FACULTY OF APPLIED SCIENCES

SYLLABUS

FOR

M.Sc. CHEMISTRY (SEMESTER: I-IV)

(Under Choice based Credit System)

Examinations: 2018 Onwards

Department of Chemical Sciences I K GUJRAL PUNJAB TECHNICAL UNIVERSITY KAPURTHALA

Note:

(i) Subject to change in the syllabi at any time. Please visit the University website time to time.

IK Gujral Punjab Technical University

VISION

To be an institution of excellence in the domain of higher technical education that serves as the fountainhead for nurturing the future leaders of technology and techno- innovation responsible for the techno-economic, social, cultural and environmental prosperity of the people of the State of Punjab, the Nation and the World.

MISSION

To provide seamless education through the pioneering use of technology, in partnership with industry and society with a view to promote research, discovery and entrepreneurship and To prepare its students to be responsible citizens of the world and the leaders of technology and techno-innovation of the 21st Century by developing in them the desirable knowledge, skill and attitudes base for the world of work and by instilling in them a culture for seamlessness in all facets of life.

OBJECTIVES

- To offer globally-relevant, industry-linked, research-focused, technology- enabled seamless education at the graduate, postgraduate and research levels in various areas of engineering & technology and applied sciences keeping in mind that the manpower so spawned is excellent in quality, is relevant to the global technological needs, is motivated to give its best and is committed to the growth of the Nation;
- To foster the creation of new and relevant technologies and to transfer them to industry for effective utilization;
- To participate in the planning and solving of engineering and managerial problems of relevance to global industry and to society at large by conducting basic and applied research in the areas of technologies. To develop and conduct continuing education programmes for practicing engineers and managers with a view to update their fundamental knowledge base and problem-solving capabilities in the various areas of core competence of the University;
- To develop strong collaborative and cooperative links with private and public sector industries and government user departments through various avenues such as undertaking

- of consultancy projects, conducting of collaborative applied research projects, manpower development programmes in cutting-edge areas of technology, etc;
- To develop comprehensive linkages with premier academic and research institutions within the country and abroad for mutual benefit;
- To provide leadership in laboratory planning and in the development of instructional resource material in the conventional as well as in the audio- visual, the video and computer-based modes;
- To develop programmes for faculty growth and development both for its own faculty as well as for the faculty of other engineering and technology institutions;
- To anticipate the global technological needs and to plan and prepare to cater to them;
- To interact and participate with the community/society at large with a view to inculcate in them a feel for scientific and technological thought and endeavour; and
- To actively participate in the technological development of the State of Punjab through the undertaking of community development programmes including training and education programmes catering to the needs of the unorganized sector as well as that of the economically and socially weaker sections of society.

ACADEMIC PHILOSOPHY

The philosophy of the education to be imparted at the University is to awaken the "deepest potential" of its students as holistic human beings by nurturing qualities of self-confidence, courage, integrity, maturity, versatility of mind as well as a capacity to face the challenges of tomorrow so as to enable them to serve humanity and its highest values in the best possible way.

Department of Chemical Sciences

VISION

The Chemical Sciences at IKGPTU campus will address the challenging and important questions in the physical and life sciences of current era using its multi-disciplinary vision, its culture of synergistic collaboration and translational science, and its excellence in the physical, medical and engineering sciences. Chemical Sciences Department continues to explore the new fields and frontiers and, with them, fundamentally new and innovative ways to address the increasingly complex scientific, health, energy and environmental problems of our time.

MISSION

- Inspiring and educating undergraduate students in chemistry and molecular-driven sciences in the core concepts of chemistry and the scientific methodology.
- To explore the new frontier area of organometallic catalysis in synthetic chemistry.
- Developing more-economic and greener strategies for chemical synthesis and production
- Understanding how molecules and materials behave, interact and transform at macroscopic, molecular, atomic and electronic levels, and exploring the contribution of geometric and electronic structure to function.
- Informing the public about the excitement of science, its impact on everyday life, and the crucial role it plays in human health, energy and environmental stewardship
- Building centralized, state-of-the-science facilities designed to promote collaborative synergies among faculty, staff and students and across disciplinary boundaries.
- Sharing the excitement of new chemical knowledge across IKGPTU and to other institutions, educators, and the global community through scientific communications and outreach.

TITLE OF THE PROGRAM: M.Sc. CHEMISTRY

YEAR OF IMPLIMENTATION: New Syllabus will be implemented from June 2018 onwards.

DURATION: The course shall be two years, with semester system (4 semesters, with two semesters in a year). The Choice based credit system will be applicable to all the semesters.

ELGIBILITY FOR ADMISSION: Candidates with 50% marks (5% relaxation for reserved categories) in Bachelors Degree with Chemistry as one of the subject are eligible for admission to this course.

INTAKE CAPACITY: 25 (Twenty five)

MEDIUM OF INSTRUCTION: English.

PROGRAM EDUCATIONAL OBJECTIVES:

The Program Educational Objectives are the knowledge skills and attitudes which the students will acquire during post-graduation.

PEO1	Apply the scientific knowledge of Physics, Mathematics and Chemistry specialization for deeper understanding of the nature.				
PEO2	Identify, formulate, research literature, and analyze advanced scientific problems reaching substantiated conclusions using first principles of mathematics, natural sciences, and engineering sciences.				
PEO3	Design solutions for advanced scientific problems and design system components or processes.				
PEO4	Use research-based knowledge and research methods including design of experiments, analysis and interpretation of data, and synthesis of the information to provide valid conclusions.				
PEO5	Create, select, and apply appropriate techniques, resources and modern scientific methods with an understanding of the limitations.				
PEO6	Apply reasoning using contextual knowledge to assess health, safety, legal and cultural issues of society.				
PEO7	Communicate effectively on research based activities with the scientific community and society at large so as to comprehend and write effective reports and design documentation.				
PEO8	Recognize the need for, and have the preparation and ability to engage in independent and life-long learning in the broadest context of scientific and technological change.				

PROGRAM OUTCOMES: At the end of the program, the student will be able to:

PO1	Apply principles of various concepts in understanding, analysis and prediction of scientific problems.
	1
PO2	Development of problem solving skill, critical thinking and analytical reasoning as
	applied to scientific problems.
PO3	To introduce advanced ideas and techniques required in emerging scientific areas.
PO4	To develop human resource with specialization in science along with various
	experimental techniques required for career in academia and industry.
PO5	Engage in lifelong learning and adapt to changing professional and societal needs.
PO6	Communicate effectively scientific information both in written and oral formats.

PROGRAM SPECIFIC OUTCOMES:

At the end of the program,

PSO1	Students will be competent to provide solutions for challenges related to energy,			
	environment, materials and health/medicine.			
PSO2	Students will be skilled in problem solving, critical thinking and analytical			
	reasoning as applied to problems related to chemical sciences.			
PSO3	The students will acquire in-depth knowledge to understand and critically interpret			
	the chemical literature.			
PSO4	Students will be able to address social, economic, and environmental issues.			
PSO5	Students will be able to design and carry out scientific experiments and analyze the			
	results of such experiments.			
PSO6	Students will be able to explore new areas of research in both chemistry and allied			
	fields of science and technology.			
PSO7	Students will be able to integrate knowledge of mathematics, physics and other			
	disciplines to solve social and technological issues.			

SCHEME OF THE PROGRAM:

Semester-I									
Sr. No	Code	Code Theory Papers Hours L-T-P Credi Marks ts Distribution			Marks				
						Internal	External	1	
1.	CHL401-18	Inorganic Chemistry-I	45	4-0-0	4	30	70	100	
2.	CHL402-18	Reactive Intermediates-I	45	4-0-0	4	30	70	100	
3.	CHL403-18	Physical Chemistry-I	45	4-0-0	4	30	70	100	
4.	CHL404-18	Spectroscopy - I	45	4-0-0	4	30	70	100	
5.	CHL405-18	Environmental Chemistry	45	3-0-0	3	25	50	75	
6.	CHL406A-18	Human Physiology * Or	45	3-0-0	3	25	50	75	
	CHL406B-18	Numerical Methods for chemists*							
7.	CHP407-18	Inorganic Chemistry Lab	60	0-0-6	3	50	25	75	
8.	CHP408-18	Organic Synthesis Lab	60	0-0-6	3	50	25	75	
		Total	28 (Theory 22, Practical 6)			270	430	700	

	Semester-II										
Sr. No	Code	Theory Papers	Hours	L-T-P	Credi ts	Marks Distribution		Marks			
						Internal	External				
1.	CHL411-18	Inorganic Chemistry-II	45	4-0-0	4	30	70	100			
2.	CHL412-18	Reactive Intermediates-II	45	4-0-0	4	30	70	100			
3.	CHL413-18	Physical Chemistry-II	45	4-0-0	4	30	70	100			
4.	CHL414-18	Spectroscopy - II	45	4-0-0	4	30	70	100			
5.	CHL415A-18 CHL415B-18	Chemistry of Materials Or Chemical Biology	45	4-0-0	4	30	70	100			
6.	CHP416-18	Physical Chemistry Lab	60	0-0-6	3	50	25	75			
7.	CHP417-18	Advanced Chemistry Lab-I	60	0-0-6	3	50	25	75			
		Total	26 (Theory 20, Practical 6)			250	400	650			

Semester-III									
Sr. No	Code	Theory Papers	Hours	L-T-P	Credi ts		Marks Distribution		
						Internal	External		
1.	CHL501-18	Inorganic Chemistry-III	45	4-0-0	4	30	70	100	
2.	CHL502-18	Advanced Organic Chemistry –I	45	4-0-0	4	30	70	100	
3.	CHL503-18	Physical Chemistry-III	45	4-0-0	4	30	70	100	
4.	CHL504-18	Advanced Characterization Techniques	45	4-0-0	4	30	70	100	
5.	CHL505A-18 CHL505B-18	Biophysical chemistry Or Medicinal Chemistry	45	4-0-0	4	30	70	100	
	CHL505C-18	Or Advanced Functional Materials							
6.	CHP506-18	Advanced Chemistry Lab- II	60	0-0-6	3	50	25	75	
7.	CHP507-18	Dissertation**		0-0-8	4				
		Total	27 (Theory 20, Practical 7)			200	375	575	

	Semester-IV									
Sr. No	Code	Theory Papers	Hours	L-T-P	Credi ts		Marks Distribution			
						Internal	External			
1.	CHL511-18	Advanced Organic Chemistry- II	45	4-0-0	4	30	70	100		
2.	CHL512A-18	Advanced physical Chemistry Or	45	4-0-0	4	30	70	100		
	CHL512B-18	Chemical Toxicology Or								
	CHL512C-18	Supramolecular Chemistry Or								
	CHL512D-18	Chemistry of Natural Products								
	CHL512E-18	Or Green Chemistry Or								
	CHL512F-18	Computational Chemistry								
3.	CHP513-18	Research Seminar	30		3					
4.	CHP514-18	Dissertation**		0-0-24	12					
		Total	23 (Theory 8, Practical 12, Seminar 3)			60	140	200		

^{*} Human Physiology for students with mathematical background and Numerical methods for chemists for students with medical background.

** Dissertation work will begin in third semester and will be continued in fourth semester. At the end of third semester, students will submit their literature work in the form of a review on the topic selected. There will be a presentation before a panel of teachers from the department.

EXAMINATION AND EVALUATION

THEC	ORY				
S.No.		Weight Marks	tage in	Remarks	
1	Mid-Semester Examination	20	15	MSTs, Quizzes, assignments, attendance, etc. Constitute internal	
2	Attendance	5	5	evaluation. Average of two mid- semester exams will be considered for	
3	Assignments	5	5	evaluation	
4	End-Semester Examination	70	50	Conduct and checking of the answer sheets will be at the department level in case of university teaching department of Autonomous institutions. For affiliated colleges examination will be conducted at the university level	
	Total	100	75		
PRAC	CTICAL				
1	Daily evaluation of practical performance/ record/ viva voce	3	0	Internal Evaluation	
2	Attendance	5	5		
3	Internal Practical	1	5		
	Examination				
4	Final Practical Examination	2	5	External Evaluation	
	Total	7	5		

PATTERN OF END-SEMESTER EXAMINATION

- I. **Part A** will be One Compulsory question consisting of short answer type questions [Q No. 1(a-j)] covering whole syllabus. There will be no choice in this question. It will be of 20 marks comprising of **10 questions of 2 marks each**.
- II. **Part B** will be comprising of eight questions [2-9]. Student will have to attempt any six questions from this part. It will be of 30 marks with **6 questions of 5 marks each**.
- III. **Part C** will be comprising of two compulsory questions with internal choice in both these questions [10-11]. It will be of 20 marks with **2 questions of 10 marks each**.

SYLLABUS OF THE PROGRAM

The syllabus has been upgraded as per provision of the UGC module and demand of the academic environment. The contents of the syllabus have been duly arranged unit wise and included in such a manner so that due importance is given to requisite intellectual and laboratory skills. The application part of the respective contents has been appropriately emphasized.

SEMESTER-I

I.K.	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY						
				NT OF CHEMICAL SCIENCES			
Course Name	M.S	c. Cl	nemis	stry			
Subject Code:	CHI	.401- 1	18				
Subject Title:	INO	RGAN	IC CI	HEMISTRY-I			
Contact Hours:	L:4	T:0	P:0	Credits:4			
Examination	3						
Duration (hours)	ırs)						
Objective(s):	The aim and objective of this course is to teach the fundamental and						
	adva	advanced concepts of chemistry of transition metals and their magnetic					
	chem	nistry	to the	students.			

Unit	Contents	Contact
I	Coordination Chemistry: Coordination complexes, ligands and their classification, chelation and chelate effect, Werner's coordination theory, nomenclature, stability of complex and stability constants, stereochemistry, isomerism, Valence bond theory: postulates, examples of complexes, shortcomings. Crystal Field Theory d-orbital by electrostatic field (octahedral, tetrahedral and square planar geometry), and magnetic properties (high spin and low spin complexes); factors affecting crystal field. splitting energy (10 Dq value), nephelauxetic effect and spectrochemical series; Structural and thermodynamic effects of dorbital splitting (variation of ionic radii, Jahn-Teller effect,	Hours 12
II	hydration and lattice energies of first row transition metal ions) Transition Metals Chemistry I: LS coupling, derivation of spectroscopic terms for d¹ to d9 electronic configurations, correlation diagram for d² ion in octahedral field, splitting of d¹ to d9 terms in an octahedral and tetrahedral field. Selection rules of d-d transitions. Vibronic and spin orbit coupling, effecting of weak to strong cubic fields on R-S terms, Comparison of CFSE values of d¹ to d9 ions in terms of orbit splitting and R-S term splitting. Orgel and Tenabe Sugano diagrams, Calculation of β and 10 Dq from spectral data.	12
III	Transition Metals Chemistry II: Molecular orbital theory-	11

	composition of ligand groups, orbitals, sigma and π -molecular orbitals MOEL, diagrams of Oh, T_d and D_{4h} complexes with and without pi-bonds, charge transfer spectra.	
	Complexes of π -Acceptor Ligands: π - acceptor character of CO, N ₂ , O ₂ , NO molecules in terms of MOEL diagrams, acid ligands of other groups of periodic table, Semi-bridging in metal carbonyls and isocyanides of metals. Magnetic, IR and X-ray diffraction	
	evidence of their structure, acidity and softness, Symbiosis and antisymbiosis, pi complexes of unsaturated organic molecules (bonding with C ₂ H ₄ only). Structures & the IR spectral properties representative transition metal carbonyl complexes	
IV	Magnetochemistry of Inorganic Compounds: Explanations of diamagnetism, paramagnetism, ferromagnetism and antiferromagnetism, origin of paramagnetic moment: electron spin moment, and orbital angular moment, magnetic susceptibility, Curie law, Curie-Weiss law, Bohr Magneton, magnetic susceptibility measurement using Gouy and Faraday methods, explanation of magnetic behaviours of transition metal complexes, Quenching of orbital angular momentum by crystal fields in complexes in terms of term-splitting. Effect of spin-orbit coupling and A, E & T states, Mixing in effect, first order and second order zeeman effects	10

S.No.	Author(s)	Title of the Book	Publisher/Year
1	B.N. Figgis	Introduction to Ligand Fields,	John Wiley and Sons Ltd,
		First Edition	United States (1999)
2	F.A. Cotton & G.	Advanced Inorganic	John Wiley New York
	Wilkinson,	Chemistry, 3 rd Edition	
3	F. Basolo and R.C.	Coordination Chemistry, 1 st	W A Benjamin. INC,
	Johnson	Edition	New York
4	J.E. Huheey, Ellen A.	Inorganic Chemistry,	Harper Collins College
	Keiter, Richard L.	Principles of Structure and	Publishers
	Keiter	Reactivity, 4 th Edition	
5	A.B.P. Lever	Inorganic Electronic-	Amsterdam, The
		Spectroscopy, 2 nd Edition	Netherlands: Elsevier,
			1984
6	A. Earnshaw	Introduction to	Academic Press, London
		Magnetochemistry, 1 st Edition	and New York
7	R.S. Drago	Physical Methods in Inorg.	London, 1977
		Chem., I st and 2 nd Edition	

Course Outcomes and Mapping

At the end of	At the end of the course, the student will be able to					
CO1.	Understand the fundamental concepts and postulates of various theories of					
	coordination complexes.					
CO2.	Learn the stereochemistry and stability of the coordination complexes.					
CO3.	Derive spectroscopic terms for various electronic configurations and their					

CO4. CO5.	Interpret Learn a	correlation diagrams. Interpret electronic and magnetic properties of coordination compounds. Learn about the complexes of π -Acceptor ligands and analysis of their structural and spectral properties.						
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	
CO1	2	2	3	2	1	3	3	
CO2	2	3	4	3	1	3	2	
CO3	1	4	1	1	1	1	2	
CO4	2	2	2	1	4	2	-	
CO5	2	2	_	-	1	2	-	

I.K. C	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES						
Course Name		M.Sc. Chemistry					
Subject Code:	CHL4	02-18					
Subject Title:	REAC	TIVE I	NTERM	EDIATES-I			
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4					
Examination	3						
Duration (hours)							
Objective(s):	1. To p	redict th	e relation	nships between organic chemical structures and			
	their re	their reactivity.					
				amental and advanced concepts in reaction			
	mechanisms in organic chemistry along with the study of reaction						
		mechanisms in various types of substitution and elimination reactions.					
				nt for the most commonly encountered reaction			
	mechar	nisms in	organic c	hemistry.			

