Indian Institute of Technology Kanpur

COURSES OF STUDY

2024

Indian Institute of Technology Kanpur
KANPUR-208016

CHEMISTRY

CHEMISTRY

BS							Template No. CHM-1
COURSES	SEMESTER						
	1st	2nd	3rd	4th	5th	6th	7th	8th
	MTH101A [11]	MTH102A [11]	CHM201A [09]**	CHM202A [09]	CHM303A [09]	CHM322A [09]	CHM423A [06]	HSS-5 (Level-2) [09]
	PHY101A [03]	PHY103A [11]	ESO/SO-1 [~10]*	CHM222A [09]	CHM305A [06]	CHM342A [09]	HSS-4 (Level-2) [09]	OE-4 [09]
	PHY102A [11]	ESC101A [14]	ESO/SO [~10]*	CHM242A [09]	CHM321A [09]	CHM344A [06]	OE-1 [09]	OE-5 [09]
	LIF101A [06]	CHM101A [03]	HSS-2 (Level-1) [11]	ESC201A [14]	CHM345A [09]	DE-1 [09]	OE-2 [09]	OE-6 [09]
	ENG112A/HSS-1 (Level-1) [11]	CHM102A [08]	TA202A [06]	ESO/SO-3 [~10]*	ESO/SO-4 [~10]*	DE-2 [09]	OE-3 [09]	OE-7 [09]
	PE101A [03]	PE102A [03]	COM200A [05]	TA201A [06]	CHM361A [02]	HSS-3 (Level-2) [09]	UGP-3/DE [09] (CHM491A)	UGP-4 [09] (CHM492A) (Extra Credits)
	TA101A [09]	-	-	-	UGP-1 [04] (CHM391A) (Extra Credits)	UGP-2/DE [09]/ (CHM392A)	-	-
	54	50	51*	57*	45/49*	60	51	45/54

MINIMUM CREDIT REQUIREMENT FOR GRADUATION:

Institute Core (IC)	:	124	Credits
Department Compulsory (DC)	:	101	Credits
Department Elective (DE)	:	36	Credits
Open Elective (OE)	:	63	Credits
*SO/ ESO	:	40	Credits
HSS (Level-I)	:	22	Credits
HSS (Level-II)	:	27	Credits
Total	:	**413**	**Credits**

REMARKS:

1) *ESO/SO courses are available in a range from 6 to 14 credits each. CHM students may choose any four courses EXCEPT CSO201A, ensuring a minimum of 8 SO credits and totalling up to a minimum of 40 ESO/SO credits.
2) DE credits may include 18 credits of UGP-2 and UGP-3.
3) UGP-1 and UGP-4 are optional and does not count towards DE/OE credits.
4) Upto 36 OE credits may be waived from the minimum requirements for students opting for either Dual Degree or Double Major programme.
5) **EXCEPTION: CHM201A to be done by Y14 and onward batches. Y11, Y12 and Y13 batches shall do CHM203A. Course title, content and credits are same. Just the course number has been changed.

BS-MS (Category – A) *(from the same department)*				Template No. BS-CHM-2
COURSES	UG Pre-Requisites		PG Component	
	Odd Semester	Even Semester	9th	10th
	CHM503A [06]	CHM402A [09]	CHM611A [09]	MS Project [48]
	-	CHM443A [06]	CHM621A [09]	-
		-	CHM664A [09]	
			DE PG-1 [09]	
			DE PG-2 [09]	
			DE PG-3 [09]	
	06	15	54	48

MINIMUM CREDIT REQUIREMENT IN MS PART FOR GRADUATION:

PG Component	:	54	Credits
MS Project component	:	48	Credits

REMARKS:

1) All courses to be taken with the permission of Supervisor/ DUGC Convener.
2) DE PG-1, 2 and 3 may include any CHM6XX level course EXCEPT CHM609A, CHM629A, and CHM640A.
3) Mandatory UG component must be completed before the 9th semester.
4) Course credits and Thesis credits mentioned under the dual degree template are only for the MS part of the programme. In addition to these credits, students are required to follow and complete all their graduation requirements for their UG programme.
5) Upto 36 OE credits may be used from the BS minimum requirements to fulfil requirements for the BS-MS dual degree programme. These will be waived from the BS programme and counted towards PG requirements.

BS/BT-MS (Category – B) *(from other departments)*			Template No. BS-CHM-3
	Mandatory UG Component	PG Component	
		9(t)	10(t)
COURSES	UG CHM DE-1 (09)	MS Project -1 (24)	MS Project -2 (24)
	UG CHM DE-2 (09)	CHM305A (06)	CHM344A (06)
	UG CHM DE-3 (09)	CHM423A (06)	CHM DE-8 (09)
	UG CHM DE-4 (09)	CHM DE-6 (09)	CHM DE-9 (09)
	UG CHM DE-5 (09)	CHM DE-7 (09)	
	45	54	48

MINIMUM CREDIT REQUIREMENT IN MS PART FOR GRADUATION:

PG Component : 54 Credits
MS Project component : 48 Credits

REMARKS:

1) All courses to be taken with the permission of Supervisor/DUGC Convener.
2) All UG DE (from 1 to 5) should be selected from Basket –A.
3) *EXCEPTION: CHM201A to be done by Y13 and onward batches. Y11 and Y12 batch shall do CHM203A. Course title, content and credits are same. Just the course number has been changed.
4) Courses in DE-6 to DE-9 may be any from CHM department core or electives (including any CHM6XX level course EXCEPT CHM609A, CHM629A, and CHM649A), which have not been credited by the student as SO / UG CHM DE during the student's UG program.
5) Course credits and Thesis credits mentioned under the dual degree template are only for the MS part of the programme. In addition to these credits, students are required to follow and complete all their graduation requirements for their UG programme.
6) Upto 36 OE credits may be used from the parent department's BT/BS minimum requirements to fulfil requirements for the dual degree programme. These will be waived from the parent department's BT/BS programme requirements and counted towards PG requirements.

Basket – A

CHM201A (09)*
CHM202A (09)
CHM222A (09)
CHM242A (09)
CHM303A (09)
CHM321A (09)
CHM345A (09)
CHM322A (09)
CHM342A (09)

DOUBLE MAJOR	Template No. CHM-4
Odd Semester	Even Semester
CHM201A (09)*	CHM222A (09)
CHM303A (09)**	CHM242A (09)
CHM321A (09)	CHM202A (09)
CHM345A (09)	CHM322A (09)
CHM305A (06)	CHM342A (09)
CHM423A (06)	CHM344A (06)
48	51

TOTAL MANDATORY CREDITS FOR SECOND MAJOR IN CHEMISTRY: 99 CREDITS

REMARKS:

1. *EXCEPTION: CHM201A to be done by Y13 and onward batches. Y11 and Y12 batch shall do CHM203A. Course title, content and credits are same. Just the course number has been changed.
2. **Pre-requisite for CHM308A is waived for double major students.
3. Upto 36 OE credits may be waived from the parent department BT/BS graduation requirements when they are used to fulfill requirements for the double major.

MINOR			Template No. CHM-5
Title	PHYSICAL CHEMISTRY *	INORGANIC CHEMISTRY	ORGANIC CHEMISTRY
COURSES	CHM321A [09] CHM322A [09] Any TWO from: CHM621A [09] CHM622A [09] CHM626A [09] CHM636A [09] CHM637A [09] CHM650A [09] CHM664A [09] CHM685A [09] CHM689A [09] CHM695A [09] CHM696A [09] CHM699A [09]	CHM345A [09] CHM342A [09] Any TWO from: CHM616A [09] CHM631A [09] CHM646A [09] CHM647A [09] CHM651A [09] CHM654A [09] CHM668A [09] CHM691A [09]	CHM201A [09]** CHM202A [09] CHM303A [09] CHM402A [09] -
	36	36	36

REMARKS:

1) *CSO202A is a pre-requisite for Minor in Physical Chemistry
2) **EXCEPTION: CHM201A to be done by Y13 and onward batches. Y11 and Y12 batch shall do CHM203A. Course title, content and credits are same. Just the course number has been changed.

New MSc template (as per the recommendation of the UGARC implementation committee).

Blue highlight is the change in the course numbers (courses with dual numbers) compared to old template.

Year I				Year II			
Semester I		Semester II		Semester III		Semester IV	
Courses	**L-T-P-D (C)**	**Courses**	**L-T-P-D (C)**	**Courses**	**L-T-P-D (C)**	**Courses**	**L-T-P-D (C)**
CHM401A	3-0-0-0 (9)	CHM402A	3-0-0-0 (9)	CHM611A	3-0-0-0 (9)	CHM700A	0-0-0-27 (27)
CHM321A	3-0-0-0 (9)	CHM322A	3-0-0-0 (9)	CHM621A	3-0-0-0 (9)	DE-3	3-0-0-0 (9)
CHM345A	3-0-0-0 (9)	CHM342A	3-0-0-0 (9)	CHM631A	3-0-0-0 (9)	DE-4	3-0-0-0 (9)
CHM503A	0-0-6-0 (6)	CHM443A	0-0-6-0 (6)	CHM699A/ 2 x DE	0-0-0-18 (18)	OE-2	3-0-0-0 (9)
CHM423A	0-0-6-0 (6)	DE-1	3-0-0-0 (9)	DE-2	3-0-0-0 (9)		
CHM521A	2-0-0-0 (6)	OE-1	3-0-0-0 (9)				
CHM361A	2-0-0-0 (6)						
Total credits: 51		Total credits: 51		Total credits: 54		Total credits: 54	

DEPARTMENT OF CHM

Courses ID	Course Title	Credits L-T-P-D-[C]	Content
CHM101	CHEMISTRY LABORATORY	0-0-3-0-3	Chemical analysis with relevance to everyday life 1. Determination of amount of Ca2+ in milk by complexometric titration; 2. Estimation of iodine in common iodized salt by iodometry; 3. Estimation of phosphoric acid in cola drinks by molybdenum blue method; 4. Analysis of kidney stone model chemical compounds by permanganometric titration; 5. Extraction of DNA from green peas or onions and its identification; 6. Extraction of caffeine, an alkaloid from tea leaves; 7. How many pigments are there in the green portion of spinach? A paper chromatography experiment to separate the various pigments including chlorophyll Synthesis of Chemical Compounds. I. Preparation and characterization of aspirin, a common medicine; 2. DielsAlder reaction a versatile organic reaction to form CC bonds: a reaction between anthracene and maleic anhydride;3. Preparation and characterization of an inorganic coordination complex compound: [Ni[NH3]6f+ 2cr; 4. Organometallic compounds: bridges between inorganic and organic compounds. Acetylation of Ferrocene; 5. An environment related synthesis: Preparation of potash alum from scrap aluminum Photochemistry: Light as a reagent in chemistry; I. Photochemical reduction of ferric oxalate and its use in blueprinting Experiments on Physical Chemistry Concepts I. Partition of solutes in mixture of solvents: Acetic acid inwater/nbutanol; 2. Kinetics of reactions: An example using the iodide hydrogen peroxide clock reaction; 3. Determining the pi of amino acids by using potentiometry; 4. Weak and strong acids and bases: conductometry A. J. Elias; A Collection of Interesting General Chemistry Experiments. Universities Press, Hyderabad 2009
CHM112	GENERAL CHEMISTRY: PHYSICAL CHEMISTRY	3-1-0-0-4	Quantum theory, Quantum mechanics of simple systems, Particle in a box, Harmonic oscillator, Rigid rotor, Hydrogen atom, Many-electron atoms, Molecular orbital theory, Spectroscopy of simple molecules. [Modular Course*] **Reference Books:** [1] P. W. Atkins and Julio de Paula, Physical Chemistry [2] D. A. McQuarrie and J. D. Simon, Physical Chemistry A Molecular Approach [3] I. N. Levine, Quantum Chemistry
CHM113	GENERAL CHEMISTRY: INORGANIC & ORGANIC CHEMISTRY	3-1-0-0-4	Inorganic Chemistry: Crystal Field Theory and Structure of Coordination Complexes, Oxidative Addition, Reductive Elimination, Insertion Reactions, Hydrogenation, Hydroformylation, Monsanto Acetic Acid Process and Ziegler-Natta Polymerization, Metalloenzymes Organic Chemistry: Conformational Analysis of Alkanes and Cycloalkanes, Chirality, Substitution and Elimination Reactions, Introduction to Biomolecules. [Modular Course*] **Course Reference**:[1] Shriver and Atkins' Inorganic Chemistry [2] J. E. Huheey, Inorganic Chemistry: Principles of Structure

			and Reactivity [3] L. Wade, Organic Chemistry [4] J. Clayden, N. Greeves, and S. Warren, Organic Chemistry [5] E. L. Eliel, Stereochemistry
CHM202	BASIC ORGANIC CHEMISTRY -II	3-0-0-0-9	Oxidation: With Cr and Mn compounds; with peracids and other peroxides; with periodic acid, Pb $(OAc)_4$, $Hg(OAc)_2$ and SeO_2. Reduction: Catalytic hydrogenation; metal hydride, dissolving metal and hydrazine-based reductions. CramFelkin Anh model. CC Bond Formation: Acyloin, Aldol, Stobbe, Claisen, Knovenagel and Benzoin condensations, Darzens glycidic estersynthesis; Dieckmann reactions, Wittig reaction, DielsAlder and ene reactions, Reformatsky reaction. Acetoacetic ester and malonic ester synthesis. Acylation reactions. Enamine reactions. Gattermannaldehyde synthesis. Michael and Mannich reactions. Synthesis of Polynuclear Hydrocarbons: Carbohydrate Chemistry: Introduction, Structural elucidation and some typical eactions of mono and dischharides. Heterocyclic Chemistry: Furan, Pyrrole, Thiophene, Pyridine, Indole, quinolines etc. Problems: Based on multistep reactions involving CC bond formation, oxidation and Reduction (to be solved in the class and supplemented by home assignments). **Course Reference**: 1. Carruthers, W., Coldham, I. Some Modern Methods of Organic Synthesis, 2008; 2. House, H. O., Modern Synthetic Reactions; 3. March, J., Advanced Organic Chemistry, 4th ed, 1999; 4. Clayden, Greeves, Warren, and Wothers, Organic Chemistry, 1st ed, 2001; 5. R. Bruckner, Advanced Organic Chemistry, 2002; 6. R. Bruckner, Organic Mechanisms, 2010; 7. M. B. Smith, Organic Synthesis, 3rd Ed. 2010
CHM203	BASIC ORGANIC CHEMISTRY -I	3-0-0-0-9	Nomenclature of Organic molecules: Brief revision, Nomenclature of polycyclic compounds including bridged, spiro and other special structures. Structure and Bonding: Nature of bonding in aliphatic, alicyclic, aromatic and heterocyclic compounds; Aromaticity in benzenoid and nonbenzenoid compounds. Alternant and nonalternant hydrocarbons; Dipole moment; Resonance; Inductive and Field effects, hyperconjugation, Steric inhibition of resonance, structural effects on acidity and basicity. Stereochemistry: Conformational analysis of acyclic systems (Pitzer strain, A strain, etc.) and cyclohexane systems (brief review as studied in Chm 201). Introduction of terminologies such as erythro, threo, exo, endo, epimers, etc. Conformational analysis of decalins and other polycyclic compounds related to steroids. A brief introduction to asymmetric synthesis; Induction of chirality on a prochiral carbon atom; R and S nomenclature in (i) cyclic systems (ii) in compounds with more than one chiral centre and (iii) in biphenyls, allenes and spiro compounds. Optical isomerism in compounds without an asymmetric atom, Racemic modifications. Conformation of acyclic molecules, topicity and prostereoisomerism (topicity of ligands and faces), chemical and biochemical transformations of heterotopic lignds and faces. Conformations of cyclic, fused and bridged ring compounds. Allylic strain (A1,2 and A1,3) and other strains. Reactive Intermediates: Carbocations; carbanions; free radicals, radical anions and cations; arynes; carbenes and nitrenes

			(Introduction to structure, stability, and reactions). Substitution and Elimination Reactions: Electrophilic aromatic substitution (in detail); Aliphatic substitutions: S_N1, S_N2, S_N2' and S_Ni reactions; neighbouring group participation. Nucleophilic aromatic substitution (brief); Free radical substitutions (both aliphatic and aromatic). Eliminations: E_1, E_2, E_1CB reactions (in detail). Elimination vs Substitution. Molecular Rearrangement: Benzidine, Pinacol, Benzilic acid, Favorskii, Wolff, Hofmann, Cartius, Schmidt, Lossen, Beckman, Dienone phenol, Fries (Some idea of migratory aptitude), Demyanov, BaeyerVilliger, Claisen, Cope and Wagner-Meerwein (only in brief). Photochemistry: 1Brief introduction, Norrish type I and type II cleavage, photoreduction, Patterno-Buchi reaction, cis trans isomerisation, Chemistry of vision. **Course Reference**: 1. March, J., Advanced Organic Chemistry, 4th ed, 1999; 2. Nasipuri, D., Stereochemistry of Organic Compounds, 2nd ed., 1995; 3. Solomons, T. W. G., Organic Chemistry 6th ed, 1996; 4. Sykes, Peter, A guide book to Mechanism in Organic Chemistry; 5. R. Bruckner, Advanced Organic Chemistry, 2002; 6. R. Bruckner, Organic Mechanisms, 2010; 7. M. B. Smith, Organic Synthesis, 3rd Ed. 2010.
CHM205	INDUSTRIAL ORGANIC CHEMISTRY	3-0-0-0-9	**Various aspects of the energy and raw material supply:** Coal, oil, natural gas,nuclear, and biomass as energy sources; Basic products of industrial synthesis: synthesis gas, methanol, formaldehyde, halogen derivatives of methane,chlorofluoro hydrocarbons; Olefins:Historical perspective, cracking of hydrocarbons,ethylene, butanes, higher olefins, unbranched higher olefins and their use inmetathesis reactions, Acetylene: Significance and manufacturing process for acetylene, manufacture through calcium carbide, thermal process, applications of acetylene, 1,3Dioolefins:1,3Butadiene, industrial manufacture from cracking, dehydrogenation, applications of butadiene, Synthesis using carbon monoxide: Hydroformylation, industrial operations,utilization of oxo products, carbonylation of olefins; Oxidation products of ethylene: Ethylene oxide, process operation, ethyleneglycol, ethylene glycol ethers, acetaldehyde, acetic acid, acetic anhydride, Alcohols: Ethanol, propanol, butanols, amyl alcohols, aldol synthesis, polyhydric alcohols, neopentyl glycol. Vinylhalogen and oxygen compounds: Vinyl chloride, vinylidene chloridevinyl acetate, binyl ethers; Polyamides: Adipic acid, hexamethylenediamine, adiponitrile, lactams; Propene conversion products; Propylene oxide, acetone, acrolein, allylchloride, acrylonitrile.; Aromatics: Source of feedstocks, coking of hard coal, isolation, special separation techniques, condensed aromatics, naphthalene, anthracene, hydrodealkylation. Benzene derivatives; Styrene, cumene, cyclohexane, phenol, maleic anhydride, nitrobenzene, aniline, diisocyanates. Oxidation products of xylene and naphthalene; Phthalic anhydride, esters of phthalic acid and derivatives, terephthalic acid.
CHM221	BASIC PHYSICAL CHEMISTRY I	3-0-0-0-9	Thermodynamic Preliminaries: System, Surroundings, Extensive and Intensive Properties, Laws of Thermodynamics, Heat Engines.

