(6 pages) **Reg. No. :** .....

Code No. : 7882 **Sub. Code : PCHM 33**

M.Sc. (CBCS) DEGREE EXAMINATION,
NOVEMBER 2019.

Third Semester

Chemistry — Core

PHYSICAL CHEMISTRY — III

(For those who joined in July 2017 onwards)

Time : Three hours Maximum : 75 marks

PART A — (10 × 1 = 10 marks)

Answer ALL questions.

Choose the correct answer :

1. Point group of molecule with only reflection symmetry is
   (a) σ_v (b) C_0
   (c) C_i (d) C_1

2. Total number of irreducible representations in ammonia is
   (a) 3 (b) 6
   (c) 4 (d) 2

3. In reduction formula 'h' refers to
   (a) plank's constant (b) class
   (c) order (d) none

4. Based on HMO theory, H_{14} is
   (a) 1 (b) α
   (c) 0 (d) β

5. Solvent used in NMR is
   (a) DMSO (b) $CHCl_3$
   (c) $CDCl_3$ (d) All

6. FID means
   (a) Fourier Interaction Decay
   (b) Frequency Induction Decay
   (c) Fourier Induction Decay
   (d) Fourier Inversion Decay

7. ESR is mainly depends on
   (a) J value
   (b) anisotropy
   (c) g-value
   (d) double resonance

8. Which one is related to NQR spectra?

(a) SPI (b) NOE

(c) Anisotropy (d) Asymmetry

9. Which of the following is used in Electronic spectra?

(a) Kramer's degeneracy

(b) Isomer shift

(c) Magnetic hyper fine interaction

(d) Franck-Condon principle

10. Which of the following is not related to mass spectra?

(a) Doppler shift (b) Fragmentation

(c) Anisotropy (d) Asymmetry

PART B — (5 × 5 = 25 marks)

Answer ALL questions, choosing either (a) or (b).

Each answer should not exceed 250 words.

11. (a) List the symmetry elements and point group for the following molecules (i) Ferrocene (ii) XeF_4.

Or

(b) Write the rules of irreducible representations.

12. (a) Deduce the vibrational modes of water molecule.

Or

(b) Determine the delocalization energy of trans-1, 3-butadiene.

13. (a) How chemical shift vary with solvent, concentration of the compound and temperature?

Or

(b) Compare the principles of ^{13}C and ^{31}P NMR spectra.

14. (a) Differentiate NMR and EPR spectra.

Or

(b) Write the selection rules and energy levels of NQR spectroscopy.

15. (a) Write the applications of Born-Oppenheimer approximation and Frank-Condon principle in electronic spectroscopy.

Or

(b) How isotopes affects the appearance of mass spectrum?

PART C — (5 × 8 = 40 marks)

Answer ALL questions choosing either (a) or (b).

Each answer should not exceed 600 words.

16. (a) How will you determine point group for a molecule?

Or

(b) Construct the character table for C_4V point group.

17. (a) Determine the hybrid atomic orbitals in PF_5 molecule.

Or

(b) Construct projection operators and molecular orbitals by SALC.

18. (a) How will you characterise your sample by ^{1}HNMR spectroscopy?

Or

(b) Discuss the role of NMR spectroscopy in MRI.

19. (a) Discuss zerofield splitting and Kramer's degeneracy.

Or

(b) Write the quadrupole transitions in axially symmetric fields.

20. (a) Write the role of fortrat diagram in Electronic Spectroscopy.

Or

(b) How will you determine molecular weight of a compound by mass spectrum?

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