QP CODE: 25022632

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Reg No : .....

Name : .....

M.Sc DEGREE (CSS) SPECIAL REAPPEARANCE EXAMINATION, APRIL 2025

Third Semester

M.Sc INDUSTRIAL CHEMISTRY

CORE - CH060301 - THEORETICAL CHEMISTRY - II

2020 ADMISSION ONWARDS

90B7B27F

Time: 3 Hours Weightage: 30

Part A (Short Answer Questions)

*Answer any **eight** questions.*

*Weight **1** each.*

1. Construct the Hamiltonian for any two-electron system and explain the terms involved.
2. Two angular momenta with quantum numbers $j_1 = 3/2$ and $j_2 = 5/2$ are added together. What are the possible values of J for the resultant angular momentum states?
3. Write down the form of the Hartree potential for the interaction between the 2nd and 4th electron in a ten-electron system.
4. Describe the important features of the Gaussian orbitals.
5. Express the Hamiltonian operator for a hydrogen molecule in atomic units.
6. Adopting the LCAO-MO scheme, obtain the wavefunction for the BMO for a heteronuclear diatomic molecule AB, assuming that the electron on an average spends 90% of its time on nucleus A and 10% of its time on nucleus B.
7. Find the inverse of the matrix
$$A = \begin{bmatrix} -1 & 2 & 4 \\ 0 & 1 & 1 \\ 5 & 2 & 3 \end{bmatrix}$$
8. Is it possible to assign the symmetry of the p orbitals of oxygen in H_2O molecule? If so, what is their symmetry?
9. Discuss the principle of electronic spectroscopy.
10. Calculate the ionization energy of a helium atom by using the Hartree-Fock energy of the helium and the exact energy of a helium ion.

(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. Obtain the derivation of the Hohenberg theorem.

13. Construct the three normalized sp^2 hybrid orbitals and specify their directional properties.

14. Calculate the energy levels for benzene molecule using the HMO theory and find the wavelength of the light for the lowest energy transition.

15. Distinguish between D_nh and D_nd point groups.

16. Reduce the following total representation using the character table (Character table is given below).

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$
Γ	8	-1	4	0	2

Character Table for Td point group

	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	linear, rotations	quadratic
A_1	1	1	1	1	1		
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		z^2, x^2-y^2
T_1	3	0	-1	1	-1	(R_x,R_y,R_z)	
T_2	3	0	-1	-1	1	(x,y,z)	xy, xz, yz

17. Discuss the significance of transition moment integral and transition moment operator in vibrational spectroscopy.

18. How are the number of infrared active and Raman active vibrations are identified using group theory?

(6×2=12 weightage)

Part C (Essay Type Questions)

*Answer any **two** questions.*

*Weight **5** each.*

19. Elaborate on the Hartree-Fock method of the self-consistent field (HF-SCF) and evaluate the important results of this approximation to closed-shell multielectron systems.

20. Compare and contrast the basic principles of different computational methods in chemistry and discuss the important applications of computational chemistry.

21. Solve the Schrodinger equation for the hydrogen molecule-ion, adopting the LCAO method, to obtain expressions for the normalized bonding and antibonding MO wavefunctions. Pictorially illustrate the these wavefunctions and their squares.

22. Explain the construction and content of a character table and give its important applications. Construct the character table for C_2v point group.

(2×5=10 weightage)