			Thermodynamic Potentials: Energy, Entropy, Legendre Transforms, Free energies, Stability criteria Applications of Thermodynamics: Partial Molar Quantities, Chemical Potential, Gibbs-Duhem Equation, Clapeyron Equation, Gibbs Phase Rule Applied to Reactive and Nonreactive Mixtures, Partial Molar Quantities, Chemical Potential, Phase Transitions, LiquidSolid-Vapor, Solid-Solid Phases, Eutectic Mixtures. Ideal and Nonideal Systems: Ideal and Nonideal Gases, Liquids, Binary Mixtures, Solutions. Electrochemistry: Electrochemical Cell, Cell Potential, Nernst Equation, Electrochemical Series, Electrolytic Cells, Electrode Kinetics, Butler-Volmer Equation, Nernst Planck Equation, Li-Ion Batteries, Intercalation and Deintercalation. Finite-Time Thermodynamics and Nonequilibrium Thermodynamics: Flexible module with possible topics like Endo Reversible Engine Cycle, Introduction to FiniteTime Engine Cycle, Curzon-Ahlborn Efficiency, Concept of Local Equilibrium, Prigogine's Entropy Production Rate, Molecular Motors etc. **Course Reference**: 1. P. W. Atkins and Julio de Paula, Physical Chemistry. 2. N. Levine, Physical Chemistry. 3. R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Physical Chemistry. 4. D. A. McQuarrie, J. D. Simon, Physical Chemistry: A molecular approach
CHM222	BASIC PHYSICAL CHEMISTRY-II	3-0-0-0-9	Kinetic Preliminaries: Local equilibrium, phenomenological laws, parallel and consecutive reactions, steady state approximation, preequilibrium. Kinetics of complex reactions: Enzyme kinetics, free radical chain reaction, polymerization. Kinetic theory of Gases: Taxonomy of collisions, derivation of mechanical pressure equation and ideal gas equation from kinetic theory. Transport properties: transport coefficients, thermal conductivity, viscosity, diffusion, calculation of transport coefficients from kinetic theory. Theory of electrolytic solutions, ionic conductivity, Kohlrausch's law, transport numbers. Surfaces and Interfaces: Gibbs dividing surfaces and interfaces, solids and surfaces, structure and morphology of surfaces, adsorption, adsorption isotherms, mechanisms of surface catalyzed reactions, Flexible topics in surfaces and interfaces: modern surface analytical tools like STM and AFM, catalytic converters, Haber-Bosch synthesis, 2D materials etc. **Course Reference**: 1. P. W. Atkins and Julio de Paula, Physical Chemistry; 2. I. N. Levine, Physical Chemistry; 3. R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Physical Chemistry. 4. D. A. McQuarrie, J. D. Simon, Physical Chemistry: A molecular approach
CHM241	BASIC INORGANIC CHEMISTRY I	3-0-0-0-9	1. Chemical bonding and Forces: Chemical bonding and various theories of covalency, types of bonding: ionic, covalent and metallic; valence bond theory, hybridization of atomic orbitals, molecular geometry and shape, fluxional behaviour of

			molecules, MO theory: Linear combination of atomic orbitals (LCAO), diatomic homonuclear species (O2, N2), involvement of d-orbitals and CFT, bond energy, sigma (σ), pi (π), delta (δ) bonds, polarity, Fajan's rule, deformation of ions, Non-covalent interactions, supramolecules, hydrogen bonding. 2. Solid State Structures: Born-Haber cycle, Lattice energy, crystal packing, radius ratio rules, Crystal systems and lattices, Structure of basic ionic crystals (AB, AB_2, AB_3, A_2B_3 types), X-ray diffraction and Bragg's law, crystal defects, band theory, perovskite and hybrid perovskite, superconductivity. 3. Oxidation Reduction Reactions: Redox reactions, Nernst equation, oxidation-reduction potentials, formal potentials, equilibrium constants, over potentials, disproportionation and comproportionation reactions, Latimer and Frost diagrams, Electrochemical cells. 4. Acids and Bases Acid-base concepts and principles (Arrhenius, BronstedLowry, conjugate acids-bases, Lewis, HSAB), strength of acids and bases, acid-base equilibrium, indicator, Henderson equation, pH and buffer, non-aqueous solvents. 5. Inorganic Chemistry in Biology, Health, Energy, and Environment Inorganic elements in life related processes, oxygen carrying proteins, therapy and diagnosis, nitrogen fixation from air Inorganic elements in energy production and storage, hydrogen fuel cells, battery, Li-ion battery, sustainability. [1] Inorganic Chemistry-Principles of Structure and Reactivity, 4th Edn., J. E. Huheey, E. A. Keiter and R. L. Keiter, Harper-Collins, NY, 1993. [2] Concepts and Models of Inorganic Chemsitry, 3rd Edn., B. Douglas, D. McDaniel and J. Alexander, John Wiley, New York. 1993. [3] Shriver and Atkins Inorganic Chemistry, 5th Edn., Oxford University Press, 2009. [4] Chemistry of the Elements, 2ndEdn., N. N. Greenwood and A. Earnshaw, Pergamon, Oxford, 2005. [5] Advanced Inorganic Chemistry, 6th Edn., F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Wiley, 1999. [6] Principles Of Bioinorganic Chemistry, I. Bertini & J. M. Berg, University Science Books, California. [7] Modern Inorganic Chemistry. 2nd Edn. Jolly, W. L. McGraw-Hill, NY, 1991. [8] Chemistry of High-Energy Materials, T. M. Klapötke, 4th Edn., 2009
CHM242	BASIC INORGANIC CHEMISTRY II	3-0-0-0-9	1.Molecular symmetry, point groups and character tables. 2. Chemistry of selective main group elements and their compounds.3. Transition metal chemistry, isomerism, structure and bonding, crystal field, and ligand field theory of transition metal complexes, thermodynamic and kinetic stability. 3. Electronic spectroscopy and magnetic behavior of transition metal complex, Chemistry of f-block elements. 4.Transuranium elements, radiations and radioactive decay, magic number, nuclear spin, half-life, nuclear fission & fusion, practical application of radioisotopes. 5. Organometallic Chemistry: Sigma bonded ligands (Metal-Alkyl, Aryl, M-hydrides, M-X (X=Si, B, etc). Pi-bonded ligands (Alkynes, alkenes) Sigma and Pi-bonded ligands (CO, Phosphines, Carbenes, etc). 6.

			Homogeneous Catalysis: Elementary organometallic reactions, Hydrogenation, Cross-coupling, Carbonylation, Reductive Amination. Heterogeneous Catalysis: Modern trends in hydrogenation of various functional groups (Acid, ester, nitrile, etc). Polymerization reaction. **Course Reference**: ggested text and reference material: 1. Inorganic Chemistry-Principles of Structure and Reactivity, 4th Edn., J. E. Huheey, E. A. Keiter and R. L. Keiter, Harper-Collins, NY, 1993. 2. Concepts and Models of Inorganic Chemsitry, 3rdEdn., B. Douglas, D. McDaniel and J. Alexander, John Wiley, New York. 1993. 3. Shriver and Atkins Inorganic Chemistry, 5th Edn., Oxford University Press, 2009. 4. Chemistry of the Elements, 2ndEdn., N. N. Greenwood and A. Earnshaw, Pergamon, Oxford, 2005. 5. F. A. Cotton, Chemical applications of Group Theory 3rd ed., John Wiley and Sons, 2003. 6. A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edition, John Wiley and Sons 2001. 7. F. Albert Cotton, Carlos A. Murillo, and Manfred Bochmann, Advanced Inorganic Chemistry, 6th Ed. Wiley Interscience Publication 2001. 8. Christoph Elschenbroich, Organometallics (Third edition); Wiley-VCH, Weinheim, 2006. ISBN: 3527293906. 9. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4th Ed.; Wiley Interscience, 2005. ISBN: 0471662569
CHM303	ORGANIC CHEMISTRY I	3-0-0-0-9	Stereochemistry: Dynamic stereochemistry: Conformation and Reactivity. Various chemo, regio and stereo selective reactions. Reactive Intermediates: Carbenes and carbenoids; Radicals: Structure, reactivity, selectivity and mechanisms of radicals and radical based reactions, involving various functional groups. Radical cations and radical anions. Carbocations: Non classical carbonation. Sigma and piparticipation. Mechanistic and Stereo chemical Aspects of: Baeyer Villiger, Claisen (including Johnson Claisen, Ireland Claisen, Eschenomser, Over man modifications) Cope, and oxy Cope, Wittig rearrangements (both 1,2 and 2,3 Wittig rearrangements); ene and metalloene reactions; (2+2), (3+2) and (4+2) cycloadditions; Barton reaction. Organometallic Chemistry: Mechanism and stereochemistry of various reactions. Palladium based reactions such as Heck, Stille, Suzuki, Sonogashira, Buchwald Hartwig couplings; Tsuji Trost C-C bond formations; Ni and Sn-catlysed reactions. Enzymatic Reactions: Mecahnistic and stereo chemical aspects of hydrolases (including esterases and lipases), oxido reductases. Green Chemistry: Concepts and applications. Classification and Structures of some natural products such as terpenoids, steroids, alkaloids and prostaglandins. **References/Text Books**: 1. March, J., Advanced Organic Chemistry, 4th ed, 1999; 2. Nasipuri, D., Stereochemistry of Organic Compounds, 2nd ed., 1995; 3. Solomons, T. W. G., Organic Chemistry 6th ed, 1996; 4. Sykes, Peter, A guide book to Mechanism in Organic Chemistry; 5. R. Bruckner, Advanced Organic Chemistry, 2002; 6. R. Bruckner, Organic Mechanisms, 2010; 7. M. B. Smith, Organic Synthesis, 3rd Ed. 2010; 8.

			Clayden, Greeves, Warren, and Wothers, Organic Chemistry, 1st ed, 2001
CHM305	ORGANIC QUALITATIVE & QUANTITATIVE ANALYSIS	0-0-6-0-6	1. **Experimental Techniques** (A) Purification of Organic Compounds a. Recrystallisation b. Sublimation at atmospheric pressure and under reduced pressure c. Separation or organic compounds by Steam distillation d. Distillation of organic compounds under reduced pressure e. Bulb-to-bulb distillation under reduced pressure (B) Chromatography a. Thin layer chromatography (TLC) and calculation of Rf values, b. Column Chromatography: separation of organic mixture. c. Preparative TLC: preparation of plates and separation of organic mixtures (C) Physical Constants a. Melting Points and Boiling Points b. Optical rotation and calculation of specific rotation and molecular rotation (D) Spectroscopic Methods, a. Preparation of an ester and its confirmation by IR and NMR, b. Structure illucidation of unknown compounds based on the given spectral data 2. **Investigation and Characterization of Organic Compoundsa**. Detection of elements present in a given organic compound. b. Identification of functional groups in a given organic compound. c. Identification of unknown organic compounds. d. Separation of organic mixture by chemical methods, preparation of derivatives, and identification of the material.
CHM321	PHYSICAL CHEMISTRY I	3-0-0-0-9	1. **Introduction:** importance, historic background, quantum mechanics vs classical mechanics, waveparticle duality, uncertainty principle; 2. **Schroedinger equation:** wavefunction and interpretation, time dependent and time independent Schroedinger equation, eigenvalue problem; 3. **Quantum mechanics of some simple systems**: free particle, particle in a box , harmonicoscillator, one dimensional potential step and barrier; 4. **Angular Momentum:** rigid rotor, orbital and spin angular momentum; 5. **Hydrogen and hydrogen like atoms;** 6. **Approximate methods:** perturbation theory, variational method, some simple examples; 7. **Many electron atom**: Pauli antisymmetry principle, Slater determinant, He atom, Li atom. **Course Reference**: 1. I. N. Levine, Quantum Chemistry; 2. J. P. Lowe and K. A. Peterson, Quantum Chemistry; 3. D. A. McQuarrie, Quantum Chemistry; 4. D. A. McQuarrie, J. D. Simon, Physical Chemistry: A molecular approach; 5. P. W. Atkins, Molecular Quantum Mechanics
CHM322	PHYSICAL CHEMISTRY -II	3-0-0-0-9	Equilibrium Thermodynamics: Laws of thermodynamics, the equilibrium state, thermodynamic variables, conjugate quantities, thermodynamic potentials Statistical Mechanics: Kinetic Theory of gases, Boltzmann distribution,the ensemble postulate, partition function, canonical ensemble, other ensembles, fluctuations, ideal monatomic, diatomic and polyatomic gases, chemical equilibrium, quantum statistics, Transport Phenomena: Transport coefficients, thermal conductivity, diffusivity, viscosity, ionic conductivity, Limiting law of DebyeHckelOnsager, Nernst Einstein relation, Stokes Einstein relation Molecular Reaction Dynamics: Collision theory, activation energy,transitionstate theory, reactions as trajectories, molecular beam experiments,reactions in liquid phase, Kramers theory, Diffusion limited reactions

			Course Reference: 1. P.W. Atkins and Julio de Paula: Physical Chemistry; 2. I.N. Levine: Physical Chemistry; 3. D.A. McQuarrie and J. D. Simon: Physical Chemistry A Molecular Approach; 4. D. A. McQuarrie, Statistical Mechanics; 5. H. B. Callen: Thermodynamics and an introduction to Thermostatistics; 6. David Chandler: Introduction to Modern Statistical Mechanics; 7. R.S. Berry, S.A. Rice and John Ross: Physical Chemistry
CHM324	BASIC PHYSICAL CHEMISTRY LABORATORY	0-0-6-0-6	**1. Solutions, Thermodynamics and Phase equilibrium**: Calibration of volumetric apparatus. (One day). Determination of partial molal volume. (One day) Determination of the isotherm for a threecomponent system. (Two days), The measurement of electrical conductance for the determination of the equivalent conductance at infinite dilution. (Two days) Determination of transport number by moving boundary method. (One day) Polarizability from refractive index measurements. (One day) **2. Kinetics:** Kinetics of fast reactions by stopped-flow technique. (One day) Rate of the hydrolysis of sucrose using polarimeter. (Two days), Determination of pKa of poly-basic acid with the pH meter. (One day) **3. Spectroscopy:** Analysis of the rotational-vibrational spectra of HCl molecules. (One day) Spectrophotometric determination of the acid dissociation constant (Two days) Fluorescence quantum yield determination of an unknown molecule. (One day) IR and Raman spectroscopy of solvent mixtures. (Two days) Formula and stability constant of a complex by spectrophotometry. (One day) Fluorescence spectrum and stern-volmer quenching constant. (One day) Determination of critical miceller concentration. (One day). **4. Quantum mechanics:** Computing Potential Energy Surface of molecules using Quantum Mechanics. (Two days). **Course Reference**: 1. Experimental physical chemistry, F. A. Bettelheim 2. Experimental physical chemistry, G. P. Matthews 3. Experimental physical chemistry, F. Daniels 4. Experimental physical chemistry, A. Halpern and G. McBane 5. Experimental Physical Chemistry, D. P. Shoemaker, C. W. Garland, and J. W. Nibler
CHM342	INORGANIC CHEMISTRY -II	3-0-0-0-9	1. Symmetry, point groups, character tables, concepts of orbital symmetries for dorbital splitting diagrams in different stereochemistry; 2. Synthesis and structure of mononuclear and multinuclear transition metal complexes; 3. Theories of bonding. Crystalfield and Molecular orbital, effects of ligandfield (spectrochemical series, consequences of dorbital splitting); 4. Spectroscopy of transitionmetal complexes: Russell Saunders coupling scheme, Term Symbols; 5. Magnetism of transitionmetal complexes: Curie law, para, ferro, antiferro and ferromagnetic systems; 6. Reaction mechanism of transition metal complexes and electrontransfer reactions; 7. Introduction of bioinorganic chemistry: heme, nonheme, FeS proteins; 8. New trends of research: supramolecular chemistry, metalorganic frameworks, gasstorage,nanochemistry, the renaissance of carbon; 9. Transition metalbased inorganic materials (magnetic, optical and biomaterials)

