Total No. of Questions : 6]

SEAT No :

P2870

[Total No. of Pages : 3

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M.Sc.

PHYSICAL CHEMISTRY

CHP-310 : Quantum Chemistry and Solid State Chemistry

(2013 Pattern) (Semester - III) (New)

Time : 3Hours] *[Max. Marks : 50*

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 precisely the following : **[10]**

a) State the condition for the acceptable wave function.

b) Define Hermitian operator giving example.

c) Explain, what is term symbol?

d) Are the following operators meet the requirements for a quantum-mechanical operator that is to represent a physical quantity : i) $\frac{d^2}{dx^2}$ and ii) $i\left(\frac{d}{dx}\right)$? Why?

e) Write the Schrodinger time - dependent equation. State the significance of the terms involved in it.

Q2) Attempt any two of the following: **[10]**

a) Apply the variation method to the system of He atom to calculate its energy.

b) Construct the Hamiltonian operator for Be^{+2} ion in atomic units. State the terms involved in it.

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

d) Explain Hückel approximations. What is their need?

Q3) Attempt any one of the following: **[5]**

a) If $g = \hat{A}F$, find g for each of the following choices of $\hat{A}$ and F.

i) $\hat{A} = \frac{d}{dx}$ and $F = \cos(x^2+1)$

ii) $\hat{A} = 5$ and $F = \sin x$

iii) $\hat{A} = (\,)^2$ and $F = \sin x$

iv) $\hat{A} = \frac{d^2}{dx^2}$ and $F = \ln 3x$

v) $\hat{A} = \exp$ and $F = \ln x$

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

SECTION -II

Q4) Attempt precisely the following: **[10]**

a) Write the equation for Frenkel defects and explain the terms involved in it.

b) State the third power law of Debye for solids.

c) Define induction period for the decomposition reaction of a single solid.

d) What is Van-Arkel process?

e) Give steps in the photographic process.

Q5) Attempt Any Two of the following : **[10]**

a) Discuss the mechanism of diffusion in solids.

b) Explain the mechanism of the following solid-solid reactions:

i) $MgO(s)+Al_2O_3(s) \rightarrow MgA1_2O_4(s)$

ii) $AgCl(s)+NaI(s) \rightarrow AgI(s)+NaCl(s)$

c) State and explain Kirkendall effect.

d) What is a colour centre? Explain the origin of colour centers in halide crystals.

Q6) Attempt any one of the following : **[5]**

a) How deep will Aluminium penetrate in silicon at 1450^oC in one hour?

[Given : $\triangle H=73$ Kcal/mole, $D_o=1.55\ cm^2/s$]

b) A certain alkali halide($A^+ X^-$) with molecular weight 74.6 has the NaCl structure. If the interionic distance $A^+–X^-$ is 0.32nm, calculate the density of the salt for the 0.1% Frenkel defects.

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