Total No. of Questions :5]

SEAT No. :

P1460

[Total No. of Pages : 3

[5223]-31
M.Sc.
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) *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	=	6.022×10^{23} mol^{-1}
2.	Boltzmann Constant	k	=	1.38×10^{-16} erg K^{-1} molecule^{-1}
			=	1.38×10^{-23} J K^{-1} molecule^{-1}
3.	Planck Constant	h	=	6.626×10^{-27} erg s
			=	6.626×10^{-34} J s
4.	Electronic Charge	e	=	4.803×10^{-10} esu
			=	1.602×10^{-19} C
5.	1 eV		=	23.06 k cal mol^{-1}
			=	1.602×10^{-12} erg
			=	1.602×10^{-19} J
			=	8065.5 cm^{-1}
6.	Gas Constant	R	=	8.314×10^{7} erg K^{-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	=	2.997×10^{10} cm s^{-1}
			=	2.997×10^{8} m s^{-1}
9.	1 cal		=	4.184×10^{7} erg
			=	4.184 J
10.	1 amu		=	1.673×10^{-27} kg
11.	Bohr magneton	β_e	=	-9.274×10^{-24} J T^{-1}
12.	Nuclear magneton	β_n	=	5.051×10^{-27} J T^{-1}
13.	Mass of an electron	m_e	=	9.11×10^{-31} kg

P.T.O.

SECTION - I

Q1) Attempt <u>any four</u> of the following: **[20]**

a) Show that the wave functions for a particle in a one dimensionel box are orthogonal

b) Formulate the Hamiltonian operators for

i) He atom

ii) H_2 molecule

iii) H_2^+ ion

c) Explain the properties of quantum mechanical operators.

d) Explain the historical origin of quantum theory.

e) Deduce the eigenvalues for sin$x$, cos$x$, sin$x$ + cos$x$ when $\frac{d^2}{dx^2}$ is the operator, in the cases where possible.

f) Find term symbols for the ground state configuration of He and C atoms.

Q2) Attempt <u>any four</u> of the following: **[20]**

a) State and prove the variation theorem.

b) Obtain an expression of the ground state energy of He atom using first order perturbation theory.

c) Distinguish between variation and perturbation theories.

d) Deduce the Secular equation for butadiene and state the energies of the first two excited states.

e) Write a note on Hückel 's approximations.

f) Derive the expression for the first order perturbation correction to the wave function for a non-degenarate system.

SECTION - II

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

a) Write a note on p-n junction.

b) State and explain the Kirkendall effect.

c) What is a colour centres? Explain the origin of Colour centres in halide crystals.

d) Define defects. Describe the various types of point defects found in crystalline solids.

e) Discuss the conditions for crystal grouth from a moltan salt.

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

a) Derive the expression for the number of Schottky defects present in a crystal at a given temperature.

b) Describe any one experimental method adopted to study the kinetics of decomposition of a single solid.

c) Discuss the mechanism of diffusion in crystalline solids.

d) Write a note on Brillouin zones.

e) Discuss the factors that affect the progress of a chemical change in solid -solid reactions.

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

a) The number of free electrons in a monovalent crystal is 10^{19} per cm^3 at 300K. Evalnate E_0 in eV.

b) Calculate the drift mobility of charge carrier for semiconductor having donor concentration of 10^{22} per metre cube. [Given: Conductivity = 100 mhos m^{-1}]

c) Calculate the mean free time for an electron in semiconductor crystal having drift mobility 625 cm^2/ Volt. Sec.