**BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI**
**(END SEMESTER EXAMINATION)**

**CLASS: IMSc** **SEMESTER : IX**
**BRANCH: CHEMISTRY** **SESSION : MO/2024**

**SUBJECT: CH503 MOLECULAR SPECTROSCOPY**

**TIME: 3 Hours** **FULL MARKS: 50**

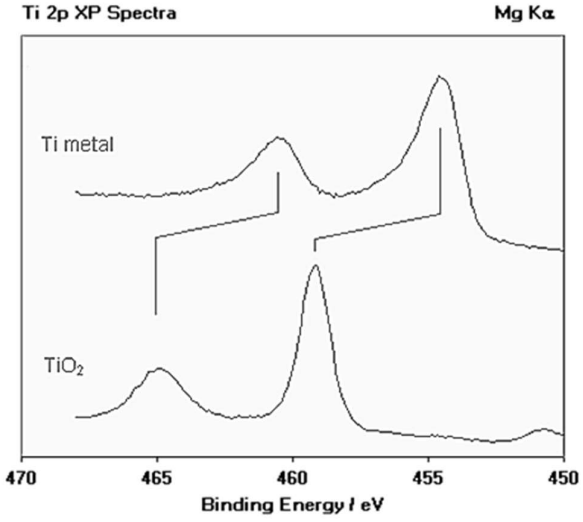
**INSTRUCTIONS:**
**1. The question paper contains 5 questions each of 10 marks and total 50 marks.**
**2. Attempt all questions.**
**3. The missing data, if any, may be assumed suitably.**
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**

---

| | | | CO | BL |
|---|---|---|---|---|
| Q.1(a) | Derive the expression for the line positions in the rotational spectra of the symmetric top molecules. | [5] | 1 | III |
| Q.1(b) | Discuss the effect of nuclear spin statistics on the intensities of rotational Raman lines. | [5] | 1 | II |
| Q.2(a) | Derive the selection rules for vibrational transitions. Assume it to be a simple harmonic oscillator. | [5] | 2 | II |
| Q.2(b) | Show that the R branch lines get crowded whereas P branch lines get widely spaced as J increases. When do you expect a reverse trend? | [5] | 2 | II |
| Q.3(a) | Show the relationship between transition moment integral and the intensity of absorption. How does the Franck-Condon factor govern the intensity of absorption? | [5] | 3 | II |
| Q.3(b) | Show that n $\rightarrow$ π* transition is symmetry forbidden in formaldehyde ($CH_2O$). | [5] | 3 | III |

| $C_{2v}$ | $E$ | $C_2$ | $\sigma_v(xz)$ | $\sigma_v'(yz)$ | | |
|---|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 | $z$ | $x^2, y^2, z^2$ |
| $A_2$ | 1 | 1 | −1 | −1 | $R_z$ | $xy$ |
| $B_1$ | 1 | −1 | 1 | −1 | $x, R_y$ | $xz$ |
| $B_2$ | 1 | −1 | −1 | 1 | $y, R_x$ | $yz$ |

| | | | | | |
|---|---|---|---|---|---|
| Q.4(a) | Photoelectron spectra were acquired from a sample of gaseous oxygen using X-ray radiation with energy of 1253.6 eV. The spectrum contained a large peak for photoelectrons with speed of $1.57 \times 10^7$ m/s. Calculate the ionization energy of these electrons. [$m_e = 9.19 \times 10^{-31}$ kg] | [5] | 4 | III |
| Q.4(b) | What is chemical shift in X-ray photoelectron spectroscopy? Explain the chemical shift observed in Ti 2p binding energy in the following spectra. | [5] | 4 | III |




| | | | | |
|---|---|---|---|---|
| Q.5(a) | Discuss the possible magnetic interactions in the H-atom in the presence of an external magnetic field. | [5] | 5 | II |
| Q.5(b) | Discuss longitudinal and transverse relaxation time in NMR spectroscopy. | [5] | 5 | II |

**::::::20/11/2024::::::E**