# **Department of Chemistry**

# M.Sc. Chemistry Curriculum and Syllabus

(Applicable to the students admitted from AY: 2023 onwards)



School of Engineering and Sciences SRM University *AP*, Andhra Pradesh

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Department Vision**

To emerge as a world-class research and teaching department which equips students with creative thinking and social skills to positively impact the scientific community, industry, and society by generating new knowledge and fostering innovations.

#### **Department Mission**

- 1. Deliver high-quality education at various levels to promote a deep understanding of chemical principles.
- 2. Contribute to scientific knowledge and industry through cutting-edge chemistry research.
- **3.** Create an atmosphere that encourages innovation and entrepreneurship, leading to the development of modern technologies and applications.

# **Program Educational Objectives (PEO)**

- 1. Equip the post-graduates with a strong understanding of the fundamental principles of chemical science, as well as practical applications in various contemporary sub-branches.
- 2. Train the post-graduates to design experiments and conduct independent research in laboratories.
- **3.** Prepare the postgraduates to apply critical thinking and problem-solving skills to solve complex research problems by making research-based presentations and carrying out research-based projects.

#### Mission of the Department to Program Educational Objectives (PEO) Mapping

	PEO 1	PEO 2	PEO 3
Mission Statement 1	3	1	2
Mission Statement 2	3	3	2
Mission Statement 3	2	1	3

#### **Program Specific Outcomes (PSO)**

- 1. We will have post-graduates who are thorough knowledge of the concepts of chemistry and be able apply chemical principles to solve problems in a variety of contexts.
- 2. We will have post-graduates who can design and conduct research in a systematic manner.
- **3.** We will have post-graduates who can demonstrate entrepreneurial and employability skills in academic and in R&D settings

#### Mapping Program Educational Objectives (PEO) to Program Learning Outcomes (PLO)

	Program Learning Outcomes (PLO)														
	POs												PSOs		
PEOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
PEO 1	3	3	1	3	2	1	1	1	3	1	3	2	3	3	1
PEO 2	1	2	1	3	3	3	3	3	2	1	2	2	3	2	1
PEO 3	3	3	3	1	1	1	1	1	2	1	3	3	2	3	3

Category Wise Credit			
Course Sub-Category	Sub-Category Credits	Category Credits	Learning Hours
Ability Enhancement Courses (AEC)		3	
University AEC	0		90
School AEC	3		
Value Added Courses (VAC)		3	
University VAC	1		90
School VAC	2		
Skill Enhancement Courses (SEC)		6	
School SEC	6		100
Department SEC	0		180
SEC Elective	0		
Foundation / Interdisciplinary courses (FIC)	100	9	
School FIC	9	N	270
Department FIC	0		
Core + Core Elective including Specialization (CC)	105 10 1	42	
Core	30		1260
Core Elective (Inc Specialization)	12	14	
Minor (MC) + Open Elective (OE)	0	0	0
Research / Design / Internship/ Project (RDIP)		19	
Internship / Design Project / Startup / NGO	0		570
Internship / Research / Thesis	19		-
Total		82	2460

Semester wise Course Credit Distribution Under	r Va	riou	s Cat	egor	ies	
Category			Se	meste	r	
Category	I	II	III	IV	Total	%
Ability Enhancement Courses - AEC	2	0	1	0	3	4
Value Added Courses - VAC	0	3	0	0	3	4
Skill Enhancement Courses - SEC	3	3	0	0	6	7
Foundation / Interdisciplinary Courses - FIC	3	3	3	0	9	11
CC / SE / CE / TE / DE / HSS	15	15	12	0	42	51
Minor / Open Elective - OE	0	0	0	0	0	0
(Research/ Design/ Industrial Practice/Project/Thesis/Internship) -RDIP	0	0	5	14	19	23
Grand Total	23	24	21	14	82	100

# Note: L-T/D-P/Pr and the class allocation is as follows.

a) Learning Hours : 30 learning hours are equal to 1 credit.

b) Lecture/Tutorial : 15 contact hours (60 minutes each) per semester are equal to 1 credit.
c) Discussion : 30 contact hours (60 minutes each) per semester are equal to 1 credit.
d) Practical : 30 contact hours (60 minutes each) per semester are equal to 1 credit.
e) Project : 30 project hours (60 minutes each) per semester are equal to 1 credit.

AP

				SEMESTER - I				
S. No	Category	Sub- Category	Course Code	Course Title	L	T/D	P/Pr	С
1	AEC	U AEC	AEC 501	Effective communication for impactful interview	2	0	0	2
2	VAC	U VAC	VAC 501	Community Engagement and Social Responsibility	0	0	1	1*
3	SEC	S SEC	SEC 501	Introduction to R and Python	1	1	1	3
4	FIC	S FIC	FIC 501	Data Science for Beginners	3	0	0	3
5	Core	CC	CHE 501	Structure Bonding and Reaction Mechanism	3	0	1	4
6	Core	CC	CHE 502	Chemistry of Main Group and Transition Metals	3	0	1	4
7	Core	CC	CHE 503	Thermodynamic Systems and States of Matter	3	0	1	4
8	Core	CC	CHE 504	Introduction to Quantum Chemistry: Concepts and Applications	3	0	0	3
				Semester Total				23
		7/	A .	o Treatment of the Control		•		

				SEMESTER - II						
S. No	Category	Sub- Category	Course Code	Course Title	L	T/D	P/Pr	С		
1	VAC	U VAC	VAC 502	Community Engagement and Social Responsibility	0	0	1	1		
2	VAC	S VAC	VAC 503	Entrepreneurial Mindset	2	0	0	2		
3	SEC	S SEC	SEC 105	Research Design and Methods	2	1	0	3		
4	FIC	S FIC	FIC 108	Design Thinking	3	0	0	3		
5	Core	CC	CHE 505	Organic reactions	3	0	1	4		
6	Core	CC	CHE 506	Solid - State Nanomaterials and Inorganic Photochemistry	3	0	1	4		
7	Core	CC	CHE 507	Reaction Kinetics and Electrochemistry	3	0	1	4		
8	Core	CC	CHE 508	Analytical Chemistry - Principles, Instrumentation and Applications	3	0	0	3		
	Semester Total 19 1 4 24									

				SEMESTER - III				
S. No	Category	Sub- Category	Course Code	Course Title	L	T/D	P/Pr	C
1	AEC	S AEC	AEC 503	Research Seminar	0	0	1	1
2	FIC	S FIC	FIC 124	Psychology for Everyday Living	3	0	0	3
3	Elective	CE		Core Elective	3	0	1	4
4	Elective	CE		Core Elective	3	0	1	4
5	Elective	CE		Core Elective	3	0	1	4
6	RDIP	RDIP	CHE 510	Project - I	0	0	3	3
7	RDIP	RDIP	CHE 509	Summer Internship	0	0	2	2
	1		No. of Street, or other Persons and the Street, or other Persons a	Semester Total	12	0	9	21

			47	100	Post Call							
SEMESTER - IV												
S. No	Category	Sub- Category	Course Code		Course Title	L	T/D	P/Pr	C			
1	RDIP	RDIP	CHE 511	Project - II	ASTAN S	0	0	14	14			
			41	E W	Semester Total	0	0	14	14			
			Physical Property of the Party	// A I								

	Specialization Elective (Industrial)												
S. No	Category	Sub- Category	Course Code	Course Title	L	T/D	P/Pr	C					
1	Elective	SE	CHE 631	Instrumental Methods of Analysis	3	0	1	4					
2	Elective	SE	CHE 632	Industrial Chemistry	3	0	1	4					
3	Elective	SE	CHE 633	Environmental and Electroanalytical Techniques	3	0	1	4					

	Specialization Elective (Computational)											
S. No	Category	Sub- Category	Course Code	Course Title	L	T/D	P/Pr	C				
1	Elective	SE	CHE 634	Advanced Quantum Chemistry	4	0	0	4				
2	Elective	SE	CHE 635	Molecular Modelling and Simulations	2	0	2	4				
3	Elective	SE	CHE 636	Data Science and Machine Learning in Chemistry	2	0	2	4				
			200									

	Specialization Elective (Organic Chemistry)												
S. No	Category	Sub- Category	Course Code	Course Title	L	T/D	P/Pr	C					
1	Elective	SE	CHE 637	Advanced Organic Chemistry (Organometallics)	4	0	0	4					
2	Elective	SE	CHE 638	Organic Synthesis and Stereochemistry	3	0	1	4					
3	Elective	SE	CHE 639	Organic Spectroscopy	4	0	0	4					

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Effective Communication for Impactful Interviews**

Course Code	AEC 501	Course Category	AEC		L 2	T 0	<b>P</b> 0	<b>C</b> 2
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)				
Course Offering Department	Literature & Languages	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

> This course equips the learners for successful job hunting by fostering a comprehensive understanding and application of the KASB Model in professional communication, enhancing verbal communication skills to excel in interviews, mastering non-verbal communication for a positive first impression, and guiding them in customizing application materials to stand out from the crowd.

#### **Course Outcomes / Course Learning Outcomes (CLOs)**

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Identify key components of verbal and non-verbal communication and their significance in the interview process.	1	50%	50%
Outcome 2	Develop the skill to articulate thoughts clearly and concisely, using effective interview responses.	2	65%	60%
Outcome 3	Exhibit proficiency in the art of storytelling as a communication tool in interviews.	2	65%	60%
Outcome 4	Create personalized and tailored resumes, cover letters, and SOPs to align with specific job or educational opportunities.	3	70%	60%

					Pro	ogram L	earning	g Outco	mes (PL	<b>O</b> )					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	1	1	1	3	1		3	2	3	2	3			
Outcome 2	2	3	3	1	3	1		3	2	3	3	3			
Outcome 3	2	1	3	2	3	2		3	2	3	3	3			
Outcome 4	2	3	3	2	3	3		3	2	3	3	3			
Average	2	2	2.5	1.5	3	1.75		3	2	3	2.75	3			

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used
Unit 1	Introduction: An Overview	9		
	Types of interview	2	1	4
	Communication as a strategy	3	1	4,5
	The KASB Model	4	1	4
Unit 2	Articulation Skills	8		
	The 3 Vs of Communication	2	1	1,4
	Tone, Pitch and Modulation	4	2	4,5
	Practice session	4	2	
Unit 3	Story Telling	6		
	The Importance of story telling	2	3	6
	Creating stories around' Tell Me About Yourself'	2	3	6,7
	Group Discussion	2	3	8
Unit 4	Written Strategy	10		
	Resume	4	4	2,4
	Cover Letter	4	4	2,4
	SOP	2	4	2,4
Unit 5	Mock Interview Sessions	12	1,2,3.4	
	Total Hours	45		

#### **Learning Assessment**

Bloom's Le	vel of Cognitive Task	Cor	50%)	Interview Handling		
Dioom's Lc	ver or cognitive rask	CLA-1 15%	Mid-1	CLA-2 15%	CLA-3 15%	Process (40%)
Level 1	Remember	100%		30%	50%	20%
Level 1	Understand	10070		3070	3070	2070
Level 2	Apply			70%	50%	50%
Level 2	Analyse			7070	3070	3070
Level 3	Evaluate					30%
Level 3	Create					3070
	Total		100%	100%	100%	100%

#### **Recommended Resources**

- 1. Cialdini, R. B. (2021). Influence: The psychology of persuasion (Revised edition). Harper Perennial Modern Classics.
- 2. Dipboye, R. L., & Cole, C. H. (2019). Secrets of a hiring manager: How to land any job and win over any boss. HarperBusiness.
- 3. LaFare, M. (2013). Veritas: A game of lies. Penguin Books.
- 4. Mock, P., & Turner, L. (2019). The interview for dummies (6th edition). John Wiley & Sons.
- 5. Stone, D. D., Patton, B., & Heen, S. (2000). Difficult conversations: How to discuss what matters most (2nd edition). Viking.
- 6. Dolan, G. (2019). Storytelling for job interviews: How to use stories, nail an interview and land your dream job. BookBaby.
- 7. Pink, S. (2014). To sell is human: The science of persuasion. Penguin Books.
- 8. Lewis, V. J. (2018). Group discussion: A practical guide (7th edition). Kogan Page

#### **Other Resources**

1. -

#### **Course Designers**

1. -

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### Introduction to R and Python

Course Code	SEC 501	Course Category		L	T	P	C
Course Coue	SEC 301	Course Category		1	1	1	3
Pre-Requisite Course(s)		Co-Requisite Course(s)	Progressive Course(s)				
Course Offering Department	Mathematics	Professional / Licensing Standards					

#### **Course Objectives / Course Learning Rationales (CLRs)**

- In Python, identify and describe essential elements such as syntax, keywords, variables, indentation, data types, lists, tuples, sets, dictionaries, operators, control statements, and loops.
- Understand the significance of built-in functions, user input-output, matrix computations, linear equations, and graphing curves and surfaces using Matplotlib and file handling in Python.
- Implement R programming fundamentals, including objects, vectors, matrices, arrays, data manipulation techniques (subsetting, filtering, merging), and data frames, and create visualisations using ggplot2 in R.
- > Synthesise knowledge from Python and R to perform comprehensive data analysis and create reports that include descriptive statistics, linear regression, hypothesis testing, and time series forecasting.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Demonstrate an understanding of Python programming fundamentals, including syntax, keywords, variables, data types, lists, tuples, sets, dictionaries, operators, and control statements.	2	80	70
Outcome 2	Grasp core programming concepts by comprehending the role of built-in functions, user input-output, file handling and graphing curves and surfaces using Matplotlib in Python.	3	75	70
Outcome 3	Apply programming skills in R by effectively using objects, vectors, matrices, arrays, and data frames, and will demonstrate the practical application of data manipulation techniques, including sub-setting, filtering, and merging, and create visualizations using ggplot2 in R.	4	75	70
Outcome 4	Integrate Python and R knowledge to perform sophisticated data analysis that incorporates descriptive statistics, linear regression, hypothesis testing, and time series forecasting, showcasing a synthesis of programming skills across both languages.	4	75	70
Outcome 5	Demonstrate an understanding of Python programming fundamentals, including syntax, keywords, variables, data types, lists, tuples, sets, dictionaries, operators, and control statements.	2	80	70

															1	
		Program Learning Outcomes (PLO)														
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3	
Outcome 1	3	3	3	3					1			2	3	1	2	
Outcome 2	3	3	3	2	1				2			2	3	2	2	
Outcome 3	3	3	3	3	1				2			2	3	2	2	
Outcome 4	3	3	3	3	3				3			2	3	2	2	
Outcome 5	3	2	3	3	3				2			3	2	2	2	
Average	3	3	3	3	2				2			2	3	2	2	

# **Course Unitization Plan Theory**

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used
		6		
Unit 1	Introduction to data and its different types of scales.	3	1,2	1
	Summarising data, different types of descriptive statistics	3	1,2	1
		9		
	Introduction to Vectors, matrices	3	2,3	1
Unit 2	Recursive functions, Matrix computations and linear equations	3	2,3	1
	Solving system of Linear Equations. Consistency, transpose, determinants, inverses, trace,	3	2,3	1
		15		
	Basic principles of probability, Random variables.	2	3,4	2
	The Binomial, Normal and other popular distributions.	2	3,4	2
Unit 3	Inference for one or two samples means using the t-distribution, statistical power for comparing two groups	2	3,4	2
	Introduction to Correlation Analysis, Correlation coefficient for Categorical and Continuous data.	2	4	2
	Introduction to the logistics regression.	4	4	2
	Total Contact Hours		30	

# **Course Unitization Plan Lab**

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used
1	Write a program to demonstrate the use of Python syntax, keywords, and variables.	2	1	1
2	Create a program that uses indentation and comments to improve code readability.	2	1	1
3	Implement a program that showcases different data types in Python (int, float, string, Boolean).	2	1	1
4	Write a program that manipulates lists (e.g., sorting, appending, slicing).	2	1	1
5	Create a program that demonstrates using tuples and sets in Python.	2	2	1
6	Implement a dictionary to store and retrieve information.		2	1
7	Write a program that uses different operators in Python (+, -, *, /, //, %, **).	2	2	1
8	Create a program that includes control statements (if-else, nested if-else, switch-case) and loops (for, while).	2	2	1
9	Write a program to create and manipulate objects in R.	2	3	2
10	Implement a program that demonstrates using vectors and matrices in R.	2	3	2
11	Create a program that works with arrays and lists in R.	2	3	2
12	Write a program to handle missing data in a data frame.	2	3	2
13	Implement a program that reads and writes data to CSV or text files.	2	4	2
14	Create a program that performs data manipulation tasks (subsetting, filtering, merging) on a data frame.	2	4	2
15	Write a program that uses ggplot2 to create a plot in R.	2	3,4	2
	Total Contact Hours	30		

#### **Learning Assessment**

Dloom?a	Level of		(	Continuous	Learning .	Assessme	nts (60%	)		End Semester		
2100111 5	ive Task	CLA-1 20%		Mid-1	20%	CLA-	2 10%	CLA-	3 10%	Exam	(40%)	
Cogmit	ive Iusii	Th	Pr	Th	Pr	Th	Pr	Th	Pr	Th	Pr	
Laval 1	Remember	35%	40%	20%	20%	30%	15%	25%		20%	15%	
Level 1	Understand	35%	40%	20%	20%	30%	15%	25%		20%	15%	
Level 2	Apply	15%	10%	20%	20%	20%	20%	25%		25%	25%	
Level 2	Analyse	15%	10%	20%	20%	20%	20%	25%		25%	25%	
Level 3	Evaluate			10%	10%		15%			5%	10%	
Level 3	Create			10%	10%		15%			5%	10%	
To	Total		100%	100%	100%	100%	100%	100%	100%	100%	100%	

#### **Recommended Resources**

- 1. Guido van Rossum and the Python development team Python Tutorial Release 3.7.0.
- 2. W. N. Venables, D. M. Smith and the R Core Team, An Introduction to R
- 3. R in Action, Robert L. Kabacoff, Second Edition, Paperback, Dreamtech Press
- 4. A Beginner's Guide to R, Alain F. Zuur, Elena N. Ieno, Erik H. W. G. Meesters, Springer New York.
- 5. The Absolute Beginner's Guide to Python Programming, A Step-by-Step Guide with Examples and Lab Exercises, Kevin Wilson, Apress Berkeley, CA
- 6. Python Programming Fundamentals, Kent D. Lee, Springer London

#### **Other Resources**

#### **Course Designers**

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Data Science for Beginners**

Course Code	FIC 501	Course Category	FIC		<u>L</u>	<b>T</b>	<b>P</b> 0	<b>C</b> 3
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)		I		
Course Offering Department	Mathematics	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- After completing this course, students will fully grasp different data types and representations. Also, they have a basic understanding of descriptive statistics for the given datasets.
- > Students will understand linear algebra concepts well, enabling them to manipulate vectors and matrices and solve linear systems efficiently.
- > Upon completing the course, students will be proficient in applying probability principles and conducting statistical inference, including point estimation, confidence intervals, and hypothesis testing for various scenarios.
- Equip the Students with the knowledge and skills necessary to apply regression techniques for modelling numerical outcomes and logistic regression for classification tasks, both for numerical and categorical data

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Explain the different types of data and graphical representation of data.	2	70%	65%
Outcome 2	Compute descriptive statistics for any given dataset, such as different measures of central tendency and variation in the data.	3	70%	65%
Outcome 3	Interpret different definitions of probability and the different types of random variables. Illustrate the application of the central limit theorem. Draw inferences about the population parameters.	3	70%	65%
Outcome 4	Describe regression analysis using the concept of matrices and the solution of the system of equations.	2	70%	65%

					Pro	ogram L	earning	g Outco	mes (PL	O)					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	3	2	2	1	-	-	-	-	-	-	-	-	-	-
Outcome 2	1	2	2	2	1	-	-	ı	-	-	-	-	-	-	-
Outcome 3	2	2	1	1	1	-	-	-	-	ı	-	-	-	-	-
Outcome 4	2	2	2	1	2	-	-	-	-	-	-	-	-	-	-
Average	2	2	2	1	1	-	-	-	-	-	-	-	-	-	-

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used
	Introduction to data, data structures	1	1	1,3
	Variables and Basic data collection techniques	1	1	1,3
Unit 1	Summarizing data, Descriptive Statistics	2	1,2	1,3
	Graphics, Histograms, and Popular database software.	2	1,2	1,3
	A glimpse inside the mind of a data scientist	1	1	1,3
	Discussion and Tutorial	2	1	1,3
	Introduction to Vectors, matrices and linear systems,	1	4	1,2
	Solving systems of Linear Equations. Consistency, transpose, determinants, inverses, trace,	1	4	2
	Vector space, subspaces,	1	4	2
Unit 2	Independence of vectors, basis and dimension, dot product, inner product, Eigenvalues and Eigenvectors.	2	4	1,2
	Dot product, inner product and its application	2	4	2
	Eigenvalues and Eigenvectors.	1	4	2
	Discussion on Practical applications of vector spaces and Matrices.	2	2,4	1,2,4
	Basic principles of probability, Different approaches for defining the probability.	1	3	1,3
	Random variables, Types of random Variables and their distribution.	1	3	1,3
	The Binomial, Normal and other popular distributions.	1	3	1,3
	Foundations for Statistical inference, Point and Interval Estimates.	1	3	1,3
	Discussion and Tutorial	1		1,3
Unit 3	General ideas for statistical inference in estimating the population proportion, Central Limit theorem and its application.	2	3	1,3
	Inference for proportions and tables using the normal and chi-square distributions.	1	3	1,3
	Inference for categorical data,	1	3	1,3
	Inference for one or two samples means using the t-distribution, statistical power for comparing two groups	2	3	1,3
	Tutorial	1	3	1,3,4
	Introduction to Correlation Analysis, Correlation coefficient for Categorical and Continuous data.	2	4	1,4
	Introduction to linear regression, Scatter Plot.	1	4	1,4
	Regression for a numerical outcome with one predictor Variable,	2	4	1,4
Unit 4	Brief Discussion about Model Adequacy, accuracy, and validation.	2	4	1,3,4
	Regression for numerical and categorical data using many Predictors,	1	4	1,4
	Logistic regression for classification,	2	4	1,4
	Tutorial and Doubt Clearing Session	1	4	1,4
Unit 5	Practical applications of Regression and Classification in prediction and forecasting	2	4	1,4
	Tutorial	1	4	1,4

#### **Learning Assessment**

Dloom's Lo	vel of Cognitive Task	Co	End Semester			
Diooni 8 Le	ver of Cognitive Task	CLA-1 10%	Mid-1 20%	CLA-2 10%	CLA-3 10%	Exam (50%)
Level 1	Remember	30%	25%	30%	20%	20%
Level 1	Understand	30%	25%	30%	20%	30%
I amal 2	Apply	20%	25%	20%	30%	25%
Level 2	Analyse	20%	25%	20%	30%	25%
Level 3	Evaluate					
Level 3	Create					
	Total	100%	100%	100%	100%	100%

#### **Recommended Resources**

- 1. Openintro Statistics (4th edition), Diez David M Christopher D Barr and Çetinkaya, 2019.
- 2. Linear Algebra and its Applications, Gilbert Strang, Publisher Cengage India Private Limited, 2005.
- 3. First Course in Probability (11th Edition), Sheldon Ross, Academic Press, 2014.

