2024/12

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: 15mins. **Marks: 10**

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

1. The frequency of fundamental band is given by which of the following?
   a. $\bar{\upsilon} = 2\overline{\omega_e}(1 - x_e)$
   b. $\bar{\upsilon} = \overline{\omega_e}(1 - 2x_e)$
   c. $\bar{\upsilon} = 2\overline{\omega_e}(1 - 3x_e)$
   d. $\bar{\upsilon} = 3\overline{\omega_e}(1 - 4x_e)$
2. The number of degrees of freedom of a chemical compound of N-atoms is
   a. N
   b. 3N-5
   c. 3N-6
   d. 3N
3. Which of the following molecule is infrared active?
   a. Cl_2
   b. H_2
   c. HCl
   d. O_2
4. The number of vibrational degrees of freedom for the molecule SO_2 is
   a. 2
   b. 3
   c. 4
   d. 1
5. In the rotational Raman spectrum of a diatomic molecule, the energy difference between the first Stokes and first anti-Stokes lines is (B denotes rotational constant)
   a. 4B
   b. 6B
   c. 2B
   d. 12B
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. Microwave radiation is primarily used in
   a. X-ray imaging
   b. Nuclear magnetic resonance
   c. Rotational spectroscopy
   d. UV-Vis spectroscopy
8. The selection rule for rotational transitions is
   a. $\Delta J = 0$
   b. $\Delta J = \pm 1$
   c. $\Delta J = \pm 2$
   d. $\Delta J = \pm 3$
9. Which molecule is rotationally inactive
   a. CO
   b. HCl
   c. O_2
   d. H_2O

10. For a rigid rotor, the energy levels are given by which expression?

a. $E = J(J + 1)B$
b. $E = J^2B$
c. $E = h\nu(J + 1)$
d. $E = h\nu(J^2)$

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Descriptive

Time : 1 hr. 15 mins. Marks: 25

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

1. a. Write the relation between fundamental frequency ($\bar{\upsilon}$) and force constant (k). What do you mean by anharmonic vibration? 2+3=5

   b. What do you mean by Symmetric top molecules? Explain by giving examples.

2. a. The fundamental vibrational frequency of $^{1}H^{127}I$ is 2309 cm^{-1}. Calculate the force constant (Nm^{-1}) for this molecule. (Given N = 6.022×10^{23}, c = 3.0×10^{8} ms^{-1}) 5+5=10

   b. For a diatomic molecule acting as an anharmonic oscillator, the oscillator frequency ($\overline{\omega_e}$) is given as 440.0 cm^{-1}. The observed value of the fundamental frequency is 432.7 cm^{-1}. Calculate the observed frequency for the second overtone.

3. a. What do you mean by Rayleigh scattering and Raman scattering? What is the selection rule for pure rotational Raman spectra? What do you mean by mutual exclusion principle? Explain with Example. 2+1+2 =5

   b. Explain the normal modes of vibration for a molecule. Assign the infrared active and inactive vibrations of H_2O molecule with proper pictorial depiction. How many Raman active vibrations are there for H_2O molecule? 2+2+1 =5

4. a. Draw the rotational energy level diagram and the rotational lines diagram. 2+2+4+ 2 =10

   b. What do you mean by J_{max}?

   c. The rotational spectrum of HI is found to contain a series of lines with a separation of 12.8 cm^{-1}. What is the moment of inertia for this molecule?

d. What is the J_{max} for a rigid diatomic molecule at 300 K having the rotational constant value of 1.566 cm^{-1}?

5. **a.** Deduce and explain the rotational spectra for non-rigid rotator. **3+2+3+2=10**

b. Explain what you mean by 1st order and 2nd order stark effect.

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. The 1st rotational line of CO molecule occurs at 3.84 cm^{-1}. Calculate the rotational constant.

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