Unit	Contents	Contact
I	Reaction Mechanism: Structure and Reactivity: Type of	Hours 10
	mechanisms, types of reactions, thermodynamic and kinetic	10
	requirements, kinetic and thermodynamic control, Hammond's	
	postulate, Curtin-Hammett principle, Potential energy diagrams,	
	transition states and intermediates, methods of determining	
	mechanisms, isotope effects. The Hammett equation and linear free	
	energy relationship, substituent and reaction constants, Taft equation.	
	Reactive intermediates: Formation and stability of Carbocations,	
	Carbanions, Free Radicals, Carbenes, Nitrenes, and Arynes.	
	Aromaticity: Huckel's rule and Concept of Aromaticity,	
	Annulences and Heteroannulenes, Fullerenes (C60).	
II	Nucleophilic Substitution : Introduction, S_N1 and S_N2 Mechanism	13
	and evidence, Stereochemistry of nucleophilic substitution,	
	Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, Ambient	
	system, common carbocation rearrangements, Ambient Nucleophiles, SET Mechanism, Neighboring Group Participation	
	reaction (NGP). The S_Ni mechanism, mixed S_N1 and S_N2 Reactions,	
	Effect of substrate structure; attacking nucleophile; leaving group	
	and reaction medium in S_N1 and S_N2 reactions, phase-transfer	
	catalysis, regioselectivity. Nucleophilic Substitution of allylic	
	systems Nucleophilic displacements at Allylic halides/tosylates,	
	Benzylic position, allylic, aliphatic trigonal and a vinylic carbon, &	
	Aryl halide. Nucleophilic aromatic substitution : Nucleophilic aromatic	
	substitution by addition—elimination mechanism and Elimination	
	addition mechanism (SNAr, S _N 1, benzyne and SR _N 1 mechanisms),	
	effect of substrate, structure, leaving group and attacking	
	nucleophile, Von Richter, Sommelet-Hauser, and Smiles	

	rearrangements.	
III	Electrophilic Substitutions: Introduction, Different mechanism for aliphatic electrophilic substitution (Bimolecular mechanisms- SE2 and SEi The SE1 mechanism), Electrophilic Substitution accompanied by double bond shift, Aliphatic Electrophilic Substitution in relation to substrate structure, Leaving group & solvent polarity, Effect of substrates, leaving group and the solvent polarity on the reactivity,	12
	Aromatic electrophilic substitution: Structure-Reactivity relationship: arenium ion mechanism; orientation and reactivity in mono substitution and disubstituted aromatics; energy profile diagram; the ortho/para ratio; ipso attack; orientation in different ring systems; quantitative treatment of reactivity in substrates and electrophiles; Diazo coupling, Vilsmeir reaction, Gatterman-Koch reaction, Bechmann reaction, Hoben-Hoesch reaction.	
IV	Free Radical Substitution: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead, Reactvity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, Free radical rearrangement, Hunsdiecker reaction. Elimination Reactions: E1, E2 and E1cb mechanisms - E1, E2 and E1cB spectrum, Regiochemistry and stereochemistry of elimination reactions, Orientation of the double bond, Hoffman and Saytzeff rules, Competition between elimination and substitution. Typical eliminations reactions - dehydration, dehydrohalogenation and dehalogenation. Stereochemistry of E2 eliminations in cyclohexane systems. Mechanism of pyrolytic eliminations. Chugaev and Cope eliminations.	10

S.No.	Author(s)	Title of the Book	Publisher
1	Francis A. Carey	Advanced Organic Chemistry	Kluwer Academic
	and Richard J.	Vol. A and Vol. B, fourth	publishers, New York
	Sundberg	Edition	2002
2	Jerry March	Organic Reaction Mechanism	John Wiley Ed. 5, 2002
3	W. Carruthers	Some Modern Methods of	Cambridge University
		Organic Synthesis, IV Edition	Press, 2004
4	H.O. House	Modern Synthetic Reactions	The Benjamin Cummings
		-	Publishing Company,
			London, 1972
5	R.O.C. Norman	Principles of organic synthesis	Chapman and Hall,
			London. 1980
6	John McMurry and	Fundamentals of Organic	Cengage Learnings
	Eric Simanek	Chemistry	
7	T.L. Gilchrist and	Carbenes, Nitrenes and Arynes	Thomas Nelson and Sons
	C.W. Rees	-	Ltd., London

Course Outcomes and Mapping

At the end of the course, the student will be able

- **CO1.** to study the various known reactive intermediate in organic synthesis
- **CO2.** to predict the relationships between organic chemical structures and their reactivity.
- CO3. to learn the fundamental and advanced concepts in reaction mechanisms in organic chemistry along with the study of reaction mechanisms in various types of substitution and elimination reactions.
- **CO4.** to study the new methodologies for altering the reactivity patterns of reactive intermediates
- **CO5.** to synthesize various molecules using combinations of reactive intermediates

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	2	3	4	1	•••	3	2
CO2	1	3	4	1	3	2	2
CO3	1	3	3	1		2	3
CO4	1	4	4	1	1	3	2
CO5	2	4	2	1	1	3	2

I.K. C	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY						
	<u>DEPA</u>	RTMEN	NT OF C	HEMICAL SCIENCES			
Course Name	M.Sc.	M.Sc. Chemistry					
Subject Code:	CHL4	03-18					
Subject Title:	PHYS	ICAL C	HEMIST	ΓRY-I			
Contact Hours:	L:4	T:0	P:0	Credits:4			
Examination	3	3					
Duration (hours)							
Objective(s):	This co	ourse wil	l equip st	tudents with the necessary chemical knowledge			
	concern	concerning the fundamentals in the basic areas of physical chemistry					
	viz. th	ermodyn	namics, e	electrochemistry and chemical kinetics, with			
	regard	regard to various theories developed and their applicability for various					
	system	systems under consideration. The problem solving skills of students are					
	expecte	ed to be	enhance	ed through due weightage given to numerical			
	probler	ns in eac	h unit.				

Unit	Contents	Contact
		Hours
I	Classical Thermodynamics: Brief introduction, partial molar properties; partial molar free energy, chemical potential, partial molar volume, partial molar heat content and their significance. Gibbs-Duhem equation. Determination of partial molar volume by method of intercept. Concept of fugacity and determination of fugacity in liquids and gases. Non-ideal solutions; activity and activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, Determination of activity and activity coefficients, ionic strength, Numerical Problems.	10
II	Electrochemistry-I: Electrolytic conductance and its measurement; Kohlrausch's Law and its applications; Conductometric titrations, Anomaly of strong electrolytes, Debye-Huckel theory, Onsager equation and its verification, Debye-Falkenhagen effect, Wien effect, Thermodynamics of electrifield interface equation, Derivation of electrocapillary, Lippmann equation. Structure of electrified interfaces, Electrical double layer, Theories of structure of electrical double layer: Helmoholtz-Perrin model, Gouy-Chapman model and Stern model. Polarography: Ilkovic equation and its derivation, concentration polarization, instrumentation, advantages of DME, half wave potential, Applications of polarography. Numericals.	13
III	Chemical Dynamics: Collision theory, modified collision theory, weakness of the collision theory, theory of absolute reaction rates, equilibrium hypothesis, Derivation of the rate equation, statistical mechanical derivation and thermodynamic formulation. Isotope effect on reaction rate; Primary isotope effect, secondary isotope effect. Dynamics of unimolecular reactions; Lindemann, Hinschelwood and RRKM theories for unimolecular reactions.	12

IV	Kinetics of Reactions: Kinetics of Complex Reactions; Opposing	10
	Reactions, Consecutive reactions, Chain Reactions. Kinetics of	
	reactions in solution: Reaction between ions, influence of solvent-	
	double sphere model, single sphere model, influence of ionic	
	strength. Kinetics of fast reactions; Flow methods for study of fast	
	reactions, pulse methods, flash photolysis and NMR method.	
	Numericals.	

S.No.	Author(s)	Title of the Book	Publisher/Year
1	P.W. Atkins	Physical Chemistry, 3 rd	ELBS (1987)
		edition	
2	S.H. Maron & C.F. Prutton	Principles of Physical	Oxford and IBH
		Chemistry, 1 st edition	(1958)
3	G.W. Castellan	Physical Chemistry, 4 th	Narosa (2004)
		edition	
4	S. Glasstone	Thermodynamics for	Affiliated East-West
		Chemists	Press Pvt. Ltd.
5	S. Glasstone	An introduction to	Affiliated East-West
		Electrochemistry	Press Pvt. Ltd.
6	K.J. Laidler	Chemical kinetics	Harper and Row,
			New York (1987)
7	D.R. Crow	Principles and Applications of	Blackie academic,
		Electro-chemistry	Glasgow (1988)

Course Outcomes and Mapping

At the end of the course,	the student will be able to
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- CO1. Understand the basic principles and theories pertaining to thermodynamics, electrochemistry and chemical kinetics.
- **CO2.** Solve various problems related to non ideal systems.
- **CO3.** Define the dynamics of various types of reactions.
- **CO4.** Familiar with the various techniques used for determination of rates of reactions.
- **CO5.** Rationalise bulk properties and processes using thermodynamic considerations.
- **CO6.** Apply the concepts related to conductance in solving problems related to electrolytes.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	2	4	5	3		2	4
CO2	2	5	5	2	3	2	5
CO3	2	2	3	2	1	1	2
CO4	2	2	2	3	4	2	2
CO5	2	4	5	3		2	4
CO6	2	5	5	2	3	2	5

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES								
Course Name		M.Sc. Chemistry						
Subject Code:	CHL40	CHL404-18						
Subject Title:	SPECT	SPECTROSCOPY-I						
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4						
Examination	3							
Duration (hours)								
Objective(s):	1. To le	1. To learn various techniques of spectrometric identification of organic						
	compounds							
	2. To c	haracteri	ze organ	ic compounds by applying various techniques				
	togethe	r		-				

Unit	Contents			
		Hours		
I	General Features of Spectroscopy: Introduction to spectroscopy, Nature of radiation, Energies corresponding to various kinds of radiation, Experimental techniques, intensities of spectral lines, Selection rules and transition moments, Line widths, Broadening. UV and Visible Spectroscopy of organic molecules: Measurement techniques, Beer – Lambert's Law, molar extinction coefficient, oscillatorstrength and intensity of the electronic transition, Frank Condon Principle, Ground andfirst excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra, Chromophores, auxochromes, blue shift, red shift, hypo andhyperchromic effect, σ - σ *, π - π *, n - π * transitions in organic molecules, Woodward rules for conjugated dienes and α , β - unsaturated carbonyl groups, extended conjugation and aromatic sterically hindered	10		
II	Infrared Spectroscopy: Introduction, Principle of IR spectroscopy, modes of vibrations, Vibrational frequency, fundamental vibrations, Selection rules, factors affecting vibrational frequencies, IR spectrophotometer, sampling techniques, special features of different classes of organic compounds pertaining to IR spectroscopy (such as aliphatic and aromatic hydrocarbons, halogen compounds, alcohols and phenols, ethers, carbonyl compounds, acids and its derivatives, amines and amides, nitro and nitrides, nitrile compounds, heteroaromatic compounds etc.) and interpretation of IR spectrum, quantitative applications.	10		
III	Nuclear Magnetic Resonance Spectroscopy: PMR: Natural abundance of ¹³ C, ¹⁹ F and ³¹ P nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, proton exchange, spin-spin coupling- splitting theory, one, two and three bond coupling, virtual, long range and allylic coupling, magnitude of coupling constant; factors affecting the coupling constant, Chemical and magnetic equivalence,	15		

	First and second order spectra, A2, AB, AX, AB2, AX2, A2B2 and A2X2 spin systems, Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents), CW and FT NMR, Relaxation processes, T1 and T2measurements, Applications of PMR in structural elucidation of simple and complex compounds. 13C-NMR: Resolution and multiplicity of 13C NMR, 1H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE and origin of nuclear overhauser effect. off-resonance, proton decoupling, Structural applications of 13C-NMR., pulse sequences, pulse widths, spins and magnetization vectors, DEPT,INEPT, Introduction to 2D-NMR, COSY, NOESY, HMBC and HSQC spectra.	
IV	Mass Spectrometry: Introduction, methods of ionization EI & CI, Brief description of LD, FAB, SIMS, FD etc., Ion analysis methods (in brief), isotope abundance, Metastable ions, general rules predicting the fragmentation patterns. Nitrogen rule, determination of molecular ion peak, index of H eficiency, fragmentation patterns for aliphatic compounds, alkyl halides, aryl halides, alcohols, amines, aldehydes, Ketones, esters, amides, nitriles, carboxylic acids, ethers, monocyclic aromatic compounds.	10

S.No.	Author(s)	Title of the Book	Publisher/Year
1	Donald L. Pavia, Gary M.	Spectroscopy	Cengage learnings
	Lampman, George S. Kriz &		
	James R. Vyvyanz		
2	Robert. M. Silverstein,	Spectrometic Identification of	Wiley, 2007
	Francis X. Webster, David J.	Organic Compounds.	
	Kiemle & David L. Bryce		
3	W. Kemp	Organic Spectroscopy	Palgrave Macmillan
4	D.H. Williams, I. Fleming	Spectroscopic Methods in	New Age
		Organic Chemistry	International
5	R. F. Barrow, Derek A.	Molecular Spectroscopy	Royal Society of
	Long, D. J. Millen		Chemistry
6	C.N Banwell	Fundamentals of Molecular	Tata Mc Graw Hill
		Spectroscopy	

Course Outcomes and Mapping

At the end of	the course, the student will be able to
CO1.	Solve structural problems based on UV-Vis, IR, ¹ H-NMR, ¹³ C-NMR and mass spectral data.
CO2.	Elucidate the structures of various organic compounds on the basis of spectral data.
CO3.	Understand various involved processes responsible for NMR chemical shifts and splitting patterns and mass spectrometry.
CO4.	Illustrate the mechanisms that give rise to the infrared and UV-Visible absorption bands and identify to which functional groups each correspond.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	3	5	3	1	5	4	2
CO2	3	4	3	1	5	3	2
CO3	2	4	3	_	4	2	2
CO4	3	4	3	2	3	2	2

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES									
Course Name		M.Sc. Chemistry							
Subject Code:		CHL405-18							
Subject Title:	ENVIRONMENTAL CHEMISTRY								
Contact Hours:	L:3	L:3 T:0 P:0 Credits:3							
Examination	3	3							
Duration (hours)									
Objective(s):	The spe	ecialisati	on in "E	nvironmental Chemistry," gives an insight to					
	the rol	the role of various environmentally harmful substances for the							
	degrada	degradation of the environment. The students will learn what is toxic,							
	and mo	st import	tantly, wi	ll become an expert on what we can do to find					
		-	•	s of toxic substances in the environment.					

Unit	Contents	
I	Air Pollution: Chemical composition of atmosphere- particles, ions and radicals and their formation, Sources and sinks of gases pollutants, classification & effects of air pollutants on living and nonliving things, Air pollution problems in India, pollution problems in industrial area, global air pollution problems, smog, green house effect, global warming, acid rain, ozone depletion and their consequences on Environment. Major air pollution disasters. Water pollution: Chemical composition of water bodies-lakes, streams, rivers and wet lands, Types, sources and classification of water pollutants, Industrial water pollution, constituents of aquatic Environment, oxygen contents of water and aquatic life, oxygen	4 4
	electrode, and its use, mercury pollution and estimation of organomercurials, Effects of water pollutants on life and Environment.	
II	Analysis of air and water pollutants: Water analysis: Color, odour, conductivity, TDS, pH, acidity, alkalinity, chloride, residual chlorine, hardness, trace metal analysis, elemental analysis, ammonia, nitrite, nitrate, fluoride, sulphide, phosphate, phenols, surfactants, BOD, COD, DO, TOC, non-dispersive IR spectroscopy, anode stripping, ICP, AES, Chromatography, ion-selective electrodes, neutron activation analysis.	12
III	Soil pollution: Soil humus, soil fertility, inorganic and organic components in soil, acid-base and ion exchange reactions in soils, micro and macro nutrients, wastes and pollutants in soil, introduction to geochemistry, treatment and recycling soil analysis, radioactive pollution, disposal of radioactive waste. Pesticide, residue analysis soil pollution, Sources of pesticides residue in the Environment, pesticides degradation by natural forces, effect of pesticide residue on life, Analytical techniques (HPLC, GC-MS) for pesticides residue analysis.	12
IV	Radiation pollution: Classification & effects of radiation, effects of ionizing radiation on man, Effects of non ionizing radiation on	13

life, radioactivity and Nuclear fall out, protection and control from
radiation. Environmental toxicology, chemical solutions to
environmental problems, biodegradability, principles of
decomposition, better industrial processes, Bhopal gas tragedy,
Chernobyl, three mile island, sewozo and minamata disasters.

