M.Sc. DEGREE END SEMESTER EXAMINATION - MARCH 2024
SEMESTER 2 - CHEMISTRY / PHARMACEUTICAL CHEMISTRY
COURSE : **21P2CHET08 / 21P2CPHT08 - THEORETICAL AND COMPUTATIONAL CHEMISTRY**
(For Regular - 2023 Admission and Supplementary 2022/2021 Admissions)

Duration : Three Hours   Max. Weights: 30

PART A
Answer any 8 questions   Weight: 1

1.	State the mutual exclusion principle based on group theory?	(R, CO 1)
2.	Illustrate non-crossing rule with an example.	(A, CO 3)
3.	Explain the notation MP2/6-31G(d,p)//HF/6-31G(d,p).	(E, CO 4)
4.	What are pseudo potentials? Give example.	(U, CO 4)
5.	What is the significance of approximate methods in quantum mechanics?	(U, CO 2)
6.	What are the allowable spin functions for a two-electron system?	(U, CO 3)
7.	Write down the complete Schrödinger equation for the He atom and indicate the ground state energy of the Helium atom.	(A, CO 2)
8.	The vibrational mode of a molecule of C_{3v} point group belong to E symmetry. Can this vibrational mode be IR active? Justify.	(An, CO 1)
9.	What is the concept of correlation diagrams in chemical bonding?	(U, CO 3)
10.	Write the Z matrix of a linear triatomic molecule?	(A, CO 4)

(1 x 8 = 8)

PART B
Answer any 6 questions   Weights: 2

11.	Normally n $\rightarrow$ $\pi*$ electronic transitions in formaldehyde is spectroscopically forbidden. But a weak band corresponding to n $\rightarrow$ $\pi*$ transition is observed in uv-visible spectrum of formaldehyde. How?	(An, CO 1)
12.	What are double zeta and triple zeta basis sets? Which one is better and why? How many basis functions used to prepare the double and triple zeta basis sets of Ethane molecule?	(An, CO 4)
13.	Elaborate on different exchange and correlation functionals with examples.	(U, CO 4)
14.	What is configuration interaction? Derive the configuration interaction wave function for H_2 molecule.	(A, CO 3)
15.	Calculate the ground state energy of the Helium atom using the variation method.	(A, CO 2)
16.	What are the advantages of MO theory over VB theory?	(U, CO 3)
17.	Use a trail wave function x(a-x); 0 < x < a, and calculate the ground state energy of a particle in 1-D box.	(A, CO 2)
18.	Deduce the hybrid orbitals of B in BF_3 molecule using the applications of group theory.	(A, CO 1)

(2 x 6 = 12)

Answer any 2 questions   **Weights: 5**

19. Discuss the Molecular Orbital treatment of hetero-nuclear diatomic molecules LiH, NO and HF.   (U, CO 3)

20. Starting from internal coordinates as basis find out IRR's corresponding to ground state and excited states of vibrational transitions in water molecule. Predict whether these transitions are allowed or forbidden using symmetry selection rules based on triple direct products.   (A, CO 1)

21. State and explain Helmann – Feynmann theorem. Find the expectation value of 1/r for the hydrogen atoms.   (A, CO 2)

22. Predict the order of consumption of time for geometry optimization calculation of the following molecules with a DFT method and a minimal basis set. Water, Ammonia and Benzene. Justify your answer.Write the input for the calculations in all cases? Plot a rough graph for all output of geometry optimization.   (An, CO 4)

                                                                        (5 x 2 = 10)

OBE: Questions to Course Outcome Mapping

CO	Course Outcome Description	CL	Questions	Total Wt.
CO 1	Apply the principles of group theory in spectroscopy and hybridization.	A	1, 8, 11, 18, 20	11
CO 2	Explain the approximation methods in quantum mechanics.	U	5, 7, 15, 17, 21	11
CO 3	Describe the quantum mechanical explanation of chemical bonding.	U	2, 6, 9, 14, 16, 19	12
CO 4	Explain the methods of computational quantum chemistry.	U	3, 4, 10, 12, 13, 22	12

Cognitive Level (CL): Cr - CREATE; E - EVALUATE; An - ANALYZE; A - APPLY; U - UNDERSTAND; R - REMEMBER;