Total No. of Questions : 6]

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P1905

[5323]-401 M.Sc. - II

PHYSICAL CHEMISTRY

CHP-410: Molecular Structure and Spectroscopy (2013 Pattern) (Semester - IV) (New)

Time: 3 Hours] [Max. Marks: 50

Instructions to the candidates:

- 1) All questions are compulsory.
- 2) Answers to the two sections should be written in separate answer books.
- 3) Neat diagrams must be drawn wherever necessary.
- 4) Figures to the right side indicate full marks.
- 5) Use of Logarithmic table / calculator is allowed.

Physico - Chemical Constants

1.	Avogadro Number	N	=	$6.022 \times 10^{23} \text{ mol}^{-1}$
2.	Boltzmann Constant	k	=	
			=	4 0 0 4 0 00 7 7 7 1 4 4 1
3.	Planck Constant	h	=	$6.626 \times 10^{-27} \text{ erg s}$
			=	6 60 6 10 21 T
4.	Electronic Charge	e	=	$4.803 \times 10^{-10} \text{ esu}$
	٥		=	$1.602 \times 10^{-19} \text{ C}$
5.	1 eV		=	23.06 k cal mol ⁻¹
			=	$1.602 \times 10^{-12} \text{ erg}$
			=	$1.602 \times 10^{-19} \text{ J}$
			=	8065.5 cm ⁻¹
6.	Gas Constant	R	=	$8.314 \times 10^7 \text{ erg K}^{-1} \text{ mol}^{-1}$
			=	8.314 J K ⁻¹ mol ⁻¹
			=	1.987 cal K ⁻¹ mol ⁻¹
7.	Faraday Constant	F	=	96487 C equiv ⁻¹
8.	Speed of light	c	=	$2.997 \times 10^{10} \text{ cm s}^{-1}$
			=	$2.997 \times 10^8 \text{ m s}^{-1}$
9.	1 cal		=	$4.184 \times 10^7 \text{erg}$
			=	4.184 J
10.	1 amu		=	$1.673 \times 10^{-27} \text{ kg}$
11.	Bohr magneton	$\beta_{\rm e}$	=	$-9.274 \times 10^{-24} \text{ J T}^{-1}$
12.	Nuclear magneton	β_n	=	$5.051 \times 10^{-27} \text{ J T}^{-1}$
13.	Mass of an electron	m_e	=	$9.11 \times 10^{-31} \text{ kg}$

SECTION - I

Q1) Attempt the following:

[10]

- a) Distinguish between δ and τ Chemical Shift Scales.
- b) Explain the terms with respect to nmr spectroscopy.
 - i) Deshielding and
 - ii) Coupling constant.
- c) What is kramers degeneracy?
- d) Write the applications of nqr.
- e) Why esr spectra are always recorded in the derivative form? Explain.

Q2) Attempt any two of the following:

[10]

- a) Explain the instrumentation involved in high resolution nmr spectroscopy.
- b) What is g-value? Explain the factors affecting it.
- c) What is the need of reference for recording high resolution nmr? Explain the advantages of TMS.
- d) Explain the concept of electric field gradient and quadrupole coupling constant.

Q3) Solve any one of the following:

[5]

a) Differentiate among the following compounds from ¹⁹F spectra at high field.

$$CH_3-CH_2F$$
, CH_2F-CH_2F , CH_3-CF_3

b) Calculate the precessional frequency of a proton in a field of 1.8T. The *g* factor for proton is 5.585.

SECTION - II

Q4) Attempt the following:

[10]

- a) What is the principle of X-ray diffraction?
- b) Explain how the Wierl equation is used to deduce molecular geometry.
- c) Write Van-Vlecks formula and explain the terms therein.
- d) Enlist the applications of neutron diffraction technique.
- e) State the phase, problems in XRD.

Q5) Attempt any two of the following:

[10]

- a) Give a brief account of main XRD methods used in the elucidation of the crystal structure of NaCl and KCl. What are limitations of Bragg's method?
- b) Distinguish between ferrimagnetism and antiferromagnetism with suitable examples.
- c) Describe the instrumentation of neutron diffraction technique with a suitable diagram.
- d) Explain the cause of electron diffraction. How is it experimentally studied?

Q6) Solve any one of the following:

[5]

- a) The mass and density of copper atom are 63.5 and 8.94 gcm⁻³ respectively. It has FCC structure. Calculate the atomic radius of copper atom.
- b) Calculate molar susceptibility of phenanthroline ($C_{12} H_8 N_2$) and pyridine ($C_5 H_5 N$) from following data.

* pascal constant (χ_A) in cgs unit

$$C = -6.0 \times 10^{-6}$$
, $H = -2.93 \times 10^{-6}$, ring $N = -4.61 \times 10^{-6}$

* Constitutive corrections (λ)

C in one ring = -0.24×10^{-6}

C shared by two rings = -3.07×10^{-6}

HHH