K25P 3529

Reg. No. : .....

Name : .....

I Semester M.Sc. Degree (C.B.C.S.S. – O.B.E.-Reg./Supple./Imp.) Examination, October 2025
(2023 Admission Onwards)
CHEMISTRY/CHEMISTRY WITH DRUG CHEMISTRY SPECIALIZATION
MSCHD01C01/MSCHE01C01 : Theoretical Chemistry – I

Time : 3 Hours Max. Marks : 60

SECTION – A

Short answer questions. Answer **any five** questions and **each** carries **three** marks.

1. Explain Compton effect with a diagram.
2. Explain Einstein's theory of photoelectric effect.
3. Illustrate the energy level diagram of a particle in a cubical box.
4. Explain how the spacing of vibrational levels varies with an increase in vibrational quantum number.
5. State and explain Variation theorem.
6. Explain why oxygen molecule is attracted in a magnetic field. **(5×3=15)**

SECTION – B

Paragraph questions. Answer **any three** questions and **each** carries **six** marks.

7. Explain the experimental setup of Davisson-Germer experiment. What is its significance ?
8. Give the quantum mechanical treatment of a planar rigid rotor.
9. Discuss the significance of spin-orbit coupling in quantum mechanical systems.

P.T.O.

10. Derive the commutation relation for [Lx, Ly].

11. Evaluate the significance of *ab initio* calculations in modern quantum chemistry and describe how the choice of basis sets affects the accuracy of results.

(3×6=18)

SECTION – C

Essay type questions. Answer **any three** questions and **each** carries **nine** marks.

12. Discuss the fundamental postulates of quantum mechanics and elaborate on their implications in understanding microscopic systems. Illustrate your answer with relevant examples and mathematical expressions.

13. Describe how Legendre polynomials, Rodrigues' formula and spherical harmonics are used in quantum mechanics to understand the rotation of particles.

14. Explain why time-independent perturbation theory is needed in quantum chemistry.

15. Explain the method for constructing spectroscopic term symbols for diatomic molecules. Illustrate with five examples. Discuss the significance of spectroscopic term symbols.

16. Derive the expressions for energy of atomic orbitals of H_2^+ using quantum mechanical treatment of MO theory. **(3×9=27)**

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