S.No.	Author(s)	Title of the Book	Publisher/Year
1	A.K. De	Environmental Pollution	Wiley Eastern
2	Wark & Werner	Air Pollution	IEP
3	S.P. Mahajan	Environmental Pollution Control	Tata Mc-graw Hill
		in Process Industries	Education
4	B.K. Sharma & H.Kaur	Environmental Pollution	Krishna
5	P.K. Trivedi	Introduction to Air Pollution	
6	S.M. Khopkar	Environmental Pollution Analysis	Wiley Eastern
7	F. J. Welcher	Standard method of chemical	Van-Nostrand
		analysis	Reinhold
8	B.K. Sharma & H.Kaur	Environmental Chemistry	Krishna
9	T. D. Biswas & S. K.	Text book of soil science	Tata Mc-graw Hill
	Mukherjee		Education

Course Outcomes and Mapping

At the end of	f the course	the student	will be able to
At the chu o	i inc course.	tile student	will be able to

- CO1. Acquire fundamental knowledge and understanding of the physical environment (land, water, air and climate) and will develop insights into key concepts in the field of environmental Chemistry.
- CO2. Understand the basic phenomena of atmospheric sciences, hydrology of different aquatic ecosystems and soil science.
- CO3. Develop sound theoretical background of basic chemistry associated with toxicology of environmental pollutants
- **CO4.** Get acquainted with the sources, properties and ill-effects of important air, water, soil and radioactive pollutants in air, water and soil and apply analytical tools to determine and measure pollutants in various environmental samples

CO5. Become aware of the local, regional and global environmental problems.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	3	4	3	2	3	4	4
CO2	2	3	3	3	2	3	5
CO3	3	3	3	2	2	2	3
CO4	3	5	3	4	4	4	3
CO5	3	1	2	5	2	2	3

I.K. G	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES				
Course Name	M.Sc.	Chemi	stry		
Subject Code:	CHL40	6A-18			
Subject Title:	HUMA	N PHYS	SIOLOG	Y	
Contact Hours:	L:3	T:0	P:0	Credits:3	
Examination	3				
Duration (hours)					
Objective(s):	Chemis	try has it	ts large a	pplications in Human functioning. Most of the	
	1			a human body performs from molecular to	
	organ system level follows the basic principles of Chemistry & Physics.				
	Therefore the major objective of teaching this subject is to understand				
	the various chemical functions which involve mechanisms underlying				
	communication & coordination within an organism and to elucidate the				
	structur	e of var	rious par	ts in relationship with its functions to bring	
	about h	omeostas	sis within	the body.	

Unit	Contents	Contact
		Hours
I	Introduction : General Introduction to anatomy, physiology and its	2
	related sciences. Physico-chemical laws and their applications in	
	Physiology. Elementary Composition of a Human Body	
	Cell Structure and Functions- A Basis of Physiology: Structure	
	and functions of subcellular organelles, Elementary tissues	
	(Epithelial, Muscular, Connective & Nervous) of the Human Body,	
	their structure & functions, molecular mechanism of skeletal muscle	8
	contraction, nerve conduction, membrane transport and cell division	
II	Digestive System: Physiological anatomy and histology of the	
	digestive system, Functions of Digestive system, Digestive juices	8
	(Saliva, Gastric, Pancreatic Bile and Intestinal), their composition,	
	functions and mechanism of secretions, movements of alimentary	
	canal and gut reflexes, digestion of carbohydrates, proteins, lipids	
	and their absorption	
	Vitamins: History, characteristics, composition and functions of	
	various vitamins (Vitamins A, D, E, K, C B ₁ , B ₂ , B ₃ B ₆ and B ₁₂) etc.	2
III	Cardiovascular System: Systemic & Pulmonary Circulation;	
	Hepatic, Renal & Hypophyseal portal circulation. Anatomy of Heart	8
	and properties of cardiac muscles. Origin and conduction of Heart	
	beat. Nervous & chemical regulation of Heart beat. Cardiac cycle,	
	heart sounds, ECG, Cardiac output. Blood pressure and its	
	regulation.	
	Respiratory System: Anatomy of respiratory system, mechanism	
	of pulmonary ventilation, pulmonary volumes and lung capacities,	
	physical principles and mechanisms of gaseous exchange and	6
	transport, regulation of respiration.	
IV	Excretory System: Physiological anatomy of the kidneys and	
	urinary tract, urine formation (glomerular filtration, tubular	5

reabsorption and secretion) and its regulation.	
Endocrine System: Introduction and General Mechanisms of	
physiological action of Pituitary hormones, Thyroid hormones,	
Adrenocortical hormones, Pancreatic hormones, Parathormone and	6
Calcitonin, Gonadal hormones.	

S.No.	Author(s)	Title of the Book	Publisher/Year
1.	Anne Waugh & Alison	Ross & Wilson Human	Churchil Livingstone
	Grant	Anatomy & Physiology	Elsevier Publishers,
			China. 2014
2.	C.C. Chatterjee	Human Physiology Vol. I & II	Medical Allied
			Agency, Calcutta.
			2000
3.	A.C. Guyton & J.E. Hall	Textbook of Medical	Prism Book Pvt Ltd.
		Physiology. 9 th edition	India. 1996
4.	Gerard G. Tortora & Bryan	Principles of Anatomy &	John Wiley & Sons,
	Derrickson	Physiology. 12th edition.	USA. 2009

Course Outcomes and Mapping

At the end of the course.	the student will be ab	le to
ALUIC CHA OLUIC COULSC.	. the student will be ab	וטוטו

- **CO1.** Understand basic structure and functioning of human organs.
- CO2. Learn various physiological processes to understand functioning of important organ systems.
- **CO3.** Know how various organs bring about homeostasis.
- **CO4.** Describe the relationship between structure & functions of cells, tissues & organs.
- CO5. Understand how the hormones effect the working of whole body organs.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	2	-	1	-	1	3	2
CO2	3	-	3	-	1	4	3
CO3	3		2	1	1	4	2
CO4	-	2	1	1	1	2	2
CO5	3	2	3	1	1	3	3

I.K. (I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES				
Course Name	Course Name M.Sc. Chemistry				
Subject Code:	CHL4	CHL406B-18			
Subject Title:	NUMERICAL METHODS FOR CHEMISTS				
Contact Hours:	L:3	L:3 T:0 P:0 Credits:3			
Examination	3	3			
Duration (hours)					
Objective(s):	To make students familiar with the basic concepts of mathematics for				
	understanding theoretical treatments and solving numerical problems in				
	other c	ourses be	eing taug	ght in the class.	

Unit	Contents	Contact
_		Hours
I	Matrix Algebra: Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-	11
	symmetric, Hermitian, skew-hermitian, unit, diagonal, unitary etc.)	
	and their properties. Matrix equations: Homogeneous, non-	
	homogeneous linear equations and introduction to vector spaces,	
	matrix eigenvalues, diagonalization, determinants (examples from	
	Huckel theory).	
II	Differential Calculus: Functions, continuity and differentiability,	12
	applications of differential calculus including maxima and minima (
	examples related to maximally populated rotational energy levels,	
	Bohr's radius and most probable velocity from Maxwell's	
	distribution etc), exact and inexact differentials with their	
	applications to thermodynamic properties.	
	Integral calculus, basic rules for integration, integration by parts,	
	partial fraction and substitution. Reduction formulae, applications of	
	integral calculus.	
	Functions of several variables, partial differentiation, co- ordinate	
	transformations (e.g. Cartesian to spherical polar).	
III	Elementary Differential Equations: Variables-separable and exact	11
	first-order differential equations, homogeneous, exact and linear	
	equations. Applications to chemical kinetics, secular equilibria,	
	quantum chemistry etc. Solutions of differential equations by the	
	power series method, order differential equations and their	
	solutions.	
IV	Permutation and Probability: Permutations and combinations,	11
	probability and probability theorems, average, root mean square and	
	most probable errors, examples from the kinetic theory of gases etc,	
	curve fitting (including least squares fit etc) with a general	
	polynomial fit.	

S.No.	Author(s)	Title of the Book	Publisher/Year
1	E.Steiner	The Chemistry Mathematics	Oxford University
		Book	Press
2	Doggett and Sutcliffe	Mathematics for Chemistry	Longman
3	F. Daniels	Mathematical Preparation for	McGraw Hill
		Physical Chemistry	
4	D.M. Hirst	Chemical Mathematics	Longman
5	J.R. Barrante	Chemical Mathematics for	Prentice Hall
		Physical Chemistry	
6	Tebbutt	Basic Mathematics for	Wiley
		Chemist	

Course Outcomes and Mapping

At the end of the course, the student will be able to

- CO1. Learn the use of derivatives in chemistry is when they want to find the concentration of an element in a product. Differentiation is used to calculate rate of reaction and compressibility in chemistry.
- CO2. Understand the various basic mathematical methods for chemists. The methods involve matrices, differentiation, integration, first and second order differential equations and their solutions.
- CO3. Students will be able to explore the idea how to use basic math, probability in chemistry to enhance the physical chemistry courses like quantum mechanics and statistics mechanics.
- Develop understanding and fluency in mathematics through inquiry, exploring and connecting mathematical concepts in chemistry and applying problem-solving skills and mathematical techniques. The theory of matrices which are used in solving equations related to chemical reactions.
- **CO5.** Develop the ability to use a variety of representations, in written, graphical form, to formulate and express mathematical ideas. They will communicate mathematically terminology and notations.
- CO6. Understand the concept of permutations and combinations during defining of structures of reactions. Applications of differential equations as chemical kinetics, secular equilibria, quantum chemistry.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	4	4	2	4	3	3	2
CO2	3	3	4	2	3	4	3
CO3	4	5	3	2	2	3	2
CO4	4	4	4	3	4	5	5
CO5	4	3	3	3	4	4	3
CO6	5	2	4	3	5	4	3

I,l	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY					
	DEPA	RTMEN	VT OF C	CHEMICAL SCIENCES		
Course Name	M.Sc.	Chemi	istry			
Subject Code:	CHP4	07-18				
Subject Title:	INORGANIC CHEMISTRY LAB					
Contact Hours:	L:0	L:0 T:0 P:6 Credits:3				
Examination	6					
Duration (hours)						
Objective(s):	The objective of this course is to provide practical knowledge and					
		illustrative experiments about synthesis and characterization of				
	inorgai	nic comp	lexes and	d estimation of metal ions.		

Unit	Contents
I	Synthesis and characterization of following complexes and estimation of metal
	ions:
	1. Synthesis of tris(ethylenediamine)nickel(II) dichloride, [Ni(en) ₃]Cl ₂ , and
	estimation of Ni(II). Record and interpret its IR, UV-vis and magnetic susceptibilty.
	2. Synthesis of hexaaminenickel(II) dichloride [Ni(NH ₃) ₆]Cl ₂ and estimation
	of Ni(II). Record and interpret its IR, UV-vis and magnetic susceptibilty.
	3. Synthesis of [Cu(NH ₃) ₄]SO ₄ .H ₂ O and estimation of Copper.
	4. To prepare cis and trans copper glycine complexes.
	5. Preparation of [VO(acac) ₂]. Record and interpret its IR, UV-vis and magnetic susceptibility.
	6. To prepare a pure sample of tris(acetylacetone)cobalt(III), Co(acac) ₃ .
	Record and interpret its IR, UV-vis spectrum.
	7. Preparation of tris(nitro-acetylacetonato)cobalt(III), Co(acac-NO ₂) ₃ , record
	and interpret its proton NMR spectrum.
	8. To prepare [Fe(NO)(S ₂ CNEt ₂) ₂]. Record and interpret its IR and UV-vis
	spectrum, Magnetic Susceptibility and Analysis of Fe(II).
II	Gravimetric Analysis
	1. Determination of Ba ²⁺ as its chromate.
	2. Estimation of lead as its lead molybdate.
	3. Estimation of chromium (III) as its lead chromate.
	4. Estimation of Cu ²⁺ using Ammonium/Sodium thiocyanate

Reference Books

S.No.	Author(s)	Title of the Book
1	J.R. Barrante G. Marr and B.W. Rockett	Practical Inorganic Chemistry
2	Vogel	Inorganic Quantitative Analysis

Course Outcomes and Mapping

At the end of the course, the students will learn

- **CO1.** Preparation of different inorganic complexes.
- **CO2.** Purification and crystallisation of inorganic compounds.
- CO3. Interpretation of compounds using UV-Vis, FT-IR techniques.
- **CO4.** Measurement of various physical properties such as magnetic moment of complexes.

CO5. Gravimetric analysis of various cations.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	5	1	4	2	5	2	-
CO2	5	1	4	1	5	2	-
CO3	5	4	5	-	5	3	4
CO4	3	4	5	-	4	2	2
CO5	5	2	2	-	5	1	-

I.K. C	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES						
Course Name	M.Sc.	Chemi	stry				
Subject Code:	CHP40	8-18	-				
Subject Title:	ORGA	NIC SY	NTHESI	S LAB			
Contact Hours:	L:0	L:0 T:0 P:6 Credits:3					
Examination	6						
Duration (hours)							
Objective(s):	1. To learn various practical techniques for synthesis, identification,						
	isolation, purification and characterization of organic compounds.						
	2. To 0	carry out	hand or	n experience the various methods of organic			
	synthes	is.		-			

Unit	Contents				
I	Techniques : (At least One Practical of Each Technique)				
	Crystallization, Purification by Sublimation, Distillation, Fractional Distillation,				
	Steam Distillation, Vacuum Distillation, Preparative chromatography, Column				
	Chromatography, TLC stains preparation and Thin Layer Chromatography.				
	(Purity is to be checked by m.p. and mixed m.p.)				
II	Preparation of Derivatives: (Each Derivative of at least one Compound) Oxime,				
	2,4-DNP, Acetyl, Benzoyl, Semicarbazone, Anilide, Amide, Aryloxyacetic acid.				
III	Preparations:				
	(a) At least eight single stage preparations from the following should be carried				
	out. The preparations should be carried out on micro scale.				
	i) Cyclohexanone to Adipic acid				
	ii) Benzophenone to Benzhydral				
	iii) Anthracene to Anthraquinone				
	iv) Chlorobenzene to 2,4-Dinitrochlorobenzene				
	v) 2,4-Dinitrochlorobenzene to 2,4-Dinitrophenol				
	vi) Acetoacetic ester to 1-Phenyl-3-methyl-5 pyrazolone				
	vii) Benzaldehyde to Cinnamic acid				
	viii) 4-Chlorobenzaldehyde to 4-Chlorobenzoic acid and 4-Chlorobenzyl alcohol				
	ix) Benzene to β-Benzoyl propionic acid				
	x) Benzaldehyde to Dibenzylidene acetone				
	xi) p-Aminobenzoic acid to p-Chlorobenzoic acid				
	xii) N,N-Dimethylaniline to 4-Formyl-N, N-dimethyl aniline				
	xiii) Benzophenone to Benzpinacol				
	xiv) p-Nitrotoluene to p-Nitro benzoic acid				
	xv) Anisole to 2,4-Dinitroanisole				
	xvi) Phthalic anhydride to phthalimide				
	xvii) Phthalimide to Anthranilic acid				
	xviii) Acetanilide to p-Bromoacetanide				
	xix) p-Bromoacetanide to p-Bromoaniline				
	xx) m-Dinitrobenzene to m-Nitroaniline				
	(b) Minimum 2 two stage and 2 three stage preparations to reveal how to develop a				
	synthetic sequence.				
	(c) Interpretation of NMR, IR and Mass Spectra of about 10 compounds.				

S.No.	Author(s)	Title of the Book	Publisher
1	Brian S. Furniss, Antony J.	Vogel's Textbook of Practical	Longman, London
	Hannaford, Peter W.G.	Organic Chemistry, 5 th	
	Smith and Austin R. Tatchell	Edition	
2	F.G. Mann and B. C.	Practical Organic Chemistry	Longman, New York
	Saunders		
3	John Leonard, Barry Lygo	Advanced Practical Organic	CRC Press, London
	and Garry Procter	Chemistry, Third Edition	
4	J.T. Sharp	Practical Organic	Springer
		Chemistry: A student	
		handbook of techniques	
5	Philippa B. Cranwell,	Experimental Organic	Wiley
	Laurence M. Harwood and	Chemistry, 3 rd Edition	
	Cristopher J. Moody		
6	Robert. M. Silverstein,	Spectrometric Identification	Wiley, 2007
	Francis X. Webster, David J.	of Organic Compounds.	
	Kiemle & David L. Bryce		

Course Outcomes and Mapping

At the end of the	course the	students	will be	able to
The thic cha of the	course, are	Students	WIII OC	aute to

- **CO1.** Apply various methods techniques in organic synthesis to build organic molecules.
- CO2. Understand the fundamental mechanistic pathways of organic synthesis involving various practical lab techniques together.
- **CO3.** Apply the spectroscopic techniques for the determination of molecular structures of organic molecules.
- **CO4.** Present their work with practical skills and the awareness of health and safety procedures.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	1	3	5	3	5	5	2
CO2	2	3	5	3	3	4	3
CO3	1	3	5	2	3	3	2
CO4	4	3	3	4	5	3	3

SEMESTER-II

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES							
Course Name	M.Sc.	Chemi	stry				
Subject Code:	CHL41	1-18					
Subject Title:	INORG	SANIC (CHEMIS	TRY-II			
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4					
Examination	3						
Duration (hours)	uration (hours)						
Objective(s):	To impart concepts in organometallic chemistry and structural aspects						
	of inorganic chains, rings, cages and clusters, inorganic reaction						
	mechan	ism and	nuclear c	hemistry			

Unit	Contents	Contact Hours
I	Organometallic Chemistry: 18 electron rule, Exceptions to	12
1	eighteen electron rule, Synthesis, structure, bonding and reactivity	12
	of transition metal complexes with olefins, Cylobutadiene	
	Cyclopentadienyl, Cyclopentadiene, Benzenoid (metallocenes), π -	
	allyl and Enyl System, Dynamic equilibria in allyl complexes,	
	Differences between unconjugated & conjugated olefin ligands.	
	Transition metal-carbon bond: Metal-alkyls (Organomercury and Grignard reagent), metal-carbenes (chromium complexes) and	
	metal-carbides (Tungsten carbide).	
II	Inorganic Reaction Mechanism: Lability and inertness of metal	13
	complexes, Factors effecting reaction rate, Substitution	
	reactions in octahedral complexes, types of intermediate formed in	
	substitution reactions, Details of mechanism of hydrolysis (under	
	acidic and basic condition) and the stereochemistry of	
	intermediate formed, Trans effect and their theories,	
	oxidation-reduction reactions, Outer sphere and inner sphere reactions. Mechanism of electron transfer reaction.	
III	Chains, Rings and Cages: Catenation, Heterocatenation,	10
111	Isopolyanions, Heteropolyanions, Preparation, structure and	10
	properties of Boranes, Diboranes, Carboranes, Borazenes,	
	metallocene-carboranes.	
	Metal clusters: Geometric and electronic structure, three, four and	
	higher connect clusters, closo-, nido-, arachno-borane structural	
	paradigm, Wade rules, Metal carbonyl cluster, heteronuclear cluster,	
***	capping rules, isolobal relationships, Zintle ions.	10
IV	Nuclear Chemistry: Nuclear particles, forces, size, nuclear	10
	binding energy; Detection and measurement of radioactivity (G.M.	
	Counter method); Decay kinetics-first order rate equation for radioactive disintegration; Theory of Radioactive disintegration;	
	Radioactive series- Uranium; magic number concept; uses of	

radioactive	and non-radioactive isotopes; transmutation of
elements; pur	ity and strength of radio isotopes, Basic principles
and types of n	uclear reactors; atomic energy and Q values.

