

(8 pages)

Reg. No. :

Code No. : 7475

Sub. Code : WCHE 14/
VCHE 14

M.Sc. (CBCS) DEGREE EXAMINATION,
NOVEMBER 2025

First Semester

Chemistry

Elective II – MOLECULAR SPECTROSCOPY

(For those who joined in July 2023 onwards)

Time : Three hours

Maximum : 75 marks

PART A — (15 × 1 = 15 marks)

Answer ALL questions.

Choose the correct answer :

1. The selection rule for the translational energy levels in the Raman spectrum [ΔJ] is
- (a) ± 1 (b) ± 2
(c) $+1$ (d) $+2$

2. Which of the following diatomic molecule will not give a rotational spectrum?
- (a) N_2 (b) CO
(c) NO (d) HF
3. Which of the following molecule may show absorption in the infrared?
- (a) N_2 (b) H_2
(c) Cl_2 (d) Ethane
4. The spectra caused in the infrared region by the transition in the vibrational levels in different modes of vibrations are called as
- (a) Vibration spectra
(b) Electronic Spectra
(c) Rotational spectra
(d) None of the above
5. The vibrational and rotational spectra was observed in _____ region.
- (a) Near IR
(b) Microwave
(c) Visible
(d) Radiofrequency

6. The number normal mode of vibrations in N_2O molecule is
 (a) 1 (b) 3
 (c) 4 (d) 7
7. Gamma ray laser are called as _____.
 (a) Maser (b) Normal laser
 (c) Grasers (d) All the above
8. What does binding energy measure?
 (a) Amount of energy needed to remove an electron from an atom
 (b) The amount of kinetic energy an electron
 (c) The effective nuclear charge
 (d) The charge carried by electron in motion
9. What are the possible x-axis coordinates in graphs made from PES data?
 (a) eV (b) MJ per mole
 (c) energy (d) All of the above
10. Which of these gives only one NMR signals in their ^{19}F NMR spectra
 (a) BF_3 (b) Chloroform
 (c) CF_3Cl (d) All the above
11. The multiplicity of ^{31}P of H_3PO_2
 (a) Doublet (b) Singlet
 (c) Triplet (d) Quartet
12. The distance between the center of the peak of doublet is called as
 (a) coupling constant
 (b) chemical shift
 (c) spin coupling
 (d) spin-spin splitting
13. For a free electron, value of Lande' factor (g-factor) will be equal to
 (a) 1.0098 (b) 2.0023
 (c) 3.0015 (d) 6.0821
14. The oxidation state of metal ion catalyst can be deduced by
 (a) AAS
 (b) HPLC
 (c) Mössbauer
 (d) GC-MS

15. The correct order of isomeric shift of iron complexes

- (a) $\text{Fe}^{2+} > \text{Fe}^{3+} > \text{Fe}^{4+}$
- (b) $\text{Fe}^{3+} > \text{Fe}^{2+} > \text{Fe}^{4+}$
- (c) $\text{Fe}^{4+} > \text{Fe}^{3+} > \text{Fe}^{2+}$
- (d) $\text{Fe}^{4+} > \text{Fe}^{2+} > \text{Fe}^{3+}$

PART B — (5 × 4 = 20 marks)

Answer ALL questions, choosing either (a) or (b).
Each answer should not exceed 250 words.

16. (a) Describe briefly about the characteristics of Raman Lines and Raman Shifts.

Or

(b) Classify the molecule on the basis of principal moments of inertia.

17. (a) Derive an expression for vibrational energy for harmonic oscillator of simple molecules.

Or

(b) Explain the statement 'Breakdown of Born oppenheimer approximation'.

Page 5 Code No. : 7475

18. (a) Predict the kind electronic transition in chlorine and Carbonyl group.

Or

(b) Sketch and explain the dissociation spectra.

19. (a) Explain the Nuclear Over Hauser Effect.

Or

(b) What is TMS? Why TMS is used as a standard compound in NMR spectroscopy?

20. (a) Explain the term isomer shift in Mössbauer spectroscopy.

Or

(b) How to differentiate the low and high spin complexes by using Mossbauer spectroscopy.

PART C — (5 × 8 = 40 marks)

Answer ALL questions, choosing either (a) or (b).
Each answer should not exceed 600 words.

21. (a) Describe the Quantum theory of Raman effect.

Or

(b) Derive an expression for rotational spectra of diatomic molecules.

Page 6 Code No. : 7475

22. (a) Sketch and explain the PQR line for perpendicular and parallel vibrations of symmetry top molecules.

Or

- (b) What are the differences between Raman and infrared spectra?

23. (a) Discuss the principles and applications of photoelectron spectroscopy.

Or

- (b) Describe the principle and construction of simple laser system.

24. (a) Discuss the factors which affecting the coupling constant in NMR spectroscopy.

Or

- (b) A compound containing C, H, O and halogen shows molecular ion peak at m/e 108 / 110 in the intensity ratio 3:1. The IR spectrum shows a very broad band in the range of $2500-3300\text{ cm}^{-1}$ and centering around 2900 cm^{-1} and a strong intensity band at 1705 cm^{-1} . In the ^1H NMR spectrum of the compound, two triplets at δ 2.8 and 3.8 and

a singlet at 12 are found in the intensity ratio 2 : 2: 1. One of the ^{13}C NMR peaks (proton-noise decoupled) is a low intensity peak at 170. Deduce the structure of the compound and explain the spectral data.

25. (a) Discuss Kramer's degeneracy and ZFS with suitable examples.

Or

- (b) Sketch and explain the Mossbauer spectrum of any two iron and tin complexes.