Marks | CO# | Blooms<br>Level |
|---|-------|-----|-----------------|
| a. What is point groups symmetry of H <sub>3</sub> PO <sub>4</sub> with and without lone pairs.   | 2     | CO1 | K2              |
| b. Define components and determine the number of components for the following system:<br>$\text{NH}_4\text{Cl (S)} \rightleftharpoons \text{NH}_3 \text{ (g)} + \text{HCl (g)}$ | 2     | CO2 | K2              |
| c. Calculate the degeneracy of particle in 2D box.  | 2     | CO3 | K2              |
| d. What are the different parts of function?  | 2     | CO4 | K2              |
| e. The point group symmetry of the given structure:   | 2     | CO1 | K2              |



- |   |   |     |    |
|---|---|-----|----|
| f. Define triple point and critical point.  | 2 | CO2 | K2 |
| g. Using Laplacian operator find the Eigen value of Cos ax.Cos by.Cos cz  | 2 | CO3 | K2 |
| h. Define array with declaration.   | 2 | CO4 | K2 |
| i. The product of (C <sub>2</sub> <sup>x</sup> .σ <sub>xy</sub> ) and (σ <sub>xy</sub> .S <sub>4</sub> <sup>2</sup> ) is; | 2 | CO1 | K2 |
| j. The value of commutator [x,[x,P <sub>x</sub> ]] is equal to:   | 2 | CO3 | K2 |

**PART – B****(10 x 5 = 50 Marks)**Answer ANY FIVE questions

- |   | Marks | CO# | Blooms<br>Level |
|---|-------|-----|-----------------|
| 2. a. Represent the Group multiplication table of H <sub>2</sub> O & NH <sub>3</sub> molecule.  | 7     | CO1 | K4              |
| b. Define Plane of symmetry and its types with examples.  | 3     | CO1 | K3              |
| 3. State the phase rule with different case studies.  | 10    | CO2 | K4              |
| 4. The probability of finding a free particle inside the left half of 1D box in between L/4 to 3L/4   | 10    | CO3 | K4              |
| 5.a. Programme for Computer Pressure from Vander Waal's Equation.   | 10    | CO4 | K4              |
| $P = \frac{nRT}{V - nb} - \frac{n^2 a}{V^2}$  |       |     |                 |
| 6. a. Consider the pyridine molecule and find its normal modes of vibration and classify them as IR active, Raman active, IR and Raman both active. | 7     | CO1 | K4              |
| b. Character table of point group D <sub>8</sub> is given below: Calculate the value of a + b + c + d + e + f + g + h + i + j + k =?                | 3     | CO1 | K2              |

D <sub>8</sub>	E	2C <sub>8</sub>	2C <sub>4</sub>	2C <sub>8</sub> <sup>3</sup>	C <sub>2</sub>	4C <sub>2</sub> '	4C <sub>2</sub> ''
A <sub>1</sub>	<b>a</b>	1	1	1	1	1	1
A <sub>2</sub>	<b>b</b>	1	1	1	1	<b>h</b>	<b>i</b>
B <sub>1</sub>	<b>c</b>	-1	1	-1	1	1	<b>j</b>
B <sub>2</sub>	<b>d</b>	-1	1	-1	1	-1	1
E <sub>1</sub>	<b>e</b>	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0
E <sub>2</sub>	<b>f</b>	0	-2	0	<b>k</b>	0	0
E <sub>3</sub>	<b>g</b>	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0

- 7.a. Calculate the delocalisation energy of cyclopropene cation and anion. 7 CO3 K4
- b. Calculate the delocalisation energy of cyclobutadiene system. 3 CO3 K3
8. Discuss Clausius-Claperon equation and explain effect of pressure on the melting point of ice. 10 CO2 K4

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