			Course Reference: 1. Huheey, J. E.; Keiter, K. E.; Keiter, R. L., Inorganic Chemistry Principles of Structure and Reactivity: 4th Edn, Pearson Education, 2008; 2. Shriver. D. F.; Atkins. P. W.; Langford, C. G., Inorganic Chemistry. 3rd Edn., OxfordUniversity, Oxford, 1999; 3. Cotton, F. A.; Murillo, C. A.; and Bochmann, M., Advanced Inorganic Chemistry 6th Edn. ,Wiley Interscience, 2001; 4. Cotton, F. A., Chemical Applications of Group Theory 3rd ed., John Wiley and Sons, 2003; 5. Carter, R. L., Molecular Symmetry and Group Theory, John Wiley and Sons, 3rdEdn.,1998; 6. Kahn, O., Molecular Magnetism, VCH, Weinheim, 1993; 7. Lehn, J. M., Supramolecular Chemistry: Concepts and Perspectives, VCH, Weinheim,1995; 8. Berg, J. M.; Lippard, S. J., Principles of Bioinorganic Chemistry, University Science Books,CA, 1995.
CHM344	INORGANIC CHEMISTRY LABORATORY EXPERIMENTS	0-0-6-0-6	Estimation of iron in minute quantities by UV-vis spectrophotometry, Principles of colorimetric analysis: determination of iron content of an unknown sample.Preparation of hexamine nickel (II) chloride: estimation of ammonia and nickel bytitrimetric and gravimetric methods Determination of complex composition using simple techniques Preparation of diamagnetic and paramagnetic maingroup and transition metalacetylacetonates Synthesis, isolation and spectroscopic characterization of the complexes Synthesis and characterization of ferrocene and acetyl ferrocene Synthesis of the complex and their purification using chromatography Acidbase and redox titration of tablets containing Vitamin C Estimation of ascorbic acid in Vitamin C tablets Paper chromatographic separation of Cu2+, Fe3+ and Ni2+. Utilization of paper chromatographic techniques to separate the metal salts, Spectrophotometric determination of phosphate: estimation of phosphate in coladrinks Determination of concentration of phosphates applying Beer Lambert law 8. Potassium trisoxalatoferrate (III): synthesis, analysis and photochemistry Synthesis of the complex and its utilization in blueprinting experiment **References/Text Books:** Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press (India) Pvt. Ltd., 2002. Roesky, H. W.; Mckel, K., Chemical Curiosities: spectacular experiments and inspired quotes, VCH, 1996. Handouts prepared for the laboratory experiments: collections from various literature sources
CHM345	INORGANIC CHEMISTRY I	3-0-0-0-9	1. Representative Chemistry of Main Group Elements (a) Organometallic Chemistry of Lithium and Magnesium: synthesis, structure and reactivity (b) Chemistry of Boron: boranes, bonding in boranes, topology of boranes, synthesis and reactivity, carboranes and metallacarboranes. New Lewis acids based on boron; polymer supported Lewis acids (c) Chemistry of Aluminum: Aluminum alkyls, use of aluminum alkyls in polymerization ofolefins (d) C60 and carbon nanotubes: discovery, preparation and selected reactions (e) Chemistry of Silicon: organosilicon compounds, silicates and aluminosilicates; 2. Unusual Compounds of MainGroup Elements (a) Multiple bonding in heavier main group elements, unusual compounds of

			maingroupelements: (i) SiSi double bond, SiSi triple bond, PP double bond, BiBi double bond,synthesis, structure and reactivity (b) Chemistry of lowvalent compounds: Synthesis, structure and bonding models andreactivity of Al(I), Si(II) low valent compounds(c) Chemistry of stable N heterocyclic carbenes, use of carbenes in catalysis(d) Inorganic rings and polymers: cyclo and heterocyclophosphazenes, polysilanes, borazine and boron nitride 3. Chemistry of halogens and noble gases: recent trends, CFCs and ozone layer 4. Organometallic Chemistry:(a) bonded systems: metal alkyls, aryls and hydrides, stability, preparation and reactivity, metalcarbonyls, metalphosphines, metalnitrosyls, metalisocyanides: structures, reactivity and bonding Metal carbenes, metal carbynes, Fischer carbenes, Schrock carbenes, complexes with N-heterocyclic carbenes, olefin metathesis (b) bonded systems: metalolefins, alkyls, alkynes, dienes, Cp and Cp*, structure, bonding and reactivity(c) Applications of organometallics in organic synthesis: CC bond coupling reactions (Heck, Sonogashira, Suzuki), reduction using transition metal hydrides, asymmetric hydrogenation. **Course Reference**: 1. Elschenbroich, C.; and Salzer, A., Organometallics: A Concise Introduction, 3rd Edn. 1999; 2. Greenwood, N. N.; Earnshaw, A., Chemistry of the Elements, Pergamon Press, 2nd Edn.,2002; 3. Douglas, B.; McDaniel, D.; and Alexander, J., Concepts and Models of InorganicChemsitry. 3rd Edn., John Wiley, New York. 1993; 4. Crabtree, R. H. The Organometallic Chemistry of the Transition Metals, 5th Edn., JohnWiley and Sons, 2009
CHM361	CHEMISTRY COMMUNICATION SKILLS	2-0-0-0-6	**Course Contents:** **Oral and written communication:** How to write news and views related to chemistry? Writing review on current topics in chemistry (e.g.: Nobel prize in chemistry, recent advances, etc.). Prepare a technical writing in Latex (Including equations, derivations, tables etc.) and Microsoft word. Presentation of slides on a project work. Presentation of reviews to audience. **Tools related to Chemistry:** Draw chemical structures using CHEMDRAW (Exercise: draw chemical structure of different natural products as per instruction), Mercury (drawing crystal structures of molecular crystals). How to find compound related data in the literature? Example: SciFinder. Finding commercial sources and databases for chemicals. Use and management of mined data (Scopus, Web of Sciences). Making literature library for scientific writing and citation with reference management tools such as Endnote, BibTex, Mendeley, Zotero etc. Data fitting (Igor, Origin, etc.). Number precision and numerical data presentation, error analysis. Making figures and technical drawings for journals. **Databases in chemistry:** Use of specialized databases like CCDC, PDB, SDBS, other nuclei NMR databases (Exercise: find crystal structures in CCDC for different known compounds as instructed, downloading spectrum from SDBS and report proton and carbon spectra in different journal format). How to report/write compound data and chemical procedures?

			(Exercise: prepare experimental procedures and synthetic procedures for different journals). **Scientific Ethics:** Plagiarism. Scientific integrity. Data integrity and recording experiments in lab notebook. How to make/prepare a text similarity report using Turnitin and ithenticate? **Flexible topics in communication skills.**
CHM391	UNDER GRADUATE PROJECT-I	0-0-4-0-4	5th Semester Undergraduate Project: UG Research project under the supervision/co-supervision of a faculty in Chemistry.
CHM392	UG PROJECT II	0-0-0-0-9	UG PROJECT II: UG Research project under the supervision/co-supervision of a faculty in Chemistry.
CHM399A	CHEMISTRY COMMUNICATION SKILLS	0-0-0-2-2	**CHEMISTRY COMMUNICATION SKILLS** **Oral and written communication:** • How to write news and views related to chemistry? • Writing review on current topics in chemistry (eg.: Nobel prize in chemistry, recent advances, etc.) • Prepare a technical writing in Latex (Including equations, derivations, tables etc.) and Microsoft word. • Presentation of slides on a project work. • Presentation of reviews to audience. **Tools related to chemistry:** • Draw chemical structures using CHEMDRAW (Exercise: draw chemical structure of different natural products as per instruction), Mercury (drawing crystal structures of molecular crystals). • How to find compound related data in the literature? Example: SciFinder • Finding commercial sources and databases for chemicals. • Use and management of mined data (Scopus, Web of Sciences). • Making literature library for scientific writing and citation with reference management tools such as Endnote, BibTex, Mendeley, Zotero etc. • Data fitting (Igor, Origin, etc.) • Number precision and numerical data presentation, error analysis. • Making figures and technical drawing for journals. Databases in chemistry: • Use of specialized databases like CCDC, PDB, SDBS, other nuclei NMR databases (Exercise: find crystal structures in CCDC for different known compounds as instructed, downloading spectrum from SDBS and report proton and carbon spectra in different journal format) • How to report/write compound data and chemical procedures? (Exercise: prepare experimental procedures and synthetic procedures for different journals). **Scientific Ethics:** • Plagiarism. • Scientific integrity. • Data integrity and recording experiments in lab notebook. • How to make/prepare text similarity report using turnitin and ithenticate? 5 **Flexible topics in communication skills.**
CHM401	ORGANIC CHEMISTRY I	3-0-0-0-9	Stereochemistry, Dynamic stereochemistry, Mechanistic and Stereo chemical aspects, Reactive Intermediates: Carbenes, Nitrenes, Radicals, Carbocations.Mechanistic and Stereochemical Aspects of: (10) Baeyer-Villiger, Claisen (including Johnson-Claisen, Ireland-Claisen, Eschenomser, Overman modifications) Cope, and oxy-Cope, Wittig rearrangements (both 1,2 and 2,3 Wittig rearrangements); ene and metalloene reactions; (2+2), (3+2) and (4+2) cycloadditions; Barton reaction. Organometallic Chemistry: (5) Mechanism and stereochemistry of various reactions. Palladium based reactions such as Heck, Stille, Suzuki, Sonogashira, Buchwald-Hartwig couplings; Tsuji-Trost C-C bond formations; Ni and Sn catlysed

			reactions.Enzymatic Reactions: (3) Mecahnistic and stereochemical aspects of hydrolases (including esterases and lipases), oxido-reductases.Green Chemistry: Concepts and applications (3) Classification and Structures of some natural products such as terpenoids, steroids, alkaloids and prostaglandins (5) **Course Reference**: 1. March, J., Advanced Organic Chemistry, 4th ed, 1999. 2. Nasipuri, D., Stereochemistry of Organic Compounds, 2nd ed., 1995. 3. Solomons, T. W. G., Organic Chemistry 6th ed, 1996. 4. Sykes, Peter, A guide book to Mechanism in Organic Chemistry. 5. R. Bruckner, Advanced Organic Chemistry, 2002 6. R. Bruckner, Organic Mechanisms, 2010 7. M. B. Smith, Organic Synthesis, 3rd Ed. 2010 8. Clayden, Greeves, Warren, and Wothers, Organic Chemistry, 1st ed, 2001
CHM402A	ORGANIC CHEMISTRY II	3-0-0-0-9	Oxidation: Oxidation involving organosulfur (such as Swern) and organoselenium compounds; DessMartin, IBXand related hypervalent iodine based oxidations, Ag2CO3/celite Prevost, photosensitised oxidation, dimethyldioxirane, RuO4, 2sulfonyl oxaziridne, transition metal catalysed oxidation, oxidation atunfunctionalised carbons, Fleming Tamao oxidation, and microbial oxidations.Reduction: (6)Using silanes, Al and B based reagents (e.g. DIBAL, Lselectride, Kselectride, RedAl etc.), low valentTi species, microbial reductions (NADH model etc.) Asymmetric Synthesis: (8) Sharpless epoxidation and dihydroxylation, Jacobsens epoxidation, Coreys oxazaborolidinecatalyzed reduction, Noyoris BINAP reduction, SAMP, RAMP, Evans oxazoline and Oppolzer sultams, Aldol reaction (in brief: only principles using models).CC Bond Formation: (14) via anions to electron withdrawing groups (carbonyl group, esters, NO2, SO2Ph, CN etc.) via B and Si enolates via imines Michael additions (cuprates etc.) Via allyl boron, allyl tin, allyl and vinyl silanes Metal catalyzed Cyclopropanation reactions (including Simmons Smith reaction) Ringclosing, ringopening and cross metathesisOrganic Synthesis: (8) Application of above reactions and the ones studied in CHM 401 in synthesis of natural products. **Course Reference**: 1. Carruthers, W., Coldham, I. Some Modern Methods of Organic Synthesis, 2008; 2. Smith, M. B., Organic Synthesis, 2nd ed., 2002; 3. Carreira, E. M.; Kvaerno, L. Classics in stereoselective synthesis, 2009; 4. Nicolaou, K. C.; Sorenson, E. J., Classics in total synthesis, 1996; 5. Nicolaou, K. C.; Snyder, S. A., Classics in total synthesis II, 2003; 6. Tsuji, J., Transition metal reagents and catalysts, 2000.
CHM423	PHYSICAL CHEMISTRY LAB	0-0-6-0-6	1. Calibration of volumetric apparatus. (One day); 2. Analysis of the rotationalvibrational spectra of HCl molecules. (One day; 3. Determination of partial molal volume. (One day); 4. Determination of the isotherm for a three omponent system. (Two days); 5. Kinetics of fast reactions by stoppedflow technique. (One day); 6. Spectrophotometric determination of the acid dissociation constant (Two day); 7. The measurement of electrical conductance for the determination of the

			equivalentconductance at infinite dilution (Two days); 8. Rate of the hydrolysis of sucrose using polarimeter. (Two day); 9. Determination of pKa of polybasic acid with the pH meter. (One day); 10. Determination of critical miceller concentration. (One day); 11. Determination of transport number by moving boundary method. (One day); 12. Polarizability from refractive index measurements. (One day); 13. Formula and stability constant of a complex by spectrophotometry. (One day); 14. Fluorescence quantum yield determination of an unknown molecule. (One day); 15. Fluorescence spectrum and sternvolmer quenching constant. (One day); 16. IR and Raman spectroscopy of solvent mixtures. (Two days); 17. Computing Potential Energy Surface of molecules using Quantum Mechanics. (Twodays) **Course Reference**: 1. Experimental physical chemistry, F. A. Bettelheim; 2. Experimental physical chemistry, G. P. Matthews; 3. Experimental physical chemistry, F. Daniels; 4. Experimental physical chemistry, A. Halpern and G. McBane; 5. Experimental Physical Chemistry, D. P. Shoemaker, C. W. Garland, and J. W. Nibler
CHM443	INORGANIC CHEMISTRY LABORATORY	0-0-6-0-6	Invisible ink: Utilization of coordination chemistry to demonstrate invisible ink in laboratory. Color effects due to ligand-exchange in nickel complexes: Demonstration of ligand-field strength in the spectrochemical series Color effects in aqueous systems containing divalent 3d metalions: Demonstration of crystal-field splitting parameters of 3d metal ions Acidic and basic salts: Hydrolysis of salts and its consequences Preparation of nitro- and nitrito-pentamminecobalt(III) chloride: Linkage isomers: synthesis and identification using various spectroscopic techniques The preparation of hexamminecobalt(III) chloride and pentammineaquocobalt(III) chloride: Synthesis, isolation and characterization of the complex The preparation of *cis*-and *trans* -potassiumdioxalatodiaquochromate(III): Geometrical isomers: synthesis and identification using various spectroscopic techniques Aquation of *trans*-dichloro-*bis*(1,2-diamminoethane)cobalt(III)chloride: Investigation of acid hydrolysis of the complex: The preparation and resolution of *tris*(ethylenediamine)cobalt(III)ion into its optical antipodes Optical isomers: synthesis, isolation and characterization: Preparation of hexamminenickel(II) chloride: estimation of ammonia and nickel by titrimetric and gravimetric methods Determination of complex composition using simple techniques:Synthesis and reactions of organo cobaloximes Synthesis of an air-sensitive organometallic complex at low temperature under inert atmosphere: Synthesis and characterization of ferrocene and acetylferrocene: Synthesis, purification using chromatography and characterization **References/Text Books**: Roesky, H. W.; Möckel, K., Chemical