S.No.	Author(s)	Title of the Book	Publisher/Year
1	J.E. Huheey, Ellen A.	Inorganic Chemistry	Harper Collins <i>College</i>
	Keiter, Richard L. Keiter	Principles of Structure and	Publishers
		Reactivity, Fourth edition	
2	Cotton, Wilkinson	Advanced Inorganic	Wiley
	Murillo and Bochmann	Chemistry, Sixth edition	
3	J.D. Lee	Concise Inorganic	Oxford
		Chemistry, Fifth edition	
4	Duward Shriver, Peter	Inorganic Chemistry, 3rd	W. H. Freeman and
	Atkins, W. H. Freeman	edition	Company, New York
5	R.S. Drago	Physical Methods in	Affiliated East-West Press
		inorganic Chemistry, 2nd	(Section 1 & 2), Reinhold
		Edition,	New York (1968)
6	H.B. Gray	Electrons and Chemical	(Section 2), W.A.
		Bonding	Benjamin, London (1965)
7	A.B.P. Lever	Inorganic Electronic-	Amsterdam, The
		Spectroscopy, 2 nd Edition	Netherlands: Elsevier,
			1984
8	N.N. Greenwood and A.	Chemistry of Elements	Earnshaw, Pergamon
	Earnshaw		Press, (Section 7) (1984)

Course Outcomes and Mapping

At the end of the course, the student will be able to

- CO1. Understand the method of synthesis, bonding and reactivity of organometallic compounds.
- CO2. Learn the factors responsible for the stability of organometallic compounds and clusters.
- CO3. Understand the structures and properties of various types of inorganic chain, rings and cages.
- CO4. Knowledge of various reaction mechanisms (substitution reactions or electron transfer reactions) in inorganic complexes
- CO5. Understand the basics of nuclear chemistry and radio analytical techniques.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	1	1	4	1	5	3	-
CO2	1	-	4	1	5	3	-
CO3	1	1	4	1	4	3	-
CO4	1	-	3	1	4	1	-
CO5	1	4	2	1	1	3	1

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES							
Course Name	M.Sc.	Chemi	stry				
Subject Code:	CHL41	2-18					
Subject Title:	REAC'	TIVE IN	TERMI	EDIATES-II			
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4					
Examination	3						
Duration (hours)	Duration (hours)						
Objective(s):	1. To study the reaction mechanisms in various types of addition						
	reactions, redox reactions and rearrangement reactions.						
	2. To predict and account for the most commonly encountered reaction						
	mechanisms in organic chemistry.						

Unit	Contents	Contact Hours
I	Addition to carbon-carbon and carbon-hetero multiple bonds:	12
1	Mechanistic and stereochemical outcome in the addition of	12
	electrophile, nucleophile, free radicals, Hydration of olefins and	
	acetylenes, addition of halogens, Electrophilic additions involving	
	metal ions, oxymercuration, hydroxylation, Michael addition,	
	Sharpless asymmetric epoxidation. Free-Radical addition of	
	hydrogen halides, halomethanes, thiols <i>etc</i> . to carbon-carbon multiple bonds	
	Hydration and addition of alcohols to aldehydes and ketones.	
	Addition of nucleophilic carbon to carbonyl groups: Grignard	
	reagents, organozinc, organolithium and Gillman reagents to	
	carbonyl and unsaturated carbonyl compounds.	
	Carbenes and their additions to double bonds, Simmon-Smith	
	reaction, Mannich, Stobbe, Darzen, Wittig, Wittig-Horner and	
	Benzoin reactions.	
II	Oxidation reactions: Introduction, different oxidative processes,	12
	Mechanistic study of the oxidation reactions. Oxidation of	
	hydrocarbons: oxidation of methylene, oxidation of aryl methanes,	
	allylic oxidation of olefins, dehydrogenation by quinones, SeO ₂ and	
	Pb(OAc) ₄ , Formation of C-C bond in phenol coupling- acetylene coupling-allylic oxidation.	
	Oxidation of alcohols: Swern Oxidations , PCC, PDC oxidation,	
	oxidation using different metal based and non-metal based	
	reagents, oxidation of glycols, halides and amines to aldehydes and	
	ketones, ozonolysis-oxidation of olefinic double bonds, oxidation of	
	α,β -unsaturated carbonyl compounds, ketones, Baeyer-Villiger	
	oxidation.	
III	Reduction reactions: Introduction. Different reductive processes,	12
	Catalytic hydrogenation: selectivity, hydrogenation of alkenes and	
	its stereochemical and mechanistic aspects, hydrogenation of	
	alkynes, aromatic compounds, carbonyl compounds-aldehydes,	
	ketones, acids, ester and nitriles, epoxides, nitro, nitroso, azo and	

	oxime groups. homogenous hydrogenation, reduction by dissolving metals: reduction of carbonyl compounds, conjugated systems, alkynes, aromatic compounds, clemmensen reduction. Reduction by hydride transfer reagents: Lithium aluminium hydride, alkoxy substituted LAH, disobutyl aluminium hydride, Sodium borohydride, Sodium cyanoborohydride, Sodium triacetoxyborohydride, tin hydride, trialkyl tin hydride, trialkyl silanes, diborane, diisoamyl borane, hexyl borane, 9-BBN, isopinocamphenyl and disiopinocamphenyl borane. Wolf-Kishner reduction.	
IV	Rearrangements: General mechanistic consideration: Types of migration, Rearrangements on deficient carbons: Wagner-Meerwein rearrangement, Pinacol-pinacolone, Favorskii rearrangement, Allylic rearrangement, Isonitrile-Nitrile rearrangement. Rearrangements on carbonyl group: Benzil-Benzilic acid rearrangement. Rearrangements on heteroatoms: Hofmann rearrangement, Beckmann, Schmidt, Baeyer-Villiger, Criegee rearrangement. Rearrangements in pericyclic reactions: Cope rearrangement, Claisen rearrangement. Other rearrangements: Demjanov, Arndt-Eistert synthesis, Neber, Curtius, Shapiro reaction, Fries rearrangement, dienone-phenol, Wolf, Stevens (in cyclic systems).	9

S.No.	Author(s)	Title of the Book	Publisher	
1	W. Carruthers and I.	Some Modern Methods of	Cambridge University	
	Coldham	Organic Synthesis, IV Edition	Press, 2004	
2	Francis A. Carey and	Advanced Organic Chemistry	Kluwer Academic	
	Richard J. Sundberg	Vol. A and Vol. B, fourth	publishers, New York	
		Edition	2002	
3	Jerry March	Organic Reaction Mechanism	John Wiley Ed. 5, 2002	
4	John McMurry and	Fundamentals of Organic	Cengage Learnings	
	Eric Simanek	Chemistry		
5	R.O.C. Norman	Principles of organic synthesis	Chapman and Hall,	
			London. 1980	
6	T.L. Gilchrist and	Carbenes, Nitrenes and Arynes	Thomas Nelson and Sons	
	C.W. Rees		Ltd., London	
7	H.O. House	Modern Synthetic Reactions	The Benjamin Cummings	
			Publishing Company,	
			London, 1972	

Course Outcomes and Mapping

At the end of	At the end of the course, the student will be able to						
CO1.	predict and account for the most commonly encountered reaction mechanisms						
CO2.	in organic chemistry predict the relationships between organic chemical structures and their reactivity.						
CO3.	learn the fundamental and advanced concepts in reaction mechanisms in						

organic chemistry along with the study of reaction mechanisms in various types of addition, redox and rearrangement reactions.

CO4. study the new methodologies for altering the reactivity patterns of reactive intermediates.

CO5. synthesize various molecules using combinations of reactive intermediates.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	1	3	4	1	1	3	2
CO2	1	3	4	1	3	3	3
CO3	2	3	4	1	1	3	3
CO4	1	4	4	1	2	5	2
CO5	1	4	4	1	3	5	2

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES						
Course Name						
Subject Code:	CHL41	3-18				
Subject Title:	PHYSI	CAL C	HEMIST	TRY-II		
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4				
Examination 3						
Duration (hours)	Duration (hours)					
Objective(s):	To impart students knowledge regarding basics of Quantum mechanics					
	and th	and their applications for solving various problems in physical				
	chemis	ry.				

Unit	Contents	
		Hours
I	An introduction to quantum mechanics; quantum mechanics vs. classical mechanics, wave–particle duality, and uncertainty principle. Postulates of Quantum mechanics, Operators and observables, Hermitian operators, Normality and orthogonality of functions. Wave function and interpretation; time-dependent and time-independent Schrödinger equation, Problems related to eigen value. Solution of Schrodinger equation for particle in one and three dimensional box.	13
II	Application of Schrodinger wave equation to Harmonic oscillator and Rigid rotor; orbital and spin angular momentum; ordinary angular momentum; Eigen functions and Eigen values of angular momentum; ladder operator; addition of angular momenta; spin and antisymmetry; and Pauli exclusion principle.	10
III	Outline of various steps in the solution of the electronic Schrödinger equation for hydrogen atom; Radial and angular parts of the hydrogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals; Significance of Quantum numbers; Need for approximation methods; Perturbation theory; variation theorem; linear variation principle; and application of variation method and perturbation to helium.	12
IV	Electronic configuration; Russel-Saunders terms and coupling schemes; Slater-Condon parameters; Term separation energies of the p ⁿ and d ⁿ configurations; magnetic effects like spin orbit coupling and Zeeman splitting; and introduction to methods of self-consistent virial theorem. Huckel theory of conjugates systems; application to ethylene and butadiene; bond order and charge density calculations.	10

S.No.	Author(s)	Title of the Book	Publisher/Year
1	I.N. Levine	Quantum Chemistry, 5 th	Prentice Hall (2006)
		edition	
2	F.L. Pilar	Elementary Quantum	McGraw Hill (1968)
		Chemistry	
3	N.H. March	Self-Consistent Fields in	Pergamon Press
		Atoms	(1975)
4	A.K. Chandra	Introductory Quantum	Tata-McGraw Hill
		Chemistry	(1988)
5	P.W. Atkins and R.S.	Molecular Quantum	Oxford University
	Friedman	Mechanics, 4 th edition	Press (2004)

Course Outcomes and Mapping

At the end of the course, the student will be able to

- **CO1.** Understand the need for quantum mechanical formalism and basic principles.
- **CO2.** Appreciate the importance and implication of generalized uncertainty principle in quantum mechanics.
- **CO3.** Solve the eigen value problems.
- CO4. Have a better understanding of the mathematical foundations of angular momentum of microscopic particles.
- **CO5.** Apply Schrodinger wave equation and approximation methods for problem solving in quantum mechanics.

CO6. Rationalise the concept of bonding in conjugated polyenes.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	1	4	4	2		2	4
CO2	1	2	4	2		2	4
CO3	2	5	3			3	4
CO4	1	5	3	2	1	3	4
CO5		5	3		2	3	4
CO6		4	3	2	1	2	3

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY						
D	EPART	MENT	OF C	HEMICAL SCIENCES		
Course Name	M.Sc.	M.Sc. Chemistry				
Subject Code:	CHL41	CHL414-18				
Subject Title:	SPECT	ROSCO	PY-II			
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4				
Examination	3	3				
Duration (hours)						
Objective(s):		To provide knowledge of advanced spectroscopic techniques for				
	identific	cation and	d elucida	tion of structures of molecules		

Unit	Contents	Contact Hours
I	Microwave spectroscopy: Rigid and non-rigid rotator, Intensities of spectral lines, isotopic substitution effects, polyatomic linear and symmetric top molecules, Stark effect Vibrational Spectroscopy: Types of vibrations, overtones, combination and difference bands, Fermi resonance, group vibrations, Harmonic and anharmonic oscillators, absorptions of radiation by molecular vibrations, selection rules, force constant, frequency of vibrational transitions of HCl, vibrations in a polyatomic molecule, 3N-6 and 3N-5 rules, Applications	12
II	Raman Spectroscopy: Introduction, vibrational-rotational Raman Spectra, selection rules, mutual exclusion principle, anisotropic polarizabilty, Stokes, anti-Stokes lines, vibrational Raman spectra of CO ₂ and H ₂ O, polarised and depolarised Raman Lines. Mössbauer Spectroscopy: Basic principles, Spectral parameters and display, simple spin states (I 1/2, 3/2), higher spin states (I > 3/2), magnetic splitting, quadruple splitting, additive model application to ⁵⁷ Fe, ¹¹⁹ Sn	10
III	Nuclear Quadruple Resonance Spectroscopy: Introduction, experimental considerations, fundamentals of NOR spectroscopy, origin of EFG, measurement of energy differences between two nuclear spin states, the asymmetry parameter, effects of the magnetic field, interpretation of the spectra, application of NQR spectroscopy Photoelectron Spectroscopy-I: Introduction, photoelectron spectroscopy, chemical shift, X-ray photoelectron spectroscopy, molecular orbital diagrams of nitrogen and oxygen and their XPS spectra-ESCA.	11
IV	Photoelectron Spectroscopy-II: Ultraviolet photoelectron spectroscopy (UPS), PES spectrum of nitrogen sample, vibrational structure in the N2 UPS spectrum, chemical shifts in XPS, exchange splitting and shake up process. Electron Paramagnetic Resonance Spectroscopy: Principle, Spectral display, hyperfine splitting in isotropic systems involving more than one nucleus, Factors affecting magnitude of g values,	12

zero field splitting and Krammer's degeneracy, Spectrum of benzene
radical anion, methyl radical, CH ₂ OH, cyclopentedienyl,
cycloheptatrienyl radical, pyrazine anion, pyrazine anion, Spectra
of triplet states.

S.No.	Author(s)	Title of the Book	Publisher/Year
1	R.S. Drago	Physical Methods in inorganic	Affiliated East-West
		Chemistry	Press (Section 1& 2)
			2nd Edition,
			Reinhold New York
			(1968)
2	C. N. Banwell	Fundamentals of Molecular	McGraw-Hill, 1966
		Spectroscopy	
3	R. V. Parish	NMR, NQR, EPR &	Ellis Horwood,
		Mossbauer spectroscopy in	London, 1990
		Inorganic Chemistry	,
4	G. M. Barrow	Introduction to Molecular	McGraw-Hill
		Spectroscopy	
5	E. A. Ebsworth, S.Craddock	Structural methods in	Blackwell Scientific
	and D.W. H. Rankin	Inorganic Chemistry	Publications (1991)
			` ,
6	C.N.R. Rao and J.R. Ferraro	Spectroscopy in Organic	Vol. I, Academic
		Chemistry	Press, 1971
			,

Course Outcomes and Mapping

At the end of the course, the student will be able to

- CO1. Learn the fundamental and advanced concepts of Microwave, Infrared-Vibration-rotation Raman and infra-red Spectroscopy and their applications for chemical analysis
- CO2. Understand Electronic spectroscopy of different elements and simple molecules.
- CO3. Study the concepts and principles of Mössbauer Spectroscopy and its application.
- **CO4.** Apply Nuclear Quadruple Resonance and Electron Spin Resonance Spectroscopy for organic compounds analysis.

CO5. Solve structural problems based on these techniques.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	3	3	3	1	3	3	3
CO2	3	4	3	1	3	3	3
CO3	3	4	2	-	3	4	3
CO4	3	3	2	-	3	4	4
CO5	3	5	2	2	4	4	3

	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY				
D :	EPAR'	<u>rment</u>	OF CH	EMICAL SCIENCES	
Course Name	M.Sc.	Chemis	stry		
Subject Code:	CHL4	15A-18			
Subject Title:	CHEM	CHEMISTRY OF MATERIALS			
Contact Hours:	L:4	T:0	P:0	Credits:4	
Examination	3				
Duration (hours)					
Objective(s):	To intr	To introduce the students in the area of liquid crystalline materials and			
	solid state material chemistry and also to impart fundamental and				
	advanc	advance understanding on nanoscale materials, their properties and			
	applica	tions.			