#### **Other Resources**

1. -

#### **Course Designers**

1. -

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Chemistry of Main Group and Transition Metals**

Course Code	CHE 502	Course Cotegowy	Inougov	sia Chamiatur	L	T	P	C
Course Code	CHE 302	Course Category	morgai	nic Chemistry	3	0	1	4
Pre-Requisite Course(s)	NILL	Co-Requisite Course(s)	NILL	Progressive Course(s)	·			
Course Offering Department	Chemistry	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- > The objective of the course is to make students understand theories of chemical bonding, reaction mechanisms, and magnetic properties of main group & transition elements
- > The course enables students to learn structure and bonding aspects of inorganic and organometallic compounds derived using main group elements
- > Additionally, students develop theoretical and practical knowledge by making complex compounds in the laboratory and characterise them using different instrumental techniques

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Gain knowledge on various theories of Acids & Bases and remember different concepts. Able to recognise and classify different Acids/Bases	1, 2	90%	85%
Outcome 2	Connecting the theories to explain how a molecule forms a specific geometry. Understand Crystal field theory (CFT) for different complexes. Find various limitations of CFT	2, 3	90%	80%
Outcome 3	Identify various types of magnetic solid by remembering Curie and other laws. Understanding of different free electron theories relate them to observed material properties	2,3	90%	80%
Outcome 4	Categorise various chemical reactions based on reaction mechanisms involved and employ the same to understand their stability and formation of various complex compounds. Compare different electron transfer mechanisms involved in complexes, such as inner vs. outer sphere electron transfer	2, 3, 4	85%	75%
Outcome 5	Extend the learned knowledge in understanding the structure, bonding, and reactivity of Boran, Silicon, Phosphorus, Sulfur, and halogen compounds	2, 3	85%	75%
Outcome 6	Adapt classroom theory in making different metal complexes and evaluate their physical properties like UV-Visible absorption, IR, X-ray diffraction, NMR etc	5, 6	90%	80%

# Course Articulation Matrix (CLO) to Program Learning Outcomes (PLO)

					Pr	ogram L	earning	g Outco	mes (PI	LO)					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self Directed and Life long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	2	1	1						2	1	2	2		
Outcome 2	2	3	3	1	1				1	2	2	2	2	1	
Outcome 3	3	3	3	2	1				1	2	2	2	2	2	
Outcome 4	2	2	2	2	1				1	2	2	2	2		
Outcome 5	2	2	2	2	1				1	2	2	2	2		
Outcome 6	3	3	3	2	3	2			2	2	1	2		2	2
Average	2	3	2	2	1				1	2	2	2	2	1	

# **Course Unitization Plan - Theory**

ourse U	<u>nitization Plan - Theory</u>			
Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
	Acid-Base Concept – Bronsted concept of Acid & Bases – Lewis concept – Classification of Lewis acids – acid/base reaction	1	1	1, 2, 3
II	Solvolysis and formation of coordination compounds – Molecular structure and bonding behaviour	1	1	1, 2, 3
Unit No.	Lux-Flood concept of acids and bases. The strength of oxyacids  - Pauling's rule - Acidity of cations in aqueous solution.	2	1	1, 2, 3
1	Hard and Soft Acids and Bases (HASB) – Person's principle – Applications of HASB theory.	2	1	1, 2, 3
	Acid-base titrations, Acid-base properties of salt hydrolysis - Polyprotic Acids.	1	1	1, 2, 3
	Transition Metal Chemistry (Bonding) - Structure and bonding in metal complexes – geometry, coordination number, thermodynamic stability.	1	2	1, 2, 3
	Stability constants & determination and factors influencing stability constants.	1	2	1, 2, 3
	Irving – William series, chelate and macrocyclic effect.	1	2	1, 2, 3
Unit No.	Theories of bonding - Crystal field theory (CFT) - Crystal field splitting in octahedral, tetrahedral, and square planar complexes.	2	2	1, 2, 3
2	Crystal field stabilisation energy and its applications in stereochemistry.	1	2	1, 2, 3
	Stability of oxidation states, trends in heats of hydration & lattice energy and colour & magnetic properties.	1	2	1, 2, 3
	Weak and strong fields – Pairing energy – Factors affecting the magnitude of crystal field splitting.	1	2	1, 2, 3
	Jahn – Teller theorem – Limitations of CFT. Molecular orbital theory of selected octahedral and tetrahedral complexes.	2	2	1, 2, 3
Unit	Transition Metal Chemistry (Properties & Electronic spectra) Magnetic properties – Dia, para, Ferro and Antiferro magnetism.	2	3	3, 4
No.	Curie's law – Spin/transition isomerism	1	3	3, 4
3	UV-Vis, charge transfer, colours, intensities and origin of transitions, interpretation	2	3	3, 4

	Term symbols and splitting of terms in free atoms, selection rules for electronic transitions	2	3	3, 4
	Russell-Sanders coupling; L-S coupling Orgel and Tanabe- Sugano diagram for d1 to d9 ions, calculation of Dq, Nephelauxetic ratio.	3	3	3, 4
Unit	Transition Metal Chemistry (Reaction mechanism) - Substitution reactions in octahedral and square planar complexes.	2	4	2, 3
No.	Trans effect and its influence lability and water exchange.	2	4	2, 3
4	Base hydrolysis stereochemistry, inner and outer sphere electron transfer mechanism.	2	4	2, 3
	The limiting rate law – Theoretical treatment of electron transfer.	2	4	2, 3
Unit	Chemistry of the main group elements – (Condensed syllabus for s, p – block elements) Structure, bonding and reactivity (synthesis) of Boran.	2	5	2, 3, 4
	Structure, bonding and reactivity (synthesis) of Silicon.	2	5	2, 3, 4
No. 5	Structure, bonding and reactivity (synthesis) of Phosphorus.	2	5	2, 3, 4
3	Structure, bonding and reactivity (synthesis) of Sulfur.	2	5	2, 3, 4
	Structure, bonding and reactivity (synthesis) of Halogens compounds.	2	5	2, 3, 4
	Total Contact Hours	45 Hours		

#### **Course Unitization Plan - Lab**

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	References Used
1.	Synthesis and analysis of tris(ethylene diamine)nickel(II) chloride 2-hydrate, [Ni(en)3]Cl2×2H2O	5	6	5
2.	Synthesis and analysis of zinc (II) (tris)thiourea sulfate, [Zn(SC(NH2)2)3OSO3]	5	6	5
3.	One Metal, Many Colors: Solvatochromism of Dirhodium Tetraacetate	5	6	5
4.	Synthesis and analysis of sodium percarbonate (SPC): An environment-friendly bleach in the detergent industry	5	6	5
5.	Synthesis and analysis of transition metal complexes of Cobalt (II)	5	6	5
6.	Synthesis and analysis of Optical Isomers of a Cobalt (III) compound. Synthesis and Characterisation of the following compounds.	5	6	5
	Total Contact Hours	30 Hours	•	•

#### **Learning Assessment**

			Continuous Learning Assessments (60%)								ster Exam
Bloom's l	Bloom's Level of Cognitive Task		CLA-1 (10%)		CLA-2 (20%)		CLA-3 (10%)		rm (20%)	(40%)	
			Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level 1	Remember	50%	40%	53%	40%	50%	40%	40%	40%	40%	
	Understand										40%
Level 2	Apply	50%	60%	47%	60%	30%	50%	40%	50%	40%	40%
Level 2	Analyse										
Level 3	Evaluate					20%	10%	20%	10%	20%	20%
Level 3	Create										
	Total	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%

#### **Recommended Resources**

- 1. J.E. Huheey, E.A. Keiter, R.L. Keiter and O.K. Mehdi, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Pearson, 2006.
- 2. J.D. Lee, Concise Inorganic Chemistry, 5th Edition, Blackwell Science, 2008.
- 3. D.F. Shriver, P.W. Atkins and Ch. Langford, Inorganic Chemistry, ELBS, Oxford University Press, 2000.
- 4. F. A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edition, Wiley, 2007.
- 5. Vogel's textbook of Macro and semi-micro qualitative inorganic analysis, Fifth edition, Longman publishers.

#### **Other Resources**

#### **Course Designers**

- 1. Internal (Institutional) Subject Matter Experts Prof. C.P Rao, Sr Professor, SRM University AP
- 2. and Dr. Pardha Saradhi Maram, Associate Professor, SRM University AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### Thermodynamic Systems and States of Matter

Course Code	CHE 503	Course Category	Core (Phys	v)	L	T	P	C	
Course Coue	CIIE 505	Course Category	core (rilys	,,	3	0	1	4	
Pre-Requisite Course(s)	NILL	Co-Requisite Course(s)		Progressive Course(s)					
Course Offering Department	Department of Chemistry	Professional / Licensing Standards							

#### Course Objectives / Course Learning Rationales (CLRs)

- > To distinguish the types of matters in various phases and can predict the effect of chemical potential and chemical equilibrium towards thermodynamic consideration of a system.
- > To understand the behaviour in liquid mixtures in both ideal and non-ideal mixtures and to learn the kinetic theory of gasses and solid states.
- > To gain knowledge on different kinds of quantitative and titrimetric analyses.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Understand phase behaviour and chemical equilibrium	2	80	70
Outcome 2	Apply thermodynamic principles to solutions	3	75	65
Outcome 3	Analyse the behaviour of ideal, real gases and solids	4	80	65
Outcome 4	Understand, apply, and remember the experimental techniques in physical chemistry	1,2,3	80	75

					Pro	ogram L	earning	g Outco	mes (PL	<b>(O</b> )					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	2	2	2	1	1	-	-	1	1	-	1	2	1	2
Outcome 2	3	2	2	2	1	1	-	-	1	1	-	1	2	1	2
Outcome 3	3	3	1	3	1	1	-	-	1	1	-	1	3	3	3
Outcome 4	2	3	3	3	1	1	-	-	1	1	-	1	3	2	3
Average	3	3	2	3	1	1	-	-	1	1	-	1	3	2	3

# **Course Unitization Plan - Theory**

Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
	Phase behaviour of one and two-component systems, Fundamental equations for open systems, Partial molar quantities	5	1	1,2
Unit No.	Chemical potential	2	1	1,2
1	Chemical equilibrium	3	1	1,2
	Ehrenfest classification of phase transitions	1	1	1,2
	Thermodynamics of ideal and non-ideal solutions	2	2	1,2
Unit No.	Liquid-liquid solutions, liquid-solid solutions, multicomponent systems	3	2	1,2
2	Excess thermodynamic properties	2	2	1,2
	Activity of ideal, regular, and ionic solutions	2	2	1,2
	Introduction: Concept of ensembles, partition functions and distributions, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions.	2	3	1,2,3
	Concept of pressure and temperature.	1	3	1,2,3
Unit No. 3	Maxwell's distribution of speeds. Kinetic energy distribution in one, two, and three dimensions, calculations of average, root mean square and most probable values in each case; calculation of the number of molecules having energy $\geq \epsilon$	3	3	1,2,3
_	Principle of the equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases.  Collision of gas molecules; collision diameter; collision number and mean free path; frequency of binary collisions (similar and different molecules); wall collision and rate of effusion. Viscosity of gases from kinetic theory of gas.	4	3	1,2,3
	Deviations from ideal gas behaviour, compressibility factor, Z, virial coefficient and its variation with pressure and temperature for different gases.	2	3	1,2,3
Unit No.	Causes of deviation from ideal behaviour. van der Waals equation of state, its derivation and application in explaining real gas behaviour	3	3	1,2,3
4	Intermolecular potential (Lennard-Jones, Hard-sphere and Square-well)	1	3	1,2,3
	Virial coefficients. Temperature dependence of the second virial coefficient.	2	3	1,2,3
Unit	Nature and different types of the solids including covalent, non- covalent ionic and metallic solids and their bonding, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups,	2	3	1,2,3
No. 5	Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. Glasses and liquid crystals.	2	3	1,3
	Band theory: metals, insulators, and semiconductors. Band gaps, doping, and devices.	2	3	1,3
	Fermi function, Fermi energy, free electron model and density of states	1	3	1,3
	Total Contact Hours	45		

#### Course Unitization Plan - Laboratory

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	References Used
1.	Determination of hardness of water by EDTA method	4	4	1,2
2.	Kinetics of Iodine Clock Reaction	4	4	1,2
3.	Adsorption of Acetic Acid on Charcoal	4	4	1,2
4.	Fluorescence Study of Critical Micellar Concentration	4	4	1,2
5.	Determination of the Change in Dipole Moment on Electronic Excitation	4	4	1,2
6.	Study of an Oscillating Reaction	4	4	1,2
7.	Spectrophotometric Determination of pKa	6	4	1,2

#### <u>Learning Assessment - Theory & Laboratory</u>

			Coi	ntinuous	Learning	g Assessr	nents (60	1%)		End Semester		
Bloom's Level of Cognitive Task		CLA-1 (10%)		CLA-2 (20%)		CLA-3 (10%)		Mid Term (20%)		Exam (40%)		
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac	
Level 1	Remember	50%	40%	53%	40%	50%	40%	40%	40%	40%		
Level 1	Understand										40%	
Level 2	Apply	50%	60%	47%	60%	30%	50%	40%	50%	40%	40%	
Level 2	Analyse											
Laval 2	Evaluate					20%	10%	20%	10%	20%	20%	
Level 3	Create											
	Total	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	

#### **Recommended Resources**

- 1. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford 2014
- 2. D. A. McQuarrie and J. D. Simon, Molecular Thermodynamics, University Science Books, California 2004
- 3. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press, Oxford, 2007
- 4. Viswanathan, and P. S. Raghavan, Practical Physical Chemistry, Viva Books, 2010
- 5. M. Halpern, and G. C. McBane, Experimental Physical Chemistry: A Laboratory Text Book, 3rd Edition, W. H. Freeman, 2006

#### **Additional Readings**

- 6. D. A. McQuarrie, Statistical Mechanics, University Science Books, California 2005
- 7. B. Widom, Statistical Mechanics A Concise Introduction for Chemists, Cambridge, University Press, 2002
- 8. Lab 2. http://www.kbcc.cuny.edu/academicDepartments/PHYSCI/PL/chm12/Documents/CHM1 2 Experiment 5 Kinetics.pdf
- 9. Lab 3. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford 2014.
- 10. Lab 4. a. Photochemistry in Micro-heterogeneous Systems, K. Kalyanasundaram, b. Any other book on fluorescence spectroscopy or photochemistry
- 11. Lab 5. M. Ravi, A. Samanta, T. P. Radhakrishnan, J. Phys. Chem. 1994, 98, 9133.
- 12. Lab 6. a. O. Benini, C. Rinaldo, P. Fetto, J. Chem. Ed. 1996, 73, 865, b. https://www.rose-hulman.edu/mathjournal/archives/2002/vol3-n1/paper1/v3n1-1pd.pdf
- 13. Lab 7. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford 2014

#### **Other Resources**

#### **Course Designers**

1. Internal (Institutional) Subject Matter Experts Dr. Sabyasachi Chakraborty, Associate Professor, SRM University – AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Introduction To Quantum Chemistry: Concepts and Applications**

Course Code	CHE 504	Course Category	Core			L	T	P	C
Course coue	CILLOUI	course category	Core			3	0	0	3
Pre-Requisite Course(s)	Nil	Co-Requisite Course(s)		Progressive Course(s)	·				
Course Offering Department	Chemistry	Professional / Licensing Standards							

#### Course Objectives / Course Learning Rationales (CLRs)

- > Facilitate students in cultivating a thorough comprehension of the fundamental principles of quantum mechanics in the context of exploring atomic and molecular structures.
- > This includes the application of quantum postulates to solve problems involving particles in one, two, and three-dimensional boxes.
- Additionally, the course will introduce the concept of operators and elucidate their application in solving problems related to Hydrogen or Hydrogen-like atoms.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Explain basic principles and mathematical aspects of quantum mechanics and applications to chemistry.	3	80	85
Outcome 2	Apply operator algebra to calculate eigen values and eigen functions.	4	75	80
Outcome 3	Solve Schrodinger equation for Set up Schrodinger equation and solve it for simple systems.	5	75	80
Outcome 4	Realize the requirements of quantum chemistry for chemical systems.	6	75	80

					Pro	ogram L	earning	g Outco	mes (PL	<b>.O</b> )					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self Directed and Life long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	2	2	1	2	2	3	1	2	2	2	1	2		
Outcome 2	1	2	2	1	2	2	3	1	2	2	2	1	2		
Outcome 3	2	2	2	2	2	2	3	1	3	2	2	1		2	2
Outcome 4	2	2	2	2	3	3	3	1	3	2	2	1		2	2
Average	2	2	2	2	2	2	3	1	3	2	2	1	2	2	2

Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
	Introduction to Quantum Chemistry: Inadequacy of classical mechanics, the concept of matter-waves, Schrodinger's and Heisenberg's formulation of quantum mechanics.	3	1	1,2
Unit No. 1	Postulates of quantum mechanics need for operators, Linear and Hermitian operators, operator algebra.	3	1	1,2
	Eigenvalue and eigenfunctions, and commutation relations.	3	1	1,2
	Preliminary Mathematical Principles: Introduction to matrices, vector algebra, Dirac notation, Differential equations, integrations in series.	3	1	1,2
	Elementary Applications of Quantum Mechanics: Solution of Schrodinger's equation for the following systems-(1) particle in ID.	3	2	1,2
Unit No. 2	2D- and 3D-boxes and applications.	3	2	1,2
	Particle in a ring and sphere, spherical harmonics.	3	2	1,2
	Rigid rotator, Simple harmonic oscillator, and Hydrogen atom.	3	2	1,2
	Approximation Methods: Variation and Perturbation methods and examples.	2	3	3,4
Unit No. 3	Antisymmetric wave functions of many-electron atoms.	2	3	3,4
	Slater determinants, Hartree and Hartree-Fock self- consistent field model for atoms.	2	3	3,4
	Electronic configuration of atoms.	2	3	3,4
	Chemical Bonding: BO approximation, LCAO,	2	4	3,4
Unit No. 4	Molecular orbital theory	2	4	3,4
	Valance bond theory	2	4	3,4
	Differences and limitations.	2	4	3,4
Unit No. 5	Review of Electronic Structure Theories: Hartree-Fock, Application of Hartree-Fock,	3	4	3,4
	DFT and configuration interaction.	2	4	3,4
	Total Contact Hours	45		

#### **Learning Assessment**

			uous Lea	rning A	ssessmen	ts (60 %	)			End Semester		
Bloom's Level of Cognitive Task		CLA-1 (20%)		CLA-2 (20%)		CLA-3 (20%)		Mid Term (0%)		Exam (40%)		
			Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac	
Level 1	Remember	50%	0	25%	0	25%	0	0	0	30%	0	
Level I	Understand				U	2370	U		U	3070	U	
Level 2	Apply	25%	0	50%	0	25%	0	0	0	40%	0	
Level 2	Analyse	25/0				2370	0	0	0	4070	U	
Level 3	Evaluate	25%	0	25%	0	50%	0	0	0	30%	0	
Level 3	Create	25%	0	2370	U	3070	0	U	U	3070	U	
	Total	100	0	100	0	100	0	0	0	100	0	

#### **Recommended Resources**

- 1. D. A. McQuarrie, Quantum Chemistry, 2nd ed., University Science Books, 2008, ISBN 978-1-891389-50-4.
- 2. I. N. Levine, Quantum Chemistry. 7th ed., Pearson, 2016, ISBN: 978-0321890603.
- 3. P. W., Atkins, R. S. Friedman, Molecular quantum mechanics, 4th ed., Oxford University Press, 2004, ISBN: 978-0199274987.
- 4. T. Engel, Quantum Chemistry and Spectroscopy, 4th ed., Pearson, 2018, ISBN: 978-0134813981

#### **Recommended Online Resources**

5. A. Szabo, and N. S. Ostlund, Modern quantum chemistry: Introduction to advanced electronic structure theory, 2<sup>nd</sup> ed., Dover Publications, 1996, ISBN: 978-0486691862

#### **Other Resources**

#### **Course Designers**

1. Internal (Institutional) Subject Matter Experts Dr. Mahesh Kumar Ravva, Associate Professor, SRM University - AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### COMMUNITY SERVICE AND SOCIAL RESPONSIBILITY

Course Code	VAC 502 Course Category		VAC		L	T	P	C
Course Code	VAC 302	Course Category	VAC	0	0	2	2	
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)				
Course Offering Department	CEL	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- 1. Encourage initiatives that address local needs, foster self-sufficiency, and promote environmental sustainability within the community.
- 2. Equip participants with a deeper understanding of social issues and a sense of responsibility towards marginalized communities.
- 3. Inspire active participation in community service programs and foster a culture of giving back among individuals and organizations.
- **4.** Develop and implement programs that contribute to skill development, economic empowerment, and equal opportunities for underprivileged sections of society.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Develop effective strategies for identifying and addressing community needs.	3	80%	80%
Outcome 2	Demonstrate empathy and cultural sensitivity when engaging with diverse community groups.	4	80%	75%
Outcome 3	Implement sustainable solutions and evaluate their impact on social well-being.	5	90%	85%
Outcome 4	Collaborate effectively within teams to design and lead community service projects.	6	90%	80%

#### **Learning Assessment**

Bloom's Level of Cognitive Task		C	End Semester			
		CLA-1 20% Mid-1 20% CLA-2		CLA-2 20%	CLA-3 20%	Exam 50%
Level 1	Remember	10%	10%			20%
LEVELI	Understand	1070	1070			2070
Level 2	Apply		10%	10%		20%
Level 2	Analyse		1070	1070		2070
Loyal 3	Evaluate				10%	10%
Level 3	Create				10/0	1070
	Total	10%	20%	10%	10%	50%

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Entrepreneurial Mindset**

Course Code	SEC 503	Course Category	SEC		L 2	T 0	P 0	C 2
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)				
Course Offering Department	Management	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- > Foster creativity and innovation skills to generate entrepreneurial solutions effectively.
- > Cultivate risk management strategies and resilience for navigating entrepreneurial challenges.

# Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Discuss the significance of entrepreneurship and assess inherent traits and skills essential for entrepreneurial success and family Business	2	80%	80%
Outcome 2	Apply strategic thinking frameworks for analyzing opportunities and creating startup strategies.	3	70%	70%
Outcome 3	Discuss potential challenges and reasons for failure in entrepreneurial ventures	2	80%	80%
Outcome 4	Analyze various business models, and differentiate between different types of entrepreneurs and intrapreneurs.	3	70%	70%

	Program Learning Outcomes (PLO)														
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self Directed and Life long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3												2		
Outcome 2	3	2	2	2				2		2	3		3	2	3
Outcome 3	3			1						2	2		3	3	
Outcome 4	3	2	2	2				2		2	3		3	3	3
Average	3	2	2	2				2		2	3		2	2	2

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used
Unit 1	Introduction	6		
	Significance of Entrepreneurship	2	1	1,2
	Inherent Traits and Skills required to be possessed by a Potential Entrepreneur	2	1	1,2
	Taxonomy of Entrepreneurship: Types of Entrepreneurs, Distinction between Entrepreneurs and Intrapreneurs	2	1	1,2
Unit 2	Entrepreneurial Opportunity	10		
	Opportunities and Challenges (Pros and Cons) of Entrepreneurship	2	2,3	1,2
	Reasons for Failure of Entrepreneurial Ventures	3	2,3	1,2
	<b>Exploring Entrepreneurial Opportunities</b>	5	2,3	1,2
Unit 3	Entrepreneurial Strategy	10		
	Ideation and idea testing	4	2,3	1,2
	Starting up Strategy: Five-Question Framework and Porter's Five Forces	4	2	1,2
	Entrepreneurial Support	2	2	1,2
Unit 4	Business Model	15		
	Understanding Business Models	5	4	1,2
	Preparing a Business Plan	5	4	1,2
	Basics of Startup finance	5	4	1,2
Unit 5	Family Business	4		
	Introduction to Family Business	2	1	3
	Entrepreneurship in Family Business	2	1	3
	Total Contact Hours	45		

#### **Learning Assessment (Theory)**

Ploom's I	evel of Cognitive Task	Continuo	us Learning Assessm	End Semester Exam (70%)	
DIOUIII S L	ever of Cognitive Task	CLA-1 (10%)	CLA-2 (10%)	CLA-3 (10%)	
Level 1	Remember	80%	70%	70%	60%
Level 1	Understand	30 /0	7070		0070
Level 2	Apply	20%	30%	30%	40%
ECVCI 2	Analyse	2070	3070		<b>40</b> / 0
Level 3	Evaluate				
Level 3	Create				
	Total	100%	100%	100%	100%

#### **Recommended Resources**

- 1. Entrepreneurship, Rajeev Roy, Oxford University Press
- 2. Entrepreneurship: A Small Business Approach, Charles E. Bramford & Garry D. Bruton, McGraw Hill Education

#### **Other Resources**

#### **Course Designers**

1. Dr Prabal Sen, Visiting Faculty, Paari School of business, SRM University-AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# **Research Design and Methods**

Course Code	SEC 105	Course Category	Foundation Course (FC)			T	P	C
					3	0	0	3
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)				
Course Offering Department	Chemistry	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- > To understand and apply various research designs and methodologies.
- > Equip students with the practical skills necessary to conduct research independently.
- Foster an understanding of ethical considerations in research.

# Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Students will be able to identify a research problem	2	85%	80%
Outcome 2	Students will develop the ability to critically evaluate and compare different research designs and methodologies.	3	80%	75%
Outcome 3	Students will demonstrate an understanding of ethical considerations in research.	5	80%	75%

	Program Learning Outcomes (PLO)														
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	2	3	2	3		3	2	3	3	3		2	1	3
Outcome 2	2	1	2	2	1		2	2	1	2	3		3	2	2
Outcome 3	3	3	3	3	2		2	1	2	2	1		1	3	1
Average	3	2	3	2	2		2	2	2	2	2		2	2	2

Unit	Unit Name	Required	CLOs	References
No.		Contact Hours	Addressed	Used
Unit 1	Introduction to Research Design and Methods	10	1	1,2
	Overview of research: Definition, significance, purpose, and	4		
	types.	4		
	Types of Research: Basic and applied research.	4		
	Google scholar, ResearchGate, Citations, h-index, i10 index	2		
	Bibliography, Reference manager	2		
Unit 2	Formulating Research Questions and Hypotheses	10	2	1,3
	Developing clear and focused research questions	2		
	Literature survey, various sources of research information	2		
	Methodology of research	2		
	Importance of research design	2		
	Steps in conducting research	2		
Unit 3	Introduction to scientific ethics	10	3	1,2,3
	Key ethical principles: Honesty, integrity, transparency.	4		
	The role of ethics in experimental design	2		
	Ethical considerations in data collection and analysis.	2		
	Human and animal research ethics.	2		
Unit 4	Report your findings	10	3	1,2,3
	Writing reports, Structuring reports	2		
	Writing journal articles,	3		
	Writing research proposals	3		
	Producing oral presentations	2		
Total Co	ontact Hours		45	

#### **Learning Assessment**

Bloom's Level of Cognitive Task		Co	End Semester			
		CLA-1 10% Mid-1 15% CLA-2 15% CI		CLA-3 10%	Exam (50%)	
Level 1	Remember	40%	60%	40%	60%	30%
Level 1	Understand	4070	0070	40 /0	00 /0	30 /0
Level 2	Apply	60%	40%	60%	40%	70%
Level 2	Analyse	0070	4070	00 /0	40 /0	7070
Level 3	Evaluate					
Level 3	Create					
	Total	100%	100%	100%	100%	100%

#### **Recommended Resources**

- 1. Bordens K.S. and Abbott, B.b.: Research Design and Methods, McGraw Hill, 2008.
- John W. Creswell and J. David Creswell Research Design: Qualitative, Quantitative, and Mixed Methods Approaches" SAGE Publications, 2017
- **3.** Wayne C. Booth, Gregory G. Colomb, Joseph M. Williams, Joseph Bizup and William T. FitzGerald, The Craft of Research, Fourth Edition, University of Chicago Press, 2016

#### **Other Resources**

1. -

#### **Course Designers**

1. Dr. Rajapandiyan J P, Assistant Professor, Department of Chemistry, SRM University AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# **Design Thinking**

Course Code	FIC 108	Course Category	FIC		L	T	P	C
Course Coue	110 100	Course Category	110		3	0	0	3
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)				
Course Offering Department	Management	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- Familiarize with the principles of Design Thinking
- ➤ Learn to apply the principles of Design Thinking
- Apply Design Thinking to solve problems.

# Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Importance of Design Thinking	1	75%	90%
Outcome 2	Grasp the Concepts and process of Design Thinking	3	75%	90%
Outcome 3	Learn the process of Design Thinking	2	85%	90%
Outcome 4	Solve a problem using Design Thinking Principles	3	75%	65%

	Program Learning Outcomes (PLO)														
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3					-	-	-	-	-	-	-	3	3	3
Outcome 2	3					-	-	-	-	-	-	1	3	1	3
Outcome 3	3					-	-	-	3	-	-	2	3	2	3
Outcome 4	3	3	3	3		-	-	-	3	3	3	3	3	3	3
Average	3	3	3	3		-	-	-	3	3	3	2	3	2	3

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used
TT '44	An Introduction to the innovation Process	15		1,2
Unit 1	Understanding of Design Thinking & its Importance, Pillars of Design Thinking		2	1,2
Unit 2	Process – Understanding the Stages of Design Thinking	15	2	1,2
Unit 3	Identifying Opportunity Areas: Problem Framing & Definition	10	2	1,2,3
Unit 4	Idea Generation and Concept Development	10	2	1,2,3
Unit 5	Implementation and Managing Innovation	10	4	1,2,3

#### **Learning Assessment**

Bloom's Level of Cognitive Task		Continuo	Continuous Learning Assessments (50%)			
		CLA-1 20%	CLA-2 15%	CLA-3 15%		
Level 1	Remember	60%	60%	40%	30%	
Level 1	Understand	0070	0070	4070	3070	
Level 2	Apply	40%	40%	60%	40%	30%
Level 2	Analyse	4070	4070	0070	7070	3070
Level 3	Evaluate					
Level 3	Create					
	Total	100%	100%	100%	70%	30%

#### **Recommended Resources**

- 1. Design Thinking Techniques and Approaches, N. Siva Prasad
- 2. Design Thinking, Nigel Cross, BERG Publishing
- Design Thinking- Integrating Innovation, Customer Experience and Brand Value, Thomas Lockwood, De-sign Management Institute, 2009

#### **Other Resources**

- 1. HBS Online Design Thinking & Innovation course material
- 2. Case studies

#### **Course Designers**

1. -

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Organic Chemistry-II: Organic Reactions**

Course Code CHE 505		Course Category	Core			T	P	C
			, and the same of				1	4
Pre-Requisite Course(s)	Nil	Co-Requisite Course(s)	Progressive Course(s)	·				
Course Offering Department	Chemistry	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- > Gain a thorough understanding of the mechanisms and synthetic applications of cycloaddition, electrocyclic, sigmatropic, and related pericyclic reactions, and the principles underlying these processes.
- Explore and comprehend the fundamental principles of organic photochemistry, including key reactions involving alkenes, arenes, carbonyl, and azide functional groups, and their applications in organic synthesis.
- > Investigate and study rearrangement reactions in organic molecules and oxidation/reduction reactions using various reagents for synthesis.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Explain the mechanisms and synthetic applications of cycloaddition, electrocyclic, sigmatropic, and related pericyclic reactions using frontier orbital, correlation diagram, and Huckel-Mobius approaches.	2	80%	70%
Outcome 2	Describe basic organic photochemical reactions involving alkenes, arenes, carbonyl, and azide functional groups, and apply this knowledge to propose synthetic routes for organic molecules.	2	70%	70%
Outcome 3	Sketch the mechanisms of rearrangement reactions involving carbocations, carbenes, carbanions, and nitrene intermediates, and apply this understanding to design synthetic strategies.	3	85%	75%
Outcome 4	Apply various oxidation and reduction reactions with specific reagents to synthesize target organic compounds, demonstrating a clear understanding of the underlying principles and mechanisms	3	80%	70%

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Guntur District, Mangalagiri, Andhra Pradesh – 522240.



		Program Learning Outcomes (PLO)													
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	1	1	2	1	1			1			1	3	1	2
Outcome 2	3	2	1	2	1	1			1			1	3	1	1
Outcome 3	3	2	2	2	2	1			3			2	3	2	2
Outcome 4	3	2	3	3	2	2			3			2	3	2	3
Average	3	2	2	2	2	1			2			2	3	2	2

Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
Unit	Concerted Reactions	8		
No. 1	Mechanism and synthetic applications of cycloaddition, electrocyclic, sigmatropic and related pericyclic reactions.	4	1	
	Explanation based on frontier orbital, correlation diagram and Huckel-Mobius approaches.	4	1	2
Unit	Organic Photochemistry	10		
No.	Introduction - Frank-Condon principle - Jablonski diagram	3	2	
2	Basic organic photochemical reactions involving alkenes, arenes, carbonyl and azide functional groups	4	2	1,2
	Remote functionalization	1	2	ŕ
	Application of photochemical reactions in organic synthesis	2	2	
Unit	Rearrangement Reactions	8		
No.	Rearrangement of organic molecules and their synthetic potential	4		
3	Rearrangement reactions involving carbo-cations, carbene, carbanion, and nitrene intermediates	4	3,4	2
Unit	Oxidation and Reduction Reactions	7		
No. 4	Oxidation of organic compounds with reagents based on peroxides, peracids, ozone, osmium, chromium, ruthenium, silver, dimethyl sulfoxide iodine, and selenium dioxide	4	3,4	
	Reduction of organic compounds with reagents based on boron, aluminium, hydrogen, hydrazine, formic acid and dissolving metals.	3	3,4	2
Unit	Named Reactions and Reagents in Organic Synthesis	12		
No. 5	Aldol, Perkin, Benzoin, Cannizaro, Wittig, Grignard, Reformatsky-Meerwein, Hoffmann Claisen and Favorskii rearrangements	3	3,4	
	Hydroboration-oppenauer oxidation, clemmensen reduction- Meerwein – Pondorf and verley and Birch reductions.	3	3,4	2
	Stork enamine reactions, Michael addition, Mannich Reaction, Diels-Alder reaction, Ene-reaction, Baeyer-Villiger Reaction	3	3,4	2
	Introductory treatment to the application of silicon, boron (organo boranes), phosphorus, palladium, samarium, ruthenium, indium reagents in organic synthesis	3	3,4	
	Total Contact Hours	45		

# **Course Unitization Plan-Lab**

Exp	Experiment Name	Required	CLOs	References
No.		<b>Contact Hours</b>	Addressed	Used
1	Preparation of oxabenzonorbornadiene	4	3,4	3
2	Synthesis of 1,2,3,4-tetrahydrocarbazole	4	3,4	3
3	Preparation of caprolactam from cyclohexanone	4	3,4	3
	oxime by Beckmann Rearrangement			
4	Synthesis of β-Nitro Styrene	4	3,4	3
5	Preparation of benzaldehyde from benzyl alcohol	4	3,4	3
	using pyridinium chlorochromate (PCC)			
6	Preparation of benzonitrile from aniline	4	3,4	3
7	Synthesis of alkenes from carbonyl compounds	6	3,4	3
	(Wittig Reaction)			
	<b>Total Contact Hours</b>		30	

#### **Learning Assessment**

			End Semester								
	Bloom's Level of Cognitive Task		CLA-1 (10%)		CLA-2 (20%)		CLA-3 (10%)		rm (20%)	Exam (40%)	
<u> </u>		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level	Remember	20	20	20	20			20	20	20	
1	Understand	20	20	20	20	20	20	20	20	20	20
Level	Apply	60	60	30	30			30	30	30	40
2	Analyse			30	30	30	30	30	30	30	40
Level	Evaluate					20	20				
3	Create										
	Total		100	100	100	100	100	100	100	100	100

#### **Recommended Resources**

- 1. J.D. Coyle, Organic Photochemistry Wiley, 1985.
- 2. Carruthers, Modern Methods in Organic Synthesis, Academic Press, 1989.
- 3. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- 4. Recommended Additional Resources
- 5. Li, Jie Jack. Name Reactions: A Collection of Detailed Reaction Mechanisms, Springer, 2003.
- 6. F. A. Carey and R. Sundberg, Advanced Organic Chemistry, Vol. 1 and 2 (2002)

## **Other Resources**

# **Course Designers**

1. Dr. E. Satheesh

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# Solid state, Nanomaterials and Inorganic Photochemistry

Course Code	CHE 506	Course Category	Inorgan	ic Chemistry		1 3	T 0	P 1	C 4	1
Pre-Requisite Course(s)	CHE 502	Co-Requisite Course(s)	NILL	Progressive Course(s)	·					1
Course Offering Department	Chemistry	Professional / Licensing Standards								

# Course Objectives / Course Learning Rationales (CLRs)

- > Detailed discussion on atomic arrangements in crystalline and amorphous solids: metals ceramics, and semiconductors
- > Introduce the concept of nanomaterials, chemical synthesis, and characterisation of solids and nanomaterials
- > The topic of inorganic photochemistry, principles of light absorption; physical and chemical processes involved in inorganic compounds

## Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Learning the concepts of the unit cells, radius ratio rules, and packing fraction. Extend the understanding of the structure of various inorganic compounds	1, 2	90%	85%
Outcome 2	The learner will be able to describe the background and concepts of nanoscience and compare the types and properties of different nanostructures using quantitative and qualitative methods.	3, 4	90%	80%
Outcome 3	Compare different synthesis methods in making materials and learn various characterisation techniques	3, 4	85%	75%
Outcome 4	Describe principles of various experimental techniques, for example, X-ray diffraction, thermal analysis, spectroscopy, and electron microscopy. Apply the methods to investigate multiple materials' structure and composition and interpret the results using relevant theories and models	1, 3	85%	70%
Outcome 5	Principles of light absorption and various theories involved in electronic transitions. Apply theories to different metal complexes	3	85%	80%
Outcome 6	Apply classroom theory in making different metal oxides, using different synthesis methods and characterise the same. Analyse the data and interpret the results	4, 5	90%	80%

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# Course Articulation Matrix (CLO) to Program Learning Outcomes (PLO)

					P	rogram I	Learning	Outcon	nes (PLC	D)					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	2	1	1						2	1	2	2		
Outcome 2	2	3	3	1	1				1	2	2	2	2	1	
Outcome 3	3	3	3	2	1				1	2	2	2	2	2	
Outcome 4	2	2	2	2	1				1	2	2	2	2		
Outcome 5	2	2	2	2	1				1	2	2	2	2		
Outcome 6	3	3	3	2	3	2			2	2	1	2		2	2
Course Average	2	3	2	2	1				1	2	2	2	2	1	

# **Course Unitization Plan-Theory**

Unit No.	Syllabus Topics	Required Contact	CLOs Addressed	References Used
INO.		Hours	Addressed	Useu
	Solid State Chemistry - Unit cell and Crystal structure description -			
	Relative density of packing in simple cubic, CCP, HCP, and BCC -	2	1	1,2,3
	Tetrahedral and octahedral holes.			
	Radius ratio for trigonal, tetrahedral, octahedral and cubic sites -	1	1	1,2,3
	Radius ratio and shape of ionic crystals			7 7-
Unit	Crystal chemistry of the prominent inorganic structural families, for			
No.	example, crystal structures of MX, MO, MH, and MS type solids,	2	1	1,2,3
1	including examples (M – Metal, X-halides, H-hydrides, S- Sulphides, O-			
	Oxides).			
	Discussion of NiAs, ZnS, MX2, CdCl2, ReO3, perovskite ABO3, YBa2Cu3O7, K2NiF4, Ag2HgI4, spinel and olivine.	2	1	1,2,3
	Frenkel and Schottky defects, colour centers, Crystallographic shear			
	(CS) in WO3-x structures.	1	1	1,2,3
	Introduction to Nanoscale & Nanomaterials			
	Background to Nanoscience:			
	Definition of Nano, Scientific Revolution-Atomic Structure and atomic	1	2	4,5
	size, emergence and challenges of nanoscience and nanotechnology.			
	Carbon age-new form of carbon (CNT to Graphene), the influence of	2	2	4.5
Unit	nano over micro/macro, size effects and crystals.	2	2	4,5
No.	Large surface to volume ration, surface effects on the properties. Types	2	2	4.5
2	of nanostructure and properties of nanomaterials.	2	2	4,5
	One-dimensional, 2D and 3D dimensional nanostructured materials,	2	2	4,5
	Quantum Dots shell structures.	2	2	4,5
	Metal oxides, semiconductors, composites, mechanical-physical-	1	2	4,5
	chemical properties.	•		-1,0
	Preparative methods of solids - Ceramic method (solid state reaction),	2	3	2,3
	Atmospheric controlled method, Quartz tube method,		-	_,-
Unit	Co-precipitation, Hydrothermal, Sol-gel, Combustion, Microwave,	•	_	2.2
No.3	Chimie douce, Vapour phase deposition and Molten salt synthesis	2	3	2,3
	methods.			
	Synthesis methods of dimensionally modulated Inorganic nanostructured materials	1	3	2,3
	nanosti uctureu materiais			

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Guntur District, Mangalagiri, Andhra Pradesh – 522240.



