REV-01
MSC/01/05

2025/12

SET A

M.Sc. CHEMISTRY
FIRST SEMESTER
MOLECULAR SPECTROSCOPY I
MSC – 105 [REPEAT]

[USE OMR FOR OBJECTIVE PART]

Duration: 1:30 hrs. **Full Marks: 35**

Objective

Time: 15 mins. **Marks: 10**

Choose the correct answer from the following: ***1×10=10***

1. A vibration is Raman active if:
   a. It causes a change in dipole moment
   b. It is surface-enhanced
   c. It causes a change in polarizability
   d. It involves spin flipping

2. Which of the following is Raman active but IR inactive?
   a. OH stretch
   b. Asymmetric stretch of CO_2
   c. Symmetric stretch of CO_2
   d. CO stretch

3. Vibrational spectroscopy typically occurs in which region?
   a. UV region
   b. IR region
   c. Visible region
   d. Radio wave region

4. A molecule with 4 atoms (non-linear) has how many vibrational modes?
   a. 3
   b. 9
   c. 6
   d. 12

5. The R-branch in a vibrational-rotational spectrum corresponds to transitions with:
   a. $\Delta J = +2$
   b. $\Delta J = +1$
   c. $\Delta J = 0$
   d. $\Delta J = -1$

6. Which of the following molecules belong to asymmetric top type?
   a. SO_2
   b. NH_3
   c. CO_2
   d. None of the above

7. Which of the following is NOT a requirement for a molecule to exhibit a pure rotational spectrum?
   a. The molecule must have a permanent dipole moment.
   b. The molecule must be in the gas phase.
   c. The molecule must be at a low temperature.
   d. The molecule must be in a non-polar solvent.

8. The rotational energy levels of a non-rigid rotor are given by:
   a. $E_J = BJ(J+1)$
   b. $E_J = BJ(J+1) - DJ^2(J+1)^2$
   c. $E_J = BJ^2(J+1)^2$
   d. $E_J = B(J+1)^2 - DJ^2$

9. For microwave spectroscopy, the sample should be -
   a. Solid
   b. Liquid
   c. Gaseous
   d. Plasma

10. Microwave radiation is primarily used in
   a. X-ray imaging
   b. Nuclear magnetic resonance
   c. Rotational spectroscopy
   d. UV-Vis spectroscopy

-- --- --

Descriptive

Time : 1 hr. 15 mins

Marks : 25

[Answer question no.1 & any two (2) from the rest]

1. a. The vibrational frequency of HBr is $\nu = 2649\ cm^{-1}$. Convert this frequency to the unit of Hz. 2+3=5

   b. Find which of the molecules are rotationally active and explain why: CH_4, C_2H_4, SF_6

2. a. A diatomic molecule has spectroscopic constants $\bar{\omega}_e = 3000\ cm^{-1}$ $\bar{\omega}_e\chi_e = 20\ cm^{-1}$. Using the anharmonic oscillator energy expression (in wavenumbers, cm^{-1}), find the fundamental transition wavenumber (ΔE). 3+3+3+1=10

   b. Describe the types of vibrational motions in a triatomic molecule (both linear and non-linear). Illustrate using CO_2 and H_2O as examples.

   c. What do you mean by Stokes and anti-Stokes lines?

   d. Write the selection rule for pure rotational Raman spectra of a diatomic molecule.

3. **a.** The rotational Raman spectrum of $^{35}Cl_2$ shows a series of Stokes lines separated by 0.9752 cm^{-1}. Calculate the bond length of the molecule. (Isotopic mass of Cl-35 is 34.97 amu). **4+3+2+1=10**

   b. The fundamental vibrational frequency of a diatomic molecule is $\upsilon = 1.2\times10^{13}$ Hz. Calculate the energy of the first vibrational level (v = 0) and the second vibrational level (v = 1) using the harmonic oscillator model.

   c. What are P, Q, and R branches in a vibrational-rotational spectra of a diatomic molecule?

   d. What do you mean by Mutual exclusion principle?

4. **a.** Write the conditions for a molecule to be Symmetric top by giving example. **2+3+3+2=10**

   b. What is stark effect? Explain in Brief.

   c. Draw the rotational energy level diagram of CO molecule by Calculating all the energy values up to j=5.

   d. Deduce and explain the rotational spectra for non-rigid rotator.

5. **a.** The rotational spectrum of HI is found to contain a series of lines with a separation of 12.8 cm^{-1}. Moment of Inertia for the molecule is? **3+2+4+1=10**

   b. What do you mean by isotopic substitution? Explain with an example.

   c. The pure rotational spectrum of gaseous HCl consists of a series of equally spaced lines separated by 20.8 cm^{-1}. Calculate the internuclear distance of the molecule. The atomic masses are, H= 1.673×10^{-28} kg and Cl= 58.06×10^{-27} respectively.

   d. Write the conditions for a molecule to be an Asymmetric top molecule.

= = *** = =