ARSD College, University of Delhi

Model Course Handout/Lesson Plan

Course Name : B.Sc. (H) Chemistry						
Semester	**Course Code**	**Course Title**	**Lecture (L)**	**Tutorial (T)**	**Practical (P)**	**Credit (C)**
VI	32177905	Molecular Modelling and Drug Design	-	NA	60	2
Teacher/Instructor(s)		**Dr. Neeta Azad**				
Session		**2021-22**				

Course Objective:

Objective of this course is to make students learn the theoretical background of principles of computational techniques in molecular modelling, evaluation and applications of different methods for various molecular systems, energy minimization techniques, analysis of Mulliken Charge & ESP Plots and elementary idea of drug design. **Course Learning Outcomes:**

Learning Outcomes: By the end of this course, students will be able to:
• Understand theoretical background of computational techniques and selective application to various molecular systems.
• Learn Energy minimization methods through use of different force fields.
• Learn ESP Plots by suitable soft wares, electron rich and electron deficient sites, • Compare computational and experimental results and explain deviations.
• Carry out Molecular dynamics (MD) and Monte Carlo (MC) simulations on several molecules and polymers.
• Learn QSAR properties and their role in molecular modelling, cheminformatics and drug discovery.
• Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.

Details of the Lab Course		
Session	**Name of Experiment**	**Contact Hours**
1	Plotting a 3D graph depicting a saddle point in a spreadsheet software	4
2	2. Determine the enthalpy of isomerization of cis and trans 2-butene. 3. Determine the heat of hydrogenation of ethylene.	4
3	Compare the optimized C-C bond lengths and Wiberg bond orders in ethane, ethene, ethyne and benzene using PM3. Is there any relationship between the bond lengths and bond orders? Visualize the highest occupied and lowest unoccupied molecular orbitals of ethane, ethene, ethyne, benzene and pyridine.	4
4	Perform a conformational analysis of butane.	4

5	Study the kinetics of iodination of propanone in acidic medium	4
6	Determine the amount of iron present in a sample using 1, 10-phenathroline	4
7	Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine by comparison of their Mulliken charges and ESP maps.	4
8	Compare the gas phase basicities of the methylamines by comparing the enthalpies of the given equations.	4
9	Arrange 1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3- dimethyl-2-butene in order of increasing stability.	4
10	Compare the optimized bond angles H2O, H2S, H2Se using PM3.	4
11	Compare the HAH bond angles for the second row hydrides (BeH2, CH4, NH3, H2O) and compare with the results from qualitative MO theory.	4
12	(a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2- propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, respectively)	4
13	Predict the aromaticity of thiophene with respect to benzene by comparing the enthalpies of the given reactions. Docking of Sulfonamide-type D-Glu inhibitor into MurD active site using Argus lab.	**4**

Suggested Books:

Sl. No.	Name of Authors/Books/Publishers	Year of Publication/Reprint
1.	Lewars, E. G. (2011),Computational Chemistry, Springer (India) Pvt. Ltd. Chapter 1 & 2.	2011
2.	Engel, T.; Reid, P.(2012),Physical Chemistry, Prentice-Hall. Chapter 26.	2012
3.	Hinchliff, components of molecular modelling	2005
Mode of Evaluation	Internal Assessment / End Semester Exam	

Evaluation Scheme:

No.	Component	Duration	Marks
1.	Internal Assessment		25
	• Quiz/Viva		
	• Observation & Record		
	• Attendance		
	• Model Exam		
2.	End Semester Examination	4 hr	50