| QP Code: D153276 | Total Pages: 2 | Name: |
|---|---|---|
| | | Register No. |

**FIFTH SEMESTER (CUFYUGP) DEGREE EXAMINATION, NOVEMBER 2026**

**CHEMISTRY**

**CHE5CJ301 Theoretical Chemistry - II: Group Theory and Molecular Spectroscopy**

**2024 Admission onwards**

**Maximum Time :2 Hours** | **Maximum Marks :70**

## Section A

**All Questions can be answered. Each Question carries 3 marks (Ceiling : 24 Marks)**

| | |
|---|---|
| 1 | Show that the symmetry operations of $C_{2v}$ form an Abelian group under multiplication. |
| 2 | List the symmetry operations and assign the point group to $NH_3$ and $BF_3$ molecules |
| 3 | Distinguish between a symmetry element and the corresponding symmetry operation with suitable examples. |
| 4 | Explain why the rotational spectrum of a homonuclear diatomic molecule consists of equally spaced lines. |
| 5 | How does the rotational spectrum of a molecule permit the determination of its bond length? |
| 6 | Explain the origin of Stokes and anti-Stokes lines in Raman spectroscopy and compare their intensities. |
| 7 | Write the mutual exclusion principle? |
| 8 | Explain the term spin-spin coupling in proton NMR spectrum. |
| 9 | How can proton NMR distinguish chemically equivalent and chemically non-equivalent protons in a molecule? |
| 10 | Explain the origin of hyperfine structure in the ESR spectrum of an organic radical. |

## Section B

**All Questions can be answered. Each Question carries 6 marks (Ceiling : 36 Marks)**

| | |
|---|---|
| 11 | Construct the multiplication table for $C_{3v}$ and identify its classes of symmetry operations. |
| 12 | Explain a systematic procedure for assigning the Schoenflies point group of a molecule from its symmetry elements. |
| 13 | For a molecule belonging to $C_{2v}$, explain how matrices can be used to represent its symmetry operations and obtain the corresponding characters. |
| 14 | Derive the rotational energy expression for a rigid diatomic rotor and explain the factors affecting line intensity. |
| 15 | Explain the vibrational energy levels of a simple harmonic oscillator and discuss the origin of anharmonicity, overtones and combination bands. |
| 16 | Explain the classical origin of Raman scattering and show how polarizability leads to the Raman selection rule. |
| 17 | Explain the Franck–Condon principle and discuss its significance in understanding the vibrational structure of an electronic spectrum. |
| 18 | Compare $H^1$NMR, $C^{13}$NMR and ESR with respect to the nature of the nucleus or particle observed, resonance condition, spectral splitting and structural information obtained. |

| Section C | |
|---|---|
| **Answer any ONE. Each Question carries 10 marks (1x10=10 Marks)** | |
| 19 | For $H_2O$, belonging to the $C_{2v}$point group, construct the reducible representation for the $3N$Cartesian motions, reduce it into irreducible representations and identify the IR- and Raman-active vibrations. |
| 20 | a) Explain the principle of NMR spectroscopy.<br>b) A compound gives a proton NMR spectrum showing a triplet, a quartet and a broad singlet; using chemical shift, integration and spin-spin coupling, deduce the structural features responsible for these signals and explain how the spectrum can be used for structural identification. |