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B.Sc-M.Sc-Integrated program in Chemistry, V Semester
Backlog Examination 2023

Paper Name: Molecular modelling & Drug Design | **Paper Code: BCH-DSE02TH**
Time: 3 hours | **Maximum Marks: 75**

Note: This paper has 3 sections A, B, and C, Attempt all the three sections
Section A: *Answer all the questions;* ***Section B:*** *Answer any 2 out of 4;* ***Section C:*** *Answer all the questions, each question has an internal choice*

Abbreviations Used
CLO- Course Learning Outcome, PLO- Program learning Outcome, BTL- Bloom Taxonomy Level: BT level 1-Remember; BT level 2-Understand; BT level 3-Apply; BT level 4-Analyse; BT level 5-Evaluate, BT level 6-Create

Q.No		BTL	CLO	PLO
	SECTION A			
Attempt ***all*** questions		**(10 x 2 = 20) Marks**		
A 1.	What is the basic difference in underlying principle of INDO and MNDO methods?	1	1/2	1
A 2.	Why is the number of internal coordinates 6 less than the number of Cartesian coordinates required to define the structure of any molecule?	3	3/4	2
A 3.	DE abbreviate the term AMBER and TIPs.	1	1	1
A 4.	Allinger and co-workers developed a series of force fields to deal with molecular geometries and energies. Explain any one such force field. Also, explain one force field used in MM to simulate liquids.	2	2/3	2/3
A 5.	Construct a Z-matrix for acetone using appropriate labels.	6	4/5	2
A 6.	Calculate the PKa for para-chlorophenol using Hammett equation if the dissociation constant for phenol is 1068×10-10, provided σp= 0.68, ρ = 2.25, under identical conditions of solvent, temperature and pressure.	5	5	2/3
A 7.	Find the number of rat poison pills, each pill having 1.5 g of poison, that are needed to reach LD50 for a 85 kg man. Given that LD50= 317.8 mg/kg.	5	1	1
A 8.	Why are chemists rarely interested in finding and characterizing second-order and higher-order saddle points?	4	4	2
A 9.	Give and explain the order of polarizabilities of ethane, propane, butane.	3	2	1
A 10.	Should calculations from first principles (ab initio) necessarily be preferred to those which make some use of experimental data (semiempirical)?	4	4	2/3
	SECTION B			
Attempt ***any two*** out of four		**(2*10=20) Marks**		
B 1.	a. Can the Schrodinger wave equation (SWE) be solved exactly for a species with two protons and one electron? Why or why not?	1/2/3	1/2	3/4
	b. State the Antisymmetry principle.			
	c. Why is there a need to convert the SWE in terms of Cartesian coordinates to SWE in terms of polar coordinates?			
B 2.	a. How Verlet Algorithm used in molecular dynamics simulation different from Leap Frog Algorithm?	2/4	3/4	4/5
	b. What is the underlying principle of (Density functional theory) DFT?			
	c. c) Why should standard DFT methods be characterized as semiempirical and not as ab initio calculation procedures?			
B 3.	a. The SHM (Simple Huckel method) predicts the resonance energy of cyclopropenyl cation, anion and radical to be the same. Actually we expect the resonance energy to decrease as we add π electrons. Why should this be the case?	4/5	3/4	6/7
	b. What molecular feature cannot be obtained at all from simple Huckel method? And why?			

	c. How many carbons would a fully conjugated polyene have if its Fock matrix is 400 x 400?			
B 4.	Explain molecular docking and list the tools used in molecular docking. How protein to protein docking differ from protein –ligand docking?	2,1	2/3	1-3

SECTION C

Attempt ***all*** questions, each question has an ***Internal choice*** **(7 x 5 =35) Marks**

C 1.	Define the term "force field". Describe the terms of a typical molecular mechanics force field. You should write down the equation, explain the variables, and explain briefly what they represent.	1,2	2-4	3-5
	OR			
	Explain time-average and ensemble-average with the help of appropriate expressions. How are they related to each other? What is their significance in simulation studies?	1,2	2-4	3-5
C 2.	Calculate the π electron energy and delocalization energy of the cyclopropenyl radical, anion and cation using simple Hückel theory.	5	4,5	2,4,5
	OR			
	The ZPE of many molecules is greater than the energy needed to break a bond; for example, the ZPE of hexane is about 530 kJ mol^{-1} while the strength of a C – C or a C–H bond is only about 400 kJ mol^{-1}. Why then do such molecules not spontaneously decompose?	2	2,3	2,4,5
C 3.	A computational chemist carried out simulations of a molecule using a technique based on random numbers Name the technique used and explain the algorithm involved with it.	2	3,4	3-5
	OR			
	Classify the following as aromatic, nonaromatic or antiaromatic on the basis of HMO a. Cyclopentadienyl anion b. Cyclobutadiene c. Cyclopropenyl cation d. Cyclopentadienyl cation e. Cyclohepatrienyl cation	5	3,4	3,4
C 4.	Draw the potential energy diagram for all the conformers of ethane.	6	1,3,4	3,4
	OR			
	Find the number of bond stretching and angle bending terms in propane. Explain the origin of these terms with the help of its structure.	6	1,3,4	3,4
C 5.	Write down simple Hartree- Fock matrices for butadiene and cyclobutadiene	3	3-5	5-6
	OR			
	How is hydrophobicity and hydrophilicity of a molecule accounted for in QSAR analysis? Explain with the help of at least one descriptor of each	2	3-5	5-6
C 6.	Two methods that are generally used for the optimization of molecular geometries are the 'Steepest Descent' and 'Newton- Raphson' method. Briefly outline the advantages and disadvantages of these two techniques.	1	2,3	5-7
	OR			
	The occupied Hückel π molecular orbitals for C2 and C3 of 1,3- butadiene can be written as: $\Psi 2 = 0.371\varphi 1 + 0.602\varphi 2 + 0.602\varphi 3 + 0.371\varphi 4$ $\Psi 3 = 0.602\varphi 1 + 0.371\varphi 2 - 0.371\varphi 3 - 0.602\varphi 4$ Calculate the bond orders between C2 and C3 carbon atoms and atomic charges on these two-carbon atom.	5	3,4	5-7
C 7.	What do you understand by term basis set. Explain each term in 6-311G** basis set.	1	2/3	3-5
	OR			
	Draw and discuss the potential energy diagrams of cyclohexane as a function of C-C-C-C torsion angle.	6	4/5	3-5

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