

Reg. No. : .....

Name : .....

**Third Semester M.Sc. Degree Examination, February 2024**

**(Chemistry/Analytical Chemistry/Applied Chemistry/  
Medicinal Chemistry/Polymer Chemistry)**

**CH/CL/CA/CM/PC 233 : PHYSICAL CHEMISTRY – III**

**(Chemistry/Analytical Chemistry/Applied Chemistry/Medicinal Chemistry :  
2016 – 2019 Admission and Polymer Chemistry : 2018 – 2019 Admission)**

Time : 3 Hours

Max. Marks : 75

SECTION – A

Answer any **two** sub-questions among (a), (b), or (c) from each question.  
Each sub-question carries **2** marks.

1. (a) Discuss the variation theorem.  
(b) What are secular determinants?  
(c) What are the similarities between MO and VB theories?
2. (a) What is Pople's style basis sets?  
(b) What is Hohenberg – Hohn theorem?  
(c) Construct the Z-matrix of H<sub>2</sub>O
3. (a) What is spin – spin coupling in NMR?  
(b) What are the factors affecting the 'g' factor?  
(c) What is meant by nuclear resonance?

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4. (a) What is the principle of equipartition energy?  
(b) Discuss the classical theory of heat capacity. What is its limitation?  
(c) What is Dulong and Petit's law?
5. (a) What is calomel electrode? What are the characteristics of calomel electrode?  
(b) Discuss potentiometric titrations and its applications.  
(c) What is amperometry? What are its uses?

**(10 × 2 = 20 Marks)**

SECTION – B

Answer either (a) or (b) of each question. Each question carries **5** marks.

6. (a) Describe the application of HMO method to allyl systems.  
(b) Briefly explain the quantum mechanical treatment of  $sp^2$  and  $sp^3$  hybridizations.
7. (a) What are Slater functions? How it is different from Gaussian function? What are the properties of Slater functions?  
(b) Discuss the different types of 'basic sets' used in computational chemistry.
8. (a) What is the principle of NQR spectroscopy? What are its applications?  
(b) Discuss the principle and uses of X-ray photoelectron spectroscopy.
9. (a) What is Langevin function? How can it be used for the determination of dipole moment?  
(b) Discuss the Debye's theory of specific heat and the assumptions used in it.
10. (a) What is the principle of conductometric titrations? Discuss its applications.  
(b) Discuss the instrumentation and applications of flame emission spectroscopy.

**(5 × 5 = 25 Marks)**



## SECTION – C

Answer any **three** questions. Each question carries **10** marks.

11. Explain the molecular orbital treatment of  $C_2$  and  $F_2$ . What are the applications of MO theory?
12. Explain the various semi-empirical quantum mechanical computational methods.
13. Explain the instrumentation of NMR spectroscopy? What are the advantages of 2D and 3D NMRs?
14. Explain the various types of molecular partition functions.
15. Explain the principle, instrumentation and applications of Atomic absorption spectroscopy.

**(3 × 10 = 30 Marks)**

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