

QP CODE: 25047659



Reg No :

Name :

M.Sc DEGREE (CSS) EXAMINATION, NOVEMBER 2025
Third Semester
M Sc Industrial Chemistry
Core Course - CH060301 - THEORETICAL CHEMISTRY - II
2020 ADMISSION ONWARDS
726168BB

Time: 3 Hours

Weightage: 30

Part A (Short Answer Questions)

Answer any **eight** questions.

Weight 1 each.

1. What do you understand by self-consistent potential?
2. What atomic terms are possible for the electron configuration: ns^1np^1 ? Identify the lowest energy term.
3. Write down the form of the Hartree potential for the interaction between the 2nd and 4th electron in a ten-electron system.
4. Explain Roothaan's concept of basis functions.
5. Show that $c_1 = c_2$ in the ground-state Heitler-London wavefunction of H_2 .
6. Use molecular orbital theory to explain why the dissociation energy of N_2 is greater than that of N_2^+ , but the dissociation energy of O_2^+ is greater than that of O_2 .
7. Derive the reduction formula for reducing a reducible representation in to an irreducible one.
8. State and explain the great orthogonality theorem.
9. Why are electronic transitions known as electric dipole transitions?
10. In terms of the Hartree theory, determine the electron energies of the outermost shell ($n=3$) for the argon atom.

(8×1=8 weightage)

Part B (Short Essay/Problems)

Answer any **six** questions.

Weight 2 each.

11. Obtain total wavefunction for the ground state of helium atom from the spatial and spin functions.
12. Write briefly on semi empirical methods.
13. Construct the three normalized sp^2 hybrid orbitals and specify their directional properties.





14. Set up the secular determinant for butadiene molecule in the Hückel approximation and determine the energies of the HMOs and the delocalization energy.
15. Derive a general expression for the matrix form of rotational operation on the basis of (x,y,z).
16. Construct the matrices for each of the elements in C_{2v} and verify the group theoretical rules using the matrices.
17. Describe the selection rules for Raman spectroscopy.
18. How are the number of Raman active vibrations identified using group theory? Explain.

(6×2=12 weightage)

Part C (Essay Type Questions)

Answer any *two* questions.

Weight 5 each.

19. Discuss the perturbation (first-order correction) and variation (simple orbital approximation with one parameter) treatments on helium atom to obtain its ground state energy, and compare the methods in terms of the obtained ground-state energy values.
20. Compare and contrast the basic principles of different computational methods in chemistry and discuss the important applications of computational chemistry.
Solve the Schrodinger equation for the hydrogen molecule-ion, adopting the LCAO method, to obtain
21. expressions for the normalized bonding and antibonding MO wavefunctions. Pictorially illustrate these wavefunctions and their squares.
22. What do you mean by similarity transformation and classes in group theory? Illustrate using C_{3v} point groups.

(2×5=10 weightage)