	Thermolysis routes, Microwave-assisted synthesis, Sonochemical assisted synthesis	1	3	2,3
	Core-Shell nanostructure, Organic-Inorganic Hybrids, Quantum dot (QDs) synthesis	1	3	2,3
	Carbon Nanotubes (SWCNT, MWCNT), Graphene nanosheets.	1	3	2,3
	Ceramic method (solid state reaction), Atmospheric controlled method, Quartz tube method,	2	3	2,3
	Characterisation of Materials - X-Ray Diffraction Methods: Single & powder X-ray diffraction, Bragg's Law.	3	4	2,3
Unit	Applications of X-ray diffraction, Phase identification, Phase purity, Crystallite size determination etc.	3	4	2,3
No.	Thermal analysis: TGA, DTA, DSC.	2	4	2,3
4	Photoluminescence Spectroscopy, Electrochemical Impedance Spectroscopy.	2	4	2,3
	Vibrating sample Magnetometer, Brunauer-Emmett Teller surface areas, Atomic Force Microscopy.	2	4	2,3
	Inorganic photochemistry	•	•	
	Principle of light absorption – physical and chemical processes	1	5	6
Unit	Bimolecular reactions – Stern – Volmer relationship. Properties of d-d, d-p*, p*-p* and p-d energy states	2	5	6
No. 5	Photochemical reactions of metal complexes – substitution – rearrangement – isomerisation – racemisation – redox reactions.	2	5	6
	Ruthenium polypyridyls – excited state properties – electron transfer and energy transfer quenching reaction. The importance of solar energy conversion and storage.	2	5	6
	Total Contact Hours	45 Hours		

#### Course Unitization Plan - Lab

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	References Used
1.	Synthesis of ZnO and Fe3O4 oxides by co-precipitation, characterisation, XRD and UV-Vis absorption spectra	6	6	2,3
2.	Sol-gel synthesis of alkali/alkaline earth silicates, characterisation, and measurement of photoluminescence	6	6	2,3
3.	Solvothermal synthesis of LiCoO2, CV and charge/discharge study.	6	6	2,3
4.	Combustion synthesis of Al2O3, XRD and particle size analysis	6	6	2,3
5.	Solid state synthesis of YBa2Cu3O7+8 and demonstration of levitation experiment	6	6	2,3
	Total Contact Hours	30 Hours		

#### **Learning Assessment – Theory & Laboratory**

		Conti	nuous L	earning	g Assessme	ents (60	%)						
Bloom's Level of Cognitive Task		CLA-1 (10%)		CLA-2 (20%)			CLA-3 (10%)		Mid Term (20%)		End Semester Exam (40%)		
cogmuve	lusik	Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac		
Level 1	Remember 1		40	40	40	20	20	20	10	20	10		
20,011	Understand	40											
Level 2	Apply	60	60	40	0 60	60	60	60	70	60	70		
Ecvel 2	Analyse			40					'0		70		
Level 3	Evaluate [ ovel 3					20	20	20	20	20	20		
Levelo	Create			20					20		20		
Total		100	100	100	100	100	100	100	100	100	100		

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



## **Recommended Resources**

- 1. Microstructural Characterization of Materials David Brandon and Wayne Kaplan, John Wiley and Sons, New York, NY, 1999.
- 2. Elements of X-ray Diffraction BD Cullity and SR Stock, Prentice Hall, New Jersey, 2001.
- 3. R. West, Solid state chemistry and its applications, Wiley Student edition (John Wiley & Sons).
- 4. Anno chemistry: A Chemical Approach to Nanomaterials Royal Society of Chemistry, Cambridge UK 2005.
- **5.** Chemistry of Nanomaterials: Synthesis, properties and applications by CNR Rao et.al., Royal Society of Chemistry, Cambridge UK 2006.

#### **Other Resources**

#### **Course Designers**

- 1. Internal (Institutional) Subject Matter Experts Prof. C.P Rao, Sr Professor, SRM University AP
- 2. and Dr. Pardha Saradhi Maram, Associate Professor, SRM University AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Reaction Kinetics and Electrochemistry**

Course Code	CHE 507	Course Category	Core (Physi	cal Chamistr		L	T	P	C
Course Code	CHE 507	Course Category	Core (Physical Chemistry) 3 0				1	4	
Pre-Requisite Course(s)	CHE 503	Co-Requisite Course(s)		Progressive Course(s)					
Course Offering Department	Department of Chemistry	Professional / Licensing Standards							

## **Course Objectives / Course Learning Rationales (CLRs)**

- > To discuss theories of reaction rates and derive rate laws for complex reactions such as enzyme-catalysed reactions and chain reactions.
- > To explain importance of transport properties in gases and liquids and to discuss different types of electrochemical cells, electrical double layer theory, and thermodynamics of galvanic cells.
- > To gain knowledge on different kinds of quantitative and titrimetric analyses related to catalysis and redox reactions.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Understand Theories of Reaction Rates to Predict and Interpret Reaction Mechanisms	1	80	70
Outcome 2	Apply Photophysical and Photochemical Processes Using Kinetic Models	2	75	65
Outcome 3	Analyse Transport Phenomena in Gases and Liquids and Electrochemical Processes	3	80	70
Outcome 4	Understand, apply, and remember the experimental techniques in related to catalysis and redox reactions.	1,2,3	80	75

					Pr	ogram L	earning	g Outco	mes (PI	<b>.O</b> )					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	2	2	2	1	1	-	-	1	1	-	1	2	1	2
Outcome 2	3	2	2	2	1	1	-	-	1	1	-	1	2	1	2
Outcome 3	3	3	1	3	1	1	-	-	1	1	-	1	3	3	3
Outcome 4	2	3	3	3	1	1	-	-	1	1	-	1	3	2	3
Average	3	3	2	3	1	1	-	-	1	1	-	1	3	2	3

# **Course Unitization Plan-Theory**

Course	Onitization 1 Ian-1 neory			
Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
	Theories of reaction rates: Collision theory, Transition state theory, Activation/thermodynamic parameters, Erying equation	3	1	1,2
Unit	Temperature dependence of reaction rates: Linear and non-linear Arrhenius equation, Interpretation of Arrhenius parameters	3	1	1,2
No.	Complex reactions: chain reactions (free radical reaction, polymerization kinetics), enzyme reactions, inhibition kinetics	3	1	1,2
	Various theories of unimolecular reactions (Lindemann-Hinshelwood, RRKM theories), potential energy surfaces for bimolecular reactions, adiabatic and non-adiabatic curve crossing processes.	4	1	1,2
Unit	Jablonski diagram, kinetics of unimolecular and bimolecular photophysical and photochemical processes, quantum yield calculation	4	2	1,2,3
No. 2	Excited state lifetime-quenching constant, resonance energy transfer rates (RET), rate and efficiency of RET	3	2	1,2,3
	Dynamics of electron transfer, solvent re-organization energy,	2	2	1,2,3
	Marcus theory of electron transfer.	1	2	1,2,3
	Transport in gases: the phenomenological equations	1	3	1,2
Unit No.	Diffusion coefficient, thermal conductivity, viscosity, effusion	2	3	1,2
3	Motion in liquids: drift velocity, mobility and conductivity	2	3	1,2
	The Einstein relations, diffusion and the diffusion equations	1	3	1,2
	Electrochemistry of solutions: ion-solvent interactions, ion-ion interactions, ionic migration and diffusion.	3	3	1,2
Unit	Thermodynamics of galvanic cells: Equilibrium electrode potentials, IUPAC convention for electrode potentials, Thermodynamics of electrochemical cells and applications.	3	3	1,2
No. 4	Electrical Double layer: Theories of Double-Layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern Model,	2	3	1,2
	Adsorption of ions and neutral compounds, Electrocaplillary and differential capacitance measurements; Influence of double layer on charge transfer processes.	2	3	1,2
Unit	The rate of electron transfer: derivation of Butler-Volmer equation and Tafel plots	2	3	1,2
No.	Types of overpotentials: origin and minimization	1	3	1,2
5	Mechanism of electro-organic reactions	1	3	1,2
	Hydrogen evolution and oxygen reduction reactions.	2	3	1,2
	Total Contact Hours	45		

#### Course Unitization Plan - Laboratory

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	References Used
1.	Determination of rate constant for acid-catalysed ester hydrolysis	4	4	1,2
2.	Determination of the order of reaction for acid-catalysed ester hydrolysis	4	4	1,2
3.	Determination of excited-state acid dissociation constant	4	4	1,2
4.	Computational determination of rate constant for a keto- enol tautomerization reaction	4	4	1,2
5.	Potentiometric titration of a redox reaction	4	4	1,2
6.	Potentiometric titration of a redox reaction	4	4	1,2

#### <u>Learning Assessment – Theory & Laboratory</u>

			Cor	ıtinuous	Learnin	g Asses	sments (	60%)		End C	emester
Bloom's Level of Cognitive Task		CLA-1 (10%)		CLA-2	CLA-2 (20%)		CLA-3 (10%)		Term )%)	Exam (40%)	
	iask	Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level 1	Remember	40	40	40	40	20	20	20	10	20	10
	Understand										
Level 2	Apply	60	60	40	60	60	60	60	70	60	70
	Analyse										
Level 3	Evaluate					20	20	20	20	20	20
	Create			20							
	Total	100	100	100	100	100	100	100	100	100	100

#### **Recommended Resources**

- 1. P. Atkins and J. Paula, Physical Chemistry, 10th edition, Oxford University Press, Oxford 2014.
- 2. J. Laidler, Chemical Kinetics, 3rd edition, Harper & Row, New York 1998
- 3. K. Rohatgi Mukherjee, Fundamentals of Photochemistry, New Age International Pvt. Ltd.; 3rd edition, New Delhi 2014.
- 4. Viswanathan, and P. S. Raghavan, Practical Physical Chemistry, Viva Books, 2010
- 5. M. Halpern, and G. C. McBane, Experimental Physical Chemistry: A Laboratory Textbook, 3rd Edition, W. H. Freeman, 2006
- 6. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford 2014.

## **Recommended Online Resources**

- 7. S. Glasstone, An Introduction to Electrochemistry, East-West Press Pvt. Ltd., 2006.
- 8. J. Mendham, R.C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel's Quantitative Chemical Analysis, 6th Ed., Pearson Education, 2009.
- 9. H. Rieger, Electrochemistry, 2nd Edition, Springer, 1994
- 10. H. Rieger, Electrochemistry, 2nd Edition, Springer, 1994

#### **Other Resources**

# **Course Designers**

1. Dr. Sabayasachi Chakrabortty

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



## Analytical Chemistry I- Principles, Instrumentation, and Applications of Analytical Techniques

Course Code	CHE 508	Course Category		<u>L</u>	T 0	P 0	C 3
Pre-Requisite Course(s)		Co-Requisite Course(s)	Progressive Course(s)		•		
Course Offering Department	Chemistry	Professional / Licensing Standards					

## Course Objectives / Course Learning Rationales (CLRs)

- > Understand the fundamentals of analytical chemistry, including basic tools, classification of methods, and selection criteria for analytical techniques.
- > Explore analytical separation techniques, such as chromatography and electrophoresis, and their principles and applications.
- > Gain knowledge of spectroscopic methods, electron microscopy, and Mossbauer spectroscopy, including instrumentation and applications in various fields

## Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Understand the basic tools, operations, and classification of analytical methods, including sample preparation, measurement basics, and data analysis.	2	80%	75%
Outcome 2	Explain analytical separations using thin-layer chromatography, column chromatography, electrophoresis, capillary electrophoresis, and isotachophoresis.	2	80%	75%
Outcome 3	Assess the principles, instrumentation, and applications of various analytical techniques.	3	80%	70%
Outcome 4	Inspect the effectiveness and limitations of these advanced techniques in different analytical contexts, ensuring accurate and reliable results.	4	70%	60%

					Pr	ogram L	earning	g Outco	mes (PI	<b>LO</b> )					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	3	2	2	2	2	1	3	2	2			3	2	3
Outcome 2	3	3	2	2	2	2	1	2	1	2			2	3	1
Outcome 3	3	3	2	3	3	3	1	2	1	3			1	3	2
Outcome 4	3	3	3	3	3	3	3	3	2	3			3	2	1
Average	3	3	2	2	3	3	1	3	2	3			2	3	2

Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
Unit 1	Introduction to analytical chemistry	7		
	Overview and status of analytical science, basic tools and operations of analytical chemistry, classification of analytical methods, types of instrumental methods, selecting an analytical method, sample preparation, measurement basics, and data analysis. Errors in chemical analysis, and spreadsheets.	7	1	1,2
Unit 2	Analytical separation techniques	10		
	Introduction to analytical separation, migration rates of solutes, a summary of chromatographic relationships, principles, and applications of thin layer chromatography, column chromatography, electrophoresis, capillary electrophoresis, and isotachophoresis.	10	2	1,2,3
Unit 3	Spectroscopic methods and electron microscopy	10		
	Types of Optical Instruments, Theory of molecular fluorescence, instrumentation, applications of fluorescence methods, phosphorescence, and chemiluminescence methods. Introduction to microscopy, types of microscopes, electron spectroscopy, scanning tunnelling microscope, and atomic force microscope.	10	3	2,3,4
Unit 4	Mossbauer spectroscopy	7		
	Principles of Mossbauer Spectroscopy, instrumentation, interpretation of spectra. Applications of Mossbauer Spectroscopy in different fields.	7	3	3,4
Unit 5	Atomic spectroscopy and microfluidic techniques	11		
	Introduction to atomic emission spectrometry. Principles and instrumentation of inductively coupled plasma optical emission spectrometry (ICP-OES). Introduction to microfluidics. Building materials for microfluidic devices. Microfluidic platforms and analytical techniques.	11	4	3,4,5
	Total Contact Hours		45	

# **Learning Assessment**

Dloom's I	Level of Cognitive		Continuous Learning Assessments (50%)						
Diooni 8 1	Task	CLA-1 (10%)	Mid-1 (15%)	CLA-2 (10%)	Mid-2 (15%)	Exam (50%)			
Level 1	Remember	40%	40%	40%	40%	40%			
Level I	Understand	40 70	40 70	40 70	40 70	40 70			
Level 2	Apply	40%	40%	40%	40%	40%			
Level 2	Analyse	40 /0	40 /0	40 /0	40 /0	40 /0			
Level 3	Evaluate	20%	20%	20%	20%	20%			
Level 3	Create	2070	20 70	20 70	20 70	2070			
	Total	100%	100%	100%	100%	100%			

#### **Recommended Resources**

- 1. Gary D. Christian, Purnendu K. Dasgupta, Kevin A. Schug, Analytical Chemistry, John Wiley & Sons, 7th Edition, 2013
- 2. S. M. Khopkar, Basic concepts of Analytical Chemistry, New Age International Publishers, 3rd Edition, 2008
- 3. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis, Cengage Learning, 7th Edition, 2017
- 4. Hobart H. Willard, Lynne L. Merritt, John A. Dean, Frank A. Settle, Instrumental Methods of Analysis, CBS Publishers, 7th Edition, 1996
- 5. Stanley Crouch, S.; Skoog; A, F. Holler; West, W, Fundamentals of Analytical Chemistry, Brooks/Cole, 9th Edition, 2013

## **Recommended Online Resources**

- 6. ChemGuide Analytical Chemistry
- 7. MIT OpenCourseWare Principles of Chemical Science

#### **Other Resources**

#### **Course Designers**

Dr. J. P. Raja Pandiyan, Assistant Professor, SRM University - AP

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# **Research Seminar (Invited Lectures)**

Course Code	AEC 503	Course Category		L 0	T 0	P 1	C 1
Pre-Requisite Course(s)		Co-Requisite Course(s)	Progressive Course(s)				
Course Offering Department		Professional / Licensing Standards					

# Course Objectives / Course Learning Rationales (CLRs)

#### Enter Data

# **Course Outcomes / Course Learning Outcomes (CLOs)**

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1				
Outcome 2				
Outcome 3				
Outcome 4				

		Program Learning Outcomes (PLO)														
CLOs	Engineering Knowledge	Problem Analysis	Design and Development	Analysis, Design and Research	Modern Tool and CT Usage	Society and Multicultural Skills	Environment and Sustainability	Moral, and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Project Management and Finance	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3	
Outcome 1																
Outcome 2																
Outcome 3																
Outcome 4																
Average																

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used
Unit 1				
Onit 1				
Unit 2				
Unit 3				
Unit 4				
Unit 5				

# **Learning Assessment**

Bloom's Level of Cognitive Task		Co	Continuous Learning Assessments (50%)							
		CLA-1 20%	Mid-1 20%	CLA-2 20%	CLA-3 20%	Exam (50%)				
Level 1	Remember									
Level 1	Understand									
Level 2	Apply									
Level 2	Analyse									
Level 3	Evaluate									
Level 3	Create									
	Total									

# **Recommended Resources**

1. Enter Data

# **Other Resources**

1. Enter Data

# **Course Designers**

1. Enter Data

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# **Psychology for Everyday Living**

Course Code	FIC 124	Course Category	Generic Elective			T	P	C
Course Coue	FIC 124	Course Category Generic Ele		eric Elective		0	0	3
Pre-Requisite Course(s)		Co-Requisite Course(s)	Progressive Course(s)					
Course Offering Department	Psychology	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- > To understand the fundamental psychological processes in everyday living.
- To apply knowledge of psychology in improving self and others.
- To apply knowledge of psychology in enhancing quality of life.

# Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Explain fundamental psychological processes in everyday living	2	80%	70%
Outcome 2	Describe important theories in psychology in the areas of sensation, perception, personality and learning	2	75%	70%
Outcome 3	Illustrate personal, professional and social applications of psychology	4	75%	60%
Outcome 4	Interpret results from certain personality tests	5	70%	60%

		Program Learning Outcomes (PLO)													
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2							1				1			
Outcome 2	1			1					2	1					
Outcome 3	1	1	1				1	1	2	2		2			
Outcome 4	2		2		1			2	1	1		1			
Average	2	1	2	1	1		1	1	2	1		1			

Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	Referen ces
	Myths and Misconceptions in Psychology	12	1	1
Unit No.	Definition, nature and goals of psychology	4		
1	Common myths and misconceptions about psychology	4		
_	Schools of psychology; Basic and applied areas of psychology	4		
	The Role of Perception and Attitude towards Understanding the World	12	2, 3	2
Unit No.	Perception: Understanding perception, Gestalt laws of organization, common illusions	3		
2	Perceptual constancy - depth perception, size perception, perception of movement	3		
	Attitude formation	3		
	Attitude change	3		
	Intelligence and Learning	12	2, 3	2
	Definitions and nature of intelligence	3		
Unit No.	Emotional and social intelligence; Measuring IQ, EQ and SQ	3		
	Fundamentals of learning and its applications	3		
	Memory techniques	3		
	Understanding the Self	12	2, 4	1
Unit No.	Definition; Approaches to personality - trait and type	4		
4	Psychoanalytical and humanistic theory, Tests of personality – MBTI and NEO-PI	4		
	Identity; Self-concept, self-esteem and self-efficacy	4	1	
	Stress, Coping and Quality of Life	12	2, 3	1
	Nature, sources of stress and its reactions	3		
Unit No.	Factors influencing stress	3		
5	Coping with and managing stress - cognitive and behavioural techniques	3		
	Improving quality of life	3		

#### **Learning Assessment**

		Cont	inuous Learnin	End Semester Exam		
Bloom's Level of Cognitive Task		CLA-1 (15%)	Mid-1 (15%)	CLA-2 (10%)	CLA-3 (10%)	(50%)
		Th	Th	Th	Th	Th
Level 1	Remember	50%	60%	60%	30%	50%
Level 1	Understand	30%	0070	0070	3070	3078
Level 2	Apply	50%	40%	40%	70%	50%
Level 2	Analyse	3070	4070	4070	7070	3070
Level 3	Evaluate					
Level 3	Create					
	Total	100%	100%	100%	100%	100%

## **Recommended Resources**

- 1. Baron, R. A. (2001). Psychology. New Delhi: Pearson Education India.
- **2.** Nolen-Hoeksema, S., Fredrickson, B.L. & Loftus, G.R. (2014). Atkinson & Hilgard's Introduction to Psychology. 16th Ed. United Kingdom: Cengage Learning.

#### **Other Resources**

1. Morgan, C. T., King, R. A., & Schopler, J. (2004). Introduction to Psychology. New Delhi: Tata McGraw Hill.

#### **Course Designers**

1.

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### Project-I

Course Code	CHE 510	Course Category	Dissertation /	Project (P)	-	L 0	T	P	C
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)		U	U	3	3
Course Offering Department	Chemistry	Professional / Licensing Standards							

## Course Objectives / Course Learning Rationales (CLRs)

- Master advanced laboratory techniques relevant to their area of study
- > Develop the ability to design and execute independent research projects
- > Critically review existing literature to identify research gaps and propose new directions.
- > Effectively communicate research findings through written and oral presentations.