			curiosities: spectacular experiments and inspired quotes, VCH, 1996. Hand-outs prepared for the laboratory experiments: collections from various literature sources.
CHM481	BIOSYSTEMS	3-0-0-0-9	Buffers (their use in study of biomolecules), pH, pKa of amino acids, D and L amino acidnomenclature. (1) Proteins: protein sequencing by chemical and mass & NMR spectroscopic methods), Use of spectroscopic tools in studying biomolecules. Primary (single letter amino acid codes), Ramachandran plot, secondary, 310, helices, parallel and antiparallel sheets, turns, turns), circular dichroism of secondary structures, tertiary (motifs and domains: someimportant motifs like Rossman fold, helix turn helix, 4 helix bundles, beta barrel) andquaternary structure (Hemoglobin and Myoglobin). Protein Engineering (17). Nucleic acids: A, B and ZDNA structures, Method of replication, sequencing of nucleic acids (chemical, dideoxy and fluorescence), Transcription, Translation, genetic code, genomes, genes, over expression of recombinant proteins, mutagenesis (random and site directed) Polymerase chain reaction (PCR). Use of modified bases in PCR (9) Carbohydrates and Glycoproteins, proteoglycans, Membranes and lipids, bacteial cell wallsynthesis and mechanism of some important antibiotics like penicllin, antibiotic resistance. (4) Metabolism: Photosynthesis, Calvins cycle, Glycolysis, Krebs cycle, electron transport, cofactors. (4) Enzymes and their kinetics: Michaelis Menten kinetics, Reaction order, competitive, uncompetitive, noncompetitive and irreversible inhibition of enzymes. Effect of pH, temperatureon enzyme activity. (4) Biophysical techniques to purify and study proteins. Dialysis, salting out and precipitation byorganic solvents, Ion exchange, gel filtration, reversed phase, affinity chromatography, ultracentrifugation, gel electrophoresis. **Course Reference**: 1. Fundamentals of Biochemistry by Voet, Voet and Pratt; 2. Biochemistry by L. Stryer; 3. Proteins by T.E. Creighton; 4. Genes VII by B. Lewin, Introduction to protein structure by Branden and Tooze; 5. Enzyme structure and Mechanism by Alan Fersht
CHM491	UNDER GRADUATE PROJECT-III	0-0-0-0-9	UG PROJECT (UGP-III): UG Research project under the supervision/co-supervision of a faculty in Chemistry.
CHM492	UG PROJECT IV	0-0-0-0-9	UG PROJECT (UGP-IV): UG Research project under the supervision/co-supervision of a faculty in Chemistry.
CHM503	ORGANIC PREPARATION LAB	0-0-6-0-6	Preparations of various organic compounds employing different reactions willbe carried out, with a view to give the student sufficient training in syntheticorganic chemistry **Benzil – Benzilic Acid Rearrangement** (a) Prep. of benzil by oxidation of benzoin by nitric acid (b) Benzil, an ® , ¯ - diketone undergoes rearrangement to benzilic acid. **Fisher: Indole Synthesis:** Preparation of 1.2.3.4 – tetrahydrocarbazole. This compound is prepared according to the Fisher indole synthesis starting from phenylhydrazine and

			cyclohexanone. **Diazotization:** Forming a diazonium salt from an appropriate primary aromatic amine in the presence of HNO2. **Preparationof P-Iodonitrobenzene:** p-Nitroaniline is diazotized and treated with KI **PHOTOCHEMICAL REACTIONS:** By Irradiation with Sunlight OR By Reductive Coupling Prep. of Benzopinacol from benzophenone by reductive coupling **MOLECULAR REARRANGEMENT** **Pinacol – Pinacolone – rearrangement** (a) Prep. of benzopinacol (b) Prep. of benzopinacolone **REIMER – TIEMANNREACTION** Prep. of β-hydroxynapthaldehyde from β-napthal **PERKIN REACTION** Preparation of Cinnamic acid Bromination cinnamic acid i.e. Prep. of bromostryrene **ALDOLCONDENSATION AND EPOXIDATION** (a) Preparation of Chalcone (b) Preparation of Chalcone epoxide **Course Reference:** 1. Fundamentals of Biochemistry by Voet, Voet and Pratt, 2. Biochemistry by L. Stryer, 3. Proteins by T.E. Creighton, 4. Genes VII by B. Lewin, 5. Introduction to protein structure by Branden and Tooze, 6. Enzyme structure and Mechanism by Alan Fersht.
CHM521	MATHEMATICS FOR CHEMISTRY	2-0-0-0-6	Functions: Series expansion, Special functions (including plotting and sketching), contour plots/surfaces, maximum and minimum of functions (of one and many variables). Differential Equations: First Order Linear Differential Equation (Homogenous, Non-Homogenous), Second Order differential equation, Solution by Power Series Expansion, Sturm-Liouville Problem, Eigenvalue-Eigenfunction Problems. Partial Differential Equations: Method of Separation of Variables, Wave Equation, Diffusion. Fourier Series and Transform: Sine and Cosine Series, Fourier Transforms, Power Spectra, Applications in Solving Partial Differential Equations. Linear Algebra: Vector Space, Hilbert Space, Inner Products, Solving Linear Equations, Matrix Inversion, Eigenvalues and Eigenvectors, Hermitian Matrices, Matrix Equations. Coordinate Transform: Polar Coordinates, Spherical Polar Coordinates, Elliptical Coordinates.
CHM599	MS PROJECT	3-0-0-0-48	MS research project for dual-degree programme under the supervision of a faculty in the Department of Chemistry.
CHM600	MATHEMATICS FOR CHEMISTRY	3-0-0-0-9	Error Analysis, Scalars, vectors, curl, divergence and gradient, ordinary 3000[4] differential equations, symmetry and group theory, matrices, etc. **Error Analysis:** Error, precision, accuracy, significant figures, mean, standard deviation, propagation of errors. (2) **Vectors and Matrices:** Dot product, cross product, gradient, divergence, continuity equation, curl. Vector integration: Stokes' and Gauss' theorems, vector spaces. Matrices: coordinate

			transformation, Jacobian, system of linear equations, inverse of a matrix, Cramer's rule, Gaussian elimination and its variants, eigenvalues and eigenvectors. (10) **Ordinary Differential Equations and Special Functions:** General and particular solutions of a differential equation. First order equations and their applications. Separation of variables, equations reducible to separable form. Exact differential equations, non-homogeneous differential equations, integrating factors. Second order linear differential equations: homogeneous with constant coefficients, characteristic equation, general solution, particular solution. Non-homogeneous linear second order equations, Sturm-Liouville theorem, Power series method of solution of differential equations, Special functions such as Legendre and Hermite polynomials, Beta, Gamma and error functions. Non-linear differential equations. (14) Fourier series and transform, basic theorems, convolution. Laplace transform and its properties, Applications of Fourier and Laplace transforms. (6) **Numerical Methods:** Numerical differentiation and interpolation, Numerical quadrature, Newton-Cotes formulae, Simultaneous equations and matrix eigenvalues, Numerical solution of differential equations. (8) **References/Textbooks**: 1. G.B. Arfken and H.J. Weber, Mathematical Methods for Physicists, Academic Press (2001). 2. M.L. Boas, Mathematical Methods in the Physical Sciences, John Wiley, India (2007). 3. E. Kreyszig, Advanced Engineering Mathematics, John Wiley, New York (1999). D. McQuarrie, Mathematical methods for scientists and engineers, University Science Books (2003).
CHM602	ADVANCED ORGANIC CHEMISTRY II	3-0-0-0-9	Principles of retrosynthetic analysis: Linear and convergent synthesis, Synthesis under steric control, Regio and stereoselective synthesis, Basic synthetic methods. Methodologies for the construction of membered rings, medium and large rings. Application in natural product synthesis. Methodologies for the construction of membered heterocyclic rings. Application In organic synthesis. **References/Textbooks**: 1. Corey and Cheng, The Logic of Chemical Synthesis, Wiley, 1989; 2. Nicolaou and Sorensen, Classics in Total Synthesis, 1996; 3. Nicolaou and Snyder, Classics in Total Synthesis II, 2003; 4 Carey and Sundberg, Advanced Organic Chemistry, Part I and II, 4th ed., 2000.
CHM609	PRINCIPLES OF ORGANIC CHEMISTRY	3-0-0-0-9	Stereochemistry, mechanisms of selected reactions, Reactive intermediates, oxidation, Reduction, C-C bond formations, synthesis of some useful natural products. Stereochemistry: Conformation of acyclic and cyclic molecules, Geometrical and Optical Isomerism. Dynamic stereochemistry: Conformation and reactivity. Reactions: Mechanistic and Stereochemical aspects of: Baeyer-

			Villiger, Claisen (including Johnson and Ireland modifications), Wittig rearrangements. Ene and metalloene reactions, Barton reaction. Reactive Intermediates: An overview and revision of the chemistry of carbenes, nitrenes, radicals, carbocations (including non-classical carbocation), carbanions (homoenolate anion) and benzynes with emphasis on stereochemical implications wherever applicable. Oxidation: Swern, Dess-Martin, Prevost, dimethyl dioxirane, transition metal catalyzed oxidations, oxidations at unfunctionalized carbons, asymmetric Sharpless epoxidation and dihydroxylation, Jacobsen's epoxidation: Mechanism, stereochemistry and applications in organic synthesis. Reduction: Reduction of carbonyl compounds and C-C multiple bonds: Using Al and B based reagents (e.g. DIBAL, Red-Al, NaBH4-CeCl3.7H2O etc.), low valent Ti species, microbial reductions (NADH models), Qxazaborolidine, BINAP, BINAL based reductions. C-C Bond Formation: [2+2], [3+2] and [4+2] cycloadditions, Enolate chemistry (including silicon chemistry). Synthetic Applications: Synthesis of some typical natural products. Photochemistry **References/Textbooks**: 1. March, J., Advanced Organic Chemistry, 4th ed, 1999. 2. Nasipuri, D., Stereochemistry of Organic Compounds, 2nd ed, 1995. 3. Carey and Sundberg, Advanced Organic Chemistry, Part I and II, 4th ed., 2000. 4. Clayden, Greeves, Warren, and Wothers, Organic Chemistry, 1st ed, 2001
CHM611	PHYSICAL ORGANIC CHEMISTRY	3-0-0-0-9	**Pericyclic Reactions:** Conservation of orbital symmetry, and Woodward and Hoffmann rules. Cycloadditions, Electrocyclizations, Sigmatropic rearrangements, and Chelotropic reactions. Orbital overlap effects in chemical processes. **Stereoelectronic Effects in Organic Chemistry:** Acetals, Esters, Amides and related functions. Reactions at sp3, sp2, and sp carbons. Examples in synthesis and biological processes. Felkin-Ahn model, Houk model, Cieplak model, EFOE model, and Cation-complexation model as applied to π-Facial selectivity. **Reactive Intermediates:** Carbonium ions, carbanions, and radicals (formation, rearrangement, and further reactions in reference to Baldwin' rules for ring-closure) Chemical Equilibria and Chemical Reactivity: Correlation of reactivity with structure, Hammett equation, substituent constants and reaction constants. **Chemical Kinetics and Isotope Effects:** Various types of catalysis and isotope effects. Importance in the elucidation of organic reaction mechanisms. **Electron-Transfer Reactions**: Theoretical basis, Examples of photo-induced and chemically-induced electron transfer reactions (PET and CET). **Organic Photochemistry**: Energy and electronic spin states, Spectroscopic transitions, photophysical processes,

			fluorescence and phosphorescence, energy transfer and electron transfer, and properties of excited states, Representative photochemical reactions of carbonyl compounds, olefins, and aromatic compounds. **Miscellaneous:** A(1,2) and A(1,3) strain, Captodative effect, Hammond's postulate, Curtin-Hammett principle, and thermodynamic and kinetic control of reactions. **References/Textbooks**: 1. Isaacs, N. S., Physical Organic Chemistry; 2. Lowry and Richardson, Mechanism and Theory in Organic Chemistry; 3. Deslongchamps, P., Stereoelectronic Effects in Organic Chemistry
CHM612	FRONTIERS IN ORGANIC CHEMISTRY	3-0-0-0-9	**Asymmetric Synthesis:** Including organo and metal-based catalysis Synthesis using Organometallic Chemistry: Transition and main group elements based reactions involving region, stereo, and enantioselective reactions and application in organic synthesis. Supramolecular Chemistry, Combinatorial Chemistry, etc. Green Chemistry, Glycobiology, Synthetic aspects using Domino reactions, Principles of atom economy with examples, Templated and solid supported Organic Synthesis. **Course Reference**: 1. M. B. Smith Organic Synthesis Wavefunction, Inc 2000; 2. HJ. Schmalz, T. Wirth Organic Synthesis Highlights, 2003; 3. J. Tsuji, Transition metal reagents and catalyst innovations in organic synthesis JohnWiley& Sons, Ltd, New York, 2000; 4. T. K. Lidhorst, Essentiall of carbohydrate chemistry and biochemistry, WileyVCH, 2006.
CHM614	ORGANIC PHOTOCHEMISTRY	3-0-0-0-9	**An overview of basic concepts of photochemistry** Energy transfer; theoretical aspects of organic photochemistry; reaction mechanisms; photoreduction and photosubstitution reactions; photocyclo additions; photoisomerizations; photo fragmentation and elimination reactions; photolytic deprotection and activation of functional groups. Singlet oxygen: generation and reactions; photoinduced electron transfer basic concepts, illustrative examples of application to organic synthesis; photochemistry in organized media. Nanosecond and picoseconds studies of organic photoreactions. **Course Reference**: 1. Modern Molecular Photochemistry by N. J. Turro; 2. Organic Photochemistry by J. M. Coxan and B. Halton Essentials of Molecular Photochemistry by A. Gilbert and J. Baggot; 3. Organic Photochemistry and Photobiology, CRC Handbook, Edited by W. M. Horspool and P.S. Song.
CHM616	CHEMISTRY OF ORGANOMETALLIC COMPOUNDS	3-0-0-0-9	Newer aspects of organometallics derived from different elements such as Pd, Cu, Ti, Rh, Ru, Mo, Ni, Fe, Sn, Si, B, Mg, Ce, etc, including chemo-, regio-, stereoselective reactions, asymmetric induction etc, and their application in organic synthesis will be discussed. **Introduction:** History of organometallic chemistry; Werner complexes; Coordination number and geometry; Crystal field theory and ligand field theory; Bonding and molecular orbitals. **Ligands:** Bonding Types, Charges, and Donor Electrons; Ligand: chelate effect and heptaciy; 18 electron rule: Usefulness and limitation; Lewis Base Ligands: Halide donors, Oxygen ligands, Sulphur ligands, Nitrogen ligands: R_3N,R_2N^-, RN^{2-};

			Tris(pyrazolyl) borate, A Few Biologically Important N-Ligands: imidazole, purine, porphyrine; Carbonyls Phosphines, singma bound carbon ligands: hydrides, alkyls, aryls, pi-bonded carbon ligands: alkene, alkyne, allyl, diene, arenes, arenes, metalacyles, Metallocene and sandwich complexes/ bonded carbon ligands: carbenes, carbines; Bimetallic complexes and Metal Clusters; Metal-metal bond in bimetallic complexes; Clusters; Isolobal analogy; Metal nanoparticles; Elementary organometallic reactions: Ligand substitutions; Oxidative addition; Reductive elimination; Intramolecular insertions/eliminations; Nucleophillic/ Electrophillic attacks on coordinated ligands. Homogeneous catalysis and Catalysts: Introduction; Alkene isomerization; Hydrogenation; Hydroformylation; Monsanto acetic acidprocess; Alkene polymerization; Cross coupling reactions; Metathesis; CH activation and functionalization; Oxidation of olefins; Metal Clusters and catalysis; Physical methods in Organometallic chemistry:1H NMR spectroscopy; 13C NMR spectroscopy; 31P NMR spectroscopy; Dynamic NMR, Massspectroscopy, Isotope effect. Bioinspired Organometallic chemistry: Introduction, Coenzyme B12, Nitrogen fixation; Nickel enzyme; **Course Reference**: 1. J. Tsuji, Transition metal reagents and catalyst innovations in organic synthesis JohnWiley & Sons, Ltd, New York, 2000; 2. M. B. Smith Organic Synthesis Wavefunction, Inc 2000; 3. HJ. Schmalz, T. Wirth Organic Synthesis Highlights, 2003; 4. K. C. Nicolaou, Classics in Total Synthesis Vols IIII, WileyVCH, 1996; 2003; 2011; 5. The Organometallic Chemistry of the Transition Metals by Robert Crabtree (3rd Edition, Wiley); 6. The Principles and Applications of Transition Metal Chemistry, by Collman, Hegedus, Norton and Finke (2nd eds, University Science Books); 7. Organometallics by Christoph Elschenbroich. (3rd Edition, Wiley).
CHM621	CHEMICAL BINDING	3-0-0-0-9	**Review of basic principles of quantum theory and atomic structure.** Introduction to chemical bonding and weak intermolecular forces. Electronic structure of many electron atoms and variation principle. Electronic structure of diatomic molecules. Born Oppenheimer approximation, H2+ ion, approximate molecular orbital (MO) theory of ground and excited states of H2+, homo and heteronuclear diatomic molecules, electronic term symbols, valence bond (VB) theory of diatomic molecules, comparison of VB and MO theories. Hartree-Fock theory of atoms and extension to molecules. Self Consistent Field (SCF) wavefunctions for diatomic molecules, configuration interaction (CI) wave functions. Electronic structures of polyatomic molecules. SCF-MO treatment of closed shell systems. Basis functions. SCF-MO treatment of simple molecules like H2O, NH3, C2H6, C2H4 etc. Population analysis, Potential energy surface and equilibrium geometry, molecular vibrational frequencies. Koopmans; and Brillouin's theorems. Brief introduction to electron correlation. MllerPlesset (MP) perturbation theory and CI calculations. Virial and Hellmann Feynman theorems. Hckel theory applied to conjugated molecules. Elements of Density Fuctional Theory

