Total No. of Questions :5]

SEAT No. :

P1849

[Total No. of Pages : 3

[5323]-31
M.Sc.-II
PHYSICAL CHEMISTRY
CH-310: Quantum Chemistry & Solid State Chemistry
(2008 Pattern) (Semester-III) (Old)

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

Instructions to the candidates:

1) ***Answer 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}
		$= 1.38 \times 10^{-23}$ JK^{-1} molecule^{-1}
3)	Planck Constant	$h = 6.626 \times 10^{-27}$ erg s
		6.626×10^{-34} Js
4)	Electronic Charge	$e = 4.803 \times 10^{-10}$ esu
5)	1 eV	$= 1.602 \times 10^{-19}$ C
		= 23.06k 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 JK^{-1}mol^{-1}
		= 1.987 cal K^{-1}mol^{-1}
7)	Faraday Constant	F = 96487 equiv^{-1}
8)	Speed of light	$c = 2.997 \times 10^{10}$ cm s^{-1}
		$= 2.997 \times 10^{8}$ cm 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	$\beta_e = -9.274 \times 10^{-24}$ J T^{-1}
12)	Nuclear magneton	$\beta_n = 5.051 \times 10^{-27}$ J T^{-1}

P.T.O.

13) Mass of an electron $m_e = 9.11 \times 10^{-31}$ kg

SECTION-I

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

a) Explain the properties of ladder operators

b) Formulate the energy operators for H_2 molecule and H_2^- ion

c) Show that $\left[\hat{L}_x, \hat{L}_z\right] = -i\hbar\hat{L}_y$ for a set of angular momentum operators $\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$.

d) Which of the following functions are eigen functions of the operator d^2/dx^2 ?

i) Sin $4x$

ii) Cos $3x$

iii) x^{-3}

Give the corresponding eigen values.

e) State and prove the variation theorem.

f) State the fundamental postulates of quantum mechanics.

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

a) Discuss Huckel's 4m+2 rule citing benzene and cyclo-octatetraene as examples.

b) Comment giving examples on the positive or negative nature of REPE value for a molecule.

c) Give the comparison between perturbation and variation methods.

d) Deduce the secular determinant for ethene and Obtain the HMO energy values for molecule.

e) How Hess and schaad improved Huckel's calculations for M.O. energies?

f) Derive the expression for the first order correction to the energy of the

non degenerate unperturbed level.

SECTION-II

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

a) Derive the expression for the Frenkel defects in a crystal at a given temperature.

b) Comment on the effect of temperature on carrier density and conductivity of n-type extrinsicsemiconductor.

c) Write a note on-mechanism of a photographic process.

d) Discuss the mechanism of diffusion in crystalline solids.

e) Distinguish between the resistivities of annealed and on annealed Cu-Au alloys.

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

a) State and explain the various methods of electric breakdown in insulators.

b) Explain the parabolic rate low used to explain the mechanism of gas-solid reactions.

c) The fast growing faces are eliminated whereas slow growing faces persist in a crystal, prove this statement on the basis of geometrical considerations.

d) Write a note on : Taylor-Orowan dislocations.

e) Define 'Colour centre' and explain the fermation of F and V colour centres in crystal.

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

a) Calculate the dislocation density for a cubic crystal having 10^{-6} cm edge length and total dislocation length of 10^{-12} cm.

b) Calculate the number of electrons per cm^3 in the conduction band of semiconductor having a bandgap of 0.72 eV at 27°C.

c) If 2 eV is the energy required for the pair of ions to move from the crystal's interior to the surface, What is the proportion of vacancies (n/N) present at 400K?

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