Unit	Contents	Contact Hours
I	Interfaces and Liquid Assemblies: Order in liquids, Surfactants, Micelles, Vesicles and biological membranes, Surface self-assembled monolayers, Liquid crystals, Nature and structure, Design of liquid crystalline materials, Supramolecular liquid crystals, Liquid crystal displays, Inorganic liquid crystals	11
II	Solid-State and Materials Chemistry: Synthesis of material, The formation of bulk material, Chemical deposition, Metal oxides: Monoxides of the 3d metals, higher oxides and complex oxides: Spinal molecule, Inverse and normal, Perovskites and related phase, High temperature superconductor, Thermochromics and photochromic materials, Oxide glasses, Aluminophosphates, Silicates. Zeolites, Structure and composition, Synthesis, MFI Zeolites in petroleum industry, Layered Solids and Intercalates: Characteristics, Graphite Intercalates, Coordination Polymers: Introduction, Metal Organic Frameworks, Guest properties of metal organic framework, applications of coordination polymers	12
III	Inorganic pigments: Coloured solids, White and black pigments, Semiconductors: Group 14 semiconductors, Semiconductor system isoelectronic with Silicon. Material used in Light emitting diodes, Defects in crystals, Color Centers, Quantum dots.	10
IV	Nanochemistry and Nanomaterials: Nanotechnology: The 'Top Down' and 'Bottom Up' Approaches, Template synthesis using frameworks, supports and substrates, Microfabrication, Nanofabrication and Soft Lithography Nanoparticles: Nanoparticles and Colloids, Gold Nanoparticles, Non-Spherical Nanoparticle, Endohedral Fullerenes, Nanotubes and Graphene	12

Reference Books

S.No.	Author(s)	Title of the Book	Publisher/Year	
1	P. Oswald, P. Pieranski	Nematic and Cholesteric	Taylor and Francis	
		liquid crystals	Group, 2005	
2	Atkins, Overton, Rourke,	Inorganic chemistry	Fifth edition, 2010,	
	Weller, Armstrong	-	oxford	
3	J. W. steed, J. L. Atwood	Supramolecular Chemistry	second edition 2009,	
		_	Wiley	

Course Outcomes and Mapping

CO3

CO4

CO5

At the end	At the end of the course, the student will be able to							
CO1.		Understand the basic concepts and formation of various supramolecular assemblies.						
CO2.	Know th	ne types and	structure of	liquid crysta	als and their	applications	.	
CO3.		Learn the common and important synthesis methods, structure and composition of solid state materials and their applications in industries.						
CO4.	Underst	and the cond	cepts, mecha	nism and ap	plications of	f inorganic p	igments.	
CO5.	Learn	the vario	ous approa	iches for	the synt	thesis of	nanoscale	
	material	s/nanopartic	les and their	r properties a	and applicati	ions.		
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	
CO1	2	2	4	2	2	2	2	
CO2	1	3	4	2	3	3	4	

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY						
	DEPA	RTMEN	T OF CI	HEMICAL SCIENCES		
Course Name	M.Sc.	Chemi	stry			
Subject Code:	CHL41	5B-18				
Subject Title:	CHEM	ICAL B	IOLOG	Y		
Contact Hours:	L:3	T:0	P:0	Credits:3		
Examination	3					
Duration (hours)						
Objective(s):	chemist biologic applicat chemist macron Therefor to prep	Chemical Biology is one of the emerging interdisciplinary branch of chemistry which helps in exploring and understanding the various biological phenomena occurring at molecular level. This involves application of principles of physical, inorganic, organic and analytical chemistry to investigate the molecular properties of various macromolecular assemblies to understand the cellular behaviour. Therefore the objective of teaching this subject of Chemical Biology is to prepare the students who are interested in having their careers in Bioengineering, Pharmacology, Molecular Medicine, Biochemistry and				

Unit	Contents	Contact
		Hours
I	Fundamentals of Chemical Biology: General Introduction to	8
	Chemical Biology, Central Dogma of Molecular Biology,	
	Molecular Biology as a tool of Chemical Biology, Genes, Genomes,	
	Biooligomers, DNA libraries, protein libraries, Combinatorial	
	synthesis of biomolecules.	
II	Molecular Selection & Evolution: Chemical Biology & Origin of	
	Life, Natural selection, Evolution of Protein functions & nucleic	5
	acids, Catalytic antibodies.	
	Structure of Biomolecules: General Introduction to biological	
	macromolecules, Structure of Proteins, Carbohydrates, Nucleic	
	acids, lipids & lipid assemblies, Structural forces in biological	8
	macromolecules.	
III	Chemical & Biological synthesis of Biomolecules: General	12
	Introduction to synthesis in Chemical Biology, Chemical synthesis	
	of peptides, proteins, oligosaccharides, lipids and nucleic acids,	
	Biological synthesis of lipids, nucleic acids and proteins.	
IV	Molecular Recognition & Binding: Molecular recognition &	
1,	binding in Chemical Biology, Analysing Molecular Recognition &	6
	binding, Biological Molecular recognition studies.	U
	Application of various techniques in studying biomolecules:	_
	Mass Spectrometry, NMR, Electronic & vibrational spectroscopy,	6
	Electrophoresis, X-Ray Diffraction	

S.No.	Author(s)	Title of the Book	Publisher/Year
1.	Andrew Miller &	Essentials of Chemical	John Wiley & Sons, USA.
	Julian Tanner	Biology: Structural &	2008
		Dynamics of Biomolecules	
2.	David Van Vranken &	Introduction to Bioorganic	Taylor & Francis Group.
	Gregory Weiss	Chemistry & Chemical	2013
		Biology	
3.	D. L. Nelson & M.M.	Lehninger Principles of	WH Freeman Company,
	Cox	Biochemistry	New York. 2008

Course Outcomes & Mapping

CO4

CO5

	or many or many the second of						
At the end	of the cours	se, the studer	nt will be ab	le to			
CO1.	Underst	tand the cho	emical princ	ciples that g	govern struc	ture & fund	ctioning of
	biomole	ecules such a	as Proteins, (Carbohydrat	es, Lipids ar	nd Nucleic a	cids etc.
CO2.	Learn c	hemical syn	thesis of var	ious Biomol	lecules.		
CO3.	Acknow	vledge the	role of C	hemical Bi	ology in l	kinetics of	molecular
	recogni	tion of funct	ional & stru	ctural biomo	olecules.		
CO4.	Explore	new frontie	ers of researc	h in biology	using chem	nical method	ls.
CO5.	Learn	to apply v	various ana	lytical tech	niques to	understand	functional
	properti	ies of biomo	lecules.				
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	2	4	3	3	4	5	4
CO2	2	3	3	4	4	5	4
CO3	-	4	3	3	4	5	4

I.l	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES					
Course Name	M.Sc.	M.Sc. Chemistry				
Subject Code:	CHP41	CHP416-18				
Subject Title:	PHYS	PHYSICAL CHEMISTRY LAB				
Contact Hours:	L:0	L:0 T:0 P:6 Credits:3				
Examination	6	6				
Hours:						
Objective(s):	To pro	To provide students practical knowledge and skills about various topics				
	taught	in theory	class of	physical chemistry		

Any fifteen experiments to be performed out of the following:

- 1. Find graphically the equivalent conductance at infinite dilution of weak electrolyte and hence determine the thermodynamic dissociation constant of the weak acid.
- 2. Determine the equivalent conductance of a strong electrolyte at several concentrations and verify the Onsagar's equation.
- 3. Determine the equivalent conductance of a weak electrolyte at infinite dilution using Kohlraush law.
- 4. To determine relative strength of two acids by conductance measurements.
- 5. Determine the solubility of a sparingly soluble salt in water using conductance measurements.
- 6. Determine the end point of some typical titrations by conductometric method.
- 7. Determine the composition of a mixture of acetic acid and hydrochloric acid by conductometric titration.
- 8. Study the kinetics of saponification of ethyl acetate by sodium hydroxide and hence determine the activation energy of the reaction.
- 9. Investigate the reaction between acetone and iodine.
- 10. Determine the relative strength of two acids studying the hydrolysis of an ester.
- 11. Study the kinetics of decomposition of the complex formed between sodium sulphide and sodium nitroprusside spectrophotometrically and find the rate constant and order of the reaction.
- 12. Investigate the inversion of cane sugar in presence of an acid.
- 13. Obtain a calibration curve for a given compound and verify Beer-Lambert law.
- 14. Study the complex formation between Fe (III) and salicylic acid, and find the formula and the stability of the complex.
- 15. Determine the concentration of Nickel in solution by spectrophotometric titration.
- 16. Determination of specific and molar refraction of a liquid by Abbe refractometer.
- 17. Determine the refraction equivalents of C, H, and Cl atoms.
- 18. Determine the composition of mixture of two liquids by refractive index measurements.
- 19. Determination of surface tension of given liquid by a) drop number method and b) drop weight method using stalagmometer.
- 20. Determine the critical micellar concentration of soap (sodium or potassium lauryl sulphate) by surface tension measurements.
- 21. Determine the parachor of the mixture using surface tension measurements.
- 22. Compare the cleansing power of two samples of detergent.

- 23. Determination of transition temperature of given substance by thermometric or dilatometric method.
- 24. Find water equivalent and heat of neutralization of strong acid vs strong base, weak base vs. strong acid using Dewar's flask.

- 1. Advanced Practical Physical Chemistry by J.B. Yadav.
- 2. Findlay's Practical Physical Chemistry.

Course Outcomes and Mapping

At the end of	the course, the students will be able to
CO1.	Understand the basic procedures for carrying out a physical chemistry practical
	like preparation and standardisation of solutions, handling the equipments and
	measuring with precision.
CO2.	Correlate the theoretical and practical aspects and know about the limits of the
	experimental error.

CO3. Determine the various physical parameters for the various problems under study which in turn will enhance their problem solving and analytical skills.

CO4. Varify various laws studied in the theory part

CO4.	Verify v	various laws	studied in the	he theory pa	rt.	•	
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	1	5	5	3	5	5	3
CO2	2	4	5	3	5	2	4
CO3	2	5	5	2	4	3	5
CO4	2	5	5	1	4	2	5

	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES				
Course Name	DEPARTMENT OF CHEMICAL SCIENCES Course Name M.Sc. Chemistry				
Subject Code:	CHP417		,		
Subject Title:	ADVAN	ADVANCED CHEMISTRY LAB-I			
Contact Hours:	L:0	L:0 T:0 P:6 Credits:3			
Examination	6				
Hours:					
Objective(s):	To provide illustrative experiments to support the material taught in the				
	theory courses and to give the students practical experience in				
	techniqu	es used i	n the s	ynthesis, isolation, characterization and	
	structure	determinat	ion of in	organic compounds.	

S.No.	Contents
I	Inorganic Practicals
	 Preparation of Octahedral and Tetrahedral Complexes of dichlorodipyridylcobalt(II), Differentiate them using IR, UV and Magnetic Properties. Estimate Co(II) from one of them.
	2. Preparation of cis-and trans-potassium Dioxalato Diaquochromate (III). Interpretation of IR, UV and Magnetic Properties. Estimation of Chromium.
	3. Preparation of Salicylamide complexes of Copper(II). IR, UV, magnetic data and analysis of Cu(II).
	4. To separate the mixture of metal ions (Cr ³⁺ , Ni ⁺² ,Cu ⁺² , Zn ⁺² , Fe ⁺²) using thin layer and column chromatography.
	5. To perform the solvent extraction for the recovery of metal ions $(Cr^{3+}, Ni^{+2}, Cu^{+2}, Zn^{+2}, Fe^{+2})$ from aqueous medium.
II	Organic Practicals
	1. Synthesize (a) 2,4-dinitro-1-chlorobenzene from chlorobenzene, (b) mixture of <i>o</i> - and <i>p</i> -nitrophenols from phenol and (c) <i>p</i> -nitroacetanilide from acetanilide and make comparison of the reactivity of various substrates and reaction conditions used for performing nitration in each experiment. (Book 2, pp 978-979, 919-20)
	2. Synthesis of benzalacetophenone by condensation of benzaldehyde with acetophenone and study its bromination and subsequent de-bromination. (Book 1, pp 242-247, Book 3 pp 361-365)
	3. Synthesis of 2-chloro-4-bromo-6-iodoaniline from aniline. (Book 1, pp 292-299).
	4. The epoxidation of benzalacetophenone to its epoxide and study its reactivity

towards hydroxyl ion. (Book 3, pp 363-364).

- 5. Michael addition of aniline to benzalacetophenone. (Book 1, p 247).
- 6. Conversion of benzalacetophenone to its oxime and its transformation to amideand oxazole derivatives. (Book 1, pp 242-247, Book 3 pp 361-365)

Reference Books

S.No.	Author(s)	Title of the Book	Publisher
1	R.M. Roberts, Gilbert, L.	An Introduction to Modern	Ranehart and Winston
	B. Rodewald and A.S.	Experimental Organic	Inc., J. C New York 1969.
	Wingrove. Holt,	Chemistry,	
2	Arthur Israel	Vogel's Text Book of	Longman, 1961.
	Vogel (Author)	Practical Organic	
		Chemistry, 5th Edition.	
3	R. Adams, J.R. Johnson	Laboratory Experiments in	Macmillan; 7th edition
		Organic Chemistry	(1979)
4	G. Marr and B.W.	Practical Inorganic	
	Rockett	Chemistry	
5	W.L. Jolly	The Synthesis and	
		Characterization of	
		Inorganic Compounds	

Course Outcomes and Mapping

The students will learn	The	etudante	xvi11	laarn
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- **CO1.** Preparation of different inorganic complexes.
- **CO2.** Purification and crystallisation of inorganic compounds.
- CO3. Interpretation of compounds using UV-Vis, FT-IR techniques.
- CO4. Measurement of various physical properties such as magnetic moment of complexes.

CO5. Applying related experiments for their research work.

CO3.	rippiyiii	is related ex	periments to	i tileli resea	ich work.		
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	5	1	4	2	5	2	-
CO2	5	1	4	1	5	2	-
CO3	5	4	5	-	5	3	4
CO4	3	4	5	-	4	2	2
CO5	5	2	2	-	5	1	-

SEMESTER-III

I.K.	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES		
Course Name	M.Sc. Chemistry		
Subject Code:	CHL501-18		
Subject Title:	INORGANIC CHEMISTRY-III		
Contact Hours:	L:4 T:0 P:0 Credits:4		
Examination	3		
Duration (hours)			
Objective(s):	To provide basic concepts of group theory and the inorganic		
	biochemistry and catalysis.		

Unit	Contents					
I	Symmetry and Group Theory : Symmetry elements, Symmetry operations, Symmetry elements of commonly occurring molecules like NH ₃ , CH ₄ , SF ₆ , PF ₅ , SF ₄ , Ni(CO) ₄ , Fe(CO) ₅ , determination of point groups, genesis and use of character table, reducible and irreducible representation determination. Solid State Chemistry : Determination of points groups; types of close packing, packing efficiency, radius ratio, polyhedral discretion of solids, structure type: NaCI, ZnS, wurtzite, rutile, perovskite, spinels.	Hours 12				
II	Bio-Inorganic Chemistry : Transition elements in biology- their occurrence and function, active site structure and function of metalloproteins and metalloenzymes. O ₂ binding properties of heme and non-heme proteins, Co-operative effect, Bohr Effect, Electron transfer proteins, rubridoxin, feredoxin and cytochromes, Vitamin B ₁₂ and cytochrome P ₄₅₀ and their mechanism of action. Biological N ₂ fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.	12				
III	Catalysis: Turnover number, turnover frequency, homogenous and heterogenous catalysis, (involving oxidative addition, reductive elimination, migratory insertion, hydride elimination, trans metallation, metal carbonyls hydroformylation, Olefin metathesis, cross coupling reactions, asymmetric synthesis).	11				
IV	Inorganic Polymers : Types of inorganic polymers, Comparison with organic polymers, synthesis, structure aspects and application of silicones, polyphosphazenes, Tri- and Tetra- Phosphonitrilic halides, ultraphosphate, borophosphate and chalcogenide glasses.	10				

S.No.	Author(s)	Title of the Book	Publisher/Year
1	R.S. Drago	Physical Methods in inorganic	Affiliated East-West Press
		Chemistry	(Section 1& 2) 2nd
			Edition, Reinhold New
			York (1968)
2	H.B. Gray	Electrons and Chemical	(Section 2), W.A.
		Bonding	Benjamin, London (1965)
3	F.A. Cotton and G.W.	Advanced Inorganic	John Wiley and Sons, 6th
	Wilkinson	Chemistry	edition, John Wiley New
		•	York (1999)
4	J.E. Huheey	Inorganic Chemistry,	Harper International, SI
	-	Principles of Structure and	Edition, 3rd Edition,
		Reactivity	Harper London (1978)
5	G. Wilkinson (Ed.)	G. Wilkinson (Ed.)	Pergamon, Pergamon
	` '	, ,	Oxford (1982)
6	N.N. Greenwood and	Chemistry of Elements	Pergamon Press,
	A. Earnshaw	•	(Section7) (1984)
7	Christopher Master	Homogenous Transition metal	(Section 8) (1981)
	-	catalysis	
8	P. Atkins, T. Overton,	Inorganic Chemistry, 5 th	W. H. Freeman and
	J. Rourke, M. Weller,	edition	Company, New York
	F. Armstrong, M.		_
	Hagerman		

Course Outcomes and Mapping

The	students	xxi11	acquire	know	ledge of
1116	Students	WIII	accuune	KIIOW	ieage or

- **CO1.** Concepts of symmetry and group theory in solving chemical structural problems.
- CO2. Use of character tables and projection operator techniques.
- CO3. Structure and biological functions of biomolecules and the role of metals in biology.
- **CO4.** Basic concepts of catalysis and reaction mechanisms using various transition metal complexes.
- **CO5.** Possible types, synthetic methodology and structure of inorganic polymers and their applications.

	and their approachers.							
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	
CO1	2	3	4	-	-	2	2	
CO2	2	3	5	2	2	2	2	
CO3	3	3	3	-	-	4	4	
CO4	2	3	4	2	2	4	4	
CO5	2	4	4	-	3	4	4	

I.K.	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES						
Course Name	M.Sc	. Ch	emis	stry			
Subject Code:	CHL5	502-1	8				
Subject Title:	ADVA	NCE	D OR	RGANIC CHEMISTRY-I			
Contact Hours:	L:4	T:0	P:0	Credits:4			
Examination	3	3					
Duration (hours)							
Objective(s):	To provide the comprehensive knowledge of principles of						
	photoc applic		•	and pericyclic reactions with learning of current			

Unit	Contents	Contact Hours
I.	Photochemical Reactions: Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy. Determination of Reaction Mechanism: Classification, rate constants and life times of reactive energy states—determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions. Photochemistry of Alkenes: Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclization reactions, rearrangement of	10
II.	1,4- and 1,5-dienes. Photochemistry of Carbonyl Compounds: Intramolecular reactions of carbonyl compounds–saturated, cyclic and acyclic, β,γ-unsaturated and α,β-unsaturated compounds, Cyclohexadienones. Intermolecular cycloaddition reactions – dimerisations and oxetane formation. Photochemistry of Aromatic Compounds: Isomerisation reactions, additions and substitution reactions, cyclization reactions. Miscellaneous Photochemical Reactions: Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog, Photodegradation of polymers, Photochemistry of vision.	10
III.	Pericyclic Reactions and Molecular Orbital Symmetry: Classification of Pericyclic Reactions, Molecular Orbitals of Alkenes and Conjugated Polyene Systems, Molecular Orbitals of Conjugated Ions or Radicals, Symmetry Properties of π or σ - Molecular Orbitals, Various methods of analysis of pericyclic reactions. Electrocyclic Reactions: Conrotatory and Disrotatory Modes, Stereochemistry of Electrocyclic Reactions, Selection Rules for Electrocyclic Reactions, Analysis of Electrocyclic Reactions: Correlation-Diagram approach, Perturbation Molecular Orbital (PMO) approach, Frontier Molecular Orbital (FMO) approach. Electrocyclic Reactions of Ionic Species: Three and five atom Electrocyclization reactions.	12
IV.	Cycloaddition Reactions: Stereochemical Modes of Cycloaddition,	13

Feasibility of Cycloaddition Reactions: Orbital Symmetry Correlation-Diagram Method, Perturbation Molecular Orbital (PMO) Method, Frontier Molecular Orbital Method. [2+2] Cycloaddition reactions, [4+2] Cycloaddition reactions: Cycloaddition reactions of Diene and Dienophile, Frontier Orbital Interactions in Diels-Alder Reaction, Stereochemistry and Regiochemistry of Diels-Alder Reaction, [4+2] Cycloaddition Reactions with Allyl Cations and Allyl Anions. 1,3-dipolar cycloaddition reactions.

