REV-01
MSC/68/34/39

2023/01

SET A

M.Sc. CHEMISTRY
FIRST SEMESTER
MOLECULAR SPECTROSCOPY-I
MSC – 105

[USE OMR SHEET FOR OBJECTIVE PART]

Duration : 1.30 hrs. **Full Marks : 35**

(Objective)

Time: 15 min. **Marks: 10**

Choose the correct answer from the following: ***1X10=10***

1. Doppler broadening for fixed frequency is proportional to
   a. $\sqrt{\frac{T}{M}}$ b. $\sqrt{\frac{M}{T}}$
   c. $\frac{\sqrt{T}}{M}$ d. $\frac{T}{\sqrt{M}}$
2. The molecule having three different rotational constants is
   a. CH_4 b. H_2O
   c. BF_3 d. CH_3F
3. The selection rule for the rotational transition of rigid prolate molecule is
   a. $\Delta J = \pm 1$ and $\Delta K = \pm 1$ b. $\Delta J = \pm 1$ only
   c. $\Delta J = \pm 1$ and $\Delta K = 0$ d. $\Delta J = 0$ and $\Delta K = \pm 1$
4. For a diatomic molecule AB, if the energy of 1st rotational transition is 3.8 cm^{-1}, then the energy of transition from J = 3 to J = 4 is
   a. 3.8 cm^{-1} b. 7.6 cm^{-1}
   c. 11.4 cm^{-1} d. 15.2 cm^{-1}
5. The molecule which has two equal principal moment of inertia but greater than the third principal moment of inertia is
   a. CH_3I b. CH_3OH
   c. C_6H_6 d. HCl
6. If ν_i and ν are frequency of incident and scattered lines respectively, which of the following is true for Stokes line?
   a. $\nu_i > \nu$ b. $\nu_i < \nu$
   c. $\nu_i = \nu$ d. Does not depend on ν_i
7. The first anti-Stoke line appears at what distance from the exciting Rayleigh line?
   a. 4B b. 2B
   c. 6B d. 8B
8. How many normal modes of vibration are there for the triatomic molecule H_2O?
   a. Three b. Four
   c. Five d. Six

9. The selection rules for pure rotational Raman spectra of a diatomic molecule are
   a. $\Delta J = \pm 1$
   b. $\Delta J = 0, \pm 1, \pm 2$
   c. $\Delta J = 0, \pm 1$
   d. $\Delta J = 0, \pm 2$

10. For a particular vibrational mode to appear in the Raman spectrum, what must change?
   a. Frequency of radiation
   b. Intensity of radiation
   c. Molecule's shape
   d. Molecule's polarizability

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Descriptive

Time : 1 hrs. 15 mins. Marks : 25

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

1. a. Write the rotational energy of a rigid diatomic molecule and show that rotational spectral lines are separated by equal distance. 1+2=3

   b. Explain the different normal modes of vibration of the triatomic molecule CO_2. 2

2. a. Under what condition a diatomic molecule shows microwave spectra? Mention the selection rule of rotational transition of a diatomic molecule. Show that the separation of rotation energy levels of a rigid diatomic molecule increases with the increase of rotational quantum number. State the cause of non rigidity of the diatomic molecule. 1+1+2+1=5

   b. State the factors on which the intensity of the rotational spectral line depends. Show diagrammatically the variation of intensity of rotational spectral line for high and low value of rotational constants with the change of rotational quantum number. What change of rotational spectral line would you observe if one of the atoms of a heteronuclear diatomic molecule is replaced by its heavier isotope? 2+2+1=5

3. a. Write the rotational term value of a rigid prolate molecule and give the selection rule of rotational transition of it. 2+1=3

   b. Write the expression of energy of a non rigid diatomic molecule. State the difference of energy levels of non rigid diatomic molecule with that of rigid one. 2+2=4

   c. The rotational constant of HCl molecule is 10.366 cm-1. Find the internuclear distance of HCl molecule if the reduced mass of it is $1.627 \times 10\text{-}27$ kg. Given that $h = 6.626 \times 10\text{-}34$ Js. 3

4. a. What do you mean by Raman shift? What are Stokes and anti-Stokes lines? Explain why Stokes lines are more intense than anti-Stokes lines. **1+2+2 =5**

b. The rotational constant of $^{14}N_2$ is 2 cm^{-1}. The wave number of incident radiation in a Raman spectrometer is 20487 cm^{-1}. What is the wave number of first scattered Stokes line (in cm^{-1}) of $^{14}N_2$? **3**

c. What do you mean by law of mutual exclusion? How many normal modes of vibration is Raman active in H_2O molecule? **2**

5. a. What do you mean by overtone and hot band? Calculate the force constant for $H^{35}Cl$ from the fact that the fundamental vibrational frequency is 8.667×10^{13} s^{-1} and the reduced mass is 1.627×10^{-27} kg. **2+3=5**

b. For N_2 molecule, fundamental, first overtone and second overtone bands are given as 2345 cm^{-1}, 4661 cm^{-1} and 6983.73 cm^{-1} respectively. Calculate $\overline{\omega_e}$, x_e and k of the molecule. **5**

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