Total No. of Questions : 5]

SEAT No. :

P1955

[Total No. of Pages : 4

[4923] - 31
M.Sc. II
PHYSICAL CHEMISTRY
CH - 310 : Quantum Chemistry and Solid State Chemistry
(2008 Pattern) (Semester - III)

Time : 3 Hours] *[Max. Marks : 80*

Instructions to the candidates:

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

Physico - Chemical Constants

1)	Avogadro Number	N	$= 6.022 \times 10^{23}$ mol^{-1}
2)	Boltzmann Constant	k	$= 1.38 \times 10^{-16}$ erg K^{-1} molecule^{-1}
			$= 1.38 \times 10^{-23}$ J K^{-1} molecule^{-1}
3)	Planck Constant	h	$= 6.626 \times 10^{-27}$ erg s
			$= 6.626 \times 10^{-34}$ J s
4)	Electronic Charge	e	$= 4.803 \times 10^{-10}$ esu
			$= 1.602 \times 10^{-19}$ C
5)	1 eV		$= 23.06$ k cal mol^{-1}
			$= 1.602 \times 10^{-12}$ erg
			$= 1.602 \times 10^{-19}$ J
			$= 8065.5$ cm^{-1}
6)	Gas Constant	R	$= 8.314 \times 10^{7}$ ergK^{-1} 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	$= 2.997 \times 10^{10}$ cm s^{-1}
			$= 2.997 \times 10^{8}$ m s^{-1}
9)	1 cal		$= 4.184 \times 10^{7}$ erg
			$= 4.184$ J
10)	1 amu		$= 1.673 \times 10^{-27}$ kg
11)	Bohr magneton	β_e	$= -9.274 \times 10^{-24}$ J T^{-1}
12)	Nuclear magneton	β_n	$= 5.051 \times 10^{-27}$ J T^{-1}
13)	Mass of an electron	m_e	$= 9.11 \times 10^{-31}$ kg

P.T.O.

SECTION - I

Q1) Attempt any four of the following: **[20]**

a) Show that the function $U(x) = e^{ax^2}$ is an eigen function of operator $\left(\frac{\partial^2}{\partial x^2} - x^2\right)$ for a = 0.5.

b) Classify the operators as linear or nonlinear.

i) $\int dx$ ii) exp

iii) $\sum$ iv) $(\,)^2$

v) $2x^2 \frac{d^2}{dx^2}$

c) Find the term symbols for the following configuration.

i) $2S^1\ 2P^1$ and ii) $1s^2 2s^2 2p^2$

d) Explain the properties of Ladder operators in brief.

e) Compare the variation method with the perturbation method.

f) Show that Hermitian operators have real eigenvalues.

Q2) Attempt any four of the following: **[20]**

a) Deduce the Hückels energies for cyclobutadiene, why is the molecule not stable?

b) State Hückels (4m+2) rule and explain how it accounts for the stability of cyclooctatetraene dianion.

c) Sketch the MO for butadiene on the basis of HMO theory. Deduce the energies of these orbitals on the basis of secular determinant.

d) Explain the mnemonic Model of Frost and Musulin used to deduce HMO energies for annulenes.

e) Comment, giving examples on the positive or negative nature of REPE Value for a molecule.

f) Derive the equation for first order perturbation energy for nondegenerate systems in a generalized situation.

SECTION - II

Q3) Attempt any three of the following: **[15]**

a) What are the differences between Schottky and Frenkel defects?

b) Explain the photo conductivity in ionic crystals.

c) Discuss Einsteins specific heat theory of metals.

d) Explain the formation of F and V colour centres in crystals.

e) Write a note on Kirkendall effect.

Q4) Attempt any three of the following: **[15]**

a) What are the different methods to grow crystals from their melts? Describe the merits and demerits of any two such methods?

b) How is the parabolicrate law useful in explaining the mechanism of a gas-solid reaction?

c) Write a note on transistors.

d) What are the main types in which materials can be divided on the basis of their response to magnetic filed? Discuss briefly.

e) Explain the various mechanism of diffusion insulator.

Q5) Solve any two of the following: **[10]**

a) How long would it take for Li to penetrate in Se at 550 ^{o}C to a 0.65 mm depth? [D = 10^{-6} cm^2/sec].

b) Calculate the relaxation time for Cu having density 8.92 g/cc. [Given - At. Wt. of Cu - 63.5].

c) The number of free electrons in a monovalent crystal is 9.8×10^{18} per cm^3 at 350 K. Evaluate E_o in eV.