Sigmatropic Rearrangements: Suprafacial and Antarafacial Processes, Analysis of [i,j] Sigmatropic Rearrangements of Hydrogen: FMO & PMO analysis, FMO & PMO Analysis of [i,j] Sigmatropic Rearrangements of Alkyl Group, [3,3] Sigmatropic rearrangements: Cope Rearrangement and Claisen Rearrangement.

Reference Books

S.No.	Author(s)	Title of the Book	Publisher
1	John D. Coyle	Introduction to the organic	John Wiley & Sons
		photochemistry	Ltd.
2	Dwaine O. Cowan & Ronald	Elements of Organic	Plenum Press, New
	L. Drisko	Chemistry	York
3	K.K. Rohtagi & mukerjee	Fundamentals of	New Age
		Photochemistry	International
4	A. Gilbert, J. Baggott	Essentials of Molecular	CRC Press, London,
		Photochemistry	UK, (1991)
5	N. J. Turro	Modern Molecular	University Press,
		Photochemistry	Menlo Park, CA
6	Sunil Kumar, Vinod Kumar	Pericyclic Reactions	Elsevier (Academic
	and S.P. Singh		Press)
7	Ian Fleming	Pericyclic Reactions	Oxford Science
			Publications
8.	W. Carruthers	Cycloaddition Reactions in	Elsevier
		Organic Synthesis	

Course Outcomes and Mapping

At the end of the course, the student will be able to

- **CO1.** Understand the basics of photochemical reactions of alkenes, carbonyl and aromatic compounds.
- CO2. Understand the role of light in the organic synthetic methods and techniques for the applications in chemical reactions.
- **CO3.** Predict the concerted mechanism of the pericyclic reactions without the involvement of an intermediate.
- **CO4.** Predict the thermal or photochemical feasibility of the pericyclic reactions along with their stereo-specificity.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	1	3	4	3	2	4	2
CO2	1	4	4	4	3	5	3
CO3	1	4	4	2	1	4	3
CO4	1	5	4	2	1	4	2

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY							
	DEPA:	RTMEN	T OF C	HEMICAL SCIENCES			
Course Name	M.Sc.	Chemi	stry				
Subject Code:	CHL 5	03-18					
Subject Title:	PHYSI	CAL CI	HEMIST	RY-III			
Contact Hours:	L:4	T:0	P:0	Credits:4			
Examination	3	3					
Duration (hours)							
Objective(s):	This course will equip students with the necessary chemical knowledge						
	concerning the fundamentals in the basic areas of phase equilibrium,						
	adsorption and statistical thermodynamics; with regard to various						
	theories	develo	ped and	their applicability for various systems under			
	conside	ration.					

Unit	Contents	Contact Hours
I.	Electrochemistry-II: Oxidation reduction reactions; Electrochemical cell and its types, Electrode potentials, Standard hydrogen electrode, Nernst equation, Applications of standard electrode potentials; calculation of cell potential and redox equilibrium constants, Oxidation reduction titrations. Potentiometric Methods: Reference Electrodes, Liquid Junction Potentials, Indicator electrodes, Applications.	12
II.	Solution & Phase Equilibrium Solubility and factors affecting solubility, types of solutions, ideal solution, vapour pressure of ideal solutions, boiling point diagrams of binary miscible mixtures and their distillation diagrams, azeotropes, critical solution temperatures, solubility of gases in liquids, Henry's law, Nernst distribution law, number of extractions, solutions of solids in liquids & chemical equilibrium. Gibb's phase rule, Triangular method for graphical representation of three component systems; partially miscible three liquid systems. Applications of ternary liquid diagrams; systems composed of two solids and a liquid.	10
III.	Adsorption and Surface phenomena: Surface phenomena, capillary action, pressure difference across surface (Laplace equation), vapour pressure of droplets (Kelvin equation), physical and chemical adsorption, adsorption isotherms, Derivation of Langmur, Freundlich, Tempkin and BET absorption isotherms, Estimation of surface area by BET equation. Heterogenous catalysis, surface catalyzed unimolecular and bimolecular reactions, Retarded surface reactions, temporary and permanent catalytic poisons, activation energy for surface reactions, Numerical problems.	10
IV.	Statistical Thermodynamics: Thermodynamic probability and most probable distribution, Maxwell-Boltzmann distribution law; the ensemble averaging and its postulates; canonical, grand canonical, and microcanonical ensembles; Translational, rotational,	13

vibrational, ar	d electronic	vibration	function;	Calculation of
thermodynamic	properties	in terms	of partit	ion functions,
Comparison of	three types	of statisti	cs; Maxwe	ll- Boltzmann,
Fermi-Dirac an	d Bose-Einstei	n statistics.		

S.No.	Author(s)	Title of the Book	Publisher/Year
1.	P.W. Atkins & Julio de	Physical Chemistry	W H Freeman
	Paula		
2.	G. W. Castellan	Physical Chemistry	Narosa, 4 th ed, 2004
3.	David Chandler	Introduction to Modern	Oxford University Press
		Statistical Mechanics	
4.	E. Thomas and R. Philip	Thermodynamics: Statistical	Pearson Education, 1 st
		Thermodynamics and	ed, 2007.
		Kinetics	
5.	J.W. Moore and R.G.	Kinetics and Mechanism	John Wiley and Sons, 2 nd
	Pearson		ed, 1981
6.	Adamson and W. Arthur	Physical Chemistry of	Wiley-Interscience
		Surfaces	Publication, 4 th ed, 1982
7.	S.H. Maron & C.F.	Principles of Physical	Oxford and IBH (1958)
	Prutton	Chemistry, 1 st edition	
8.	Skoog, West, Holler and	Fundamentals of Analytical	Cengage Learning
	Crouch	Chemistry	

Course Outcomes and Mapping

- **CO1.** Solve various problems related to electrochemistry and be familiar with the various types of sensing electrodes.
- CO2. Understand and construct the phase diagrams for the ternary mixtures.
- CO3. Develop insights in the phenomenon occurring at surfaces and the theories behind them.
- CO4. Correlate classical thermodynamics with quantum mechanics by using statistical mechanical approach.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	1	5	5	3		2	3
CO2	1	5	5	2	3	2	4
CO3	2	3	3	2	1	1	3
CO4		3	3	3	2	2	4

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY								
	DEPA]	RTMEN	T OF C	HEMICAL SCIENCES				
Course Name	M.Sc.	Chemi	stry					
Subject Code:	CHL50	CHL504-18						
Subject Title:	ADVANCED CHARACTERIZATION TECHNIQUES							
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4						
Examination	3							
Duration (hours)								
Objective(s):	This co	ourse wi	ll introd	uce the students to different techniques for				
	characterisation of organic and inorganic materials. The emphasis will							
			_					
Duration (hours)	This co							

Unit	Contents						
		Hours					
I.	X-Ray diffraction: Single crystal XRD and powder XRD, Bragg's						
	diffraction law, Unit cell, space group, element of space group,						
	particle size analysis using Scherer formula.						
	Thermo-Analytical Methods: Theory, instrumental requirements						
	and methodology for thermo gravimetric analysis (TGA),						
	differential thermal analysis (DTA) and differential scanning						
	calorimetry (DSC), applications.						
II.	Scanning electron microscopy: Principle, Specimen Preparation,	10					
	Replicas Various-application of SEM.						
	Transmission electron microscopy : Instrumentation, Principle,						
	Advantage, Difference between SEM and TEM.						
III.	Chromatographic Methods: Classification of chromatographic	13					
	methods according to separation and development procedure,						
	Stationary phase, mobile phase, retention time.						
	Gas chromatography: Physical components, Types of column and						
	detector, Carrier gas, Applications, Inverse Gas chromatography,						
	GC-MS: construction and working.						
IV.	High performance liquid chromatography: Construction and	10					
	working, Partition chromatography, Normal and reverse phase						
	chromatography, Ion exchange chromatography, Isocratic and						
	gradient elution. Gel permeation chromatography. Electrophoresis						
	and electrochromatography.						

Reference Books

S.No.	Author(s)	Title of the Book	Publisher/Year
1.	J.Goldstein, D. E. Newbury,	Scanning Electron	2003
	D.C. Joy, and C.E. Lym	Microscopy and X-ray	
		Microanalysis	
2.	S.L. Flegler, J.W. Heckman	Scanning and Transmission	WH Freeman & Co,
	and K.L. Klomparens	Electron Microscopy: A	1993.

		Introduction	
3.	P.J.Goodhew, J.Humphreys,	Electron Microscopy and	
	R.Beanland	Analysis	
4.	Willard, Merritt, Dean and	Instrumental Methods of	CBS Publisher and
	Settle	Analysis	Distributors.,1986
5.	W. W. Wendlandt and L.	Thermal Analysis	
	W. Collins, Dowden		
	Hutechin and Ross		
6.	K. Tyagi, Mainak Roy, S. K.	Advanced Techniques for	
	Kulshreshtha and S.	Materials Characterization	
	Banerjee		

Course Outcomes and Mapping

At the end of the course, the student will be able to

- CO1. Understand the topography, morphology, composition, relationship between composition and material properties.
- CO2. Learn the functioning of the X-ray diffractometer, about its components and would be able to determine the crystal structure of a material, find impurity in the material, different phases present in the mixture of compound qualitative as well as functionalities
- CO3. Understand the instrumentation of TGA and also to calculate the weight loss with temperature, types of changes occurring in the material/substances during thermal breading, enthalpy changes during heat treatment of a compound.
- CO4. Apply the knowledge of various characterization techniques in material industries, metallurgy industries, electronic industries, civil Engineering.
- Apply the quantitative and qualitative separation techniques in purification and its applications in food industry, pharmaceutical industry, purification, removal of pollutants, medicinal chemistry and essential oils.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	2	2	3		3	3	3
CO2	1	2	2		3	3	3
CO3	1	2	2	1	4	3	3
CO4	2	1		4		2	
CO5	3	2	1		3	3	2

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES								
Course Name	M.Sc.	Chemi	stry					
Subject Code:	CHL50	5A-18						
Subject Title:	BIOPH	BIOPHYSICAL CHEMISTRY						
Contact Hours:	L:3	L:3 T:0 P:0 Credits:3						
Examination	3	3						
Duration (hours)								
Objective(s):	students macron chemist	Biophysical chemistry is an interdisciplinary subject which enables students to have an insight of physico-chemical properties of bio macromolecules by using principles & laws governing physics & chemistry and have an understanding of various biological processes.						
		Therefore the objective of teaching this subject of Biophysical Chemistry is to prepare the students who are interested in having their						
		careers in Bioengineering, Molecular Medicine, Biochemistry and						
	Molecu	lar Biolo	gy, Biopl	hysics.				

Unit	Contents	Contact Hours						
I	Biological macromolecules: An introduction to the configuration	6						
	and conformation of macromolecules; molecular interactions in							
	macromolecular structure, Structure of Proteins (1 ⁰ , 2 ⁰ , 3 ⁰ and 4 ⁰) & Nucleic acids.							
	Water: Weak interaction in aqueous systems, interactions of	5						
	molecules with water, ionization in weak acids and bases; buffering	3						
	against pH changes in biological systems; water as reactant; and							
	role of water in maintaining the native structure of biopolymers.							
II	Bioenergetics and thermodynamics: Biological energy	12						
	transformations and the laws of thermodynamics; concepts of							
	standard free energy, entropy, enthalpy, and chemical potential							
	changes in biochemical reactions; relationship between equilibrium							
	constant and standard free energy; the effect of temperature and pH							
	on standard free energy; free energy changes associated with							
	hydrolytic and redox (electron transfer) reactions in biological							
TTT	systems.	10						
III	Techniques to study structure and function of biomolecules: An	12						
	overview of UV-Visible, fluorescence, and circular dichroism (CD) spectroscopy; ultracentrifugation, sedimentation velocity and							
	equilibrium determination of molecular weights; Diffraction and							
	light scattering techniques; and nuclear magnetic resonance.							
IV	Study of the behaviour of biomolecules: Ligand interactions at	10						
	equilibrium and its kinetics; conformational transitions of							
	polypeptides and proteins: helix-coil transition and reversible							
	protein folding; nucleic acid structural transitions; and membrane							
	equilibria and transport.							

S.No.	Author(s)	Title of the Book	Publisher/Year		
1.	Kensel E. Van Holde,	Principles of Physical	Pearson Prentice Hall,		
	W. Curtis Johnson &	Biochemistry	USA (2006)		
	P. Shing Ho.				
2.	James P Allen	Biophysical Chemistry	John Wiley & Sons, USA		
			(2008)		
3.	H R Horton, L A	Principles of Biochemistry	Pearson Prentice Hall,		
	Moran, K G		USA (2006)		
	Scrimgeour, M D				
	Perry & J D Rawn				
4.	D. L. Nelson & M.M.	Lehninger Principles of	WH Freeman Company,		
	Cox	Biochemistry	New York. (2008)		

Course Outcomes & Mapping

At the end of	the course	e, the stu	ident will be	able to					
CO1	Learn d	ifferent	interactions	account	for	formation	αf	different	etr

- CO1. Learn different interactions account for formation of different structures of Biological Macromolecules in living systems.
- CO2. Learn applications of thermodynamics in biological systems such as macromolecules in solution and conformation equilibria.
- **CO3.** Describe how kinetic factors influence the biochemical reactions.
- **CO4.** Explain biophysical and chemical methods that are used to study the regulation and function of biomolecules.
- CO5. Learn to apply various analytical techniques to understand structural & functional properties of biomolecules.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	3	2	4	2	3	4	5
CO2	3	3	4	-	3	5	5
CO3	3	2	4	-	3	5	5
CO4	3	2	4	-	3	5	5
CO5	2	2	4	-	4	4	5

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY									
	DEPARTMENT OF CHEMICAL SCIENCES								
Course Name	M.Sc.	Chemi	stry						
Subject Code:	CHL 5	05B-18							
Subject Title:	MEDIO	MEDICINAL CHEMISTRY							
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4							
Examination	3								
Duration (hours)									
Objective(s):		The aim and objective of this course is to familiarize students with the							
	basic co	basic concept of Medicinal Chemistry. Emphasis will be made on the							
	SAR o	SAR of various drugs such as Antimicrobial, antihelmenthics,							
	antifung	gal and	their mo	de of actions. The commercial synthesis of					
	represe	ntative of	f such dru	ags will also be discussed.					

Unit	Contents	Contact Hours
I	Antibacterial Drugs: Structure, stereochemistry, Mode of action, Structure activity relationships, specific clinical applications of following classes of pharmaceuticals with synthetic/commercial route to the indicated examples. Penicillines, Cephalosporins, Tetracyclines, Aminoglycosides, Chloramphenicol, Macrolides, Lincomycins, Polypeptides antibiotics, Polyene antibiotics. Sulfonamides and Sulfones fluoroquinolines, Trimethoprim and other unclassified antibiotics. Antimycobacterials: Sulfanilamides, p-Aminosalicyclic acid derivatives, Thioamides, Thiourea, derivatives, Thiosemicarbonazones, Isoniazid, Kanamycin sulfate, Capreomycin, Rifaampin, Pyrazinamide, Anthionamide, Clofazimine, Cyclosporin, Dapsone, Sulfazem. Commercial synthetic/semi-synthetic routes to: 6-aminopenicillanic acid, ampicillin, amoxycillin, production of penicillin, 7-aminocephalsporanic acid, cephalexin, ceftizoxime,	Hours 10
	cefaclor, cephslothin, Tetracyclins: doxycycline, nalidixic acid, sulfadiazine, Norflaxacin, Ciproflexacin, O-flaxacin, Amiflaxacin, Difloxacin, Chloramphenicol, Nitroflurantion, Sulfamethyoxazole, Acetysulfoxiazole, Trimethoprim.	
II	Antiamoebic and Antiprotozoal Drugs: Emetine hydrochloride, 8-Hydroxyquinoline, Iodochlorohydroxyquinol, Metronidazole, Diloxanide furoate, Bilamical hydrochloride, Hydroxystilbamidine isothinate, Pentamidine isothionate, Nifurtimox,Suramin sodium, Carbarsone, Glycobiarsol, Melarsoprol, Sodium stibogluconate, Dimercaprool, Diethylcabamazine citrate, Centarsone, Acetarsone, Antimony potassium tartarate, Bismuth sodium thioglycollate, Sulphonamide, Stibiophen. Bismuth sodium thioglycollamate, Furazolidone. Commercial synthetic routes to: Metronidozole, ronidazole, flunidazole, iodoquinol, nifurfimax, benzindazole, tryparsamide.	15
III	a. Antimalarial Drugs:Cinchona alkaloids, 4-Aminoquinolines, 8-Aminoquinolines, 9-	10

	Aminoacridines, Biguanides, Pyramidines and Sulfones,	
	Mefloquine, Sulfonamides.	
	Commercial synthetic routes to: Chloroquine, pamaquine,	
	primaquine, proguanil, Amodiaquine, Mefloquine, Pyremethamine,	
	Sontoquine.	
	b. Anthelmintic Drugs:	
	Introduction, Tetrachloroethylene, Piperazines, Gentian violet,	
	Pyrvinium pamoate, Thiabendazole, Mabendazole, baphenium	
	hydroxynaphthoate, Dichlophene, Niclosamide, Levamisole	
	hydrochloride, Tetramisole, Niridazole, Biothional,	
	Antimonypotassium tartarate, Stibiophen, Sodium Stibiocaptate.	
IV	Antifungal Drugs: Fatty acids and their derivatives (Propionic	10
	acid, zinc propionate, sodium caprylate, zinc caprylate, undecylenic	
	acid, Zinc undecylenate, Triacetin), Salicylanilids, Salicyclic acid,	
	Tolnaftate, pchloromethoxylenol, Acrisocrin, Fluconazole,	
	Itraconazole, Haloprogin, Clotrimazole, Econazole, Miconazole,	
	Ketoconazole, Flucytosine, Griseofulvin, Polyene antibiotics	
	(Nystatin, Amphoetericin-B), Chlorophenesin, Dithranol.	
	Commercial synthetic routes to: Miconazole, Clotrimazole,	
	Econoazole, Fluconazole, Griseofulvin, Ketoconazole, Nafttidine,	
	Tolnaftate, Flucytosin.	

