Lecture Plan

Name of the college: Government College of Arts, Science and Commerce, Sanquelim- Goa

Name of Faculty: Dr. Amarja Prashant Naik	**Subject: Chemistry (Skill)**	
Paper code: CHC-241 Mathematical Aspects and Computers in Chemistry	**Program: SY BSc**	**Division: NA**
Academic year: 2024-2025	**Semester: III**	**Total Lectures: 15**

Course Objectives:

1. To apply theoretical knowledge for plotting graphs.
2. To understand the use of computers for calculations and graphical representations.

Expected Course Outcome:

To plot various mathematical functions.
2. To solve numerical problems in chemistry.
3. To apply computer software's for data analysis.
4. To explain the types of orbitals and their shapes.
5. To identify order of the reaction by graphical method.
6. To solve numericals from the given data.

Student Learning Outcome:

1. Solving numerical based on differential and partial differential equation, maxima and minima.
2. Determination of mean, median and standard deviation of given data.

Month	Lecture From	Lecture To	No. of lectures allotted	Topic, Subtopic to be covered	Exercise/ Assignment	ICT Tools	References
June	28/06/2024	29/06/2024	Nil	Nil	Exercise	Google Classroom	1. A. Bahl and G.D. Tuli, Essentials of Physical Chemistry, S. Chand Publication, 2019**,** New Delhi, 26thedition. 2. Puri, Sharma and Pathania, Principles of Physical Chemistry, Vishal Publishing Company, 2018, New Delhi, 1stedition. 3. N. Joshi, S.G. Chitale, G. Venkat, S.R. Rege, Statistical techniques, Sheth Publishers, 2010, Mumbai. 4. E. Joseph Billo, Excel for Scientists
July	04/07/2024	04/07/2024	01	Numerical problems in logarithmic functions.	Exercise	Google Classroom	
	11/07/2024	11/07/2024	01	Obtain Mean, Median, Standard deviation from the given data.	Exercise	Google Classroom	
	15/07/2024	20/07/2024	01	Introduction to chemical knineticsTo solve and plot the integrated rate law equations for a. Zeroth order	Exercise	Google Classroom	
	22/07/2024	27/07/2024	01	To solve and plot the integrated rate law equations for b. First order c. Second order	Exercise	Google Classroom	
	29/07/2024	03/08/2024	01	To plot a function and its derivative using Henderson-Hasselbalch equation.	Exercise	Google Classroom	
August	5/08/2024	10/08/2024	01	Problem solving on differentiation	Exercise	Google Classroom	
	12/08/2024	17/08/2024	01	Partial differentiation.	Exercise	Google Classroom	

	19/08/2024	24/08/2024	01	To find the critical points in a function using Henderson-Hasselbalch equation and characterize them using a. Graphical method b. Derivative method	Exercise	Google Classroom	and Engineers: Numerical methods, Wiley-Interscience, 2007, New Jersey, 1stedition. 5. D. A. McQuarrie and J. D. Simon, Physical chemistry a molecular approach, Viva Books Pvt Ltd, 2012, Mumbai 1stedition. 6. R. G. Mortimer, Mathematics for Physical Chemistry, 4th edition, Academic Press, 2013, USA.
September	2/09/2024	7/09/2024	01	To find the critical points in a radial distribution function for 2s orbital and characterize them using a. Graphical method b. Derivative method	Exercise	Google Classroom	
	9/09/2024	14/09/2024	01	Plotting atomic orbitals and finding how shapes of orbitals emerge	Exercise	Google Classroom	
	16/09/2024	21/09/2024	01	Demonstration of MS excel for calculations and graphical representations for above experiments 1-6		Google Classroom	
	23/09/2024	28/09/2024	01	Demonstration of date on MS Excel	Exercise	Google Classroom	
October	30/09/2024	5/10/2024	01	Demonstration of use of Chemdraw/ Chemsketch for drawing chemical structures.	Exercise	Google Classroom	
	7/10/2024	12/10/2024	01	Demonstration for drawing chemical structure.	Exercise	Google Classroom	
	14/10/2024	22/10/2024	01	Graphical representation on Cartesian and spherical polar coordinate. Problem solving on maxima and minima.	Exercise	Google Classroom	

***Assessment Rubrics**

Component	Max Marks
ISA 1	5
ISA 2	5
Practical	---
Project	---
Semester End Exam	40