## **Course Outcomes / Course Learning Outcomes (CLOs)**

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Mastery of complex laboratory techniques.	5	<b>75</b> %	70%
Outcome 2	Competence in designing and executing research	5	75%	70%
Outcome 3	Ability to identify gaps and propose innovative solutions	3	75%	70%
Outcome 4	Clear presentation of findings to diverse audiences	5	<b>70</b> %	65%

	Program Learning Outcomes (PLO)														
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	3	3	3	3				3			2	3	2	3
Outcome 2	3	3	3	3	2				2			3	3	3	3
Outcome 3	3	3	3	3	2				3			3	3	3	3
Outcome 4	3	3	3	3	3				3			3	3	3	3
Outcome 5	3	3	3	3	3				3			3	3	3	3
Outcome 6	3	3	3	3	3				3			3	3	3	3
Average	3	3	3	3	2				3			3	3	3	3

Unit No.	Syllabus Topics	Required Contact hours	CLOs Addressed	References Used
Unit 1	Research problem and project selection	20 hours		
	Based on interest conceive an idea	10 hours	1,4	1
	Do a feasibility check of the project	10 hours	1,4	1
Unit 2	Literature review and methodology refinement	20 hours		
	Literature survey of the related works	10 hours	2	3,4,5,7
	Write an abstract of the proposed idea	10 hours	2	1
Unit 3	Data collection and analysis	30 hours		
	Hands-on data collection using chosen methodologies	30 hours	3	1,2, 3
	Ongoing meetings with a faculty advisor to discuss progress	10 hours	3	1,6,7
Unit 4	Oral presentation, evaluation and publish results	20 hours		
	Evaluation of written reports and oral presentation	10 hours	3	1, 7
	Initiation of the process for a possible publication	10 hours	5	2,3,4,5,7
	Total		90 Hours	

## **Learning Assessment**

		Continuo	ous Learning Assessments (5	0%)	<b>End Semester Exam</b>
Bloom's Level of Cognition Task		Experiments (20%)	Record / Observation Note (10%)	Viva + Model (20%)	(50%)
Level 1	Remember				
Level 1	Understand				
Level 2	Apply	70%	70%	70%	70%
Level 2	Analyse				
Level 3	Evaluate	30%	30%	30%	30%
Level 5	Create				
	Total	100%	100%	100%	100%

## **Recommended Resources**

- 1. As recommended by Advisor pertaining to student research interest
- 2. https://pubs.acs.org/
- 3. https://www.sciencedirect.com/
- 4. www.springer.com
- 5. https://onlinelibrary.wiley.com/
- 6. Research Methodology
- 7. Reading assignment related to undergraduate project as guided by faculty

## **Other Resources**

## **Course Designers**

1. Dr. J. P. Raja Pandiyan, Assistant Professor, SRM University – AP; Dr. K. Narayanaswamy, Assistant Professor, SRM University – AP

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Guntur District, Mangalagiri, Andhra Pradesh – 522240.



**Summer Internship** 

Course Code	CHE 509	Course Category		L	T	P	C
				0	0	2	2
Pre-Requisite Course(s)		Co-Requisite Course(s)	Progressive Course(s)	·			
Course Offering Department		Professional / Licensing Standards					

# Course Objectives / Course Learning Rationales (CLRs)

# Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1				
Outcome 2				
Outcome 3				
Outcome 4				

	Program Learning Outcomes (PLO)														
CLOs	Engineering Knowledge	Problem Analysis	Design and Development	Analysis, Design and Research	Modern Tool and CT Usage	Society and Multicultural Skills	Environment and Sustainability	Moral, and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Project Management and Finance	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1															
Outcome 2															
Outcome 3															
Outcome 4															
Average															

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used
Unit 1				
Onit 1				
Unit 2				
Unit 3				
Unit 4				
Unit 5				

# **Learning Assessment**

Bloom's Lev	vel of Cognitive Task	Co	End Semester			
Diooni s Lev	er or cognitive rask	CLA-1 20%	Mid-1 20%	CLA-2 20%	CLA-3 20%	Exam (50%)
Level 1	Remember					
Level 1	Understand					
Level 2	Apply					
Level 2	Analyse					
Level 3	Evaluate					
Level 3	Create					
	Total					

# **Recommended Resources**

1. Enter Data

# **Other Resources**

1. Enter Data

# **Course Designers**

1. Enter Data

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### Project-II

Course Code	CHE 511	Course Category	Dissertation	n / Project (P)	L	Т	P	C
Course Code	CHE 311	Course Category	Dissertation	17 110/2001 (1)	0	0	14	14
Pre-Requisite Course(s)		Co-Requisite Course(s)						
Course Offering Department	Chemistry	Professional / Licensing Standards						

# Course Objectives / Course Learning Rationales (CLRs)

- Master advanced laboratory techniques relevant to their area of study.
- > Develop the ability to design and execute independent research projects.
- > Critically review existing literature to identify research gaps and propose new directions.
- > Effectively communicate research findings through written and oral presentations.

## Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Mastery of complex laboratory techniques.	5	<b>75</b> %	70%
Outcome 2	Competence in designing and executing research	5	75%	70%
Outcome 3	Ability to identify gaps and propose innovative solutions	3	<b>75</b> %	70%
Outcome 4	Clear presentation of findings to diverse audiences	5	<b>70</b> %	65%

		Program Learning Outcomes (PLO)													
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	3	3	3	3				3			2	3	2	3
Outcome 2	3	3	3	3	2				2			3	3	3	3
Outcome 3	3	3	3	3	2				3			3	3	3	3
Outcome 4	3	3	3	3	3				3			3	3	3	3
Outcome 5	3	3	3	3	3				3			3	3	3	3
Outcome 6	3	3	3	3	3				3			3	3	3	3
Average	3	3	3	3	2				3			3	3	3	3

Unit No.	Syllabus Topics	Required Contact hours	CLOs Addressed	References Used
Unit 1	Research problem and project selection	50 hours		
	Based on interest conceive an idea	25 hours	1,4	1
	Do a feasibility check of the project	25 hours	1,4	1
Unit 2	Literature review and methodology refinement	50 hours		
	Literature survey of the related works	25 hours	2	3,4,5,7
	Write an abstract of the proposed idea	25 hours	2	1
Unit 3	Data collection and analysis	270 hours		
	Hands-on data collection using chosen methodologies	200 hours	3	1,2, 3
	Ongoing meetings with a faculty advisor to discuss progress	70 hours	3	1,6,7
Unit 4	Oral presentation, evaluation, and publish results	50 hours		
	Evaluation of written reports and oral presentation	25 hours	3	1, 7
	Initiation of the process for a possible publication	25 hours	5	2,3,4,5,7
	Total		420 Hours	

#### Learning Assessment

		Continu	End Semester Exam (50%)		
Bloom's I	Level of Cognitive Task	Experiments (20%)	Record / Observation Note (10%)	Viva + Model (20%)	(**,*)
Level 1	Remember				
	Understand				
Level 2	Apply	70%	70%	70%	70%
Level 2	Analyse				
Lovel 2	Evaluate	30%	30%	30%	30%
Level 3	Create				
	Total	100%	100%	100%	100%

# **Recommended Resources**

- 1. As recommended by Advisor pertaining to student research interest
- 2. https://pubs.acs.org/
- 3. https://www.sciencedirect.com/
- 4. www.springer.com
- 5. https://onlinelibrary.wiley.com/
- 6. Research Methodology
- 7. Reading assignment related to undergraduate project as guided by faculty

# **Other Resources**

# **Course Designers**

1. Dr. J. P. Raja Pandiyan, Assistant Professor, SRM University – AP, Dr. K. Narayanaswamy, Assistant Professor, SRM University – AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



## **Instrumental Methods of Analysis**

Course Code	CHE 631	Course Category	Inorganic C	Chemistry	_	1 3	T 0	P 1	<b>C 4</b>
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)		'			
Course Offering Department	Chemistry	Professional / Licensing Standards			•				

## Course Objectives / Course Learning Rationales (CLRs)

- > Develop a comprehensive understanding of advanced spectroscopic and chromatographic techniques.
- > Learn skills in spectral interpretation for various compounds and understand different measurement modes and enhancements in spectroscopy.
- Enhance practical skills and problem-solving abilities in analytical chemistry

# Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Understand the basic principles, instrumentation, and applications of NMR, mass spectrometry, IR, Raman spectroscopy, HPLC, GC, and other analytical techniques.	2	70%	65%
Outcome 2	Explain the theoretical foundations of various spectroscopic and chromatographic methods, including the gyromagnetic ratio, chemical shift, nuclear coupling, ionization methods, molecular vibrations, and chromatographic separation principles.	3	80%	75%
Outcome 3	Utilize techniques learned in the course to interpret and analyzes NMR spectra, IR and Raman spectra, mass spectra, and chromatograms	4	75%	70%
Outcome 4	Compare and contrast different analytical methods and their suitability for various applications, including industrial and environmental analysis.	4	70%	60%

		•	,												
		Program Learning Outcomes (PLO)													
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	3	2	2	2	2	1	3	2	2			3	2	2
Outcome 2	3	3	2	2	2	2	1	2	1	2			2	3	3
Outcome 3	3	3	2	3	3	3	1	2	1	3			2	1	3
Outcome 4	3	3	3	3	3	3	3	3	2	3			1	3	1
Average	3	3	2	2	3	3	1	2	2	3			2	2	2

Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
	Nuclear Magnetic Resonance (NMR) and Mass Spectrometry-Basic principles of nuclear magnetic resonance: gyromagnetic ratio, chemical shift, nuclear coupling.	2	1	1,2
	Instrumentation, Two-Dimensional Fourier Transform NMR	2	1	1,2
Unit No.	Elucidation of NMR spectra, multi-pulse and multidimensional NMR.	2	1	1,2
	Introduction to EPR spectroscopy, Principles of mass spectrometry	2	1	1,2
	Ionisation methods in mass spectrometry, instrumentation	2	1	1,2
	Its applications, correlation of mass spectra with molecular structure.	2	1	1,2
	Molecular Spectroscopy (IR and Raman Spectroscopy) - IR spectroscopy - Molecular vibrations, vibrational modes	1	2	1, 2, 3
	Theory of IR absorption, instrumentation	1	2	1, 2, 3
Ilmit	IR sources and transducers, sample preparation, spectral interpretation of typical compounds.	1	2	1, 2, 3
Unit No.	Different measurement modes (ATR, reflectance)	2	2	1, 2, 3
2	IR microscopy, and surface-enhanced IR absorption spectroscopy.	1	2	1, 2, 3
	Raman spectroscopy - Theory, instrumentation	1	2	1, 2, 3
	Applications of Raman spectroscopy	1	2	1, 2, 3
	Spectral interpretation of Raman spectra. Other types of Raman spectroscopy (SERS and TERS).	2	2	1, 2, 3
	High-Performance Liquid Chromatography and Gas Chromatography - Principle of HPLC, the scope of HPLC, instrumentation	2	3	3, 4
Unit	Mobile phase, stationary phase, applications of HPLC.	2	3	3, 4
No. 3	Integrating HPLC with other analytical techniques (LC-MS)	2	3	3, 4
	Principle of GC, plate theory of GC, instrumentation, headspace analysis, gas-solid chromatography	2	3	3, 4
	Integrating GC with other analytical techniques (GC-MS).	1	3	3, 4
TT	XPS, XRD, SEM, TEM - Principles, instrumentation	2	4	1,2,4
Unit No.	Application of XPS, XRD, SEM, and TEM techniques	2	4	1,2,4
4	SEM imaging modes, electron detectors	2	4	1,2,4
	High-resolution imaging.	2	4	1,2,4
	Industrial Analyzers and Thermo-analytical Methods- Industrial process analysers, methods based on bulk properties, online potentiometric analysers, chemical sensors.	1	5	3,4,5
Unit No.	Process gas chromatography, automatic chemical analysers, flow injection analysis, and environmental monitoring	2	5	3,4,5
5	Introduction to particle size analysis, dynamic light scattering, and laboratory robots.	2	5	3,4,5
	Thermogravimetric Analysis, Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), and microthermal analysis.	1	5	3,4,5
	Total Contact Hours	45 Hours		

#### Course Unitization Plan - Lab

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	References Used
1.	UV-visible spectroscopy for silver nanoparticle characterization	4	6	1,3
2.	Infrared spectroscopic measurements of solvents	4	6	1, 2, 3
3.	Raman spectroscopic measurement of polymers	4	6	1,3
	Thin-layer chromatography (TLC) dye separation	4	6	1,3
4.	Spectral analysis – NMR spectra	4	6	1, 3, 4
5.	Diffraction pattern analysis (XRD)	4	6	1,3
6.	Student's seminar on real-world applications	3	6	NA
	Total Contact Hours	30 Hours		•

## **Learning Assessment**

			Cor	ntinuous								
Bloom's Level of Cognitive Task		CLA-1 (10%)		CLA-2	CLA-2 (20%)		CLA-3 (10%)		rm (20%)	End Semester Exam (40%)		
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac	
Level 1	Remember	30	30	30	30	30	30	30	30	30	30	
	Understand											
Level 2	Apply	50	40	50	40	50	40	50	40	50	40	
Level 2	Analyse	30	40	30	40	30	40	30	40	50	40	
I1 2	Evaluate	20	30	20	30	20	30	20	30	20	20	
Level 3	Create	20	30	20	30	20	30	20	30	20	30	
Total		100	100	100	100	100	100	100	100	100	100	

#### **Recommended Resources**

- 1. Gary D. Christian, Purnendu K. Dasgupta, Kevin A. Schug, Analytical Chemistry, John Wiley & Sons, 7th Edition, 2013
- 2. S. M. Khopkar, Basic concepts of Analytical Chemistry, New Age International Publishers, 3rd Edition, 2008
- 3. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis, Cengage Learning, 7th Edition, 2017
- 4. Hobart H. Willard, Lynne L. Merritt, John A. Dean, Frank A. Settle, Instrumental Methods of Analysis, CBS Publishers, 7th Edition, 1996
- 5. Stanley Crouch, S.; Skoog; A, F. Holler; West, W, Fundamentals of Analytical Chemistry, Brooks/Cole, 9th Edition, 2013

#### **Other Resources**

1. Enter Data

#### **Course Designers**

1. Enter Data

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# **Industrial Chemistry**

Course Code	CHE 632	Course Category	Inorganic Chemistry	1 3	T 0	P 1	<b>C 4</b>
Pre-Requisite Course(s)		Co-Requisite Course(s)	Progressive Course(s)				
Course Offering Department	Chemistry	Professional / Licensing Standards					

#### Course Objectives / Course Learning Rationales (CLRs)

- Gain knowledge of various industrial processes involved in chemical manufacturing, including
- > synthesis, purification, and separation techniques.
- > Understand the principles of chemical reaction engineering and apply them to analyze and design chemical reactors for industrial processes.
- > Learn the principles of product development in chemical industries, including formulation, testing, scale-up, and commercialization of chemical products.
- Familiarize with various analytical techniques used in industrial chemistry for product characterization, process monitoring, and quality assurance.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Describe the industrial process of making hydrocarbons, fuels and industrial gases	3	80	85
Outcome 2	Understand the industrial scale production of acids, glasses, fertilizers	3	75	80
Outcome 3	Analyze and design various industrial catalytic process and chemical transformations	4	75	80
Outcome 4	Develop skills in understanding dyes, pigments and colouring agents and its applications	5	75	80
Outcome 5	Perform analytical and instrumental techniques used in industries.	5	75	80

	Program Learning Outcomes (PLO)														
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	2	1	1	1			1	2	1		2	2	1	1
Outcome 2	2	2	2	1	1	1		1	2	1		2	2	1	1
Outcome 3	2	2	2	2	1	1		1	2	1		2	2	1	1
Outcome 4	2	2	1	1	1			1	2	1		2	2	1	1
Outcome 5	2	2	1	1	1	1		1	2	1		2	2	1	1
Average	2	2	1	1	1	1	1	1	2	1		2	2	1	1

Course	Unitization Tian			
Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
	Industrial Organic Chemistry			
Unit No. 1	Primary raw materials from petroleum and natural gas; petroleum refining reactions; cracking and reforming processes-reaction mechanisms	3	1	1,2
	Chemicals derived from ethylene, propylene, C4 stream, and C6 aromatics	2	1	1,2
	Surface Active Agents, Detergents -Mechanism of detergent; cationic and anionic surfactants; non-ionic surfactants; household detergents	3	1	1,2
	Industrial Inorganic Chemical Technology			
Unit No. 2	Fuel and industrial gases – production and uses of producer gas, water gas, acetylene, natural gas, and LPG	2	2	1,2
	Liquefaction of gases- noble gases, carbon dioxide, hydrogen, oxygen, nitrogen	2	2	1,2
	Chloralkali industry – soda ash, caustic soda, chlorine; Chemicals from the sea- sodium chloride, magnesium chloride	2	2	1,2
	Acids and fertilisers- sulphuric acid – nitric acid – ammonia – nitrogenous fertilisers – phosphatic fertilisers	2	2	1,2
	Silicate industries – refractories – abrasives – ceramics – glass – cement, lime, gypsum	2	2	1,2
Unit No. 3	Industrial Catalysis			
	Type of catalyst - Homogeneous catalysis, Enzyme catalysis, Heterogenous catalysis	2	2,3	1,2
	Heterogenous Catalysis - Adsorption Isotherms, Physical Adsorption, and Chemisorption. Promoters and Catalyst Poisons	3	2,3	1,2
	Porous catalytic system - Zeolites, SM-5, MCM- 41, Mesoporous AIPO's, perovskites and spinels	2	2,3	1,2
	Alkylation, isomerisation, hydrogenation/ dehydrogenation, dehydrosulphurization, oxidation, metathesis, carbonylation, polymerisation	2	2,3	1,2
	Chemical reactors – Batch reactor – Flow reactor – Fixed bed, Fluidised bed and slurry reactor	2	2,3	1,2
Unit No. 4	Natural and synthetic dyes			
	Dyes: Classification of dyes - methyl orange, fluorescein, malachite green, alizarin, crystal violet, Phthalocyanines, Cyanine dyes and uses (both textile and non-textile)	7	4	3,4
	Reaction of dyes with fibers and water-fluorescent Brightening agents	3	4	3,4
	Pigments, Leather			
Unit No. 5	Pigments: Organic and Inorganic pigments-application and their uses in paints	3	4	3,4
	Leather: Basic principles in tanning and dyeing of leather, types of tanning (chrome and vegetable tanning)	3	4	3,4
Total	Contact Hours	45 Hours	-	

#### Course Unitization Plan - Lab

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	References Used
1.	Determination of surface area, pore size, and distribution of mesoporous materials by BET surface analyser	5	5	5,6
2.	Fractional distillation of hydrocarbons	5	5	5,6
3.	Determination of critical micelle concentration of a surfactant	5	5	5,6
	Applications of Spectrophotometry - Determination of the copper content in Brass alloy	5	5	5,6
4.	Synthesis and determination of fluorescence quantum efficiency of Perovskites nanocrystals	5	5	5,6
5.	Determination of Sucrose in sugar cane juice	5	5	5,6
6.	Determination of surface area, pore size, and distribution of mesoporous materials by BET surface analyser	5	5	5,6
Total	Contact Hours	30 Hours		

#### **Learning Assessment**

		Contin	Continuous Learning Assessments (60%)								mester
Bloom's Level of Cognitive Task		CLA-1	LA-1 (10%) CLA-2		-2 (20%) CLA-3 (10%)				Mid Term Exam (40		
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level 1	Remember	30%	30%	30%	30%	30%	30%	30%	30%	30%	30%
Level 1	Understand	30%	30 /0	30 /0	30%	30%		30%	30%		30%
Level 2	Apply	50%	40%	50%	40%	50%	40%	50%	40%	50%	40%
Level 2	Analyse		40 70	30 70	40 70	30 70	40 70	30 76	40%	30 70	40 70
Level 3	Evaluate	20%	30%	20%	30%	200/-	30%	20%	30%	20%	30%
Create		20 70	30 70	2070	30 70	20%	30 70	20 /0	30 /0	20 70	30 /0
Total	·	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%

#### **Recommended Resources**

- 1. Peter Wiseman, An Introduction to Industrial Organic Chemistry, 2nd Edition, Applied Science Publishers Ltd., London (1979).
- 2. BK. Sharma Industrial Chemistry, GOEL Publishing House (1991)
- 3. Physical and Chemistry applications of dye stuffs- F.P. Schafer, Springer-Veriag N.Y.1976.
- 4. Dyes and their intermediates Abraha, Pergamon Press, 1969.
- 5. Jens Hagen, Industrial catalysis, 2nd Edition, Wiley-VCH Verlag Gambh & Co, (2006).
- 6. J. A.Kent, (ed) Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi, (1997)

# **Other Resources**

#### **Course Designers**

- a) Dr. Balaji Babu, Assistant Professor, Department of Chemistry, SRM University AP
- b) Dr. Pardha S Maram, Associate Professor, Department of Chemistry, SRM University AP
- c) Professor V Subramanian, Professor, Department of Chemistry, IIT-Madras

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# **Environmental and Electroanalytical Techniques**

<b>Course Code</b>	CHE 633	Course Category	Inorganic Chemistry		1	L 3	T 0	P 1	<b>C 4</b>
Pre-Requisite Course(s)	CHE502 & CHE506	Co-Requisite Course(s)	NILL Progressive Course(s)						
Course Offering Department	Chemistry	Professional / Licensing Standards							

#### Course Objectives / Course Learning Rationales (CLRs)

- > Introduce the basic principles of electroanalytical chemistry and apply the techniques for making electrochemical devices.
- > Followed by applications in environmental sample analysis, quality assurance and quality control.
- > Through this course, the learner will know the various electrochemical devices and electroanalytical techniques to be applied in environmental analysis and device-making

#### **Course Outcomes / Course Learning Outcomes (CLOs)**

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Understands the importance of environmental analysis and its significance. Also, various sampling techniques of different environmental pollutants	1, 2	85%	80%
Outcome 2	Learn and apply the concepts of electrochemistry, able to explain the basic principles involved in redox reactions and titrations	3	85%	80%
Outcome 3	Demonstrate proficiency in using electrochemical equipment, gathering data, and analysing the results.  Interpret electrochemical data to draw meaningful conclusions	3	80%	75%
Outcome 4	Able to explain the underlying mechanisms that allow these devices to store and convert energy, highlighting the differences and similarities among them	2, 3	85%	80%
Outcome 5	Learn the principles involved in various electrochemical testing in environmental analysis. Demonstrate using these techniques to detect and measure contaminants in environmental samples, such as water, soil, or air.	3	85%	80%
Outcome 6	Apply classroom theory in making different metal oxides, using different synthesis methods and characterise the same. Collect the data, analyse and tabulate the results	4, 5	80%	75%

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# Course Articulation Matrix (CLO) to Program Learning Outcomes (PLO)

	Program Learning Outcomes (PLO)														
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self Directed and Life long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	2	1	1						2	1	2	2		
Outcome 2	2	3	3	1	2				2	2	2	2	2	1	
Outcome 3	3	3	3	2	1				1	2	1	2	2	2	
Outcome 4	2	2	2	2	2	1			2	2	2	2	2		
Outcome 5	2	2	2	2	1	1			1	2	1	2	2		
Outcome 6	3	3	3	2	3	2			2	2	2	3		2	2
Average	2	3	2	2	2	1			1	2	2	2	2	1	

Course	Unitization Plan	n ' 1		
Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
	Introduction to Environmental Chemistry			
	Overview of environmental analysis and its significance in environmental science.	2	1	1,2
Unit No.	Basic principles of sampling techniques and sample preparation methods.	2	1	1,2
1	Introduction to various environmental pollutants (e.g., heavy metals, microplastics, organic pollutants, nutrients) and their sources.	3	1	1,2
	Discussion on environmental regulations and standards.	2	1	1,2
	Fundamentals of Electrochemistry - Basic concepts include chemistry and electricity (Galvanic Cell)	2	2	2
Unit No.	standard electrode potentials, reference electrodes, indicator electrodes, and oxidation-reduction indicators	2	2	2
2	Nernst equation for the complete reaction.	2	2	2
	Redox reactions/titrations.	2	2	2
	Electroanalytical Techniques - Electrochemical instrumentation, potential sweep methods, controlled current techniques	2	3	2,3
Unit No.	Potentiometry, Voltammetry, bulk electrolysis, spectroelectrochemistry, and other coupled characterisation techniques.	3	3	2,3
3	Introduction to electrogravimetric analysis, Coulometry	2	3	2,3
	Amperometry, Votammetry and Karl Fischer Titration of H <sub>2</sub> O	3	3	2,3
Unit No.	Electrochemical Devices - Introduction to electrochemical energy conversion processes.	3	4	3, 6
4	Principles of energy storage and conversion mechanisms in batteries, supercapacitors, electrolysers, fuel cells, and solar cells.	2	4	3, 6

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Guntur District, Mangalagiri, Andhra Pradesh – 522240.