S.No.	Author(s)	Title of the Book	Publisher
1	W.O. Foye, T.L.	Principles of Medicinal Chemistry,	Lippencott Williams and
	Lamke, D.A.	5 th Edition,	Wilkins, 2002
	Williams		
2	R.F. Deorge	Wilson and Gisvolds Textbook of	J.B. Lippincott Company,
		Organic Medicinal and	Philadelphia, 1982.
		Pharmaceuticals Chemistry,8 th ed.	
3	B.G. Reuben and	Pharmaceutical Chemicals in	John Wiley & Sons, New
	H.A.Wittcoff	Perspective	York, 1989.

Course Outcomes and Mapping

At the and of the course the student will be oble to										
	At the end of the course, the student will be able to									
CO1.	Underst	tand the nee	d of Medicir	nal Chemistr	y in curing v	arious ailm	ents.			
CO2.	Study th	ne concept o	f Antimicro	bial and Ant	i-protozoal	drugs.				
CO3.	Study th	ne SAR of A	antimicrobia (1941)	l and Anti-p	rotozoal dru	igs.				
CO4.	Underst	tand the tota	l synthesis c	of Antimicro	bial and Ant	i-protozoal	drugs.			
CO5.	Underst	tand the var	rious disease	es cured by	Antimicrob	ial and Ant	i-protozoal			
	drugs.			·			•			
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7			
CO1	5	3	3	4	1	4	4			
CO2	5	1	3	2	1	3	3			
CO3	4	2	3	3	1	4	4			
CO4	3									
CO5	4	1	3	2	1	2	2			
					ĺ					

I.K. (I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY							
	DEPA	RTME	NT OF C	HEMICAL SCIENCES				
Course Name	M.Sc.	. Chem	istry					
Subject Code:	CHL5	05C-18						
Subject Title:	ADVA	ADVANCED FUNCTIONAL MATERIALS						
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4						
Examination	3							
Duration (hours)								
Objective(s):	materia	To introduce the students in the area of various functionalized materials, their synthesis and their properties with emphasis to their applications.						

Unit	Contents	Contact Hours
I	3-D Carbon-rich p-Systems – Nanotubes and Segments:	12
	Functionalization of Carbon Nanotubes, Introduction to Carbon	
	Nanotubes – A New Carbon Allotrope, Functionalization of Carbon	
	Nanotubes, Covalent Functionalization, Halogenation of Carbon Nanotubes, Fluorination of Carbon Nanotubes, Chlorination of	
	Carbon Nanotubes, Bromination of MWCNTs, Chemical	
	Derivatization of "Fluoronanotubes", Oxidation of CNTs –	
	Oxidative Purification, Carboxylation of CNTs, Defect	
	Functionalization-Transformation of Carboxylic Functions,	
	Hydrogenation of Carbon Nanotubes, Addition of Radicals,	
	Addition of Nucleophilic Carbenes, Sidewall Functionalization	
	Through Electrophilic Addition, Functionalization Through	
11	Cycloadditions, Addition of Carbenes, Addition of Nitrenes	1.1
II	Cyclophenacene Cut Out of Fullerene:- Introduction, Synthesis of	11
	[10]Cyclophenacene β -Conjugated Systems from [60]Fullerene, Synthetic Strategy, Synthesis and Characterization of	
	[10]Cyclophenacenes, Structural Studies and Aromaticity of	
	[10]Cyclophenacene, Synthesis of Dibenzo-fused Corannulenes.	
	Strategic Advances in Chromophore and Materials Synthesis	
	Introduction, Oligomers with a Tetrahedral Core Unit, Oligomers	
	with a Tetrasubstituted Benzene Core, Oligomers with a	
	Tetrasubstituted Biaryl Core.	
III	Advanced Biodegradable Organic Polymers: Introduction,	11
	Synthesis of Biodegradable Polymers by Polycondensation, General	
	Polycondensation Technique, Post Polycondensation Technique, Chain-Extension Technique, Enzyme-Catalyzed Polycondensation,	
	Synthesis of Biodegradable Polymers by ring-opening	
	polymerization, Monomers, Polymerization with Metal Catalysts,	
	Polymerization Using Metal-Free Organic Catalysts	
IV	Antimicrobial Biopolymers: Introduction, Biopolymers, ε-Poly-l-	11
	Lysine, Chitin and Chitosan, Synthetic Biodegradable Polymers,	
	Quaternary Polymers, Polyethylenimine, Antimicrobial Peptide	
	Mimics, Metal Loading, Silver, Magnesium, Zinc, Titanium,	
	Assessment of Antimicrobial/Antifungal Testing Methods	

S.No.	Author(s)	Title of the Book	Publisher/Year
1	Thomas J.J. Müller (Editor),	Functional Organic Materials	Wiley-VCH
	Uwe H.F. Bunz (Editor)	Volume-I	
2	Hee-Gweon Woo (Editor),	Advanced Functional Material	Springer
	Hong Li (Editor)		

Course Outcomes and Mapping

At the end of the course, the student will be able to

CO1. Understand the basic concepts and formation of various carbon nano tubes and its functionalizations.

CO2. Know the types and structure of functionalized fullerenes.

CO3. Learn the common and important synthesis methods, structure and composition of organic polymers and its properties and applications.

CO4. Understand the synthesis and applications of Antimicrobial biopolymers.

nanoscale **CO5.** Learn the various approaches for the synthesis of materials/nanoparticles and their properties and applications.

	materials/nanoparticles and their properties and applications.									
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7			
CO1	2	2	4	2	2	2	2			
CO2	1	3	4	2	3	3	4			
CO3	4	3	5	4	3	4	4			
CO4	1	3	4	2	2	3	2			
CO5	3	3	4	4	3	5	4			

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES							
Course Name							
Subject Code:	CHP5	CHP506-18					
Subject Title:	ADVA	ADVANCED CHEMISTRY LAB-II					
Contact Hours:	L:0	L:0 T:0 P:6 Credits:3					
Examination	6	6					
Hours:							
Objective(s):	To pro	vide stud	dents pra	ctical knowledge and skills about various topics			
	taught	in theory	class of	physical chemistry			

Unit	Contents
I	Any 10 experiments to be performed out of the following:
	 Preparation and study of Hardy – Schulze's rule for arsenious sulphide / Ferric hydroxide sols. Verify the Freundlich adsorption isotherm for adsorption of CH₃COOH
	from its aqueous solution by activated charcoal.
	3. Composing a phase diagram for three component system.
	4. Determination of distribution coefficient of I ₂ between CCl ₄ and H ₂ O.
	5. To show that benzoic acid dimerises in benzene by distribution method.
	6. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and hence hydrolysis constant of the salt.
	7. Determination of pH of various mixtures of sodium acetate and acetic acid in aqueous solutions and hence determine the dissociation constant of the acid.
	8. Determination of equilibrium constant of a reaction potentiometrically.
	9. To construct a calibration curve for quinhydrone electrode and thus determine its standard reduction potential.
	10. Determination of dissociation constant of a dibasic acid potentiometrically.
	11. Determination of composition of KCl-KBr mixtures by potentiometric titration against silver nitrate solution.
	12. Determination of acid and basic dissociation constants of an amino acid and hence the iso- electric point of the acid.
	13. Titration of a mixture of Chloride and Iodide with AgNO ₃ potentiometrically.
	14. Titration of Phosphoric acid solution with NaOH using quinhydrone
	electrode.
	15. Determination of Solute species in a phosphate mixture potentiometrically.
II	Any 5 experiments to be performed out of the following:
	 Separation of a mixture of amino acids using thin layer chromatography. Isolation and quantitation of DNA from onion. Separation of DNA using gel electrophoresis (agarose).

- 4. Isolation, detection, and quantitation of protein (casein) from milk.
- 5. Osmosis and diffusion through semipermeable membrane.
- 6. Estimation of DNA quantity using UV-Vis spectrophotometer.
- 7. DNA/ligand interaction (Scatchard plot) using UV-Vis spectrophotometer.
- 8. Serum albumin/ligand interaction using UV-Vis spectrophotometer

- 1. Advanced Practical Physical Chemistry by J.B. Yadav.
- 2. Findlay's Practical Physical Chemistry.
- 3. Safety-Scale Laboratory Experiments for Chemistry for Today, S L Seager and M R Slabaugh, Brooks/Cole Laboratory Series for General, Organic, and Biochemistry, VII edition, Brooks/Cole, 2010

Course Outcomes and Mapping

At the end of the course, the students will be able to

- **CO1.** Emphasize the importance of different techniques used for titration viz. potentiometery, pHmetry and amperometry.
- **CO2.** Correlate the theoretical and practical aspects and know about the limits of the experimental error.
- CO3. Determine the various physical parameters for the various problems under study which in turn will enhance their problem solving and analytical skills.

CO4. Verify various laws studied in the theory part.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	1	4	4	3	5	5	3
CO2	2	4	5	3	5	2	4
CO3	2	5	5	2	4	3	5
CO4	2	4	5	1	4	2	5

SEMESTER-IV

I.K. C	I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY						
	DEPA	RTMEN	VT OF C	HEMICAL SCIENCES			
Course Name	M.Sc.	Chemi	istry				
Subject Code:	CHL5	11-18					
Subject Title:	ADVA	NCED (ORGANI	C CHEMISTRY-II			
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4					
Examination	3	3					
Duration (hours)							
Course	The ob	jective o	of this co	ourse is to familiarize the students about the			
Objective(s):	concep	concept of asymmetric synthesis, and its applications in organic					
	synthes	synthesis. Another objective of the course is to make student					
	underst	understand the use of disconnection approach in Organic Synthesis. The					
	use of	organom	etallic rea	agent in organic synthesis will also be covered			
	to give	e an em	phasis o	n importance of organometallic reagents in			
	organic	synthes	is.				

Unit	Contents	Contact Hours
I	Asymmetric synthesis: Analytical methods for determination of enantiomeric purity – GC, HPLC and NMR. Natural sources of chiral starting materials, classification and methods of formation of new chiral compounds. Non enzymatic methods of asymmetric synthesis: Methods of asymmetric synthesis using naturally occurring chiral compounds, chiral auxillaries and their functions, Diels – Alder cycloadditions, Michael reaction and addition to carbonyl compounds. Cram's rule and Felkin – Ahn model. Asymmetric oxidation and reductions.	10
II	Disconnection approach and Strategies for disconnection approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, The importance of the order of events in organic synthesis, chemoselectivity, reversal of polarity, cyclisation reactions, protecting groups, stereoselectivity, regioselectivity, use of acetylenes, carbonyl condensation and control in carbonyl condensation, use of aliphatic nitro compounds, radical reaction, reconnections, ring synthesis (3,4,5 and 6 membered), rearrangements, use of ketenes.	15
III	One group disconnections: One group C-X and C-C disconnections (alcohol and carbonyl compounds) Two group disconnections: Two group C-X disconnections in 1,2-difunctionalized compounds,1,3-difunctionalized compounds and α,β -unsaturated carbonyl compounds, 1,4-difunctionalized compounds, 1,5-difunctionalized compounds and 1,6-difunctionalized compounds.	10

IV	Organometallic Catalysis in organic synthesis:	10
	Fundamental reaction steps of transition metal catalysed reaction.	
	oxidative-addition reactions, elimination reactions, cleavage of C-H	
	bonds, migration reaction, insertion reaction, Hydrogenation	
	reactions, hydrosilylation reactions, hydroformylation of	
	unsaturated compounds, carbonylation reactions, C-C cross	
	coupling and related reaction, alkene and alkyne metathesis, C-H	
	activation using metal salts, Suzuki reaction, Heck reaction, Negishi	
	coupling, Stille reaction, Sonogashira coupling reactions.	

S.No.	Author(s)	Title of the Book	Publisher
1	Francis A. Carey	Advanced Organic Chemistry	Kluwer Academic
	and Richard J.	Vol. A and Vol. B, fourth	publishers, New York
	Sundberg	Edition	2002
2	Jerry March	Organic Reaction Mechanism	John Wiley Ed. 5, 2002
3	W. Carruthers	Some Modern Methods of	Cambridge University
		Organic Synthesis, IV Edition	Press, 2004
4	H.O. House	Modern Synthetic Reactions	The Benjamin Cummings
			Publishing Company,
			London, 1972
5	Guo-Qiang Lin	Principles and	John Wiley & sons,
	Yue-Ming Li	Applications of	
	Albert S. C. Chan	Asymmetric Synthesis	
6	J. Furhop and G.	Organic Synthesis-concept,	Verlage VCH.
	Penzillin,	methods and starting materials	
7	Stuart Warren, Paul	Organic Synthesis: The	Wiley; 2nd Edition
	Wyatt,	Disconnection Approach	edition.

Course Outcomes and Mapping

At the end	At the end of the course, the student will be able to							
CO1.	Explain	the concept	of asymme	tric synthesi	s.			
CO2.	Underst	anding the p	hysical met	hods in anal	yzing the as	ymmetricity	•	
CO3.	Underst	and the m	ethodologic	al concept	of connec	tion discon	nection in	
	organic	synthesis.	C	•				
CO4.	Emphas	size the role	of various o	rganometall	ic complexe	s in Organic	Synthesis.	
CO5.	Explore	the use of v	arious meta	ls in organic	synthesis	_		
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	
CO1	2	4	4	2		1	2	
CO2	2	2 4 4 1 1 2						
CO3	2	4	4	1		1	1	
CO4	2	4	4	1		1	4	
CO5	2	4	4	1		1	4	

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES						
Course Name		Chemi				
Subject Code:	CHL 5	12A-18				
Subject Title:	ADVANCED PHYSICAL CHEMISTRY					
Contact Hours:	L:4	T:0	P:0	Credits:4		
Examination	3					
Duration (hours)						
Objective(s):	The objective of this course is to provide an introduction to few					
	advanced topics in physical chemistry like the chemistry of colloids,					
	macron	macromolecules and the latest electroanalytical techniques, focussing				
	especia	lly on th	eir applic	ration part.		

Unit	Contents	Contact Hours
I.	Colloidal State: Classification of colloids, charge and stability of colloidal dispersions, Hardy-Schulze Law, gold number, electrical properties of colloids, zeta-potential, electrophoresis and electroosmosis, emulsions and their classification, gels and their classification, thixotropy. Micelles, Surface active agents, Classification of surface active agents, Micellization, Hydrophobic interaction, Critical micellar concentration (cmc), Factors affecting the concentration of surfactants, Counter-ion binding of micelle, Thermodynamics of micellization, Applications.	11
II.	Polymers: Types of polymers, regular and irregular polymers, electrically conducting polymers, synthesis of polymers by chain and step reaction polymerization, physical properties of solid polymers (crystallinity, plasticity & elasticity) vulcanization of rubbers, molecular mass determination by osmometry, viscometry, light scattering and ultracertrifuge methods, number and mass average molecular masses, polymer solutions, factors affecting the solubility of polymers.	12
III.	Voltammetric Techniques-I: Linear sweep voltammetry; voltammetric electrodes, voltammograms. Hydrodynamic Voltammetry; concentration profiles at electrode surfaces, voltammetric currents, current voltage relationships, voltammograms for mixtures, Applications; voltammetric detectors, amperometric sensors, amperometric titrations. Differential pulse voltammetry.	10
IV.	Voltammetric Techniques-II: Polarography: principle, instrumentation and Applications, advantages and disadvantages of DME. Cyclic Voltammetry: Electrode used in cyclic voltametry, electrochemical mechanism, Eads mechanism (Adsorption mechanism), Butler-volmer equation, Reversible one electron transfer.	12

S.No.	Author(s)	Title of the Book	Publisher/Year
1.	R.J. Young and	Introduction to Polymers	Chapman and Hall London, 2nd
	P.A.Lovell		ed., New Delhi (2004)
2.	F.W. Jr. Billmeyer	Text book of polymers	Wiley-Interscience, 3 rd ed.
		science	(1984)
3.	D. Myers	Surfactant Science and	VCH Publishers (1988)
		Technology	
4.	P.J. Flory	Priciples of polymer	Cornell Univ. Press, Ithace
		chemistry	(Indian Print 2006)
5.	M.J. Rosen	Surfactants and Interfacial	John Wiley & Sons (1989)
		Phenomena	
6.	P.H. Reiger	Electrochemistry	Prentice-Hall, New Jersey (1994)
7.	D.R. Crow	Principles and Applications	Blackie academic, Glasgow
		of Electro-chemistry	(1988)
8.	Bard &. Faulkner	Electrochemical Methods:	
		Fundamentals and	
		Applications	
9.	C.M.A. Brett and	Electrochemistry:	Oxford Uni. Press (1993)
	A.M.O. Brett	Principles, Methods and	
		Applications	

Course Outcomes and Mapping

At the end	At the end of the course, the student will be able to							
CO1.	Underst	and major a	spects of ch	nemical term	ninology rela	ated to surfa	ce science,	
	polyme	rs and electr	ode processo	es.				
CO2.	Develor	o insights	in the mid	celle forma	tion proces	s and em	ohasize its	
	applicat	ion in daily	life.		-	-	-	
CO3.	Know a	Know about polymers in detail.						
CO4.		te various t			echniques a	nd their im	portance in	
	sensing		, I		1	•		
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	
CO1	2	4	5		3	2	2	
CO2	2	3	5	2	2	2	2	
CO3	3	2	4	2		3	2	
CO4	2	3	3		2	3	3	

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES							
Course Name		Chemi		HEMICAL SCIENCES			
Subject Code:	CHL51	2B-18					
Subject Title:	CHEM	CHEMICAL TOXICOLOGY					
Contact Hours:	L:4	L:4 T:0 P:0 Credits:4					
Examination	3	3					
Duration (hours)							
Objective(s):	The course objective is to make students familiar with basic principles						
	of Chemical Toxicology including aspects of exposure, toxicity & risks						
	assessm	assessment of chemicals in the environment so that they can understand					
	hazards	& risks	associate	ed with them and handle them safely.			

