M.Sc. (Chemistry) $2^{\text {nd }}$ Semester

## SPECTROSCOPY B : TECHNIQUES FOR STRUCTURE ELUCIDATION OF INORGANIC COMPOUNDS

## Course-XII

Time Allowed-3 Hours] [Maximum Marks-75
Note :-(1) The students are allowed to use Non-Programmable Calculator. Ask for Character tables from the Supervisor.
(2) Attempt a total of five questions. Each question carries equal marks. Attempt one question from each section. The fifth question can be attempted from any section.

## SECTION-A

1. (a) Identify various symmetry elements belonging to the following molecules :
(i) $\mathrm{PtCl}_{4}^{2-}$
(ii) Allene $\mathrm{CH}_{2}=\mathrm{C}=\mathrm{CH}_{2}$
(iii) $\mathrm{Ni}(\mathrm{CO})_{4}$
(iv) $\mathrm{CO}_{3}^{2-}$
(v) $\mathrm{PCl}_{3}$.
(b) Determine the Point Groups in each of the following cases :
(i) $\mathrm{H}_{2} \mathrm{~S}$
(ii) $\mathrm{PCl}_{3}$
(iii) $\mathrm{B}_{2} \mathrm{H}_{6}$
(iv) $\mathrm{C}_{6} \mathrm{H}_{6}$
(v) $\left[\mathrm{CoCl}\left(\mathrm{NH}_{3}\right)_{5}\right]^{+}$.
2. Determine the hybridization of $\mathrm{CH}_{4}$ molecule using the following reducing representation of the molecule :

| Operation | E | $8 \mathrm{C}_{3}$ | $3 \mathrm{C}_{2}$ | $6 \mathrm{~S}_{4}$ | $6 \sigma_{\mathrm{d}}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| Character | 4 | 1 | 0 | 0 | 2 |

The character table for $T_{d}$ group is:

| $\mathrm{T}_{\mathrm{d}}$ | E | $8 \mathrm{C}_{3}$ | $3 \mathrm{C}_{2}$ | $6 \mathrm{~S}_{4}$ | $6 \sigma_{\mathrm{d}}$ |  |
| :--- | :---: | :---: | :---: | ---: | ---: | :---: |
| $\mathrm{A}_{1}$ | 1 | 1 | 1 | 1 | 1 | $\mathrm{x}^{2}+\mathrm{y}^{2}+\mathrm{z}^{2}$ |
| $\mathrm{~A}_{2}$ | 1 | 1 | 1 | -1 | -1 | - |
| E | 2 | -1 | 2 | 0 | 0 | $2 x^{2}-y^{2}-\mathrm{z}^{2}, \mathrm{x}^{2}-\mathrm{y}^{2}$ |
| $\mathrm{~T}_{1}$ | 3 | 0 | -1 | 1 | -1 | $\mathrm{R}_{\mathrm{x}}, \mathrm{R}_{\mathrm{y}}, \mathrm{R}_{\mathrm{z}}$ |
| $\mathrm{T}_{2}$ | 3 | 0 | -1 | -1 | 1 | $(x, y, z),(x y, y z, z x)$ |

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## SECTION-B

3. (a) Differentiate between harmonic and an-harmonic oscillations.
(b) Describe applications of vibrational spectroscopy.
(c) Derive an equation for the energies of rotational transitions of rigid diatomic rotor. $5 \times 3=15$
4. (a) Discuss non-rigid rotator and compare selection rules of rigid and non-rigid rotators critically.
(b) Explain polarizability and selection rules in Raman Spectroscopy.
(c) How symmetry elements are used to determine number of active IR and Raman lines ?

$$
5 \times 3=15
$$

## SECTION-C

5. (a) Explain Zeeman Effect and support your answer with diagram.
(b) What is effect of electronic spin on electronic spectra of atoms?
6. (a) Explain Larmor precession in electronic paramagnetic resonance (epr).
(b) How does spin and magnetic field interact in epr to generate signals.

## SECTION-D

7. (a) How structure elucidation of $\mathrm{I}_{2} \mathrm{Br}_{2} \mathrm{Cl}_{4}$ molecule is done by Mossbauer Spectroscopy ?
(b) Explain isomer shift in Mossbauer spectra. 7
8. (a) What information are obtained from Nuclear Quadruple Resonance spectra of $\mathrm{PCl}_{5}, \mathrm{PCl}_{4} \mathrm{Ph}$, and $\mathrm{TeCl}_{4}$ molecules.
(b) Discuss hyperfine coupling in isotropic systems in NQR spectra.