	Theory and principles of electrochemical impedance spectroscopy (EIS) for characterising electrochemical systems.	2	4	3, 6
	Voltammetric techniques for studying electrochemical reactions in energy devices.	3	4	3, 6
	Electroanalytical Techniques in Environmental Analysis			
Unit No.	Cyclic Voltammetry, chronoamperometry polarography, impedance spectroscopy, and its applications in environmental analysis.	3	5	4,5
5	Techniques for in-situ and ex-situ analysis of environmental samples.	3	5	4,5
	Quality assurance and quality control in environmental analysis.	2	5	4,5
	Total Contact Hours	45 Hours		

## Course Unitization Plan - Lab

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	Reference s Used
1.	Standard addition method for estimation of Ascorbic acid in fruit juice	5	6	6,7
2.	Determination of ascorbic acid in actual samples using Voltammetry and comparing results with traditional estimation method	5	6	6,7
3.	Electrochemical Impedence measurements (EIS) on Battery cathode and Carbon-based materials	5	6	6,7
4.	Water quality assessment - pH, TDS, DO, BOD, COD, TOC	5	6	6,7
5.	Fabrication of Li-ion coin cells and electrochemical characterisation	5	6	6,7
6.	Fabrication of a supercapacitor and electrochemical characterisation (both a three-electrode testing and a two-electrode testing)	5	6	6,7
	Total Contact Hours	30 Hours		

# **Learning Assessment**

	Contin	Continuous Learning Assessments (60%)								r Exam	
Bloom's Level of Cognitive Task		CLA-1	(10%)	(10%) CLA-2 (20%)		CLA-3 (10%)		Mid Term (20%)		(40%)	LAam
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level 1	Remember	30%	30%	30%	30%	30%	30%	30%	30%	30%	30%
Level 1	Understand	30%	30 /0	30 70	30 76	30 76	30 76	30 70			30 76
Level 2	Apply	50%	40%	50%	40%	50%	40%	50%	40%	50%	40%
Level 2	Analyse	30 76	40 70	30%	40 70	30%	40%	50%	40%		40 /6
Level 3	Evaluate	20%	30%	20%	30%	20%	30%	20%	30%	20%	30%
Create		2070	30 %	20 70	30 70	20 70	30 70	20 /0	30 /0	20 /0	30 /0
Total		100%	100%	100%	100%	100%	100%	100%	100%	100%	100%

#### **Recommended Resources**

- 1. S.S. Dara, Environmental Chemistry and Pollution Control, S. Chand
- 2. Instrumental analysis of pollutants edited by C.N. Hewitt, Elsevier Applied Science
- 3. Allen J. Bard, Larry R. Faulkner, Henry S. White, Electrochemical Methods, Fundamentals and Applications, Wiley, 3rd Edition, 2022
- 4. S. M. Khopkar, Basic Concepts of Analytical Chemistry, New Age International Publishers, 3rd Edition, 2008
- 5. Gary D. Christian, Purnendu K. Dasgupta, Kevin A. Schug, Analytical Chemistry, John Wiley & Sons, 7th Edition, 2013
- 6. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis, Cengage Learning, 7th Edition, 2017
- 7. Hobart H. Willard, Lynne L. Merritt, John A. Dean, Frank A. Settle, Instrumental Methods of Analysis, CBS Publishers, 7th Edition

#### **Other Resources**

#### **Course Designers**

- 1. Internal (Institutional) Subject Matter Experts Prof. C.P Rao, Sr Professor, SRM University AP
- 2. Dr. Pardha Saradhi Maram, Associate Professor, SRM University AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



### **Advanced Quantum Chemistry**

Course Code	CHE 634	Course Category	Core		T 0	P 0	<b>C</b>
Pre-Requisite Course(s)	CHE 504	Co-Requisite Course(s)	Progressive Course(s)				
Course Offering Department	Chemistry	Professional / Licensing Standards					

#### Course Objectives / Course Learning Rationales (CLRs)

- > Understand the fundamental principles of group theory.
- > Understand post-HF methods, including configuration interaction (CI) and coupled cluster (CC) methods.
- > Learn the principles of basis sets and their impact on the accuracy of quantum chemical calculations.
- > Learn specific quantum algorithms, such as the variational quantum eigensolver (VQE), for solving quantum chemistry problems.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Demonstrate group theory concepts and their applications in analysing molecular symmetry and selection rules.	2	80	85
Outcome 2	Comprehend the principles of Hartree-Fock theory and various post-HF methods, including CI and CC methods.	2	75	80
Outcome 3	Choose and understand the impact of basis sets on the accuracy of quantum chemical calculations.	3	75	80
Outcome 4	Understand the basics of quantum computing and apply quantum algorithms to solve problems in quantum chemistry.	2	75	80

					Pro	ogram L	earning	g Outco	mes (PI	.O)					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	2	2	1	2	2	3	1	2	2	2	1	2		
Outcome 2	1	2	2	1	2	2	3	1	2	2	2	1	2		
Outcome 3	2	2	2	2	2	2	3	1	3	2	2	1		2	2
Outcome 4	2	2	2	2	3	3	3	1	3	2	2	1		2	2
Average	2	2	2	2	2	2	3	1	3	2	2	1	2	2	2

TT*1	Chication I fan	Required	CI O-	D - (
Unit No.	Syllabus Topics	Contact Hours	CLOs Addressed	References Used
Unit	Introduction to Group Theory: Symmetry elements and operations, group axioms and examples of groups, group representations.	4	1	1
No.	Molecular symmetry and point groups, character tables and great orthogonality theorem.	4	1	1
	Applications of character tables in predicting IR-active and Raman active vibrational modes.	4	1	1
	HF and Post HF methods: Molecular Hamiltonian, BO approximation, Mean Field theory, LCAO approximation, Roothaan's equations	3	2	2
Unit	self-consistent field theory, Slater determinants, anti- symmetrization of wavefunction, Pauli exclusion principle	3	2	2
No. 2	Koopman's theorem, Open-shell and Closed-shell systems (UHF vs ROHF), spin contamination.	3	2	2
	Configuration Interaction Models, Multi Configurational Interaction models, choice of active space,	2	2	2
	Møller-Plesset perturbation theory, and Coupled Cluster Models, Size Consistency and Extensivity.	1	2	2
***	Basis Sets: Single center and multi center expansions, Slater- type orbitals, split-valence basis sets.	4	3	2,3
Unit No.	Gaussian-type orbitals, primitive and contracted basis sets, Polarization and Diffuse functions.	4	3	2,3
	Effective Core Potential (ECP); Pople's Notation, Basis set superposition Error (BSSE) – Counterpoise Correction.	4	3	2,3
	Density Functional Theory (DFT): Electron density and its importance, Hohenberg-Kohn theorems, Kohn-Sham formalism of DFT, density functional approximations (DFAs).	3	2	4
Unit No. 4	Local density approximation (LDA) and generalized gradient approximation (GGA), pure and hybrid functionals.	3	2	4
4	Meta GGA and double hybrids, Jacob's ladder, comparison of the accuracy and computational cost of different exchange-correlation functionals	3	2	4
	Introduction to TD-DFT in modeling electronic excited states	3	2	4
I Imit	Quantum Chemistry using Quantum Computers: Basics of quantum computing: Quantum states and measurements	4	4	5
Unit No. 5	Quantum superposition and entanglement, quantum gates and circuits, quantum phase estimation algorithm	4	4	5
	Variational quantum eigensolver (VQE) algorithm and its application to simulate small molecules.	4	4	5
	Total Contact Hours	60		

#### **Learning Assessment**

			Cor		End Semester						
Bloom's	Bloom's Level of Cognitive Task		CLA-1 (20%)		CLA-2 (20%)		A-3 (%)	Mid Term (0%)		Exam (40%)	
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level 1	Remember	50%	0	25%	0	25%	0	0	0	30%	0
Level 1	Understand	3070		2370	U	2370	U	U	U	3070	U
Level 2	Apply	25%	0	50%	0	25%	0	0	0	40%	0
Level 2	Analyse	2370	U	50%		25%	0	0	0	4070	U
Level 3	Evaluate	25%	0	25%	0	50%	0	0	0	30%	0
Level 3	Create	2370	0	25%	U	3070	0	U	0	3070	U
	Total	100	0	100	0	100	0	0	0	100	0

#### **Recommended Resources**

- 1. F. A. Cotton, Chemical applications of group theory, 3rd ed., John Wiley & Sons, 2017, ISBN: 978-8126519255
- 2. Szabo, and N. S. Ostlund, Modern quantum chemistry: Introduction to advanced electronic structure theory, 2nd ed., Dover Publications, 1996, ISBN: 978-0486691862.
- 3. T. Helgaker, P. Jørgensen, J. Olsen, Molecular Electronic-Structure Theory, 1st ed., John Wiley & Sons, 2000, ISBN: 978-1119019572.
- 4. W. Koch, M. C. Holthausen, A Chemist's Guide to Density Functional Theory, 2nd ed., Wiley-VCH Verlag GmbH, 2001, ISBN: 978-3527303724
- 5. T. Wong, Introduction to quantum computing, 4th ed., Rooted Grove, 2023, ISBN: 979-8985593105

#### **Recommended Online Resources**

6. R. G. Parr and W. Yang, Density-functional theory of atoms and molecules, 1st ed., Oxford University Press, 1989, ISBN: 978-0195092769.

#### **Other Resources**

## **Course Designers**

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



## **Molecular Modelling and Simulations**

Course Code	CHE 635	Course Category	Core	1. 2	T 0	P 2	<b>C 4</b>
Pre-Requisite Course(s)	CHE 504	Co-Requisite Course(s)	Progressive Course(s)	·			
Course Offering Department	Chemistry	Professional / Licensing Standards					

#### Course Objectives / Course Learning Rationales (CLRs)

- > Understand the fundamentals of molecular modelling in the context of chemistry.
- Learn the concept of potential energy surfaces in molecular systems and explore molecular properties in different phases, with a focus on the condensed phase (liquids and solids).
- > Learn how to set up and run molecular dynamics simulations for various molecular systems

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Demonstrate proficiency in various molecular modeling techniques, including molecular mechanics, docking studies, and quantum mechanics, understanding their principles and applications.	2	85%	75%
Outcome 2	Set up and run molecular dynamics simulations for different molecular systems, demonstrating competence in understanding simulation parameters and conditions.	3	85%	85%
Outcome 3	Develop strong skills in analyzing and interpreting results from molecular dynamics simulations, including the identification of molecular motion, conformational changes, and thermodynamic properties.	3	80%	75%
Outcome 4	Apply molecular modeling and simulation techniques to address real-world problems in chemistry and biology, showcasing their ability to use computational methods for practical research applications.	4	75%	85%
Outcome 5	Demonstrate an understanding of how molecular modeling and simulations can be integrated with experimental techniques, recognizing the synergies between computational predictions and experimental observations.	4	75%	85%

# SRM University *AP*, Andhra Pradesh Neerukonda, Mangalagiri Mandal,

Guntur District, Mangalagiri, Andhra Pradesh – 522240.



					Pr	ogram L	earning	g Outco	mes (PI	<b>.O</b> )					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self Directed and Life long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	2	2	2	1	2	2	3	1	2	2	2	1	2		
Outcome 2	1	2	2	1	2	2	3	1	2	2	2	1	2		
Outcome 3	2	2	2	2	2	2	3	1	3	2	2	1		2	2
Outcome 4	2	2	2	2	3	3	3	1	3	2	2	1		2	2
Outcome 5	2	2	2	2	3	3	3	1	3	2	2	1		2	2
Average	2	2	2	2	2	2	3	1	3	2	2	1	2	2	2

No.   Syllabus lopics   Contact Hours   Addressed   Used	Unit		Required	CLOs	References
Theory, Models, and Computation; Overview of Classical and Quantum Mechanical Methods.  No. Classical and Quantum Mechanical Methods.  Accuracy, cost and efficiency; Coordinate systems: Cartesian and Internal Coordinates.  Bond lengths, bond angles and torsion angles; Writing Z-matrix for small molecules.  Potential Energy Surfaces: Equilibrium points - Local and Global minima; energy minimization and geometry optimization techniques  Vibrational frequencies, Characterizing stationary Vibrational frequencies, Characterizing reaction coordinates, Calculations of reaction mechanism using computational chemistry, intrinsic reaction of coordinates, Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Molecular Interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis, of active sites in proteins, modelling protein and ligand interactions by t		Syllabus Topics	_		
Unit Classical and Quantum Mechanical Methods.  Accuracy, cost and efficiency; Coordinate systems:  Cartesian and Internal Coordinates.  Bond lengths, bond angles and torsion angles; Writing Z-matrix for small molecules.  Potential Energy Surfaces: Equilibrium points - Local and Global minima; energy minimization and geometry optimization techniques  Vibrational frequencies, Characterizing stationary points, First order and second order saddle points.  No.  Conformational search, Concept of transition state with examples: SNP reactions, Diels-Alder Reactions.  Predicting the reaction mechanism using computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electron density, Properties Related to Charge Distribution: Electric multipole moments, and the condensed Phases.  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecular interactions of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis, dactive sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dopamics Simulations and Analysis:  Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adi		Introduction to Molecular Modelling: Definitions of			
No.   Accuracy, cost and efficiency; Coordinates systems:   2		Theory, Models, and Computation; Overview of	2	1	1
Cartesian and Internal Coordinates.   2	Unit	Classical and Quantum Mechanical Methods.			
Cartesian and Internal Coordinates.   2			2	1	1.2
Writing Z -matrix for small molecules.   2	1				1,2
Potential Energy Surfaces: Equilibrium points — Local and Global minima; energy minimization and geometry optimization techniques  Vibrational frequencies, Characterizing stationary points, First order and second order saddle points.  No. Conformational search, Concept of transition state with examples: SNP reactions, Diels-Alder Reactions.  Predicting the reaction mechanism using computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Unit No. 4  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics and non-adiabate molecular dynamics and non-adiabate molecular dynamics and non-adiabate molecular			2	1	1.2
Local and Global minima; energy minimization and geometry optimization techniques  Vibrational frequencies, Characterizing stationary points, First order and second order saddle points.  Conformational search, Concept of transition state with examples: SN² reactions, Diels-Alder Reactions.  Predicting the reaction mechanism using computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Unit No.  4 Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies:  Unit No.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics		_	_	_	_,_
geometry optimization techniques  Vibrational frequencies, Characterizing stationary points, First order and second order saddle points.  Conformational search, Concept of transition state with examples: SN² reactions, Diels-Alder Reactions.  Predicting the reaction mechanism using computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of an intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis, Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics and non-adiabatic molecu			_	_	
Vibrational frequencies, Characterizing stationary points, First order and second order saddle points.			1	2	1,2
Unit No. Conformational search, Concept of transition state with examples: SN² reactions, Diels-Alder Reactions.  Predicting the reaction mechanism using computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electros density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis, Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies:  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics and non-adiabatic molecular dynamics and no					
No.   Conformational search, Concept of transition state with examples: SN² reactions, Diels-Alder Reactions.	T7 **	-	1	2	1,2
with examples: SN² reactions, Diels-Alder Reactions.  Predicting the reaction mechanism using computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron densitry, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis, Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies:  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics					
Reactions.  Predicting the reaction mechanism using computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis, Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Unit No.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics and non-adiabatic molecular dynamics and non-adiabatic molecular dynamics and non-adiabatic molecular dynamics		-	2	2	1.2
Predicting the reaction mechanism using computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics and an analysis and non-adiabatic molecular dynamics and an analysis and analysis analysis and analysis analysis analysis and analysis analysis analysis and analysis analysis analysis analysis and analysis analysis analysis analysis analysis	2	•	2	2	1,4
computational chemistry, intrinsic reaction coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Molecular Dynamics Simulations and Analysis:  Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics					
coordinates. Calculations of reaction energies.  Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis, Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Unit Molecular Dynamics Simulations and Analysis:  Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Total Charge 2  3 1,2  3 1,2  3 1,2  4 1,2  4 1,2  1 4 1,2  1 4 1,2  1 4 1,2  1 5 3 1 3 1,2  1 5 3 1 3 1,2  1 6 1 1 2 1 3 1,2  1 7 1 1 3 1,2  1 7 1 1 1 1 3 1,2  1 7 1 1 1 1 3 1,2  1 7 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		8	2	2	12
Molecular Properties and the Condensed Phase: The electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Limitations and challenges in molecular docking studies.  Dimit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics and non-adiabatic molecular dynamics of an active interaction to a properties of molecular dynamics and non-adiabatic molecula		-	_	_	1,2
electron density, Properties Related to Charge Distribution: Electric multipole moments, electrostatic potential maps.  Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis, Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Limitations and challenges in molecular docking studies.  Initroduction to ab initio molecular dynamics and non-adiabatic molec					
Distribution: Electric multipole moments, electrostatic potential maps.  No. Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Unit Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Time the partition of the moments, and the protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protei		-	_	_	
Unit No. Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Atomic charge partition schemes, characterization of 2  3 1,2  3 1,2  4 1,2  4 1,2  4 1,2  5 3 3 1,2  1 4 1,2  1 4 1,2  1 4 1,2  1 5 3 1 3 1,2  1 6 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 1 2 1 1 1 1 2 1		, -	2	3	1,2
No. Atomic charge partition schemes, characterization of intermolecular interactions, Implicit Models for Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies:  Unit Molecular Dynamics Simulations and Analysis:  Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Atomic Molecular Dynamics Simulations and Analysis:  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1	Unit	_			
Condensed Phases  Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Unit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Total Carlottion of molecular dynamics and non-adiabatic molecular dynamics of an analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Introduction to ab initio molecular dynamics and non-adiabatic molecular	No.				
Strength and weakness of Continuum solvation models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Unit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1	3	intermolecular interactions, Implicit Models for	2	3	1,2
models.  Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, onsembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Total Case studies and analysis and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Total Case studies and analysis anal		Condensed Phases			
Case studies related evaluation of molecular properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Transport of molecular dynamics and analysis and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Introduction to ab initio molecular dynamics and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Introduction to ab initio molecular dynamics and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Introduction to ab initio molecular dynamics and analysis of active sites in proteins, modelling protein and active sites in proteins, modelling protein and analysis of active sites in proteins, modelling protein and active sites in proteins, and analysis of active sites in proteins, modelling protein and analysis of active sites in proteins, and analysis of active sit		Strength and weakness of Continuum solvation	1	3	1.2
properties (ionization potentials, electronic affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Unit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1		models.	1	3	1,2
affinities, excited state energies) of small molecules in the gas phase and solvent phase.  Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization Van der Waals and electrostatic interactions, conformational analysis, Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  3 1,2  4 1,2  1,2  4 1,2  5 3		Case studies related evaluation of molecular			
Unit No. 4  Unit No. 4  Unit No. 4  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Unit No. 4  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  3  3  5  3		• •	1	3	1.2
Molecular Mechanics and Docking Studies: Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis: Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Total A 1,2  1,2  4 1,2  4 1,2  5 3		3 ,	_		_,_
Overview of molecular mechanics, force fields and their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Basic principles of molecular dynamics simulations, No. ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1					
their parameters, energy minimization  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Basic principles of molecular dynamics simulations, No. ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  their parameters, energy minimization  1		9	_	_	
Unit No. 4  Van der Waals and electrostatic interactions, conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Unit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  3		-	1	4	1,2
Conformational analysis,  Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Unit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1					
Molecular Docking, identification and analysis of active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Unit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1	Unit		1	4	1,2
active sites in proteins, modelling protein and ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Unit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1	No.	-			
ligand interactions by taking few case studies.  Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Unit Basic principles of molecular dynamics simulations, one ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1 4 3  3 5 3	4	•	3	4	2
Limitations and challenges in molecular docking studies.  Molecular Dynamics Simulations and Analysis:  Unit Basic principles of molecular dynamics simulations, ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  1 4 3  5 3			3	<b>T</b>	3
studies.  Molecular Dynamics Simulations and Analysis: Unit Basic principles of molecular dynamics simulations, No. ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  3  5  3					
Molecular Dynamics Simulations and Analysis: Unit Basic principles of molecular dynamics simulations, No. ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  3  5  3			1	4	3
Unit No. ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  Basic principles of molecular dynamics and anon-adiabatic molecular dynamics  3  5  3  5  3					
No. ensembles  Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics  3  5  3	Unit		3	5	3
5 Introduction to ab initio molecular dynamics and non-adiabatic molecular dynamics 3 5 3					
non-adiabatic molecular dynamics			•	_	2
Total Contact Hours 30		-	3	5	3
		Total Contact Hours	30		1