Unit	Contents	Contact
		Hours
I	Introduction to Toxicology: Risk Assessment & Management	12
	Definitions, Scope & Relationship with other sciences, History and	
	milestones in Toxicological Sciences; Sources of Toxic	
	Compounds; Exposure Classes (Air Pollutants, Water & Soil	
	Pollutants, Occupational Pollutants), Use Classes (Metals,	
	Agrochemicals, Food additives and Toxins). Process of Risk	
	assessment, Hazard Identification & Characterization (Types &	
	Source of Information, Dose response, Dose Effect, Human &	
	Environmental Exposure); Risk Evaluation & Management Process,	
	Risk Considerations, Criteria for Risk Evaluations (Human health &	
	Environment), Risk Management.	
II	Toxicokinetics	8
	Absorption, Distribution, Metabolism (Phase-I, Phase-II Reactions	
	& Activation Enzymes, Reactive Metabolites; Nature & Stability of	
	Reactive Metabolites, Fate of Reactive Metabolites and factors	
	affecting their toxicity) and Elimination of Toxicants.	
III	Environmental Toxicology	6
	Environmental Persistence, Bioaccumulation and Toxicity of	
	Toxicants. Sources of Toxicants: Transportation Processes,	
	Equilibrium Partitioning, Transformation Processes.	
IV	Safe Handling of Chemicals	4
	Introduction, Legislation, Toxicological Reactions (Corrosion,	
	Organic Compounds, Biological Materials, Allergens,	
	Pharmaceuticals & Radionuclides), Good Laboratory Practices,	
	Health & Safety, Protocols & Procedures	

Reference Books

S.No.	Author(s)	Title of the Book	Publisher/Year
1	John H. Duffus & Howard	Fundamental Toxicology	Royal Society of
	G.J. Worth		Chemistry (2006)
2	Earnst Hodgson	A Text Book of Modern	John Wiley & Sons

		Technology	(2004)
3	Poisoning & Toxicology	Jerrold B Leikin & Frank P.	Informa Healthcare
	Handbook	Paulocek	USA (2008)
4	Environmental Toxicants:	Morton Lippman	John Wiley & Sons
	Human Exposures & Their		(2009)
	Health Effects		
5	Handbook on the	G.A. Nordberg, B.A. Fowler,	Academic Press
	Toxicology of Metals	M. Nordberg & Lars Friberg	(2005)

Course Outcomes and Mapping

At the end of the course, the student will be able to

- **CO1.** Acquired broad knowledge of environmental toxicants & their effects on the physiological systems.
- CO2. Describe basic toxicological principles and how different chemicals are taken up by, processed in and eliminated from the body.
- CO3. To synthesize and apply concepts from various other disciplines in environmental & chemical toxicology.
- **CO4.** Apply different toxicological frameworks within the professional disciplines and have awareness about different risk assessment criteria.

CO5. Learn safe handling of chemicals in the laboratory.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	4	3		4	3	5	4
CO2	-	3	3	3	3	4	4
CO3	3	5	5	5	3	4	4
CO4	3	3	3	3	-	4	3
CO5	5	-	2	_	4	_	-

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES							
Course Name	M.Sc.	M.Sc. Chemistry					
Subject Code:	CHL5	12C-18					
Subject Title:	SUPR	SUPRAMOLECULAR CHEMISTRY					
Contact Hours:	L:4	T:0	P:0	Credits:4			
Examination	3	3					
Duration (hours)	Duration (hours)						
Objective(s):		To impart in depth knowledge of non-covalent interactions in					
	supran	nolecular	systems	and their applications			

Unit	Contents	Contact Hours
I	Host-Guest Chemistry: Definition-Supramolecular chemistry, Host-guest and Self-assembly; Selectivity, Preorganization and Complementarity of binding sites, Chelate ring size effect, Donor group and orientation; Binding constants, Thermodynamic and kinetic selectivity; Solvent effects and Non- covalent interactions	11
II	Solution Host-Guest Chemistry and Ion Recognition: Macrocyclic vs acyclic hosts, Templates effect and High dilution synthesis; Cation recognition: Crown ethers, Lariat ethers, Podands, Cryptands, Spherands, Calixarenes, Siderophore, Inclusion compounds, Molecular clefts and Tweezers; Anion recognition: Challenge in anion receptor chemistry, Charged and neutral receptors, contact ion pairs, cascade complex, remote anion and cation binding sites.	12
III	Basic concepts of self-assembly and classification: Self-Assembly in Synthetic Systems: Template effects in synthesis, Self-Assembly with covalent modification, A Thermodynamic Model: Self-assembly of zinc porphyrin complexes, Cooperativity and the extended site binding model Self-Assembly in biological Systems: Biological self-assembled fibres and layers, Amyloids, Actins and Fibrin, Bacterial S-Layers, Single molecule self-assembly: Proteins and Foldamers, Strict Self-Assembly: The Tobacco Mosaic Virus and DNA	12
IV	Catenanes and Rotaxanes: Statistical approaches to catenanes and rotaxanes, π – π and Hydrogen bonded rotaxanes and catenanes, Metal and auxiliary linkage approaches to catenanes and rotaxanes. <i>Molecular Devices:</i> , Logic gate, Molecular switches, Molecular motor.	10

Reference Books

S.No.	Author(s)	Title of the Book	Publisher/Year
1	J. W. steed, J. L. Atwood	1 1	2009, Wiley
		Second edition	

2	Jean-Marie Lehn	Supramolecular Chemistry	1995, Wiley
3	K. Ariga, T. Kunitake	Supramolecular chemistry-	2006, Springer
		fundamental and applications	

Course Outcomes and Mapping

- **CO1.** To learn the fundamental concepts of supramolecular chemistry such as Host-guest chemistry/ self-assembly.
- CO2. Various kinds of non-covalent interactions occurring in supramolecular systems.
- **CO3.** Molecular recognition and nature of bindings involved in biological systems.
- **CO4.** Structure of supramolecules of various types in solution and solid state.
- **CO5.** Applications of supramolecules in miniaturization of molecular devices.

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
CO1	3	1	3	1	4	4	2
CO2	3	-	1	2	1	4	3
CO3	3	-	1	2	1	4	3
CO4	3	-	1	2	1	4	3
CO5	5	-	3	1	1	4	4

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES							
Course Name	M.Sc. Chemistry						
Subject Code:	CHL51	2D-18					
Subject Title:	CHEMISTRY OF NATURAL PRODUCTS						
Contact Hours:	L:4	T:0	P:0	Credits:4			
Examination	3						
Duration (hours)							
Course	Course The aim and objective of this course is to make students understand			this course is to make students understand the			
Objective(s):	bjective(s): chemistry of common natural products. The course will involve			atural products. The course will involve the			
	structur	structure, chemistry and metabolic pathways involving the common					
	natural	products	•	-			

Unit	Contents	Contact Hours
I	Terpenoids and Carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination and synthesis of citral, geraniol, camphor, farsenol, santonin, abetic acid.	10
II	Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of elucidation, degradation, classification based on nitrogen heterocyclic ring, Strucuture, stereochemistry, synthesis of epheridine, nicotine, atropine, morphine.	10
III	Steroids: Occurrence, nomenclature, Isolation, structure determination and synthesis of Cholesterol, bile acids, Androsterone, testosterone, estrone, progesterone.	10
IV	Secondary Metabolism: (a) <i>Metabolites Derived from Acetate (Polyketide Pathway):</i> Biosynthesis of unsaturated and saturated fatty acids, prostaglandins, polyphenols viz. Orsellinic acid, 6-methylsalicylic acid, usnic acid, penicillic acid, patulin, citrinin, griseofluvin, alizarin, emodin, tetracyclines. (b) Metabolites Derived from Mevalonic Acid Pathway (Terpenes): Biosynthesis of mevalonic acid and the active isoprene units, monoterpenes viz. Citral, geraniol, pinene, camphor, terpineol, thujone, isobornylene, menthol, artemesia alcohol, santolina alcohol, Iridoids, viz. Loganin, iridomyrmecin, secolaganin, swerosidebisabolene, γ-cedrene, αSesquiterpenes, viz. Humulene, ovalicin, juvenile hormone, Diterpenes, viz. Phytol, Sclareol, abietic acid, taxinine. Triterpenes, squalene, lanosterol, cholesterol, cycloartenol, sitosterol, Vitamin Dcarotene,β-carotene, Biological functions of steroids. Biosynthesis of carotenoids, viz. vitamin A	15

S.No.	Author(s)	Title of the Book	Publisher
1	I. L. Finar	Organic Chemistry, Vol. 2.	Longmans Green & Co.
			1964
2	J. Mann	Secondary Metabolism	Oxford University Press,
			Oxford, 1980.
3	Kurt B. G. Torssell,	Natural Product Chemistry - A	Swadish Pharmaceutical
		Mechanistic, Biosynthetic and	Society, 1997.
		Ecological Approach	
4.	by D. Voet, J.G.	Fundamental of Biochemistry	John Willey & Sons Inc.,
	Voet and C.W. Pratt		New York,1999.
5.	A. L. Lehninger	Principles of Biochemistry	CBS Publishers, New
			Delhi.

Course outcomes and Mapping

Course of	Course outcomes and wrapping								
At the end of the course, the student will be able									
CO1.	To lear	To learn the chemistry and methods to determine structure elucidation of							
	natural	products							
CO2.	To stud	y the chemi	stry of chem	istry of terp	enoids and o	carotenoids			
CO3.	To stud	y the Chem	istry of stero	oids					
CO4.	To stud	y the chemi	stry of v me	tabolic proc	esses involv	ing such bio	chemicals		
CO5.	To und	To understand the role of such natural products in living systems							
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	P2SO7		
CO1	5	3	3	4	1	4	4		
CO2	5	1	3	2	1	3	3		
CO3	4	2	3	3	1	4	4		
CO4	3	1 3 2 1 2							
CO5	4	1	3	2	1	2	2		

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES								
Course Name	1	M.Sc. Chemistry						
Subject Code:	CHL51	2E-18						
Subject Title:	GREE	GREEN CHEMISTRY						
Contact Hours:	L:4	T:0	P:0	Credits:4				
Examination	3							
Duration (hours)	Duration (hours)							
Objective(s):	Objective(s): 1. To introduce the students of Master class about various concepts of							
	green chemistry and its technologies.							
	2. The emphasis is on the synthesis of various entities using benign							
				try (their role and advantages).				

Unit	Contents	Contact Hours
I.	Introduction to the Green Chemistry; Historical context: The Greening of Chemistry; Waste: Production, Problems, Prevention; Measuring and Controlling Environmental Performance; planning for the future for reducing carbon in the atmosphere; Emergence of Green chemistry and its environmental impact.	10
II.	Twelve Principles of green chemistry, concepts, importance and their applications with special emphasis on the use of alternative renewable feedstock (bio-fuels, biomass and their applications in green synthesis of various compounds); Use of innocuous reagents in natural processes; Alternative solvents; Design of the safer chemicals; Designing alternative reaction methodology; Minimizing energy consumption. Sustainable Polymers: The case of polylactide, using CO ₂ and other feedstock.	10
III.	Green reactions (Role, advantages and applications): Aqueous phase organic synthesis, Solvent less organic synthesis, Photochemical organic synthesis, PTC catalysed reactions, Microwave induced reactions, Enzymatic transformations, Sonication reactions & reactions in Ionic liquids.	13
IV.	Green reactions (Role & mechanism): Aldol condensation reaction (solid phase and Ionic liquid synthesis), Baeyer-Villiger oxidation (aqueous phase and solid phase synthesis), Baylis-Hillman Reaction (Microwave synthesis and Ionic liquid synthesis), Biginelli Reaction under Microwave irradiation, Cannizaro Reaction under sonication, Dakin reaction under ultrasonication, Darzen reaction in PTC, Dieckmann condensation (Polymer supported synthesis), Diels-Alder reaction (in water, ionic liquid, MW and sonication), Photo-Fries rearrangement, Stille coupling in water and SC-CO ₂ , Ullmann reaction under sonication and in aqueous medium, Sonogashira reaction.	12

S.No.	Author(s)	Title of the Book	Publisher
1	Lancaster, M.	Green Chemistry an	Royal Society of Chemistry,
		Introductory Text	Cambridge, UK 2002. ISBM
			0-85404-620-8.
2	Cann, M.C.; Connelly,	Real World Cases in Green	American Chemical Society:
	M.E.,	Chemistry	Washington DC. 2000. ISBN
			0-8412-3733-6.
3	Anastas, P. T.;	Green Chemistry: Theory	Oxford University Press:
	Warner, J. C.	and Practice	New York, 1998.

Course Outcomes and Mapping

CO5

3

At the end	At the end of the course, the student will be able to									
CO1.	Concep	Conceptualize the various syntheses using novel and greener methods.								
CO2.	Predict	the relation	nships bety	ween organ	ic chemical	structures	and their			
	reactivi	ty in differe	nt greener ar	nd benign co	nditions.					
CO3.	Learn th	he fundame	ntal and adv	anced conce	epts of green	n chemistry	in reaction			
	mechan	isms.								
CO4.	Apply t	he new metl	nodologies f	or altering th	ne reactivity	patterns of	substrates			
CO5.	Synthes	size various	molecules u	sing combin	nations of re	active speci	es in novel			
	condition	ons.								
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7			
CO1	4	4	4	4	3	5	2			
CO2	3	3 4 2 2 4 2								
CO3	3	3 3 1 3 4 3								
CO4	4	3	4	2	1	4	2			

4

4

2

5

I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY								
	DEPARTMENT OF CHEMICAL SCIENCES							
Course Name	M.Sc. Chemistry							
Subject Code:	CHL51	2F-18						
Subject Title:	COMPUTATIONAL CHEMISTRY							
Contact Hours:	L:4	T:0	P:0	Credits:4				
Examination	3							
Duration (hours)	uration (hours)							
Course	Theoretical chemistry lies at the interfaces among chemistry, physics							
Objective(s):	and mathematics. The primary goals of the present course are to							
	provide an overview of the roles that theory plays within the science of							
	chemist	ry and to	o introdu	ce the students to the modern day components				
	of theor	etical ch	emistry.					

Unit	Contents					
I	The Basics of Quantum Mechanics: Methods for solving Schrodinger equation, Exact Solution, Understanding Energy Surfaces, beyond model problems, normal modes, local modes, transition states, symmetry. An overview of theoretical chemistry: Molecular structure, types of	Hours 11				
II	bonding, symmetries groups. Numerical methods: Methods for roots of equations, numerical integration and differential equations, interpolation and extrapolation of data, matrices. Elements of Computer Programming; Introduction to Plotting softwares, Visualization of structures	11				
III	Classical Molecular dynamics: Statistical Mechanics of Molecules at or Near Equilibrium, Monte Carlo simulations, Molecular Dynamics Simulations, Theoretical Treatment of Chemical Change and Dynamics, Experimental Probes of Reaction Dynamics, Introduction to some molecular dynamics codes such as GROMAC, PACKMOLE, VMD and CHEMIRA	11				
IV	Ab initio methods and applications: Hartree Methods, Hartree Fock Methods and Geometry Optimization, Non-variational methods, density functional theory and property calculations, Quantum Monte Carlo methods, Introduction to some molecular dynamics codes such as GAUSSIAN	12				

Reference Books

S.No.	Author(s)	Title of the Book	Publisher
1	Jack Simons	An Introduction to Theoretical	Cambridge University
		Chemistry,	Press, 2003.
2	C. J. Cramer	Essentials of Computational	Wiley, 2002.
		Chemistry	
3	R. D. Levine and R.	Molecular Reaction Dynamics	Oxford University Press,

	B. Bernstein	and Chemical Reactivity,	1997.
4.	A. R. Leach,	Molecular Modeling, 2nd ed	Prentice Hall, 2001.

Course outcomes and Mapping

At the end of the course, the student will be able to									
CO6.	Bridge	Bridge the chemistry with modern day physics, material sciences.							
CO7.	Underst	tand theoreti	cal aspects	of chemical	transformati	ons.			
CO8.	Underst	tand the char	nges in the p	hysical para	ameters in cl	nemical reac	tions.		
CO9.	Rationa	lize the char	nges in chen	nical process	ses.				
CO10.	Underst	tand the feas	sibility of the	e reactions.					
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7		
CO1	3	3	2			3	4		
CO2	2	3	2			4	4		
CO3	2	4 1 3 4							
CO4	2	3	2	••		2	3		
CO5	2	2	3	••		3	4		