

PSG COLLEGE OF ARTS & SCIENCE  
(AUTONOMOUS)

MSc DEGREE EXAMINATION MAY 2023  
(Second Semester)

Branch – PHYSICS

**GROUP THEORY AND MOLECULAR SPECTROSCOPY**

Time: Three Hours

Maximum: 50 Marks

**SECTION-A (5 Marks)**

Answer ALL questions

ALL questions carry EQUAL marks (5 x 1 = 5)

- 1 The inverse of 'i' operation is  
(i) E (ii) C<sub>2</sub>  
(iii) S<sub>3</sub> (iv) i
- 2 How many irreducible representations are possible for C<sub>3v</sub> point groups?  
(i) Two (ii) Three  
(iii) Four (iv) Five
- 3 Which part of the IR spectrum is called the "fingerprint region"?  
(i) 3000-2000 cm<sup>-1</sup> (ii) 3000-1000 cm<sup>-1</sup>  
(iii) 2000-1000 cm<sup>-1</sup> (iv) 1000-600 cm<sup>-1</sup>
- 4 For the detection of aldehyde and ketones, which transition is most authentic?  
(i) π to π\* (ii) n to π\*  
(iii) σ to π\* (iv) π to σ\*
- 5 How many signals will vinyl chloride have in <sup>1</sup>H NMR spectrum?  
(i) 1 (ii) 2  
(iii) 3 (iv) 4

**SECTION - B (15 Marks)**

Answer ALL Questions

ALL Questions Carry EQUAL Marks (5 x 3 = 15)

- 6 a Justify diagrammatically that H<sub>2</sub>O molecule is Abelian whereas NH<sub>3</sub> molecule is non-abelian.  
OR  
b List out symmetry elements presents in the following molecules i) CH<sub>4</sub> and ii) H<sub>2</sub>.
- 7 a Analyze the properties of irreducible representation.  
OR  
b Illustrate mutual exclusion rule.
- 8 a Sketch normal modes of vibration of CO<sub>2</sub> and explain which of these are IR active.  
OR  
b List the three applications of IR spectroscopy.

Cont...

- 9 a Explain the following terms :  
 i) Bathochromic shift  
 ii) Hypsochromic shift  
 iii) A Chromophore  
 OR  
 b Justify : UV spectroscopy is useful for distinguishing between cis and trans-1,3,5-Hexatriene.
- 10 a Evaluate the structural formula for the compounds with the following molecular formulae showing only one PMR signal each. i)  $C_2H_6O$  ii)  $C_5H_{12}$ .  
 OR  
 b Illustrate spin-spin coupling phenomenon in NMR .

**SECTION -C (30 Marks)**

Answer ALL questions

ALL questions carry EQUAL Marks

(5 x 6 = 30)

- 11 a Develop the derivation for matrix representation for rotation and reflection operations .

OR

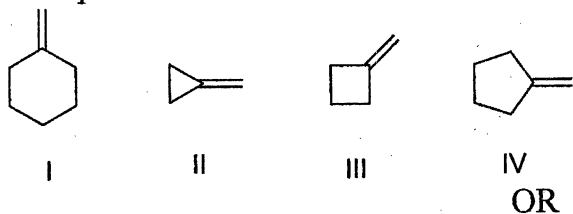
- b Explain reducible and irreducible representations.

- 12 a Construct the character table for the point group  $C_{2v}$ .

OR

- b Formulate the symmetries of the normal modes of vibration of  $NH_3$  molecule and comment on their IR and Raman activity.

- 13 a Arrange the following compounds in order of their increasing wave number of absorption due to  $C=C$  stretching. Justify your answer.

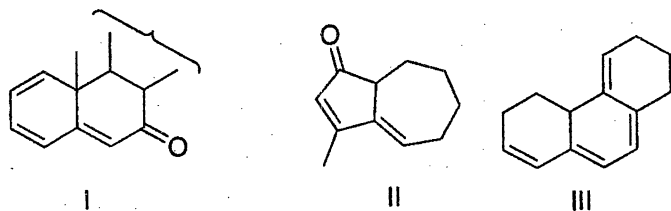


- b Discuss the classical theory of Raman effect and show how the Stokes and anti-Stokes lines appear in the Raman spectrum of a molecule.

- 14 a Interpret various types of electronic transitions in UV and explain the effect of the polarity of the solvent on each type of transition.

OR

- b Following the Woodward-Fieser rules, determine the absorption maximum for each of the following compounds. (2+2+2 Marks)



- 15 a Assess the uses of lanthanide shift reagent in NMR.

OR

- b i) Discuss term chemical shift. What are the factors affecting chemical shift? (4 Marks)  
 ii) Compare chemical shift of  $^1H$  NMR and  $^{13}C$  NMR (2 Marks)