			(DFT), Semiempirical methods (extended Hckel and CNDO), Molecular mechanics, Topological characteristics of electron density. **Course Reference**: 1. I.N. Levine, Quantum Chemistry, Fifth edition, Pearson Education (2000); 2. F.L. Pilar, Elementary Quantum Chemistry, Second edition, McGrawHill (1990); 3. J.P. Lowe, Quantum Chemistry, Second edition, Academic Press (1993); 4. P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, Third edition, OxfordUniversityPress (1997); 5 A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover (1996).
CHM622	CHEMICAL KINETICS	3-0-0-0-9	**Phenomenological Kinetics:** Simple and complex systems including opposing, concurrent and consecutive reactions, Rate law and mechanism, relation with thermodynamics, Precision in rate measurement, data analysis, Special experimental methods including flash photolysis, shock tube, molecular beam and relaxation techniques. Oscillatory reactions. Theories of reaction rates: bimolecular reactions, rate coefficient, activation energy, potential energy surfaces, trajectory methods and transition state theory. Unimolecular intermolecular reactions, Applications: photochemistry, solution kinetics, homogeneous and heterogeneous catalysis and enzyme kinetics. **Course Reference**: 1. K. J. Laidler, Chemical Kinetics, 3rd Ed. Harper & Row, New York, 1987; 2. R. D. Levine and R. B. Bernstein, Molecular Reaction Dynamics and Chemical Reactivity, Oxford Univ. Press, Oxford, 1987; 3. J. I. Steinfeld, J. S. Francisco, W. L. Hase, Chemical Kinetics and Dynamics, 2nd ed. Prentice Hall, NJ 1999.
CHM626	SOLID STATE CHEMISTRY	3-0-0-0-9	**Chemical Crystallography**: Introduction, Space lattice, Crystal point groups, space group (working knowledge), Stereographic projections, Packing in solids, Crystal structures of representative systems, Silicates and Zeolites, Cements, Glasses, Quasicrystals, Nanostructures**. Bonding in solids and Crystal energetic:** Crystal classifications, Madelung constant and Lattice energy. Characterization techniques (working knowledge) for solids: Xray diffraction, Electron microscopy (SEM, TEM, AFM), Thermal techniques (TG, DTA, DSC), Spectroscopic techniques (Mossbauer, IR, UVVIS) and Physical propertymeasurement techniques (Magnetic momentsVSM /SQUID, Electrical resistivity V Two / Fourprobe methods and thermal conductivity, Optical band gap, XPES, XAS). **Electronic properties and Band theory of solids:** Free electron model, Metals, semiconductors and insulators, doped semiconductors Solid state ionics. Defects, Nonstoichiometry and Diffusion: Point defects, Dislocations, Extended defects, Clusters and aggregates, Color centres, Nonstoichiometry of compounds, Diffusion mechanisms, Ficks law, Kirkenall effect. **Phase transitions:** Critical phenomena, variety of phase transitions (Ordered disorder, Martensiteaustenite, Spinoidal decompositions etc), Liquid crystals, Structure property relations (magnetic,electrical, superconductivity, optical and thermal). Preparative techniques: Powder synthesis by conventional and modern chemical methods, Reactivity of solids, Decomposition mechanisms, Powder processing (sintering and diffusion

			processes), Tailoring of solids, Special methods for single crystal growth and thin films depositions. **Course Reference**: 1. A R. West, Solid state chemistry and its applications, John Wiley & Sons, 1989; 2. L Smart and E. Moore, Solid state chemistry, Chapman and Hall , 1992; 3. A K. Cheetham and P. Day, Solid state chemistry compounds, Clarendon Press,Oxford 1992; 4. C N. R. Rao and J. Gopalkrishanan, New directions in solid state chemistry,Cambridge Univ. Press 1997; 5. R E. Newnham, Structure property relations, SpringerVerlag, 1975; 6. P. A. Cox, Electronic structure and chemistry of solids, Oxford Univ. Press 1987.
CHM627	METHODS OF ELECTRONIC STRUCTURE CALCULATION	3-0-0-0-9	**Hartree-Fock (HF) Theory:** Born-Oppenheimer approximation, Postulate of antisymmetry, Slater determinants, Slater-Condon rules for matrix elements, Hartree-Fock equations, Koopmans' and Brillouin's theorem, Roothaan equations, basis sets, computational aspects: direct and semi-direct methods, Molecular properties, UHF method, Pople-Nesbet equations, limitations of HF theory, MP2 method as a perturbation correction to the HF theory. **Configuration Interaction (CI) Method:** Multi-configuration wave function, full CI matrix, singly and doubly excited CI, illustrations of CI calculations on small atoms/molecules, Natural orbitals, Truncated CI and size-consistency, introduction to coupled cluster theory. **Density Functional Theory (DFT):** Introduction to electron density and functionals, Hohenberg Kohn Theorems, N- and V-representibility, Levy Functional, Kohn-Sham equations, Electronegativity and hardness in DFT. Discussion of some exchange-correlation functionals, applications. Demonstrations, Hands on Sessions and short projects with standard Electronic Structure Programs. **References/Textbooks**: 1. Modern Quantum Chemistry, A. Szabo and N. L. Ostlund, Dover, New York (1996). 2. Density Functional Theory of Atoms and Molecules, R. G. Parr and W. Yang, Oxford University Press, Oxford (1986). 3. Exploring Chemistry with Electronic Structure Methods, J. B. Foresman and A. Frisch, Gaussian, Inc. Pittsburgh (1996). 4. A Chemist's Guide to Density Functional Theory, W. Koch and M. C. Holthausen, Wiley-VCH, Weinheim (2001). 5. Molecular Electronic Structure Theory, T. Helgakar, J. Olsen and P. Jorgensen, Wiley, New York (2013).
CHM629	PRINCIPLES OF PHYSICAL CHEMISTRY	3-0-0-0-9	Atomic and Molecular structure, Molecular Spectroscopy, Concepts of Statistical Thermodynamics, Electrochemistry, Chemical Kinetics, Photochemistry. **Atomic and Molecular Structure:** Review of quantum mechanics, approximate methods in quantum chemistry and many electron atoms. Molecular orbital description, application of the variation theorem to calculate Mos, Valence bond description , sigma orbitals and pi orbitals, ionic bonds, dipole moment, resonance, delocalization, aromatic molecules and solids.

			Molecular spectroscopy: Rotational and vibrational spectra, P, Q and R branches, Raman spectra. Electronic spectra,fluorescence and phosphorescence, principle of laser action. **Concepts of Statistical Thermodynamics:** Molecular energy levels and Boltzmann distribution, partition function and calculation of thermodynamic quantities. Einstein and Debye models for solids, chemical equilibrium constant. Electrochemistry: Ionic equilibrium, activity and activity coefficients, Debye-Huckel theory, EMF of chemical cells, Nernst equation, concentration cells, applications, potentiometric titrations, solubility product, pH and pK. **Chemical Kinetics:** Rates of chemical reactions, steady state approximation, temperature dependence, activation energy, molecular reaction dynamics, collision and activated complex theory, theories of unimolecular reactions. Techniques of fast reactions and their applications. **Photochemistry:** Laws of photochemistry, quantum yield, radiative and non-radiative processes, photosensitized reactions, some applications of photochemical reactions. **References/ TextBooks:** 1. D. A. McQuarrie and J. D. Simon, Physical Chemistry A Molecular Approach, Viva, New Delhi (1998). 2. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd ed. Oxford Univ. Press, Oxford (2000). 3. R. J. Silbey, R. A. Alberty and M. G. Bawendi, Physical Chemistry, 4th Edition, Wiely (2004). 4. P. W. Atkins and Julio de Paula, Physical Chemistry, 8th Edition, Oxford University Press, (2008). 5. I. N. Levine, Physical Chemistry, 5th Edition, Tata McGraw Hill (2007)
CHM631	APPLICATIONS OF MODERN INSTRUMENTAL METHODS	3-0-0-0-9	**Infrared Spectroscopy:** Introduction. Identification of functional groups, hydrogen bonding etc., metal ligand vibrations. **Nuclear Magnetic Resonance Spectroscopy:** Introduction. Application of ^{1}H and ^{13}C NMR spectroscopy including COSY, NOESY, NOE techniques in the structural determination of complex organic systems. Application in conformational analysis. Multinuclear NMR of various inorganic and organometallic compounds. **Ultraviolet Spectroscopy**: Introduction. Studies of conjugated and extended conjugated systems etc. Woodward rules. Electronic spectra of transition metal complexes. Mass Spectrometry: Basic concepts. Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules. Isotope effects etc. Structural elucidation by joint application of UV, IR, NMR and mass spectrometry. **Electron Spin Resonance Spectroscopy:** A brief review of theory. Analysis of ESR spectra of systems in liquid phase, radicals containing single set, multiple sets of protons, triplet ground states. Transitionmetal ions. Rare earth ions, ion in solid state. Double resonance stechniques: ENDOR in liquid solution, ENDOR in powers and non-oriented solids. Biological applications: Substrate free radical, flavins and metal free flavin

			proteins, photosynthesis, Heme proteins, Iron-sulfur proteins, spin labels. **Mossbauer Spectroscopy:** Basic physical concepts, spectral line shape, isomer shift, quadrupole splitting, magnetic hyperfine interaction. Interpretation of Mossbauer parameters of ^{57}Fe, ^{99}Ru, ^{101}Ru, ^{195}Pt, ^{193}Ir and ^{110}Sn. Some special applications: Solid state reactions, thermal decomposition, ligand exchange, electron transfer, isomerism, surface studies and biological applications. **X-Ray Photo-Electron Spectroscopy:** Physical concepts. Application to determine atomic charges, oxidation numbers, catalyst surface structures and in some cases molecular structures. **CD spectroscopy:** CD of polypeptides and nucleic acids, Induced CD, magnetic circular dichroism. Fluorescence spectroscopy: Fluorescence energy transfer and its applications to measurement of distances in molecules. **Magnetism:** Introduction to Magnetism. Origin of diamagnetism. **Paramagnetism:** Van Vleck formula and its approximated forms, Curie law. Magnetic susceptibility, orbital quenching and spin-only moment. Magnetic exchange interactions in coordination compounds: ferrimagnetism and antiferromagnetism. Bulk magnetic properties and ferromagnetism. Molecule-based magnetic materials: organic magnets and single molecule magnets. **Electrochemistry:** Heterogeneous electron transfer and concept of capacitive and faradic current. Cyclic voltammogram. Instrumentation: three-electrode potentiometer and electrodes. Measurements and analyses of the voltammograms. Differential pulse voltammetry and coulometry. Application of cyclic voltammetry in inorganic and organic chemistry. **References/ TextBooks:** 1. Physical Methods in Chemistry, RS Drago, 2nd edn., Saunders, 1992. 2. Carbon-13 Nuclear Magnetic Resonance Spectroscopy, G. C. Levy, R. L. Lichter and G. L. Nelson, Wiley, 1980. 3. NMR Spectroscopy - An Introduction, H. Gunther, John Wiley, 1980. 4. Basic One- and Two-Dimensional NMR Spectroscopy, H. Friebolin, VCH, 1991. 5. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, 4th ed., 1988. 6. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley & Sons, New York, 5th Ed. 1991. 7. Interpretation of Mass Spectra, F. W. McLafferty, 1980. 8. Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Weil, John A, J. R. Bolton, and Wertz, J. E, Wiley-Interscience, New York, (1994). 9. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin, & S. Cradock, 2nd Ed. 1991, CRC Press, Boca Raton, Florida, 10. Circular Dichroism: Principles and Applications, Nakanishi, K., Berova, N., Woody, R. W., Eds.; VCH Publishers, Inc.: New York, 1994. 11. Principles of Fluorescence Spectroscopy, J. Lackowicz, Plenum Press, (New York, 1983). 12. Electrochemical Methods - Fundamentals and Applications, A. J. Baird and L. R. Faulkner, Wiley, 1980.

CHM632	ENZYME REACTIONS MECHANISM AND ENZYME KINETICS	3-0-0-0-9	Enzyme kinetics of single and multiple substrate systems including Enzyme assays and inhibition. Cooperativity and multienzyme systems. Enzyme structure and identification of active site residues labelin, chemical modification and mutagenesis. Enzyme Mechanisms. Methods of study and mechanisms of some enzymes like Serine proteases, polymerases, ribonucleases, lysozyme and ribonucleotide reductases (radical enzyme). Mechanism based enzyme inhibition and drugs fluorouracil for thymidylate synthase. **Course Reference**: 1. Allan Ferhst, Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysisand Protein Folding; 2. N. C. Price and E. Stevens, Fundamentals of Enzymology: The Cell and Molecular Biology of Catalytic Proteins; 3. I. H. Segel, Biochemical calculations, How to Solve Mathematical Problems in General Biochemistry, 2nd Edition.
CHM636	PHYSICAL PHOTOCHEMISTRY	3-0-0-0-9	1**. Theory of electronic absorption spectra**, Beers law, Absorption crosssection,Solvatochromism; 2. Radiative and nonradiative transitions, Vibrational relaxation, Internal conversion, Intersystem crossing; 3. Fluorescence, Phosphorescence, Various photophysical processes, Solvent effect onemission, Lippert equation, Dynamic stokes shift, Dynamic and static quenching, SternVolmer equation, Forster resonance energy transfer and theory, Fluorescence anisotropy and Perrin equation, Excited state proton/electron transfer, Excimer andexciplex; 4. Laser fundamentals, Stimulated emission, Population inversion, Light amplification, Pulsed laser: cavity dumping, Qswithching, modelocking; 5. Spectroscopic techniques, Spectrophotometer, Spectrofluorimeter, Time correlated single photon counting, Transient absorption, Streak camera, Fluorescence upconversion; 6. Single molecule spectroscopy, Fluorescence correlation spectroscopy, Protein fluorescence. **Course Reference**: 1. Nicholas J. Turro, Modern Molecular Photochemistry; 2. K. K. RohatgiMukherjee, Fundamentals of Photochemistry; 3. J. R. Lakowicz, Principles of Fluorescence Spectroscopy; 4. W. T. Silvast, Laser Fundamentals.
CHM637	MOLECULAR SPECTROSCOPY	3-0-0-0-9	**1. Group theory:** Review of point groups, permutation inversion and molecular symmetry groups; 2. Interaction of radiation and matter: Qualitative aspects, Einstein A, B coefficients, absorption emission and lineshapes; 3. Rotational Spectroscopy Rigid body, selection rules, vibrational angular momentum, tops; 4. Vibrational Spectroscopy: Normal modes, selection rules, Fermi and Coriolis perturbations, polyatomic molecules; 5. Electronic Spectroscopy: Introduction, symmetry aspects, vibronic effects; 6. Advanced topics: Coupling of rotational and vibrational motions, nonrigid systems, high resolution and highly excited states, Wilson Howard-Watson Hamiltonian, time dependent viewpoint. **Course Reference**: 1. Bernath, Spectra of Atoms and Molecules, 1995; 2. Bunker & Jensen, Molecular Symmetry & Spectroscopy, 1998; 3. Papousek & Aliev, Molecular Vibrational Rotational Spectra, 1982; 4. Hollas, Modern Spectroscopy, 2004; 5. McHale, Molecular Spectroscopy, 1998.