#### Course Unitization Plan - Lab

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	References Used
1.	Building three dimensional models of complex molecules using graphical user interface.	5	1	1,2
2.	Carrying out conformational analysis of amino acids and oligomers.	4	2	1,2
3.	Predicting and analysing vibrational frequencies	4	3	1,2
4.	Locating the transition state and identifying the reaction mechanism of simple nucleophilic substitution and Diels-Alder reactions.	4	3	1,2
5.	Evaluation of molecular properties of small molecules.	4	3	1,2
6.	Predicting the aromaticity in organic compounds.	4	3	1,2
7.	Modeling of protein and ligand interactions using molecular docking studies.	5	4,5	2,3
	Total Contact Hours	30 Hours		

#### **Learning Assessment**

			Co		End Semester Exam						
Bloom's Level of Cognitive Task		CLA-1 (10%)		CLA-2 (20%)		CLA-3 (10%)		Mid Term (20%)		(40%)	
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level 1	Remember	30%	30%	30%	30%	30%	30%	30%	30%	30%	30%
20,011	Understand			2070	2070	2070		2070	5070	50,0	2070
Level 2	Apply	50%	40%	50%	40%	50%	40%	50%	40%	50%	40%
LCVCI Z	Analyse	3070	4070	3070		3070	4070	3070	4070	3070	4070
Level 3	Evaluate	20%	30%	20%	30%	20%	30%	20%	30%	20%	30%
Level 3	Create	2070	3070	2070	3070	2070	3070	2070	3070	2070	3070
	Total	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%

#### **Recommended Resources**

- 1. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd ed., John Wiley and Sons, 2004, ISBN: 978-1-118-71227-6
- 2. R. Leach, Molecular Modelling: Principles and Applications, 2nd ed., Pearson, 2001, ISBN: 978-0582382107.
- 3. J. M. Haile, Molecular Dynamics Simulations: Elementary Methods, 1st ed., John Wiley & Sons, 1997, ISBN: 978-0471184393
- 4. D. C. Young, Computational Drug Design: A Guide for Computational and Medicinal Chemists, 1st ed., Wiley-Interscience, 2009, ISBN: 978-0470126851

## **Other Resources**

1. Enter Data

## **Course Designers**

1. Enter Data

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### Data Science and Machine Learning in Chemistry

Course Code	CHE 636	Course Category	Core		2	T 0	P 2	<b>C 4</b>
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)		1		
Course Offering Department	Chemistry	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- > Students will be able to apply Python programming skills to solve computational problems in chemistry.
- > Students will be able to explain the applications of LU and Cholesky decompositions in Hartree-Fock theory.
- > Students will be able to utilize machine learning and optimization methods to solve chemical problems

# Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Apply Python programming skills to solve computational problems in chemistry.	4	85%	75%
Outcome 2	Explain the applications of LU and Cholesky decompositions in Hartree-Fock theory.	3	85%	85%
Outcome 3	Apply data normalization techniques to spectroscopic data.	4	80%	75%
Outcome 4	Apply numerical optimization techniques (gradient descent, conjugate gradient, Newton-Raphson, BFGS) using SciPy.	4	75%	85%

					Pro	ogram L	earning	g Outco	mes (PI	<b>.O</b> )												
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral Multicultural and social Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3							
Outcome 1	2	2	2	1	2	2	3	1	2	2	2	1	2									
Outcome 2	1	2	2	1	2	2	3	1	2	2	2	1	2									
Outcome 3	2	2	2	2	2	2	3	1	3	2	2	1		2	2							
Outcome 4	2	2	2	2	3	3	3	1	3	2	2	1		2	2							
Average	2	2	2	2	2	2	3	1	3	2	2	1	2	2	2							

Unit No.  Syllabus Topics  Syllabus Topics  Clos Addressed Used  Used  Unit No.  Introduction to Python Programming: Introduction to Jupyter Notebook, data types and data structures.  Variables, operators, and control structures.  Variables, operators, and control structures.  Variables, operators, and control structures.  Vector Operations and Matrix Decompositions in Quantum Chemistry: Vector operations using Numpy: dot product and cross product of vectors.  Applications in quantum chemistry such as finding bond lengths, Applications in quantum chemistry such as finding bond lengths, and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming molecular orbitals,.  IU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory.  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping-binning, aggregation and filtering Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients.  Data Visualisation in Chemistry: Data visualisation using 1 4 3,4  Matplotitis:  Data Visualisation in Chemistry: Data visualisation using 1 4 3,4  Histograms and contour plots 1 4 3,4  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using 1 4 3,4  Machine Learning and Numerical Optimization energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.  Total Contact Hours 30			<b>D</b> 1 1	I	
No. Syllabus Topics Contact Hours Addressed Used Hours Notebook, data types and data structures.  1 Introduction to Python Programming: Introduction to Jupyter Notebook, data types and data structures.  2 1 1 1  Variables, operators, and control structures.  Functions, modules, and packages, classes and instances.  2 1 1 1  Vector Operations and Matrix Decompositions in Quantum Chemistry: Vector operations using Numpy: dot product and cross product of vectors.  Applications in quantum chemistry such as finding bond lengths, bond angles and dithedral angles in a molecule, Matrix operations No. and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming molecular orbitals.  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory.  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients.  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Data wisualisation in Chemistry: Data visualisation using Matplotlib:  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  No. Plotting spectroscopic data using line plots, Hotting spectroscopic data using line plots, Hotting spectroscopic data using line plots, Hotting spectroscopic data using line plots, Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and Matrix Decompson. Applications: linear regression in determining activation energy	Unit		Required	CLOs	References
Unit Notebook, data types and data structures.  Variables, operators, and control structures.  Variables, operators, and control structures.  Vector Operations and Matrix Decompositions in Quantum Chemistry: Vector operations using Numpy: dot product and cross product of vectors.  Applications in quantum chemistry such as finding bond lengths, Applications in quantum chemistry such as finding bond lengths, Applications in quantum chemistry such as finding bond lengths, and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming and elecular orbitals.  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear rand logistic regression. Numerical optimisation using Applications: linear regression in desernations in development.		Syllabus Topics	Contact		
Notebook, data types and data structures.   2	140.		Hours	Hadressea	Osca
Notebook, data types and data structures.  Variables, operators, and control structures.  Functions, modules, and packages, classes and instances.  Vector Operations and Matrix Decompositions in Quantum Chemistry: Vector operations using Numpy: dot product and cross product of vectors.  Applications in quantum chemistry such as finding bond lengths, bond angles and dihedral angles in a molecule, Matirx operations and decompositions using Numpy: matrix multiplication.  2 Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming molecular orbitals,.  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory.  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  No.  Plotting spectroscopic data using line plots,  Histograms and contour plots  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and Spellor a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.	TT *1	Introduction to Python Programming: Introduction to Jupyter	2	1	1
Tunctions, modules, and packages, classes and instances.  Vector Operations and Matrix Decompositions in Quantum Chemistry: Vector operations using Numpy: dot product and cross product of vectors.  Applications in quantum chemistry such as finding bond lengths, bond angles and dihedral angles in a molecule, Matirx operations and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2		Notebook, data types and data structures.	2	1	1
Vector Operations and Matrix Decompositions in Quantum Chemistry: Vector operations using Numpy: dot product and cross product of vectors.  Applications in quantum chemistry such as finding bond lengths, bond angles and dihedral angles in a molecule, Matrix operations bond angles and dihedral angles in a molecule, Matrix operations and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2		Variables, operators, and control structures.	2	1	1
Vector Operations and Matrix Decompositions in Quantum Chemistry: Vector operations using Numpy: dot product and cross product of vectors.   Applications in quantum chemistry such as finding bond lengths, bond angles and dihedral angles in a molecule, Matirx operations and decompositions using Numpy: matrix multiplication.   I	1	Functions, modules, and packages, classes and instances.	2	1	1
Chemistry: Vector operations using Numpy: dot product and cross product of vectors.  Applications in quantum chemistry such as finding bond lengths, bond angles and dihedral angles in a molecule, Matirx operations and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2					
product of vectors.  Applications in quantum chemistry such as finding bond lengths, bond angles and dihedral angles in a molecule, Matirx operations  no. and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming molecular orbitals,  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplottib:  1 4 3,4  Plotting spectroscopic data using line plots,  Histograms and contour plots  1 4 3,4  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimization using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  5 Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		•	1	2	2
Applications in quantum chemistry such as finding bond lengths, bond angles and dihedral angles in a molecule, Matirx operations and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2					
Unit No. and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming molecular orbitals.  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory.  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots,.  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning and Numerical Optimization in Chemistry: Supervised learning and Numerical Optimization in Chemistry: Supervised learning and Numerical Optimization using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear aregression in dose-response relationships in drug development.		•			
No. and decompositions using Numpy: matrix multiplication.  Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming molecular orbitals,.  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  No. Plotting spectroscopic data using line plots,  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.	Ilmit		1	2	2
Finding eigenvalues and eigenvectors of a matrix, unitary transformations and their applications in transforming molecular orbitals,.  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots, Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		-	1	_	2
transformations and their applications in transforming molecular orbitals,  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients.  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots,  Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots.  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.					
molecular orbitals,.  LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots, Plotting conductometry and potentiometry data using scatter plots,. Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.	2				•
LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots, Plotting conductometry and potentiometry data using scatter plots, Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.			2	2	2
Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots,  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using  Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		•			
Hartree-Fock theory  Data Manipulation and Analysis in Chemistry: Data pre-processing using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients.  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots, Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.			2	2	2
using Pandas module: normalisation and standardisation of data, application in normalising absorbance and emission intensities.  Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots, Plotting conductometry and potentiometry data using scatter plots, Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		<u> </u>	_	_	_
Unit No. 3					
Data manipulation and analysis using Pandas: indexing, grouping, binning, aggregation and filtering  Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  1 4 3,4  Plotting spectroscopic data using line plots, 1 4 3,4  Plotting conductometry and potentiometry data using scatter plots, 3 4 3,4  Histograms and contour plots 1 4 3,4  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		using Pandas module: normalisation and standardisation of data,	2	3	3,4
No. 3 binning, aggregation and filtering Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  Plotting spectroscopic data using line plots, Plotting conductometry and potentiometry data using scatter plots,. Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.	T Imit	application in normalising absorbance and emission intensities.			
Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  1 4 3,4  Plotting spectroscopic data using line plots, 4 Plotting conductometry and potentiometry data using scatter plots,. 4 Plotting conductometry and potentiometry data using scatter plots,. 5 Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and SFGS algorithms  5 Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		Data manipulation and analysis using Pandas: indexing, grouping,	2	2	2.4
Statistical measures: Normal distribution, mean, standard deviation, variance, standard error, Pearson and Spearman correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  No. Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots,  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		binning, aggregation and filtering	2	3	3,4
correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  No. Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots,  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using  Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No.  BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.	3	Statistical measures: Normal distribution, mean, standard			
correlation coefficients  Data Visualisation in Chemistry: Data visualisation using Matplotlib:  No. Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots,  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using  Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No.  BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		deviation, variance, standard error, Pearson and Spearman	2	3	3,4
Unit Matplotlib:  No. Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots,.  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		_			
Unit Matplotlib:  No. Plotting spectroscopic data using line plots,  Plotting conductometry and potentiometry data using scatter plots,.  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.		Data Visualisation in Chemistry: Data visualisation using			
No. Plotting spectroscopic data using line plots,  4 Plotting conductometry and potentiometry data using scatter plots,.  5 Histograms and contour plots  6 Machine Learning and Numerical Optimization in Chemistry:  6 Supervised learning algorithms using sci-kit learn module: linear,  7 nonlinear and logistic regression. Numerical optimisation using  8 Scipy: gradient descent, conjugate gradient, Newton-Raphson, and  8 No. BFGS algorithms  7 Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.	Unit	•	1	4	3,4
Plotting conductometry and potentiometry data using scatter plots,.  Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.			1	4	3.4
Histograms and contour plots  Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.					
Machine Learning and Numerical Optimization in Chemistry: Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.	-				
Supervised learning algorithms using sci-kit learn module: linear, nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.				<b>T</b>	3,4
nonlinear and logistic regression. Numerical optimisation using Scipy: gradient descent, conjugate gradient, Newton-Raphson, and No. BFGS algorithms Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.  3 4 3,4,5					
Unit Scipy: gradient descent, conjugate gradient, Newton-Raphson, and BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.  3 4 3,4,5			2	4	0.45
No. BFGS algorithms  Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.  3 4 3,4,5	** •.		3	4	3,4,5
Applications: linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.  3 4 3,4,5		, , ,			
a reaction, and molar extinction coefficient in Beer-Lambert law, nonlinear regression in dose-response relationships in drug development.					
nonlinear regression in dose-response relationships in drug development.	5				
development.			3	4	3.4.5
-				_	<i>2,1,0</i>
Total Contact Hours 30		•			
		Total Contact Hours	30		

#### Course Unitization Plan - Lab

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	Reference s Used	
1.	Applications of dot product and cross products in quantum chemistry such as finding bond lengths, bond angles and dihedral angles in a molecule.	5	1	1,2	
2.	Unitary transformations and their applications in transforming molecular orbitals, LU and LR (Cholesky) decompositions and their applications in Hartree-Fock theory.	4	2	1,2	
3.	Normalisation and standardisation of data, application in normalising absorbance and emission intensities.	4	3	1,2	
4.	Mean, SD and variance calculations.	4	3	1,2	
5.	Plotting Spectroscopic data using line plots, plotting conductometry and potentiometry data using scatter plots.	4	3	1,2	
6.	Linear regression in determining activation energy of a reaction, and molar extinction coefficient in Beer-Lambert law.	4	3	1,2,5	
7.	Nonlinear regression in dose-response relationships in drug development.	5	4,5	2,3,5	
	Total Contact Hours	s 30 Hours			

#### **Learning Assessment**

		Continuous Learning Assessments (60%)								- End Semester Exam		
Bloom's Level of Cognitive Task		CLA-1 (10%)		CLA-2	CLA-2 (20%)		CLA-3 (10%)		Term %)	(40%)		
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac	
Level 1	Remember	30%	30%	30%	30%	30%	30%	30%	30%	30%	30%	
Level I	Understand	3070		3070	3070	3070	3070	3070	3070	3070	3070	
Level 2	Apply	50%	40%	50%	40%	50%	40%	50%	40%	50%	40%	
Level 2	Analyse	3070	4070	3070	4070	3070	70/0	3070	7070	3070	40 / 0	
Level 3	Evaluate	20%	30%	20%	30%	20%	30%	20%	30%	20%	30%	
Level	Create	2070	3070	2070	3070	2070	3070	2070	3070	2070	3070	
Total		100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	

## **Recommended Resources**

- 1. J. VanderPlas, Python Data Science Handbook: Essential Tools For Working With Data, 1st ed., Shroff/O'Reilly, 2016, ISBN: 978-9352134915.
- 2. G. Strang, Introduction to Linear Algebra, 5th ed., Wellesley-Cambridge Press, 2016, ISBN: 978-0980232776
- 3. L. N. Trefethen and D. Bau, Numerical Linear Algebra, 1st ed., siam, 1997, ISBN: 978-0898713619
- 4. P. E. Gill, W. Murray, and M. H. Wright, Practical optimization, 2nd ed., Academic Press, 1982, ISBN: 978-0122839528
- 5. A. Geron, Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems, 3rd ed., Shroff/O'Reilly, 2022, ISBN: 978-9355421982.

#### **Other Resources**

## **Course Designers**

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Advanced Organic Chemistry (Organometallics)**

Course Code	CHE 637	Course Category	Core	4	T 0	P 0	<b>C 4</b>
Pre-Requisite Course(s)		Co-Requisite Course(s)	Progressive Course(s)				
Course Offering Department	Chemistry	Professional / Licensing Standards					

#### Course Objectives / Course Learning Rationales (CLRs)

- > To equip students with a deep understanding of organometallic reagents and the mechanisms by which they react
- > To empower students to design new chemical reactions for forming carbon-carbon and carbon-heterobond.
- > To enable students to apply these methodologies for the synthesis of molecules with potential applications in pharmaceuticals, agrochemicals, and materials science

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Describe the fundamental concepts of organometallic chemistry, including bonding theories, structural features, and reactivity patterns	2	85%	80%
Outcome 2	Explain reaction mechanisms involving organometallic reagents	2	85%	80%
Outcome 3	Discuss the applications of metal-complexes in organic synthesis	3	85%	80%
Outcome 4	Explain and apply the concept of metathesis (RCM, ROM, CM, etc.) and its applications in organic synthesis using metal carbene catalysts.	3	85%	80%
Outcome 5	Demonstrate and design various metal-catalyzed reactions using latest synthetic methodology	3	85%	75%

		Program Learning Outcomes (PLO)													
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	2	2	2	2	2	1					2	3	1	2
Outcome 2	3	2	2	2	2	2	2					2	3	1	2
Outcome 3	3	2	3	3	3	2	1					3	3	3	2
Outcome 4	3	3	3	3	3	2	2					3	3	2	3
Outcome 5	3	3	3	3	3	2	2					3	3	2	3
Average	3	2	3	3	3	2	2					3	3	2	2

Unit No.	Syllabus Topics	Required Contact Hours	CLOs Addressed	References Used
	Concepts	14		
	Ligand systems: Classification of ligands as dative or covalent, neutral or anionic, even- or odd-electron, L-type or X-type.	3	1	
	Classification by number of electrons donated to the metal. $\pi$ -bonded ligands. Combinations of $\sigma$ - and $\pi$ -donors. Cationic ligands	3	1	
Unit 1	The relationship between oxidation state and the number of d-electrons. Trends in the properties of transition metals.	2	1	1,5
	Electron counting. The 18-electron rule. Metal-metal bonding and electron counting in polynuclear complexes.	2	1	
	Geometries of transition metal complexes. Isoelectronic and isolobal analogies.	2	1	
	Molecular orbitals for transition metal complexes $\pi$ -bonding in organotransition metal complexes	2	1	
	Organometallics Reaction Mechanism	11		
	Introduction. Ligand substitution process	2	2	
	Oxidative addition/reductive elimination. Migratory insertions/ β-Hydride eliminations	2	2	
Unit 2	Nucleophilic attack on ligands coordinated to transition metals. Transmetalation.	3	2	1,2
	Electrophilic attack on transition-metal coordinated ligands	2	2	
	Catalysis: Homogeneous and Heterogeneous. Turnover number and turnover frequency.	2	2	
	Applications of Metal-Complexes in Organic Synthesis	14		
	Metal-catalyzed C-C and C-heteroatom bond forming reactions	2	3	
	Palladium-, nickel- and copper-catalyzed coupling reactions with organometallics and bimetallic reagents.	3	3	1,3
Unit 3	Coupling reactions of organic halides with terminal alkynes, amines, alcohols and thiols.	3	3	
	Carbonylation of organic halides to form ketones. Carbonylation of arenes and alkanes.	3	3	
	Dehydrogenation: Dehydrogenation catalyzed by complexes of pincer ligands.	3	3	
	Metal Carbene Complexes and its Applications	8		
Unit 4	Brief introduction to Fischer and Schrock carbene complexes	4	4	1,4
Omt 4	Metathesis: concepts and catalysts, RCM, ROM, CM, yne-metathesis, ene-yne metathesis and their applications	4	4	1/1
	Miscellaneous Transition Metal Catalyzed Reactions	13		
Unit 5	C-H activation reactions: Mechanistic pathway and scope of the catalysts. Applications of C-H activation reactions in cross-coupling and annulation reactions.	4	5	1,2,5
	Click chemistry. Hydrogenation of arenes, alkynes and alkenes.	2	5	

Hydroarylation and acylation reactions Hydrosilylation and hydroamination of alkynes and olefins.	2	5	
Hydroboration, diboration, silylboration, and stannylboration reactions.	2	5	
Allylic substitution reactions. Polymerization reactions. Asymmetric synthesis.	3	5	
Total Contact Hours		60	

#### **Learning Assessment**

		Continuous Learning Assessments (60%)								End Semester	
Bloom's Level of Cognitive Task		Mid-I (15%)			d-1I (%)	CL.	A-1 %)	(20)		Exam (	40%)
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
T 11	Remember		1140		1140		1140		1140		11
Level 1	Understand	40%		40%		40%		40%		40%	
Level 2	Apply	60%	40%	40%		40%		40%		40%	
LCVCI Z	Analyse	0070		7070		7070		TU/0		7070	
Level 3	Evaluate Evaluate			20%				20%		20%	
Level 3	Create			2070				2070		2070	
	Total			100%		100%		100%		100%	

#### **Recommended Resources**

- 1. Crabtree, R. H. The organometallic chemistry of the transition metals, John Wiley, 2005.
- 2. B. D. Gupta, Anil J. Elias Basic Organometallic Chemistry: Concepts, Syntheses and Applications, University Press, 2013
- 3. Hegedus, L. S. Transition metals in the synthesis of complex organic molecule, University Science Books, 2010 (3rd Ed).

