



K24P 3879

Reg. No. :

Name :

I Semester M.Sc. Degree (C.B.C.S.S. – OBE – Reg./Supple./Imp.)
Examination, October 2024
(2023 Admission Onwards)
CHEMISTRY/CHEMISTRY WITH DRUG CHEMISTRY SPECIALIZATION
MSCHD01C01/MSCHE01C01 : Theoretical Chemistry – 1

Time : 3 Hours

Max. Marks : 60

SECTION – A

(Answer **any five** questions. Short answer questions. **Each** question carries **three** marks.)

1. What is meant by Compton effect ? Calculate the Compton shift when scattering angle is equal to 90° .
2. Explain eigen values and eigen functions with suitable examples.
3. Explain (i) spherical harmonics and (ii) polar diagrams.
4. Explain the concept of degeneracy with respect to particle in a cubical box problem. What will be the degeneracy of the energy level ($14h^2/8ma^2$) of a cubical box with edge length 'a' ?
5. State and explain variation theorem.
6. Derive the ground state spectroscopic term symbol for O_2 molecule. **(5×3=15)**

SECTION – B

(Answer **any three** questions. Short answer questions. **Each** question carries **six** marks.)

7. Explain the Davisson-Germer experiment as a proof of wave-particle duality of matter.
8. What angular momentum operators ? Discuss their commuting property.

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9. Briefly discuss the Self Consistent Field theory.
10. Differentiate the basis sets STO and GTO.
11. Sketch the MO diagrams of heteronuclear diatomic molecules, NO and HF. Calculate their bond orders. **(3×6=18)**

SECTION – C

(Answer **any three** questions. Essay type questions. **Each** question carries **nine** marks.)

12. Discuss the postulates of quantum mechanics.
13. Give the Schrodinger wave equation for hydrogen like systems. Separate the variables and obtain the complete solution of θ (theta) equation.
14. Discuss the quantum mechanical treatment of non-planar rigid rotator.
15. Explain the perturbation method. Apply first-order time-independent perturbation method to particle in 1-D box with slanted bottom.
16. Apply the Huckel Molecular Orbital (HMO) theory to benzene. **(3×9=27)**