CHM645	ORBITAL INTERACTIONS IN CHEMISTRY	3-0-0-0-9	**Molecular Symmetry in Chemistry Symmetry:** Introduction, Symmetry operations & elements, Groups, Representations and character tables, Reduction of reducible representations, Group-Subgroup relationships: Descent and ascent in symmetry. Degeneracies, Direct products. Symmetry properties of Orbitals, Symmetry adapted wavefunctions. Molecular orbital construction: H_2, linear and angular H_3, Linear, rectangular, square planar and tetrahedral H_4, pentagonal H_5 and hexagonal H_6. Diatomic molecules A-A and A-B. Electronegativity perturbation. Ligands with -systems. AH_2, AH_3, AH_4, AH_5 and AH_6. Walsh diagram. Symmetry aspects of the d-orbital splitting by ligands. Symmetry adapted orbitals on the ligands: sigma-interactions. MH_6 (Oh), MH_5 (D_{3h} and C_{4v}), MH_4 (D_{4h} and C_{4v}), MH_3 (D_{3h} and C_{2v}). Correlation. Inclusion of p-orbitals: ML_6 P-donor and P-acceptor ligands: MCl_6 and $M(CO)_6$ Applications: Isolobal analogy, The Woodward-Hoffmann Rules– pericyclic reactions, Zeise's salt, Metal carbonyls, Kubas complex W(CO)3(PCy3)2(H2), Agostic complex, Oxidative addition and reductive elimination, Migratory insertion and b-hydride elimination, Metal-Carbene complexes (Fischer, Schrock and N-heterocyclic carbene), Bimetallic complexes: from Single to Quadruple/Quintuple bond, Magnetic interactions. **References/ Textbooks:** 1. 'Orbital Interactions in Chemistry' - Wiley-Interscience, 1st and 2nd Edition - Thomas A. Albright, 2. Jeremy K. Burdett and Myung-Hwan Whangbo. 3. 'Molecular Orbitals of Transition Metal Complexes' Oxford University Press - Yves Jean. 4. 'Molecular Symmetry and Group Theory' Wiley and Sons - Robert L. Carter. 5. Chemical Applications of Group Theory, 3rd Edition – F. A. Cotton
CHM646	BIO-INORGANIC CHEMISTRY I	3-0-0-0-9	1. **Mineral Origin of life**. Archaeal, Eucarial and Bacterial domain. (3 Lectures); 2. Transition metal ions in biology. Metalobiomolecules. Electron carriers, oxygencarriers, enzymes. Biogeoinorganic chemistry, environment. (10 Lectures); 3. Specific examples: Hemoglobin, Myoglobin, Hemocyanin, Hemrythrincytochromes, FeS proteins, Cytochrome P450, Nitrophorin, NOsynthase, peroxidase, catalase, Ferritin, cytochromeC oxidase, cerulplasmin, bluecopper proteins, di and tricopper proteins. Other enzymes like, hydrogenase, methane monooxygenase, dioxygenases, dehydratase, nitrogenase, molybdenum containing oxidase and reductase class of enzymes like sulfite oxidase, xanthine oxidase, nitrate reductase, DMSO reductase, tungsten containing formate dehydrogenase and tungsten bearing hyperthermophilic and thermophilic enzymes. Zn enzymes like carbonicanhydrase, carboxypeptidase, DNA and RNA polymerases, Nickel containingF430, role of manganese in water splitting. (15 Lectures)4. Active site analogue reaction models and structural models of theseenzymes. (5 Lectures); 5. Environmental chemistry, auto exhaust, arsenic and other heavymetal pollutions. (2 Lectures); 6. Forensic chemistry;

			inorganic chemistry in medicine, platinum complexes, MoScomplexes as anticancer drugs. **Course Reference**: 1. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books, Mill Valley, 1994; 2. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W. Kaim and B. Schwederski, John Wiley & Sons Inc., 1994.
CHM647	MACROCYCLES, RINGS AND POLYMERS	3-0-0-0-9	Inorganic Heterocyclic Rings: P-N rings: Cyclophosphazenes and Cyclophosphazanes. Synthesis, structure and reactivity. Bonding models. P-N-X rings: carbophosphazenes, thiophosphazenes, metallaphosphazenes. Si-O rings: Cyclosiloxanes. Sn-O rings: Stannoxanes B-containing rings: Boranes, carboranes, metallacarboranes, Borazine. Al-containing Rings: Al-N rings and cages, Al-C rings and cages, Alumoxanes. Inorganic Homocyclic Rings Inorganic homocyclic rings and cages containing silicon, germanium, boron, aluminum and gallium. Inorganic Macrocycles: Metalla porphyrins. Inorganic polymers: A brief review of organic polymers-methods of synthesis, polymer characteristics-molecular weights, glass-transition temperatures, stress-strain characteristics etc.: Polyphosphazenes, polysiloxanes, polysilanes, organometallic polymers. Synthetic methods, structure-property relationships, applications. **Course Reference**: Most of the material for this course will be accessed from primary literature viz., Journal articles. Some text books that will be followed are as follows: Inorganic and Organometallic Polymers. Chandrasekhar, V. Springer-Verlag, Heidelberg, 2005. Contemporary Polymer Chemistry. 3rd Edn. Allcock H.R.; , Lampe, F.W.; Mark, J. Prentice Hall, N, 2004. Inorganic Polymers. Mark, J.E.; West, R.; Allcock, H.R.; Prentice-Hall, NY, 1992. Synthetic Metal Containing Polymers. Manners, I. Wiley-VCH, Weinheim, 2004.
CHM648	THE CHEMISTRY OF METAL-CARBON BOND: STRUCTURE REACTIVITY & APPLICATIONS	3-0-0-0-9	Introduction to Organometallics: Bonding, Types of Ligands, and some basics concepts like isoelectronic and isolobal analogy Characterization techniques of Organometallic compounds (NMR and IR spectroscopy andMass spectrometry) Representative chemistry of main group Organometallics Organometallic chemistry of lithium and magnesium: synthesis, structures, fluxionality and reactivity Chemistry of Aluminum: Aluminum alkyls. Use of aluminum alkyls in polymerization of olefins. Organometallic chemistry of transition metals bonded ligands: Metal alkyls, aryls and hydrides. Stability, preparation and reactivity. Metal carbonyls / Metal phosphines / metal nitrosyls / metal isocyanide: structures,reactivity and bonding. Metal carbenes, metalcarbynes, Fischer carbenes, Schrock, carbenes, complexes with N-heterocycliccarbenes (NHCs), bonded ligand: Metal olefins, alkyls metal alkynes, dienes, Cp and Cp*, structure, bonding and reactivity. Reactions in Organometallic Chemistry: Oxidative addition, reductive elimination, insertion,elimination, and migration Applications of organometallics in organic synthesis CC bond coupling

			reactions (Heck, sangoshira, Suzuki) Reduction using transition metal hydrides, asymmetric hydrogenation.Olefin metathesis Most of the material for this course will be accessed from primary literature viz., Journal articles. Some text books that will be followed are as follows- **Course Reference**: 1. Elschenbroich, C.; Salzer, A.; Organometallics: A Concise Introduction 3rd Edn. John Wileyand sons 2005; 2 B. D. Gupta and A. J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses andApplications, First Edition, Universities Press, 2010; 3. Douglas, B.; McDaniel, D.; and Alexander, J. Concepts and Models of Inorganic Chemsitry 3rdEdn. John Wiley, New York. 1993; 4. Rober t H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley and Sons, 4th edn. John Wiley and sons 2005.
CHM649	PRINCIPALES OF INORGANIC CHEMISTRY	3-0-0-0-9	**Principles of modern inorganic chemistry** discussion of the chemistry of nontransition elements, Coordination Chemistry, organometallic chemistry, Inorganic chemistry of biological systems. General: Localized and delocalized bonding models. A review of various bonding models in inorganic chemistry with appropriate examples. Symmetry, Point Groups and applications of symmetry. Introduction to symmetry elements and operations, point groups, character tables and uses in applications such as bonding. Chemical forces including weak interactions and the basic aspects of crystal engineering. Structural characterization tools for inorganic compounds. Main-group:Inorganic rings and cages: Boranes, P-N , Si-O, Al-O systems. Low-valent compounds containing main-group elements. Multiple-bonding in compounds containing main group elements. Transition Metals: Transition metal chemistry-A review of basic theories of bonding in coordination complexes. Term symbols and electronic spectra of transition metal compounds. Magnetism of coordination complexes. Single molecule magnets. Supramolecular Chemistry. Organometallic compounds- various types of organometallic compounds including metal carbenes and their reactivity. **Course Reference:** 1. Inorganic Chemistry-Principles of Structure and Reactivity. 4th Edn. Huheey J. E.; Keiter, E. A.; and Keiter, R. L. Harper-Collins, NY, 1993. 2. Concepts and Models of Inorganic Chemistry. 3rd Edn. Douglas, B.; McDaniel, D.; and Alexander, J. John Wiley, New York. 1993. 3. The Organometallic Chemistry of the Transition Metals. 4th Edn. Crabtree, R. H. Wiley-Interscience, 2005.
CHM650	STATISTICAL MECHANICS & ITS APPLICATION TO CHEMISTRY	3-0-0-0-9	Course description: Thermodynamics, Statistical Mechanics of noninteracting systems, interacting systems, and nonequilibrium systems Course Details 1. Equilibrium Thermodynamics: Thermodynamic Equilibrium state, laws ofthermodynamics, axiomatic formulation of thermodynamics, thermodynamic potentials,stability criteria, phase equilibria (4 lectures); 2.

			Ensembles in Statistical Mechanics: Ensemble postulate and ergodicity, microcanonical,canonical and grand canonical ensembles, quantum and classical partition functions, phase space, fluctuations (6 lectures); 3. Noninteracting systems: Factorization of the partition function, quantum correlations,collective modes, occupation numbers, collections of fermions, bosons,photons, classical deal gas of spinless particles, molecular partition functions, idealparamagnets. (6 lectures); 4. Interacting Systems: Classical Liquids Interparticle potentials, Configurational Partition functions, distributions, pair correlation function, neutron scatteringexperiments, Virial equation, Meyer cluster diagrams (6 lectures); 5. Interacting Systems, Computer Simulations Ensemble averages, ergodicity, random numbers, Monte Carlo methods, Molecular Dynamics, constant temperatureMD. (5 lectures); 6. Interacting Systems 3 Phase Transitions in Lattice models Lattice gas Ising Model, order parameter, Mean Field theory, Renormalization group theory (6 lectures); 7. Nonequilibrium Statistical Mechanics (6 lectures) Linear Response theory, fluctuation dissipation theorem, time correlation functions, applications to transport phenomena. **Course Reference**: 1. D.A. McQuarrie, Statistical Mechanics2. David Chandler, Introduction to Modern Statistical Mechanics3. K.L. Huang, Statistical Mechanics4. B. Widom, Statistical Mechanics: A concise introduction for chemists
CHM651	CRYSTAL AND MOLECULAR STRUCTURE DETERMINATION	3-0-0-0-9	Generation of Xrays, monochromators, safety (1 Lecture) Concept of direct and reciprocal lattices, Braggs law of Xray diffraction in direct andreciprocal lattice, crystal systems, point groups, Bravais lattices(5 Lectures)Rotational axes of symmetry, screw axes, glide planes, equivalent points, systematicabsences, space groups (8 Lectures) Argand diagram, intensity data collection and quantitative aspects of Xray diffraction,temperature factor and scaling of data (10 Lectures)The phase problem, direct method of solving structures (8 Lectures) Patterson method, isomorphous replacement method(8 Lectures) Structure refinement and their critical evaluation (5 Lectures). **Course Reference**: 1. Xray Structure Determination A Practical Guide by G. H. Stout and H. L. Jensen, MacMillan, N.Y. 1968; 2. Contemporary Crystallography, M. J. Buerger, McGrawHill, N.Y. 1970; 3. Crystal Structure Analysis A Primer J. P. Glusker and K. N. Trueblood, OUP, N.Y. 1985; 4. Structure Determination by Xary Crystallography, M. Ladd and R. Palmer, KluwerAcademic/Plenum, N.Y. 2003
CHM654	SUPRAMOLECULAR CHEMISTRY	3-0-0-0-9	Introduction to the meaning of supramolecular chemistry, phenomenon of molecular recognitionand their quantification (2 Lectures); Building blocks of supramolecular chemistry acyclic receptors for neutral and chargedguests, macrocycles and crown ethers, macrobicycles and cryptands, macropolycycles, cucurbiturils and cyclodextrins (12 Lectures); Sensors and information processing, electrooptic phenomena, molecular machines (12Lectures); Amphiphilic molecules and their aggregation, Langmuir Blodgettry, molecular recognition atthe airwater interface. (3 Lectures); Discrete and polymeric

			metalorganic hybrid materials guest inclusion, catalysis and otherapplications. (12 Lectures); Future scopes (1 Lecture). **Course Reference**: 1. Supramolecular Chemistry: Concepts and Perspectives, J.M. Lehn, VCH, Weinheim, 1995; 2. Principles and Methods in Supramolecular Chemistry, H. J. Schneider and A. Yatsimirsky, Wiley, New York, 2000; 3. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley & Sons, Chichester,2009.
CHM656	ORGANIC STRUCTURE DETERMINATION BY SPECTROSCOPIC TECHNIQUES	3-0-0-0-9	**UV – Visible absorption spectroscopy:** General principles; instrumentation; chromophores; degree of unsaturation and conjugation; dienes, aromatic compounds, conjugated carbonyl compounds; color in compounds; quantitative aspects and what to look for in a UV – vis absorption spectrum. (3 lectures) **Infrared (IR) Spectroscopy:** Basic principles; instrumentation (dispersive IR and FT IR); absorption range and the nature of IR absorption; experimental aspects of infrared spectroscopy; general features of IR spectra; important IR chromophores. (3 lectures) **Mass Spectrometry:** Ionization processes; electron impact ionization (EI); chemical ionization (CI); fast atom bombardment (FAB); matrix assisted laser desorption ionization (MALDI); electrospray ionization (ESI). **Mass analyzers:** quadrupole, ion trap, time of flight, orbitrap, magnetic and electromagnetic, etc. Basic principles; practical considerations and instrumentations. Formation and fragmentation of ions and basic rules: electron ionization, photoionization under vaccum, proton transfer, adduct formation, formation of aggregates or clusters and reactions at the interface between source and analyser. (6 lectures) **Mass Spectrometry/Chromatography Coupling:** Elution Chromatography Coupling Techniques; Gas Chromatography/ mass spectrometry; Liquid Chromatography/ mass spectrometry. (2 lectures) **NMR Spectroscopy:** Basic principles of NMR; properties of magnetic nuclei – energy levels, transitions, relaxations, etc. spectral acquisition – old and modern ways; line width; line shape and relaxation time; symmetry considerations – homotopic, enantiotopic and diastereotopic. **Proton NMR Spectroscopy:** shielding, deshielding, chemical shift, spin – spin coupling, coupling constant, correlation of the spectral information with structure, etc. Second – order effects and different spin systems; dynamic processes by NMR. Spin Decoupling or double resonance – Homonuclear and Heteronuclear decoupling, NOE and difference NOE. C^{13} NMR: Chemical shifts, APT, DEPT, etc.; 2D techniques – HMQC, HSQC, etc. 2D NMR: COSY, NOSY, etc. (12 lectures) **HPLC – NMR Coupling:** General principle and examples. (2 lectures) **Fluorescence and Circular Dichroism** (2 lectures) **Determination of structures from comprehensive spectroscopic data:** Problem solving and practice. (10 lectures) **Course Reference**: 1. Organic structure from spectra by Field, Sternhell, Kalman, Wiley, 4th Edition 2008. 2. Mass spectrometry: Principles and applications, Edmond de Hoffmann and Vincent Stroobant, Wiley, 3rd Edition, 2007. 3. Introduction to spectroscopy, Donald L. Pavia, Gary M. Lampman and George S. Kirz,

			Brooks/Cole, 2001. 4. NMR – From spectra to structures, Terence N. Mitchell and Burkhard Costisella, Springer, 2007. 5. Mass spectral interpretation, Terrence A. Lee, John Wiley, 1998. 6. A complete introduction to modern NMR Spectroscopy, Roger S. Macomber, John Wiley, 1998. 7. Solving problems with NMR Spectroscopy, Atta – ur – Rahman abd Muhammad Iqbal Choudhary, Academic Press, 1996. 8. Nuclear Magnetic Resonance Spectroscopy: An introduction to principles and experimental methods, Joseph B. Lambert and Eugene P. Mazzola, Prentice Hall, 2003. 9. Structure Elucidation by NMR in Organic Chemistry, Eberhard Breitmaier, John Wiley, 2002.
CHM661	Computational & Electronic Structure of Solids	3-0-0-0-9	This course aims to provide broad understanding of a spectrum of state-of-the-art computational electronic structure methods and tools used in materials science and engineering. Lectures, case studies, demonstrations and hands-on exercises are planned, to provide theoretical and practical knowledge required comprehending the process-structure-property relationships and in aiding the discovery and design of new materials. **Introduction to the course:** The gist of relating electronic structure of materials to cohesion, electrical, optoelectrical, mechanical and other various physicochemical properties **The Basic Approach:** Quantum mechanical description of atomic states, molecules and extended solids – the metals and semiconductors **Unified Electronic Structure Theory for Periodic Systems:** k-mesh, Brillouin zone sampling, pseudopotentials, planewave basis set and self-consistent electronic minimizations **Total Energy and Beyond:** Cohesion, modulus of elasticity, States in k-space, phonons, and phase transitions **Codes and Testing:** Linux HPC environment, scripting -coding, graphing, error estimates – uncertainty quantification **Hands-on Numerical Experiments:** Structure description, modeling and simulations of materials – analysis of electronic structure, estimation of forces and force constants, diffusion and mechanical properties **Short Summary of the course**: Chemistry and Physics of Materials; theoretical and computational electronic structure theory; total energy calculations of periodic solid state materials; plane waves and pseudopotential model; Kohn-Sham first principles schemes; tetrahedral solids; zone integrations; band dispersion spectra; lattice vibrations; bulk modulus and elastic constants; numerical high performance computing simulations. **Recommended books/ References:** 1. Solid State Theory and Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond, Walter. A. Harrison 2. Solids and Surfaces: A Chemist's View of Bonding in Extended Structures, Roald Hoffmann 3. Atomic and Electronic Structure of Solids, Efthimios

