K23P 3072

Reg. No. : .....

Name : .....

I Semester M.Sc. Degree (CBCSS – OBE – Regular)
Examination, October 2023
(2023 Admission)
CHEMISTRY
MSCHE01C01 : Theoretical Chemistry – I

Time : 3 Hours Max. Marks : 60

SECTION – A

Answer **any 5** questions from the following. **Each** question carries **three** marks.

1. State Planck's radiation law.
2. What is meant by normalisation of a wave function ?
3. What are spherical harmonics ? Are they mutually orthogonal ?
4. State Variation theorem.
5. Show that the ground state term symbol of H_2 is $1\Sigma_g^+$.
6. What is basis set ? **(5×3=15)**

SECTION – B

Answer **any 3** questions from the following. **Each** question carries **six** marks.

7. What are eigenfunctions and eigenvalues ? Show that e^{ikx} is an eigenfunction of the momentum operator $\hat{P}_x = i\hbar\frac{\partial}{\partial x}$. What is the eigenvalue ?
8. What will happen if the walls of the one-dimensional box are suddenly removed ? Explain.

P.T.O.

9. Explain spin orbit coupling and spin orbit coupling constant. Why is it very large in heavy elements ?

10. What is meant by HFSCF procedure ? Explain.

11. What are the important problems faced in quantum mechanical calculations for many particles compared to a single particle ? How it is overcome ? **(3×6=18)**

SECTION – C

Answer **any 3** questions from the following. **Each** question carries **nine** marks.

12. Give the postulates of quantum mechanics.

13. Set up the Schrodinger wave equation for hydrogen atom in spherical polar coordinates. Separate the variables. How do the quantum numbers n, l and m emerge from the solution of three equations ?

14. Obtain the normalized wave function and energy for a particle confined in a three-dimensional box with lengths Lx, Ly and Lz. Evaluate the results.

15. Give the Molecular Orbital (MO) treatment for the following molecules
    i) Be_2
    ii) NO
    iii) LiH

16. Set up the Huckel secular equation for cyclobutadiene, calculate the energies of the π orbitals and determine the delocalization energy. **(3×9=27)**

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