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5 SEM TDC CHM M 7 (N/O)

2017

(November)

CHEMISTRY

(Major)

Course : 507

(Symmetry and Quantum Chemistry)

The figures in the margin indicate full marks for the questions

(New Course)

Full Marks : 48

Pass Marks : 14

Time : 2 hours

1. Select the correct answer from the following : 1×5=5

(a) The quantum mechanical operator for kinetic energy is

(i) $-\frac{h^2}{8\pi^2 m}\nabla^2$ *(ii)* $\frac{h}{2\pi i}\nabla$

(iii) $\frac{h}{2\pi i}\frac{d}{dx}$ *(iv)* V

(b) A particle is moving in a 1-D box, N_n is the number of nodes in a state with quantum number n. The ratio of $N_{n=2} : N_{n=1}$ has a value

(i) 1

(ii) 2

(iii) 3

(iv) ∞

(c) The energy required to excite (to first excited state) a particle of mass m confined in a length l is

(i) $\frac{3h^2}{8ml^2}$

(ii) $\frac{h^2}{8ml^2}$

(iii) 0

(iv) h^2

(d) The eigenvalue of the function $\psi = 8e^{4x}$ for the operator $\frac{d^2}{dx^2}$ is

(i) 16

(ii) 32

(iii) 8

(iv) 4

(Continue

(e) The point group of NH_3 is

(i) T_d

(ii) D_{2h}

(iii) C_{2v}

(iv) C_{3v}

2. Answer any *five* questions from the following : 2×5=10

(a) What is the matrix representation of rotation-reflection axis (S_n) in symmetry?

(b) Briefly describe Compton effect.

(c) Distinguish bonding molecular orbitals from antibonding molecular orbitals.

(d) Show that the functions $\psi_1 = \left(\frac{1}{2\pi}\right)^{1/2}$ and $\psi_2 = \left(\frac{1}{\pi}\right)^{1/2} \cos x$, in the interval $x = 0$ to $x = 2\pi$, are orthogonal to each other.

(e) Hermitian operators have real eigenvalues. Explain.

(f) Show that the energy levels in a simple harmonic oscillator are equally spaced.

(Turn Over)

UNIT—I

3. Answer any *three* questions from the following : 3×3

(a) Write the symmetry elements and point groups of the following : 1×3

(i) $CHCl_3$

(ii) NH_3

(iii) PCl_5

(b) Construct the character table for C_{2v} point group.

(c) What are dihedral planes of symmetry? Explain with example. $2+1$

(d) Distinguish Abelian groups from non-Abelian groups by taking a suitable example.

UNIT—II

Answer any *two* questions : $9\times2=$

4. *(a)* A wave function is described by $\psi(\theta) = \sin\theta$, where θ can change continuously from 0 to 2π. Show whether it is normalized or not. If it is not, then find the normalizing factor. $2+2$

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(b) Show that $\psi = \sin(k_1x)\sin(k_2y)\sin(k_3z)$ is an eigenfunction of ∇^2. What is the eigenvalue? $2+1=3$

(c) Verify that the operator ∇^2 is linear. 2

5. *(a)* Solve Schrödinger's wave equation for a particle moving freely in a one-dimensional box. Find the eigenfunction and energy also. 5

(b) A particle of mass m is confined in a one-dimensional box of length a. Calculate the probability of finding the particle in the region $0 \le x \le \frac{a}{4}$. What is the limiting probability when $n \to \infty$? $3+1=4$

6. *(a)* Define rigid rotator. Write the Schrödinger's wave equation for this system and separate the variables. $1+4=5$

(b) Sketch the variation of radial probability density against the distance from the nucleus for 2*s* state for hydrogen atom. 2

(Turn Over)

(c) Determine the degree of degeneracy of the energy level $\frac{6h^2}{8ma^2}$ of a particle in a cubical box.

UNIT—III

7. (a) Explain the valence bond treatment for H_2 molecule.

Or

Compare the MO and VB treatment of hydrogen molecule in the ground state.

(b) Write the MO configuration of CN^- ion and predict its magnetic character.

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