			Kaxiras 4. Solid State Physics, Neil W. Ashcroft, N. David Mermin and Quantum Theory of Solids, Charles Kittel 5. Reviews and discussions on subject matter will be suggested.
CHM662	CHEMISTRY OF NATURAL PRODUCTS	3-0-0-0-9	**Biosynthetic aspects and Synthesis of selected natural products of biological and structural importance:** Discussions on synthetic methods, strategies towards these natural product smostly in chiral forms will be discussed in detail. The natural products include carbacycles and heterocyclic moieties containing structures ranging from memebered to macrocyles, and complex natural products such as Taxol, rapamycin, lejimailde B etc. **Course Reference**: 1.K. C. Nicolaou, Classics in Total Synthesis Vols IIII, WileyVCH, 1996; 2003; 2011; 2.T. Hudlicky and J. W. Reed, The way of synthesis, WileyVCH, 2007; 3. E. J. Corey and XM. Cheng, The logic of chemical synthesis, JohnWiley & Sons, New York1989; 4. D.H. R. Barton, K. Nakanishi, O. MethCohn, Comprehensive natural products chemistryVols 19, Elsevier, 1999.
CHM663	ELECTRON, PROTON AND HYDRIDES	3-0-0-0-9	Short Summary: Chemical and Electrochemical Electron transfer; Chemistry of reducing and oxidizing agents; basic electrochemistry and methods; Proton management in catalysis; Metal hydrides; Organic hydrides; Covalent hydrides, Prohydrides, Ammonia-Borane, Masked hydrides; PCET; Electron, proton and hydride in small molecule activation; Electrocatalysis; Hydrogen energy. Electrons: Electron transfer – Chemical and Electrochemical; Chemistry of reducing and oxidizing agents; analytical methods in working with electrons – basic electrochemistry and methods; Protons: Proton management; keto-enol, lactam-lactim, amide-imide, amine-imine tautomerism in catalysis; special acids in studying the mechanism, analytical methods Hydrides: Metal hydrides: Synthesis, stability, thermodynamics, how hydridic is the hydride - hydridicity, analytical methods in working with hydride Organic hydrides and their stoichiometric and catalytic reactions; regeneration,Covalent hydrides, Prohydrides, Ammonia-Borane, Masked hydrides, Hydrides in biology PCET, Electron, proton and hydride in small molecule activation, Electrocatalysis - homogeneous and heterogeneous; aqueous and non-aqueous; advantages and challenges, Hydrogen - advantages and challenges. **Recommended books:** Lecture notes and study materials will be provided by the instructor.
CHM664	MODERN PHYSICAL METHODS IN CHEMISTRY	3-0-0-0-9	**Symmetry and Group Theory:** Group multiplication table, elements of a symmetry group,symmetry group classification, characters, group representation, The Great Orthogonality theorem, basis of representation, wave functions as bases of IR representations, symmetry adapted linear combinations, direct products, spectral transitions; 2. Interaction of light with matter,

			Einsteins coefficients, relationship of Einsteins coefficients with transition moments (no derivation) and transition probabilities, oscillator strength. BeerLambert law, relationship between Einsteins coefficients and total absorbance. Born Oppenheimer approximation, energy levels, potential energy curves, MO and term symbols, Franck Condon principle, symmetry and selection rules, spin and parity forbidden transitions, vibronic interaction; 3. Simple harmonic motion, anharmonicity, introduction of different coordinates (generalised, mass weighted generalized, internal and normal coordinates). Force constants, selection rules, (F and G matrix if time permits). Applications: Organic molecules, functional group versus frequency approach, Fermi resonance, frequency shifts because of substitutions, isotope effect., theory and application of Raman Spectroscopy; 4. Other spectroscopic methods like Mass Spectrometry, Magnetic Resonance, Photoelectron Spectroscopy. **Course Reference**: 1. Chemical Applications of Group Theory F.A. Cotton; 2. Theory and applications of UV spectroscopy. H.H. Jaffe and M. Orchin; 3. Quantum mechanics, CohenTannoudj, Diu and Lalo (2005); 4. Molecular Spectroscopy I. N. Levine; 5. High Resolution NMR, theory and application, E.D. Becker; 6. Modern Spectroscopy J. M. Hollas;
CHM667	QUANTUM DYNAMICS IN CHEMISTRY	3-0-0-0-9	Recapitulations of basic concepts of Quantum Mechanics. Approximation methods: Time-dependent Perturbation Theory and Dirac-Frenkel variational method with applications in reaction dynamics. Statistical perspectives of quantum dynamics for composite quantum systems. Density matrix theories for open quantum systems. The path integral approach and its applications in chemistry. Introduction to relativistic quantum mechanics. Trajectory picture of quantum dynamics. Applications: Chemical Dynamics theory. Radiation-matter interaction. Matters under strong external fields: Attosecond spectroscopy. **Course Reference**: Quantum Mechanics, Albert Messiah Modern Quantum Mechanics, J. J. Sakurai Quantum Dynamics, E. Bittner Quantum Mechanics, E. Merzbacher Quantum Mechanics and path integrals, R. P. Feynman and A. R. Hibbs
CHM668	ADVANCED MAIN GROUP CHEMISTRY	3-0-0-0-9	**A. Topics for SelfStudy** 1. VSEPR Theory and prediction of molecular geometry 2. Symmetry. Symmetry elements and symmetry operations. Point groups. Introduction to character tables. Uses of character tables. **B. Chemistry of Maingroup Elements Chemistry of boron:** Selfstudy: boranes, bonding in boranes, topology of boranes, synthesis and reactivity, Carboranes and metalla carboranes. Lowvalent boron compounds, organo boron compounds and organic synthesis. Use of 11B NMR in structure elucidation of organoboron compounds. Boron containing polymers. Borazine and Boron Nitride Organo lithium compounds. Synthesis, bonding and

			reactivity. Organo magnesiusm and organo sodium compounds. Chemistry of Aluminum. Aluminum Alkyls. Unusual organometallic compounds of aluminum. Including low oxidation state Al compounds and aluminum clusters. Chemistry of Low valent compounds: NHCs and their analogous group 13, 14 and 15 compounds and the recent advances Multiple bonding in main group elements: Compounds involving silicon, phosphorus, bismuthetc. Synthesis, structure and reactivity. Recent literature on multiple bonding models among low valent compounds Inorganic rings and polymers: Siloxanes, Cyclophosphazenes and cyclophosphazanes. Polysilanes and Polyphosphazenes Noble gas compounds Most of the material for this course will be accessed from primary literature viz., Journalarticles. Some text books that will be followed are as follows- **Course Reference**: 1. Inorganic ChemistryPrinciples of Structure and Reactivity. 4th Edn. Huheey J. E.; Keiter, E.A.; and Keiter, R. L. HarperCollins, NY, 1993; 2. Concepts and Models of Inorganic Chemsitry. 3rd Edn. Douglas, B.; McDaniel, D.; and Alexander, J. John Wiley, New York. 1993; 3. Chemistry of the Elements. 2nd Edn. Greenwood, N. N.; and Earnshaw, A. Pergamon, Oxford, 1989; 4. Elschenbroich, C.; and Salzer, A.; Organometallics: A Concise Introduction 3rd Edn. 1999; 5. Inorganic and Organometallic Polymers. Chandrasekhar, V. SpringerVerlag, Heidelberg,2005.
CHM679	MOLECULAR REACTION DYNAMICS	3-0-0-0-9	**1. Introduction:** Review of kinetic theory of gases, collisions atomic and molecular; **2. Rate theories** Transition state theory and RRKM theory, scattering classical and quantum; **3. Reactive Collisions** ,Potential energy surfaces, atomdiatom reactions, polyatomic reactions, stateselective,molecular beams, reaction rates and cross sections; **4. Dynamics in gas phase** Photodissociation, energy transfer, stereodynamics, chemistry in real time with lasers,control; **5. Dynamics in condensed phase** Solvation, diffusion, barrier crossing, Kramer Grote Hynes theory, Langevin equation,correlation functions; **6. Advanced topics** Dynamics on surfaces, spatiotemporal aspects of pattern formation, ultrafast dynamics. **Course Reference**: 1. Levine, Molecular Reaction Dynamics, 2005; 2. Henriksen & Hansen, Theories of Molecular Reaction Dynamics, 2008; 3. Schinke, Photodissociation Dynamics, 1993; 4. Manz & Wste, Femtosecond Chemistry, 1995; 5. Nitzan, Chemical Dynamics in Condensed Phases, 2006.
CHM681	BASIC BIOLOGICAL CHEMISTRY	3-0-0-0-9	Recombinant DNA techniques, Protein folding, design and Engineering, ChouFasman rules, Ramachandran plot and conformation of biopolymers. Mechanisms of important enzymes. Biosynthesis of nucleic acids and proteins. confactors. Immunology. Immune response, Innate immunity and adaptive immunity, Immune dysfunction and its consequences, Immunogenicity, antigens, antibody diversity, monoclonal antibodies, autoimmunity, Hybridoma technology Biosynthesis of lipids and fatty acids. Secondary metabolism, Membrane transport, Aminoacid biosynthesis and metabolism. Cell differenciation, Regulation of gene expression, recombination, DNA replication, signal transduction. **Course Reference**: Fundamentals of Biochemistry by Voet,

			Voet and Pratt, Biochemistry by L. Stryer, Proteins by T.E. Creighton, Genes VII by B. Lewin, Introduction toprotein structure by Branden and Tooze, Enzyme structure and Mechanism by Alan Fersht.
CHM682	MODERN CHEMISTRY AND APPLICATIONS OF LANTHANIDES	3-0-0-0-9	**Introduction to Lanthanide chemistry:** Discovery, extraction and separations, position in periodic table, Highlights of f-block elements, Differences from d-block/main group elements, why RE's are critical elements? Rare earths in modern technologies, Technical sustainable recycling of Lanthanides. **Principles, energetics and Periodic properties f-block elements:** principles, energetics, periodic properties and trends, f-orbitals, lanthanide contraction, ionic radii, oxidation states, stability. **Coordination Chemistry of Lanthanides:** Binary compounds, Cerium oxide and uses, Complexes, nature of bonding, hydration & hydrolysis, stability of complexes, ligand types and their design, geometry and structures of Ln-complexes, Structure-property relationships, Heterometallic lanthanide systems, f-f, f-f', d-f, s-f hybrid multimetallic systems. **Organometallic Chemistry of Lanthanides:** bonding, alkyls, aryls, arenes, synthesis, structure and reactivity, application of organo-lanthanide compounds in organic transformation, divalent rare earth chemistry, catalytic applications: sigma bond metathesis, olefin hydrogenation/Ziegler-Natta catalysis, Hydroamination reactions. **Spectroscopic properties of Lanthanides:** Basic f-element electronic structures, Excited state electronic properties, luminescence properties, nature of f-f transitions, sensitization mechanism: antenna effect, energy-transfer, time-resolved luminescence spectroscopy, Upconversion of Ln-luminescence, Ln-probes for bioresponsive imaging and design principles, luminescence-based applications. **Luminescence-based Chemosensors and Bio-imaging with Lanthanide Complexes:** Modulation of lanthanide luminescence and quenching, Chemosensor design principle, Time-resolved luminescence, Ln-based bioimaging, cellular imaging probes, Emissive lanthanide probes studying protein interactions. **Magnetic properties of Lanthanides:** Electronic structures, term symbols, spin-orbit coupling, magnetic moments, permanent magnets, NMR-shift reagents, Lanthanide Single-molecule-magnet (SMM), Superconductive materials. **Lanthanide-base MRI Contrast Agents:** Principles of MRI, Contrast agents, Gadolinium-chelates as MRI contrast agents, water-exchange kinetics, Relaxivity, relaxation time, molecular parameters for relaxivity in MRI probes, Sensitivity and Selectivity of MRI probes, New generation MRI contrast agents. **Lanthanides in Biology:** Bioinorganic chemistry of Ln, Emergence of lanthanide in metallobiochemistry and microbiology, Ln-dependent proteins: methanol dehydrogenase (MDH), lanmodulin as selective Ln-binding protein, mechanism of uptake by bacteria. **References/ Textbooks** 1. Lanthanide and Actinide Chemistry, Simon Cotton, John Wiley &

			Sons, Ltd. 2006. 2. Luminescence of Lanthanide Ions in Coordination Compounds and Nanomaterials, Ed. Ana de Bettencourt–Dias , John Wiley and Sons, Ltd, 2014. 3. Lanthanide-Based Multifunctional Materials, Ed. P. Martin-Ramos, M. Ramos-Silva, Elsevier 2018. 4. Lanthanide Luminescence: Photophysical, Analytical and Biological Aspects, Ed. P. Hänninen, H. Härmä, Springer, 2011. 5. Lanthanides and Actinides in Molecular Magnetism, Ed. R. A. Layfield, M. Murugesu, Wiley-VCH, 2015
CHM683	SURFACES, INTERFACES, THIN FILMS & RELATED ANALYTICAL TECHNIQUES	3-0-0-0-9	**General introduction to solid surface and interface of materials**: Why surface is different/important? Applications of surface and interfaces. **Thin films and Clusters:**Type of interfaces: solid-solid, solid-molecule, solid-liquid, gas-solid interfaces - Elementary processes of gas-surface interaction. Adsorption (physical and chemical) and interface formation. Ultra high vacuum (UHV) technology. Methods for preparation of thin films (Physical and chemical methods) **Structure, morphology and electronic properties of surfaces and interfaces:** Structure of clean surfaces, reconstructions, stepped surfaces. Electronic properties of surfaces. Adsorbates on surfaces, self-assembly, consequences of adsorbates on surface. Electronic properties of adsorbates on surfaces **Thermodynamics at surface:** Surface tension. Surface energy and surface composition. Meta stable surfaces, curves surfaces. Thermodynamics of adsorbed layers **Catalysis by surface:** Chemical reactions at surface - Few case studies **Surface morphology characterization techniques:** Electron microscopes (Scanning electron microscope, Transmission electron microscope). Near field microscopes (Scanning tunneling microscope, Atomic force microscope, Scanning electrochemical microscope, Scanning near field optical microscope). **Surface electronic properties characterization techniques:** Electron emission from surfaces by incident electron or photon. X-ray photoelectron spectroscopy (XPS). UV-Vis photoelectron spectroscopy (UPS). Auger electron spectroscopy (AES). High-Resolution Electron-Energy-Loss Spectroscopy (HREELS). Near edge X-ray absorption fine structure (NEXAFS). **Surface structure characterization techniques:**Low energy electron diffraction (LEED) - Reflection high energy electron diffraction (RHEED) **Perspectives.** **Course Reference**: 1. Introduction to solid state physics by Charles Kittel 2. Introduction to surface chemistry and catalysis by Gabor A. Somorjai, Yimin Li 3. Electronic and Photoelectron Spectroscopy by Andrew M. Ellis, Miklos Feher and Timothy G. Wright 4. Scanning Probe Microscopy by Roland Wiesendanger. Handbook of vacuum science and technology by Dorothy Hoffman 5. Solid surfaces interface and thin films by H. Lüth
CHM684	COMPUTER PROGRAMMING	3-0-0-0-9	**Fortran and Computer Programming:** Elements of Fortran programming, constants, variables and operators, control

	FOR CHEMISTRY		statements, I/O operations, functions and subprograms, common, equivalence, arrays, strings, DATA statements, Disk I/O. New features in Fortran 90 compared to Fortran 77. Programming considerations Round off and truncation errors, pitfalls and debugging. **Numerical Methods:** Roots of equations Bisection and NewtonRaphson methods, Systemof linear equations, Gaussian, Gauss Jordan elimination, Nonlinear system of equations. Regression analysis and Least square fit, Linear, Polynomial and NonLinear regressionanalysis, eigenvalues and eigenvectors, Numerical differentiation and integration, Differential equations **Applications to chemistry:** statistical thermodynamics, chemical kinetics, Curve fitting, Gaussian and Lorentzian deconvolution. Use of software packages such as visualization, semiempirical methods. **Course Reference**: 1. Michael Boillot, Understanding Fortran77, wess publishing company, New York(1987); 2. Fortran95/2003 for scientists and engineers, S.J.Chapman, McGrawHill (2008); 3. (Ed) D.F. De Tar, Computer programs for chemistry, vol 14, Academic press, New York(1972); 4. K.B. Wiberg, Computer Programming for Chemists, W.A. Benjamin Inc, New York (1965); 5. S.C.Chapra and R.P.Canale, Numerical Methods for Engineers, Tata McGraw Hill, NewDelhi (2003).
CHM685	MOLECULE RADIATION INTERACTION	3-0-0-0-9	**1. Classical Elecromagnetics:** Fields, Maxwell's equations, gauges and optics; **2. Quantization of Electromagnetic Fields.** Photons, polarizations, Stokes parameters, nontrivial role of the vector potential; **3. Interactions** of One and two photon processes, line widths and line shapes, broadening, Raman scattering; **4. Spectroscopy Born** Oppenheimer limit, time dependent view points, nonadiabatic effects; **5. Advanced topics:** Beyond dipole approximation, attosecond spectroscopy. **Course Reference**:1. Sakurai, Advanced Quantum Mechanics, 1967; 2. Cohen Tannoudji & DupontRoc, Atom Photon Interactions, 2004; 3. Landau & Lifshitz, Classical Theory of Fields, 1951; 4. CohenTannoudji, DupontRoc & Grynberg, Photons & Atoms, 1989; 5. Feynman Lectures in Physics II, 2005.
CHM689	NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY	3-0-0-0-9	**Introduction to NMR Spectroscopy.**Angular momentum, matrix representation of angular momentum operators. Density matrices, pure and mixed states, density operator and calculation of expectationvalues. Chemical shifts, coupling constants, rotating frame concept and qualitative description ofpulse experiments. Construction of hamiltonian matrix for multispin systems and the solution of AB and ABX spinsystems. Product operator formalism and vector diagrams. Analysis of multipulse experiments: INEPT, DEPT, COSY, NOESY and double quantumfiltered COSY. Multidimensional NMR and macromolecular structure determination. **Course Reference**: 1. M. Goldman, Quantum Description of High-Resolution NMR in Liquids, Clarendon Press, New York (1988). 2. J. A. Pople, W.G. Schneider and H.J. Bernstein, High Resolution NMR, McGraw Hill, NewYork (1959). 3. J. Cavanagh, W.J. Fairbrother, A.G. Palmer III and N.J. Skelton, Protein NMR Spectroscopy, Academic Press (1996). 4. C.P. Slichter,