#### **Additional Resources**

- 4. Grubbs, R. H. (Editor) Handbook of Metathesis, (Vol 1-3), Wiley-VCH, 2003.
- 5. Hartwig, J. H. Organotransition Metal Chemistry: From Bonding to Catalysis, University Science Books, 2009 (1st Ed).

### **Other Resources**

#### **Course Designers**

1. Dr. S. Mannathan, Associate Professor, SRM University - AP

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



#### **Organic Synthesis and Stereochemistry**

Course Code	CHE 638	Course Category	Elective		L	T	P	C
Course Code	CHE 030	Course Category	Liective		3	0	1	4
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)				
Course Offering Department	Chemistry	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- > Gain a comprehensive understanding of various ligand systems, electron counting methods, and the principles of metal-metal bonding and transition metal complex geometries.
- Explore and comprehend the mechanisms of key organometallic reactions, including ligand substitution, oxidative addition/reductive elimination, and catalytic processes.
- > Recognize the application of metal-catalyzed reactions for C-C and C-heteroatom bond formation

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Classify ligands by their bonding characteristics and number of electrons donated to the metal, and explain electron counting methods, the 18-electron rule, and the properties and geometries of transition metal complexes.	2	80%	75%
Outcome 2	Describe the mechanisms of ligand substitution, oxidative addition/reductive elimination, and other key organometallic reactions, and apply this understanding to propose mechanistic pathways for given reactions.	2	75%	70%
Outcome 3	Use the knowledge of palladium-, nickel-, and copper- catalyzed coupling reactions and other metal-catalyzed processes to design synthetic routes for organic molecules	3	75%	70%
Outcome 4	Understand the mechanistic pathways and synthetic applications of transition metal-catalyzed reactions such as C-H activation, hydrogenation, and polymerization, and apply this knowledge to solve synthetic problems	3	75%	70%

					Pro	ogram L	earning	g Outco	mes (PL	<b>(O</b> )					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	2	2	2	2				2			2	3	1	2
Outcome 2	3	2	3	2	3	2			2			2	3	3	2
Outcome 3	3	3	3	3	3	2			2			2	3	2	2
Outcome 4	3	3	2	2	3				2			2	3	2	2
Average	3	3	3	2	3				2			2	3	1	2

	Unitization Pian	Doguirad	Γ	Γ
Unit	Cvillahus Tonics	Required Contact	CLOs	References
No.	Syllabus Topics		Addressed	Used
	Y 1/4 A	Hours		
	Unit 1 Asymmetric Synthesis:	10		
	Principle of stereoselectivity, strategies of asymmetric synthesis,			
	substrate diastereoselectivity, product stereoselectivity, product			
	composition, determination of product composition,	2	1	
	diastereomeric excess (de), and enantiomeric excess (ee), double			
	stereo differentiating reactions.			
	Strategies for stereo control in enantio and diastereoselective			
	synthesis, small ring templates, ring formation reactions,			
Unit	pericyclic reactions coordination to metal centers, use of $\pi$ -donors	3	1	
No.	complexes, $\pi\pi$ interactions with aromatic substituents, directed $\pi$			1,2
1	facial diastereoselectivity chiral auxiliaries, achiral auxiliaries,.			1,2
1	Nucleophilic additions to cyclic and acyclic carbonyl compounds,			
	Cram's rule, Felkin's model, addition to chelated carbonyl			
	compounds, Prelog's rule and its applications, addition to chelated			
	carbonyl compounds of H and R to cyclic ketones (formation of			
	axial and equatorial alcohols), Electrophilic initiated cyclization,	5	1	
	Aldol reactions: (1) Achiral enolates with achiral aldehydes (2)			
	Achiral enolates with achiral aldehydes. (3) Chiral enolates with			
	achiral aldehyde. (4) Chiral enolates with chiral aldehydes,			
	organocatalysis.			
	Stereo-selective and Enantioselective Reactions:	10		
	Stereo-selective reactions of C=C double bond, Diastreoselective			
	transformations involving catalytic hydrogenation; Hydrogenation			
	over heterogeneous catalysts; Directed hydrogenation with soluble	1 1 2 1		
	catalysts;			
	synthetic applications of organoboranes and organosilanes,			
	hydroboration, reactions of organoboranes, reactions with alpha			
Unit	halo carbonyl compounds, reactions of alkenylboranes and	3	2	
No.	trialkenylboranes, free radical reactions of organoboranes, alkenyl		_	
2	silanes and allylsilanes,			1,2
	Stereochemistry of free radical cyclization reactions, Prevost			
	hydroxylation, Simon-Smith reaction. Enantioselective synthesis			
	with chiral catalysts, hydroboration reactions involving chiral			
	boranes, chiral organometallic complexes, chiral enolate	6	2	
	aggregates, reductions with chiral complexes hydrides. Catalysis	Ů	_	
	by chiral transition metal complexes, enantioselective epoxidation			
	of alkenes. Enantioselective hydrogenations.			
	Unit 3 Design of Organic Synthesis:	11		
	Introduction and target selection and terminology, aims and	11		
	objectives, introduction, target selection, biological activity,			
	topological studies, new reactions and reagents, retro synthetic	2	3,4	
IIn:1	analysis, terms used in retro synthetic analysis, target molecule,			
Unit No.	functionalization, functional group interchange, disconnection	2	2.4	
	synthons, synthetic equivalent transform, retron different	3	3,4	1,2
3	strategies in retro synthetic analysis,			
	C-C disconnection, introduction one group C-C disconnection, two			
	group disconnections, 1,2-, 1,3-, 1,4-, 1,5-, 1,6- difunctional	_	2.4	
	compounds, applications of some important strategies in organic	3	3,4	
	synthesis, chemo selectivity, regioselectivity, stereoselectivity,			
	cyclisation reactions(3 to 7 membered rings), reversal polarity			

	Biomimetic approach to retrosynthesis, Johnson polyene cyclization, retro mass spectral degradation, Yamaguchi esterification, Corey-Nicolaou macro lactonization. Protecting Groups.	3	3, 4	1,3
	Unit 4 C-C Single Bond and Multiple Formation Reactions:	14		
	Alkylation importance of enolate anions, alkylation of relatively acidic methylene groups, Gama alkylation of 1,3-dicarbonyl compounds; dianions in the synthesis, alkylation of ketones	2	3,4	
	the enamine related reactions under basic conditions, enamines, Alkylation and Acylation in acidic medium alkylation of alpha- thio and alpha-selenocarbanions, umpolung, allylic alkylation of alkenes	2	3,4	
Unit No. 4	reactions of lithium organocuprates: copper-catalysed reactions of Grignard reagents, synthetic applications of carbenes and carbenoids, formation of C-C bonds by addition of free radicals to alkenes, some photocyclization reactions.	2	3,4	1,3
	Wittig reaction, Phosphonium Ylide preparation, reaction mechanism, olefin synthesis, Modified Wittig reactions, stereoselective synthesis of substituted ethylenes	4	3,4	
	Wharton olefin synthesis, alkenes from tosylhydrazone, sulfone, alkenes from titanium and chromium reagents, alkene metathesis reaction, Oxidative decarboxylation of acids, stereospecific synthesis from 1,2-diols, Oxidation & electro organic oxidations.	4	3,4	

#### <u>Course Unitization Plan - Lab</u>

Exp No.	Experiment Name	Required Contact Hours	CLOs Addressed	References Used
1	Tetrahydro carbazole synthesis,	2	3,4	4
2	Synthesis of Benzylideneacetophenone from acetophenone and benzaldehyde.	4	3,4	4
3	Synthesis of 3,5 -dimethylpyrazole from acetylacetone (2,4-pentanedione) and hydrazine.	4	3,4	4
4	Synthesis of 2,4-dimethyl -3H-benzo[b][1,4] diazepine from acetylacetone (2,4pentanedione)	4	3,4	4
5	Preparation of acridone from anthranilic acid (through o-chloro benzoic acid, N-phenyl anthranilic acid),	4	3,4	4
6	Synthesis of symmetrical tribromo benzene (aniline to 2,4,6 tribromo aniline, diazotization followed by deamination).	4	3,4	4
7	Synthesis of 1 -phenylazo-2-napthol from 2-napthol.	4	3,4	4
8	Synthesis of Organic Compounds using modern techniques: Ultrasound, Sonication	4	3,4	4

#### **Learning Assessment**

			(	Continuou	s Learnin	g Assessm	ents (60%	(o)		End Se	mastau
	's Level of itive Task	CLA-1	(10%)	CLA-2	(20%)	CLA-3 (10%)			Term %)	Exam	
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level 1	Remember	40%	40%	40%	40%	20%	20%	20%	10%	20%	10%
Level 1	Understand	40%	7070	4070	4070	2070	2070	2070	1070	2070	1070
Level 2	Apply	60%	60%	40%	60%	60%	60%	60%	70%	60%	70%
Level 2	Analyse	0070	0070	4070		60%	0070	0070	/0%	0070	7070
Level 3	Evaluate					20%	20%	20%	20%	20%	20%
LCVCI 3	Create			20%		2070	2070	2070	2070	2070	2070
	Total	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%

#### **Recommended Resources**

- 1. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India, 2008.
- 2. Stereochemistry of Organic Compounds: Principles and Applications, Fourth Edition, D. Nasipuri, New Age International Publishers, 2020.
- 3. Modern Methods of Organic Synthesis, W. Carruthers, I. Coldham, Cambridge University Press, Cambridge, 2015, 4th Edition.
- 4. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)

#### **Other Resources**

- 1. Advanced Asymmetric Synthesis, edited by G. R. Stephenson. Chapman & Hall, Springer Science, 1996
- 2. Organic Synthesis, Michael B. Smith. Academic Press, 2016, 4th Edition.
- 3. Organic Synthesis, The disconnection Approach, S. Warren, Wiley India Edition, John Wiley & Sons, 2007.
- 4. Stereochemistry: Conformation and Mechanism, P.S. Kalsi, New Age Publishers, 2019, 10th Edition.

## **Course Designers**

1. Enter Data

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



## **Organic Spectroscopy**

Course Code	CHE 639	Course Category	Elective	L 4	T 0	P 0	<b>C 4</b>
Pre-Requisite Course(s)		Co-Requisite Course(s)	Progressive Course(s)				
Course Offering Department	Chemistry	Professional / Licensing Standards					

#### Course Objectives / Course Learning Rationales (CLRs)

- > Develop a foundational understanding of UV-Visible and IR spectroscopy, focusing on the electronic transitions, solvent effects, vibrational frequencies, and characteristic spectra of various organic compounds..
- > Gain insight into the principles and techniques of 1H and 13C NMR spectroscopy, including chemical shifts, spin-spin interactions, and factors influencing NMR spectra, as well as the applications of these techniques in structural determination.
- Master the concepts and applications of mass spectrometry, including ion production, fragmentation patterns, and interpretation of mass spectra to determine the structures of organic compounds.

#### Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Explain the principles of UV-Visible and IR spectroscopy, describe electronic transitions, vibrational frequencies, and their solvent effects, and apply this knowledge to interpret the spectra of various organic compounds	2	85%	80%
Outcome 2	Describe the principles of <sup>1</sup> H and <sup>13</sup> C NMR spectroscopy, including chemical shifts and spin-spin interactions, and apply these principles to interpret NMR spectra for structural determination of organic molecules.	3	90%	75%
Outcome 3	Apply mass spectrometry techniques to analyze ion production and fragmentation patterns, and apply this knowledge to determine the structures of organic compounds based on their mass spectra	3	80%	70%
Outcome 4	Apply all spectrometry techniques for the structure elucidation of the organic compounds	3	80%	70%

					Pr	ogram I	earning	g Outco	mes (PI	LO)					
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Life Long Learning	PSO 1	PSO 2	PSO 3
Outcome 1	3	2	3	3	2				2	1			2	1	2
Outcome 2	3	2	3	3	2	2			2	1			3	2	2
Outcome 3	3	3	3	3	3	2			2	1			3	3	2
Outcome 4	3	3	3	3	3				2	1			3	2	2
Average	3	3	3	3	3	1			2	1			3	2	2

	Unitization Plan		T	
Unit		Required	CLOs	References
No.	Syllabus Topics	Contact	Addressed	Used
		Hours		
	UV-Visible Spectroscopy	8		
	Various electronic transitions - Effect of solvent on electronic	2	1	
	transitions			
Unit	Ultraviolet bands for carbonyl compounds, unsaturated carbonyl	4	1	
No.	compounds, dienes and conjugated polyenes			1,2
1	Fieser- Woodward rules for conjugated dienes and carbonyl	2	1	
	compounds -			
	Ultraviolet spectra of aromatic and heterocyclic compounds - Steric	2	1	
	effect in biphenyls.			
	IR Spectroscopy	10		
	Characteristic vibrational frequencies of alkanes, alkenes, alkynes,	2	1	
TT *4	aromatic compounds, alcohols, ethers, phenols and amines.			
Unit	Detailed study of vibrational frequencies of carbonyl compounds	4	1	1.2
No.	(ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams			1,2
2	and conjugated carbonyl compounds).			
	Effect of hydrogen bonding and solvent effect on vibrational	2	1	
	frequencies, overtones, combination bands and Fermi resonance.			
	H <sup>1</sup> NMR Spectroscopy -I	10		
		2	2	
Unit	Nuclear spin - Nuclear resonance - Saturation, shielding of magnetic nuclei - Chemical shifts and its measurements.	2	2	
No.			2	100
3	Factors influencing chemical shift; De-shielding - Spin-spin	6	2	1,2,3
]	interactions. Factors influencing coupling constant 'J' - Classification			
	(ABX, AMX, ABC, A2B2 etc.) - Spin decoupling.	_	_	
	Basic ideas about the instrument - FT-NMR - Advantages of FTNMR.	2	2	
	H <sup>1</sup> NMR Spectroscopy -II and <sup>13</sup> C NMR Spectroscopy	20		
	H <sup>1</sup> NMR Spectroscopy: Shielding mechanism - Mechanism of	2	2	
	measurement.			
	Chemical shift values and correlation for protons bonded to carbon	4	2	
	(aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols,	•	_	
	phenols, enols, carboxylic acids, amines and amides)			
	Chemical exchange - Effect of deuteration - Complex spin-spin	4	2	
Unit	interaction between two, three, four and five nuclei (First order	4	2	
No.	spectra).			1,2,3
4	Virtual coupling. Stereochemistry Hindered rotation - Karplus curve	2	2	
	variation of coupling constant with dihedral angle.	2	2	
	Simplification of complex spectra: nuclear magnetic double resonance -	4	2	
	Contact shift reagents - Nuclear overhauser effect (NOE).	7		
	<u> </u>	4	2	
	<sup>13</sup> C-NMR Spectroscopy: General considerations – Chemical shift	7		
	(aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl			
	carbon) - Coupling constants			
	Mass Spectrometry	12	_	
	Mass Spectrometry: Introduction - Ion production - Types of	2	3	
	ionization; EI, CI, FD, and FAB.		_	
Unit	Factors affecting fragmentation - Ion analysis - Ion abundance. Mass	6	3	
No.	spectral fragmentation of organic compounds. Common functional			1,2,3
5	groups - Molecular-ion peak - Metastable peak - Mc.		_	- ,- ,*
	Lafferty rearrangement. Nitrogen rule - Isotope labelling - High	2	3	
	resolution mass spectrometry.	_		
	Examples of mass spectral fragmentation of organic compounds with	2	3	
	respect to their structure determination.			

#### **Learning Assessment**

			Coi	ntinuous I	earning	Assessme	ents (60%	<b>(o)</b>		End C	
	Bloom's Level of Cognitive Task		(15%)	CLA-2 (15%)		(15%) CLA-3		Mid Term (15%)		End Semester Exam (40%)	
		Th	Prac	Th	Prac	Th	Prac	Th	Prac	Th	Prac
Level 1	Remember	40%		40%		40%		40%		40%	
Level 1	Understand			1							
Level 2	Apply	50%		40%		40%		40%		40%	
Level 2	Analyse										
Level 3	Evaluate	10%		20%		20%		20%		20%	
Level 3	Create	10/0		2070							
	Total			100%		100%		100%		100%	

#### **Recommended Resources**

- 1. P.M. Silverstein, F. X. Wester, D. J. Kiemle, D. L. Bryce, Spectroscopic Identification of Organic Compounds, 8th ed., Wiley 2015.
- 2. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994
- 3. P.S. Kalsi, Spectroscopy of Organic Compounds, 6th Edition, New age international
- 4. publishers, 2007

## **Other Resources**

- 1. C.N. Banwell, Fundamentals of molecular Spectroscopy, 3rd ed., TMH, New Delhi, 1983.
- 2. J.R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall,
- 3. 1965.
- 4. Y.R. Sharma, Elementary Organic Spectroscopy Principles and Chemical applications,
- 5. S.Chand, 5th ed., 2013.

#### **Course Designers**

1. Enter Data

Neerukonda, Mangalagiri Mandal, Guntur District, Mangalagiri, Andhra Pradesh – 522240.



# BA/BA(H)/BA(Hons with research) III Semester

**Summer Immersion: Liberal Arts** 

Course Code		Course Category	RDIP		<b>L</b> 0	<b>T</b>	P 2	<b>C</b> 2
Pre-Requisite Course(s)		Co-Requisite Course(s)		Progressive Course(s)	-	umn terns		
Course Offering Department	Sociology/Anthropology	Professional / Licensing Standards						

#### Course Objectives / Course Learning Rationales (CLRs)

- > To provide students with real-world experience in understanding the challenges faced by communities working towards social development
- To help students analyse the efforts of organizations driving inclusive development in rural and urban areas.
- > To enhance students' practical skills in problem-solving and community engagement for social impact.

## Course Outcomes / Course Learning Outcomes (CLOs)

	At the end of the course the learner will be able to	Bloom's Level	Expected Proficiency Percentage	Expected Attainment Percentage
Outcome 1	Identify social and developmental issues encountered by communities in both rural and urban settings.	1,2	70	80
Outcome 2	Explain the effectiveness of interventions and strategies used by organizations to promote inclusive social change.	2	70	80
Outcome 3	Apply critical thinking skills to develop solutions for the challenges observed during their field immersion.	3	70	80
Outcome 4	Examine the functioning of civil society and development related organisations.	4	70	80

	Program Learning Outcomes (PLO)														
CLOs	Scientific and Disciplinary Knowledge	Analytical Reasoning and Problem Solving	Critical and Reflective Thinking	Scientific Reasoning and Design Thinking	Research Related Skills	Modern Tools and ICT Usage	Environment and Sustainability	Moral, Multicultural and Ethical Awareness	Individual and Teamwork Skills	Communication Skills	Leadership Readiness Skills	Self-Directed and Lifelong Learning	PSO 1	PSO 2	PSO 3
Outcome 1	0	2	1	2	3	3	2	2	2	3	3	3	2	3	3
Outcome 2	0	2	1	2	3	3	2	2	2	3	3	3	2	3	2
Outcome 3	0	2	1	2	3	3	1	2	2	3	3	3	1	3	3
Outcome 4	0	2	1	2	3	3	1	2	2	3	3	3	3	2	2
Average	0	2	1	2	3	3	1	2	2	3	3	3	2	2	2

Unit No.	Unit Name	Required Contact Hours	CLOs Addressed	References Used	
Unit 1	Fieldwork Experience		1,2		
	Students engage with communities to identify social and developmental issues in rural and urban settings.				
Unit 2	Organizational Analysis		2		
	Students explain the effectiveness of interventions and strategies used by organizations to promote inclusive social change.	,			
Unit 3	Problem-Solving Exercises		3		
	Students apply critical thinking to develop solutions for challenges observed during their field immersion.				
Unit 4	Civil Society Assessment		4		
	Students examine the functioning of civil society and development-related organizations during their engagement.				

#### **Learning Assessment**

Bloom's Level of Cognitive Task		Progress Report (Daily reflection Journal) (30%)	Internship Report/Video Documentary (40%)	Viva (Presentation) (30%)		
Level	Remember	30%	25%	25%		
1	Understand	30 %	25 /6			
Level	Apply	50%	50%	25%		
2	Analyse	30 %	30 %	25 /0		
Level	Evaluate	20%	25%	50%		
3	Create	20 /6	23 /6			
Total		100%	100%	100%		

#### **Recommended Resources**

1. Enter Data

#### **Other Resources**

1. Enter Data

## **Course Designers**

- 1. Dr Vandana Swami, Associate Dean and Professor, Eswari School of Liberal Arts, SRM University AP
- 2. Dr. Vineeth Thomas, Assistant Professor and Head, Department of Political Science, SRM University AP