# PSG COLLEGE OF ARTS & SCIENCE
## (AUTONOMOUS)

## MSc DEGREE EXAMINATION MAY 2024
### (Second Semester)

### Branch – PHYSICS

## GROUP THEORY AND MOLECULAR SPECTROSCOPY

Time: Three Hours          Maximum: 75 Marks

### SECTION-A (10 Marks)
Answer ALL questions

ALL questions carry EQUAL marks      $(10 \times 1 = 10)$

| Module No. | Question No. | Question | K Level | CO |
|---|---|---|---|---|
| 1 | 1 | Which of the following molecule possesses a centre of symmetry?<br>(a) $NH_3$        (b) $[PtCl_4]^{2-}$<br>(c) Pyridine      (d) Chlorobenzene | K1 | CO1 |
| | 2 | An example for cyclic group is<br>(a) $T_d$    (b) $O_h$    (c) $C_3$    (d) $I_h$ | K2 | CO1 |
| 2 | 3 | The number of vibrational degrees of freedom of water molecule is<br>(a) $2A_1 + B_2$      (b) $2A_2 + B_2$<br>(c) $2A_1 + B_1$      (d) $2A_2 + B_1$ | K1 | CO2 |
| | 4 | Mutual exclusion principle is applicable to<br>(a) HCl    (b) $CO_2$    (c) $H_2O$    (d) HBr | K2 | CO2 |
| 3 | 5 | For Raman spectra, the molecule must have<br>(a) Anisotropic polarizability<br>(b) Isotropic polarizability<br>(c) Oscillating dipole moment<br>(d) Permanent dipole moment | K1 | CO3 |
| | 6 | Hooke's law for the vibration of a diatomic molecule may be expressed as<br>(a) $X = -KF$      (b) $K = XF$<br>(c) $F = -KX$      (d) $K = -FX$ | K2 | CO3 |
| 4 | 7 | Blue shift is also known as<br>(a) Hypsochromic shift    (b) Hyperchromic shift<br>(c) Hypochromic shift    (d) Bathochromic shift | K1 | CO4 |
| | 8 | The energy needed for the promotion of electron follows the order:<br>(a) $\sigma < \pi < n$      (b) $\sigma > \pi > n$<br>(c) $\sigma < n < \pi$      (d) $n > \sigma > \pi$ | K2 | CO4 |
| 5 | 9 | Tell the number of $^1$H-NMR signals in case of 1,2-dibromo ethane.<br>(a) 0    (b) 1    (c) 2    (d) 3 | K1 | CO5 |
| | 10 | The chemical shift of proton on the 'δ' scale is 4. The value on the 'τ' scale is<br>(a) 10    (b) 6    (c) 5.5    (d) 4 | K2 | CO5 |

### SECTION - B (35 Marks)
Answer ALL questions

ALL questions carry EQUAL Marks      $(5 \times 7 = 35)$

| Module No. | Question No. | Question | K Level | CO |
|---|---|---|---|---|
| 1 | 11.a. | Derive the matrix representation of reflection operation. | K4 | CO1 |
| | | (OR) | | |
| | 11.b. | Examine the relationship between reducible representation and irreducible representations. | | |

| Module No. | Question No. | Question | K Level | CO |
|---|---|---|---|---|
| 2 | 12.a. | State great orthogonality theorem. Appraise its consequences. | K5 | CO2 |
| | | (OR) | | |
| | 12.b. | How are irreducible representations symbolized? Write the standard reduction formula and explain with an example. (6) | | |
| 3 | 13.a. | (i) How would you distinguish acetamide and ethyl amine using IR spectroscopy? (3) <br> (ii) Compare finger print region and functional group region. (4) | K4 | CO3 |
| | | (OR) | | |
| | 13.b. | (i) Distinguish between fundamental frequency, first overtone and second overtone. (3) <br> (ii) Contrast IR and Raman spectroscopy. (4) | | |
| 4 | 14.a. | Sketch and explain the instrumentation of UV-Visible spectroscopy. | K5 | CO4 |
| | | (OR) | | |
| | 14.b. | The wave length as well as extinction coefficient increase with increase in conjugation in the compound. Justify this statement. | | |
| 5 | 15.a. | Suggest with proper justification the expected $^{13}C$-chemical shifts for different carbons in n-butyl ethyl ketone. | K6 | CO5 |
| | | (OR) | | |
| | 15.b. | Discuss the principle and advantages of FT-NMR spectroscopy. | | |

## SECTION -C (30 Marks)
### Answer ANY THREE questions
ALL questions carry EQUAL Marks  (3 × 10 = 30)

| Module No. | Question No. | Question | K Level | CO |
|---|---|---|---|---|
| 1 | 16 | Sketch and explain the group multiplication table of the symmetry operations of $H_2O$ molecule. | K4 | CO1 |
| 2 | 17 | Construct a character table for $C_{3v}$ point group and also find the symmetries of normal modes of vibrations of ammonia molecule. | K6 | CO2 |
| 3 | 18 | (i) The reduced mass of a diatomic molecule is $2.5 \times 10^{-26}$ kg and its vibrational frequency is $2900$ cm$^{-1}$. Calculate its force constant. (5) <br> (ii) Determine the structure of ammonia molecule by Raman spectroscopy. (5) | K5 | CO3 |
| 4 | 19 | (i) Calculate the absorption maximum in the UV-Visible spectrum of 1,3-Pentadiene and 2,4- Hexadiene. (5) <br> (ii) Increase in polarity of the solvent shifts $\pi \rightarrow \pi^*$ band to longer wavelength but $n \rightarrow \pi^*$ and $n \rightarrow \sigma^*$ bands to shorter wavelength. Justify this statement. (5) | K5 | CO4 |
| 5 | 20 | (i) Compare the characteristics of spin-spin, spin-lattice and quadrupole relaxation processes in NMR spectroscopy. (5) <br> (ii) Examine the $^1H$-NMR spectrum of absolute alcohol and acidified ethanol. (5) | K4 | CO5 |

Z-Z-Z      END