

No. of Printed Pages : 9

MCH-020

M. Sc. IN CHEMISTRY

(MSCCHEM)

Term-End Examination

June, 2026

MCH-020 : ATOMIC AND MOLECULAR

SPECTROSCOPY

Time : 2 Hours

Maximum Marks : 50

Note : (i) *Question no. 1 is compulsory.*

*Attempt any **four** questions from
question nos. 2 to 7.*

*(ii) Use of simple non-scientific
calculator is allowed.*

1. Answer any *five* questions from the following : 5×2=10

- (i) Why is a triplet state ($s = 1$) not possible for the ground state of He atom having configuration $1s^2$?
- (ii) What are the disadvantages of continuous wave CW-NMR spectrum ?
- (iii) Why are NMR spectra intrinsically weak ?
- (iv) What is meant by polarizability of a molecule ?
- (v) How does the isotopic substitution affect the rotational spectrum of a molecule ?

- (vi) Write any *two* important applications of photoelectron spectroscopy in studying polyatomic molecules.
- (vii) Calculate the number of vibrational modes for a molecule of methane.
2. (a) (i) The atomic spectra are line spectra whereas the molecular spectra are band spectra, comment. 2
- (ii) Radioactive-Cobalt-60 nucleus emits γ -rays during its decay. If a photon of the radiation has an energy of 2.135×10^{-16} J, calculate the frequency and the wavelength of the radiation. 3
- (b) (i) Differentiate between Zeeman effect and Stark effect. 2

- (ii) The bond length of CO molecule is 113 pm and the masses of ^{12}C and ^{16}O atoms are 12u and 16u respectively. Calculate the (i) reduced mass, and (ii) moment of inertia for CO molecule. $[1\text{u} = 1.66 \times 10^{-27} \text{ kg}]$. 3
3. (a) (i) Predict the number of ESR lines in the spectrum of CH_3CH_2 . 2
- (ii) Briefly discuss the basic principle of photoelectron spectroscopy. 3
- (b) (i) What information about the molecule can be obtained from its rotational spectrum ? 2
- (ii) State the Franck-Condon principle and explain how it influences the intensity of electronic spectral lines. 3

4. (a) The Mössbauer spectrum of $K_4[Fe(CN)_6]$ consists of one line whereas that of $K_3[Fe(CN)_5NO]$ consists of two lines. Comment. Also draw these spectra quantitatively and account for their appearance. 3
- (b) What are *d-d* transitions and charge transfer transitions in polyatomic molecules ? 3
- (c) In the Raman spectrum of a linear triatomic molecule, the first three lines are observed at 4.86, 8.14 and 11.36 cm^{-1} from the excitation line. Determine the rotational constant *B* and moment of inertia of molecule. 4

5. (a) What makes TMS (Tetramethyl silane) a molecule of choice to act as a reference compound in proton NMR spectroscopy. 2

(b) The fundamental vibrational frequency of $^{35}\text{Cl} - ^{35}\text{Cl}$ molecule is found to be 2940.8 cm^{-1} . Determine the fundamental vibrational frequency of $^{37}\text{Cl} ^{35}\text{Cl}$ molecule. Assume the force constant to be same in both of molecules. How much is the shift in the vibration frequency ? 4

(c) What is meant by the Paschen series of hydrogen ? What will be the wave

number of the longest wavelength in the Paschen series ?

$[R_H = 109,667.58 \text{ cm}^{-1}]$ 4

6. (a) (i) What are the limitations of Raman spectroscopy. 2

(ii) The molecule X_2Y has three fundamental vibrational frequencies. One is Raman active and two are IR active. Identify the structure of molecule. 3

(b) What is meant by spin-spin coupling in NMR spectroscopy ? Explain the splitting of a proton signal having two equivalent neighboring protons. 5

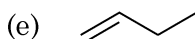
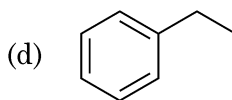
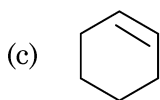
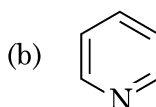
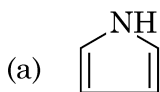
7. (a) (i) When an electron is placed in a magnetic field strength of 1 T, it splits into two energy levels. Calculate the energy differences between these two energy levels.

[Given : $g_e = 2.0023$; $h = 6.626 \times 10^{-34}$ Js and $B_z = 9.274 \times 10^{-34}$ JT⁻¹]

2

- (ii) Predict the number of signals in ¹³C-NMR spectrum in any *three* of the following :

3



- (b) What are the limitations of Beer-Lambert law ? The molar absorptivity of a substance is $2.0 \times 10^4 \text{ cm}^{-1} \text{ mol}^{-1} \text{ dm}^3$. Calculate the transmittance through a cuvette of path length 5.0 cm containing $2.0 \times 10^{-6} \text{ mol dm}^{-3}$ solution of the substance. [Given : $10^{0.2} = 1.585$]. 5

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