			Principles of Magnetic Resonance, SpringerVerlag, Berlin (1990).
CHM691	FRONTIERS IN INORGANIC CHEMISTRY	3-0-0-0-9	**Developing facets of Inorganic Chemistry** (2 Lectures) Oxidative generation of molecular oxygen from water during photosynthesis (8 Lectures)Its importance from the standpoint of nonconventional energy research (6 Lectures) Reductive cleavage of the dioxygen bond (3 Lectures) Reductive cleavage of dioxygen bond and novel organic transformations including methane tomethanol performed by a large number of Fe containing metalloenzymes (8 Lectures) Reductive cleavage of dioxygen bond and novel organic transformations performed by alarge number of Cu containing metalloenzymes and synthetic catalysts (15 Lectures) **Course Reference**: Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, University Science Books, Mill Valley, 2006.
CHM692	SPECIAL TOPICS IN PHYSICAL CHEMISTRY	3-0-0-0-9	The course contents will involve some topics of current interest in Physical Chemistry. Topics relating to quantum mechanics, thermodynamics, physical and chemical kinetics, spectroscopy, statistical mechanics, molecular simulations, continuum mechanics, solid-state and materials chemistry, biophysics, nonlinear dynamics, can be taught as part of this course. Additionally, new and emerging areas may be included from time-to-time. The exact topics for the course will be decided by the instructor at the time of offering the course. The instructor will be required to submit the course contents, reference books and list of prerequisites at the time of course registration.
CHM693	CHEMICAL SYNTHETIC STRATEGY OF ADVANCED MATERIALS	3-0-0-0-9	Chemical methods of synthesis play a crucial role in designing materials, discovering novel materials, metastable phases, nanomaterials and provide less cumbersome routes for the known materials. Chemical ingenuity is important for the synthesis of solid materials with desired structure and properties. Keeping in mind the multidisciplinary nature of the subject, a rational approach to the synthesis of materials is evolved. Indeed, soft chemistry routes/techniques are pursued with greater vigour. These include precursor technique, solgel, hydrothermal, nonaqueous liquid phase reactions, polymer pyrolysis, gas phase reactions, plasma reactions, electron beam evaporation, freeze drying, spray drying, topochemical reactions, intercalation, electrochemical methods, CVDlaser ablation, arcmethod, molten salt method, inter grown structures. Solidstate reactivity, working knowledge of characterization techniques and conventional techniques.
CHM695	MOLECULAR MODELLING IN CHEMISTRY	3-0-0-0-9	**Brief Review of the basic Principles of quantum mechanics of atoms and molecules.** Potential energy surfaces and intermolecular interactions: Quantum mechanical ab initiocalculations within Born Oppenheimer approximation and modelling of calculated energies bymodel potentials for simple atoms, molecules and ions. Energy calculations using molecular mechanics. Simple applications of molecular modelling: Study of an assembly of atoms or molecules (clusters and/or bulk phases). Approximation of the total potential energy as the sum of pair potentials. Concept of large number of microstates,

			averages and basic principles of simulations. Study of cluster and bulk properties through simulations. Modelling of water and small organic molecules: Nonpolarizable and polarizable rigid models. Flexible models and calculation of force constants. Structural, dielectric and dynamical properties of a polar medium: Continuum models versus molecular models. Calculation offree energy using molecular models. Modelling of macromolecules: Study of selforganized assemblies, biomolecules like peptides, proteins, membranes and ion channels. Concept of hydrophobic and hydrophilic interactions. Use of molecular modelling in drug design, QSAR. **Course Reference**: 1. A.R. Leach, Molecular Modeling : Principles and Applications, Longman (1996); 2. J. H. Jensen, Molecular Modeling Basics, CRC Press (2010); 3. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Ed., Wiley(2004); 4. J. Israelachvili, Intermolecular and surface Forces, Academic (1991); 5. M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Clarendon Press (1987); 6. D. Frenkel and B. Smit, Understanding Molecular Simulation : From algorithms to Applications, Academic Press (1996); 7. P.W. Atkins, Molecular Quantum Mechanics, Oxford (1997); 8. W. Koch & M. C. Holthausen, A Chemists Guide to Density Functional Theory, WileyVCH; 9. A. Szabo, Modern Quantum Chemistry: Introduction to Advanced Electronic StructureTheory, Dover Publications (1996).
CHM696	QUANTUM COMPUTING	3-0-0-0-9	**Thermodynamics of computing, Shannon Theory, elementary information theory.** Basics of computers, ChurchTuring hypothesis, basics of computing complexity. Basic of quantum mechanics, Feynman Block Pseudopolarization Vector Model, Time Dependent Schrodinger equation, basics of approximate quantum approaches (Two level Systems, Coherence, Superposition Principle, Density Matrix, Entanglement, Relaxation Processes.Quantum gates and circuits, Theory of Quantum Information and Computation, Deutsch Jozsa algorithm, Shor's algorithm for factoring, Grover's search algorithm and its applications. Quantum Complexity, Quantum Turing Machine. Physical implementations of Quantum Computation, Light polarization, NMR, Cavity QED, IonTraps, Lasermatter interaction, Coherent Control. **Course Reference:** Michael A. Nielsen and Isaac L. Chuang, Quantum Computation and Quantum Information,Cambridge University Press, 2000; b. Jozef Gruska, Quantum Computing, McGraw Hill, 1999; c. Neil Gershenfeld, Physics of Information Technology, Cambridge University Press, 2000; d. CohenTannoudji, Diu, and Lalo, Quantum Mechanics I, 200; e. Mika Hirvensalo, Quantum Computing, SpringerVerlag New York, 2000; f. G. Alber, T. Beth, M. Horodecki, P. Horodecki, R. Horodecki, M. Rotteler, H. Weinfurter, R.Werner, A. Zeilinger, Quantum Information: An Introduction to Basic Theoretical Conceptsand Experiments, Springer, 2001.
CHM697	LASERS IN CHEMISTRY AND BIOLOGY	3-0-0-0-9	**Fundamentals of lasers.** General concepts of laser spectroscopy. Laser-induced fluorescence and multiphoton ionization processes of molecules, probing IVR and dynamics of chemical reactions in liquid and molecular beam.

			Spectroscopy of single molecule, confocal microscopy and fluorescence correlation spectroscopy. Probing of proton/electron dynamics, anisotropy Optical trapping and manipulation of biological macromolecules, applications of diagnostics and biotechnology. Pulsed laser and ultrafast spectroscopy Non-linear spectroscopy. References and Textbooks: 1. Laser Chemistry, Telle, H. H. and Urena, A. G., John Wiley & Sons, New Jersey, 2007. 2. A Guide To Lasers In Chemistry, Van, H. and GERALD, R. J. Bartlett Pub., Boston, 1998. 3. Nonlinear Laser Chemistry, Letokhov, V. S., Springer-Verlag, 1983. 4. Lasers, Milonni, P. W. and Eberly, J. H., John Wiley & Sons, 1988.
CHM698	CHEMISTRY OF DRUG DESIGN AND METABOLISM	3-0-0-0-9	**Physicochemical Principles of Drug Action**; Partition Coefficients; Receptor Effector Theories; Role of Second Messengers in Drug Action; Methods of Receptor Isolation, Characterization and Modeling Principles of Drug Design: Random Screening, Analogue Synthesis, Rational Design, Combinatorial Libraries; Enantiopure Drugs and Regulatory Implications; Theoretical Approaches: QSAR, Topliss Tree, MSA, CoMFA Neuroactive Drugs: Neurons and Neurotransmitters; Brain related Disorders andChemotherapy; Drugs Interacting with Cholinergic, Adrenergic, Dopaminergic andHistaminic Receptors and Receptor subtypes. Anticancer, Antimalarial, Antiviral, and Cardiovascular Drugs; Emerging Trends in Drug Design: Inhibitors of DNA Topoisomerase and Protein Farnesylation & Prenylation; Gene Based Medicines Biopharmaceuticals: Recombinant Proteins as Medicines and Vaccines. Drug Delivery: Passive, Assisted and VectorBased Delivery of Conventional and Genetic Drugs; Tissue Specific Delivery of Antitumor Agents (8)Drug Administration, Distribution, Metabolism and Elimination (ADME); Pathways of Drug Metabolism: Enzymology and Molecular Mechanisms; Detoxification of Diverse Drug Classes; Dose Formulation (10)Induction and Inhibition of Drug Metabolism; Toxicological Aspects of Metabolism: Metabolic Activation of Environmental Carcinogens and DNA Damage; Drug Pharmacokinetics and Final Body Clearance. **Course Reference**: 1. Medicinal Chemistry: A Biochemical Approach, Thomas Nogrady; 2. Principles of Medicinal Chemistry, William O. Foye; 3. The Pharmacological Basis of Therapeutics: Goodman and Gilman; 4. Introduction to Drug Metabolism, G. Gordon Gibson and Paul Skett
CHM699	MS PROJECT	3-0-0- 0-18	M.Sc. research project in 3rd semester (Non-compulsory) with 18 credits under the supervision/co-supervision of a faculty in Chemistry. Alternatively, two DE (2 x 9 credit = 18 credits) courses to be taken.
CHM700	M.Sc. PROJECT	0-0-0-0-27	M.Sc. research project in 4th semester under the supervision/ co-supervision of a faculty in Chemistry.
CHM799	RESEARCH	0-0-0-0-36	Ph. D. Thesis
CHM800	GENERAL SEMINAR2	----0	General Seminar

CHM800A	GENERAL SEMINAR	----0	Graduate Seminar
CHM800B	GENERAL SEMINAR	----0	Graduate Seminar
CHM801	GRADUATE SEMINAR	----0	Graduate Seminar
CHM801A	GRADUATE SEMINAR	----0	Graduate Seminar
CHM801B	GRADUATE SEMINAR	----0	Graduate Seminar
CSO201	ORGANIC CHEMISTRY: FUNDAMENTALS AND APPLICATIONS	3-1-0-0-11	Basic Organic Chemistry Concepts: introduction to organic molecules and functional groups, understanding organic reactions, stereochemistry and carboncarbon bond forming reactions in organic synthesis. Drugs some examples including love drugs and molecules of death. Chemistry of odours, dyes and flavors, Green Chemistry introduction, principles, sustainability, atom economy, some green initiatives, management of resources and its effect on health and environment. Catalysis and biocatalysts in organic chemistry. enantioselectivity and chiral synthesis, organo catalysis. Enzymes as drug targets and their inhibitors as model inhibitors. Solid phase synthesis and strategies for futuristic designs in organic chemistry. Photochemistry: simple concepts and applications (semiconductor photochemistry, solarenergy conversion by photovoltaic cells, photocatalysis, etc.); supramolecular photochemistry. Organic Materials: polymers (biodegradable polymers, conducting polymers, etc.), smart materials, OLEDs, intelligent gels, dyes, etc. **Course Reference**: 1. Organic Chemistry: Structure, Mechanism,and Synthesis by R. J. Oulettle and J. D. Rawn; 2.Green Organic Chemistry: Strategies, Tools, and Laboratory Experiments by K. Doxsee and J.Hutchinson; 3. Bioorganic Chemisty: A Chemical approach to enzyme action by H. Dugas; 4. Solid Phase organic synthesis: concepts strategies and applications by P. H. Toy and Y. Lam; 5. General Organic Chemistry, Janice Smith, McGrawHill, New York, USA, 2011; 6. Organic Chemistry, W. H. Brown, C. S. Foote, B. L. Iverson and E. V. Anslyn, Brooks/Cole,Belmont, USA, 2012; 7. Principles and Applications of Photochemistry, Brian Wardle, Wiley & Sons, Chichester, UK., 2009; 8. Chemistry of New Materials, FactsOn File, Inc. New York, USA, 2007; 9. Love Drugs, Otto Snow, Thoth Press, USA, 2005; 10. Molecules of Death, R. H. Waring, G. B. Steventon, S. C. Mitchell, Imperial College Press, London, UK, 2007.
CSO202	ATOMS, MOLECULES AND PHOTONS	3-1-0-0-11	This course is dedicated to introduce to the contemporary physical chemistry for undergraduate students. The course starts by inspiring students by introducing several landmark experiments of physical chemistry. Importance of theoretical approaches to explain experimental observations will be introduced subsequently. A combination of theoretical and experimental techniques in understanding structure and dynamics of atoms and molecules are then discussed. Content: 1. Landmark experiments in physical chemistry; 2. Interplay of

			theory and experiments in modern physical chemistry; 3. Structure of atoms and molecules; 4. Dynamics of atoms and molecules5. Structure and dynamics of atoms and molecules interacting with radiation. **Course Reference**:1. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry; 2. D. A. McQuarrie, J. D. Simon, Physical Chemistry: A molecular approach; 3. K. J. Laidler, The World of Physical Chemistry; 4. C. E. Dykstra, Physical Chemistry A modern Introduction
CSO203	INORGANIC MOLECULES, MATERIALS & MEDICINE	3-1-0-0-11	**Module I: Life with Oxygen**:The aim of this module is to understand how our life is dependent on oxygen. We will start with the fundamentals related to dioxygen and need for its activation. We will then talk about its usefulness in various biological activities and applications. **Module II: Metals and Medicine**: Dmitri Ivanovich Mendeleev in 1869 delivered a remarkable contribution to arrange chemical elements in the Periodic table. This module starts with Nature's selection of elements from Periodic Table. It will provide a brief overview of metals used in the ancient times and today as therapeutic and diagnostic agents. Will discuss on the Rosenberg's accidental landmark discovery of cisplatin as blockbuster anticancer drug. Lectures will also provide mechanistic action of the drug and the current status. **Module III: Electron Transfer Process**: Nobel Prize in Chemistry in 1983 has been given to Henry Taube for his outstanding work on the mechanisms of electron transfer reactions, especially in metal complexes. We will discuss various electron transfer processes and how our life is dependent on that! **Module IV: Catalysis and Sustainability**: Catalysis is one of prime field which has attained more number of Nobel prizes (20! at least) wherein the fundamental role of catalyst and its design play a critical role. Here, catalytic activities of few selected and important catalysts will be discussed along with their industrial applications. In addition, recent development on Green Chemistry for chemical synthesis and sustainable chemical processes will be highlighted. **Module V: Inorganic Polymer**: An overview of important compounds used in rubber, adhesives, ceramic materials, sealant and inorganic polymers will be discussed. **Module VI: Inorganic Materials**:A large number of new generation materials, such as network structures, molecular (nano)machines and molecular (nano)devices based on supramolecular chemistry and molecular self-assembly (Nobel prizes in 1982 and 2016). In addition, we will also discuss selected materials used for Magnetic, Optical, Conducting and Storage materials. **Course Reference**: Inorganic Chemistry-Principles of Structure and Reactivity, 4thEdn., J. E. Huheey, E. A. Keiter and R. L. Keiter, Harper-Collins, NY, 1993 Advanced Inorganic Chemistry, 6thEdn., F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Wiley, 1999 Concepts and Models of Inorganic Chemsitry, 3rdEdn., B.

			Douglas, D. McDaniel and J. Alexander, John Wiley, New York. 1993 Concepts and Models of Inorganic Chemsitry, 3rdEdn., B. Douglas, D. McDaniel and J. Alexander, John Wiley, New York. 1993 Supramolecular Chemistry, J-M. Lehn, VCH, Weinheim, 1995 Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John-Wiley and Sons, Ltd., 2000 Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard & J. S. Valentine, Viva Books Pvt. Ltd., 2004. Shriver and Atkins Inorganic Chemistry, 5thEdn., Oxford University Press, 2009. Organotransition Metal Chemistry: From Bonding to Catalysis, 1stEdn., J. Hartwig, 2010 Molecular Magnetic Materials: Concepts and Applications, Editors(s): B. Sieklucka and D. Pinkowicz, Wiley-VCH, 2016 Molecular Magnetic Materials: Concepts and Applications, Editors(s): B. Sieklucka and D. Pinkowicz, Wiley-VCH, 2016.