Department of Chemistry
Central University of Rajasthan
M. Sc. (2 Year) Syllabus

The purpose of the master's program is to further develop knowledge and skills in Chemistry and to prepare students for a professional career in academia, industry or for doctoral studies. This is achieved through various fundamental as well as advanced theory courses coupled with a number of laboratory courses that allows students to gain hands-on experience with chemical phenomena, gather data and propose models and explanations for their observations. The program provides an opportunity for students to take modules from a wide range of cutting-edge fields in chemistry, encompassing sessions on theory, laboratory, scientific writing, communication and presentation, besides a semester long research project.

Program Objectives:

- To deliver advanced concepts in Chemistry covering topics in Analytical, Inorganic, Organic and Physical Chemistry, while also reinforcing the fundamental concepts.
- To make students proficient in advanced laboratory techniques, enabling them to independently plan and conduct experiments at a higher level as well as to work as a team.
- To expose the students to a range of analytical methods using modern instrumentation, enabling them to analyse results at a higher level.
- To enable students develop the skills required to succeed in graduate school, chemical industry or any government organization.
- To develop critical thinking and skills like effective scientific communication, time management, and multi-tasking aptitude.

Learning Outcomes:

1. The graduating students would have an in-depth knowledge of the molecular principles of Chemistry that empower them to understand and solve complex problems and effectively articulate their ideas in the scientific community.
2. They would progress and mature to become increasingly independent learners, moving beyond textbooks and courses and into learning directly from the primary literature, especially within the context of independent research.
3. They would have a deeper understanding about inter-disciplinary topics, encouraging them to take up research in inter-disciplinary and frontier research domains.
4. They develop an adaptability skill to work in teams as well as independently to deliver the outcomes effectively.
5. Interested students would be well-equipped to join the chemical industry in either Research & Development units or the process & manufacturing streams.
6. Students would be expected to compete for various National and International level exam such as NET-JRF, GATE, GRE, etc.
7. They would also be able to communicate scientific results, both written and oral, for specialized and non-specialized audiences.

Structure of the M.Sc. (2 yr) programme

Semester I

S. No.	Course Code	Title of Course	Type of course	h/week	Credits
1.	CHM-401	Chemistry of Main Group Elements	Core	3	3
2.	CHM-402	Stereochemistry and Reaction Mechanism	Core	3	3
3.	CHM-403	Quantum Chemistry	Core	3	3
4.	CHM-404	Group Theory and Molecular Spectroscopy	Core	3	3
5.		**Elective-I**	**DSE**	**3**	**3**
6.	CHM-430	Inorganic Chemistry Laboratory I	Core Lab	4	2
7.	CHM-440	Organic Chemistry Laboratory I	Core Lab	4	2
8.	CHM-450	Physical Chemistry Laboratory I	Core Lab	4	2
			Total Semester Credits		**21**

Semester II

S. No.	Course Code	Title of Course	Type of course	h/week	Credits
1.	CHM-405	Coordination Chemistry	Core	3	3
2.	CHM-406	Synthetic Methods in Organic Chemistry	Core	3	3
3.	CHM-407	Thermodynamics	Core	3	3
4.	CHM-408	Spectroscopic Methods of Structure Determination	Core	3	3
5.		**Elective-II**	**DSE**	**3**	**3**
6.	CHM-460	Inorganic Chemistry Laboratory II	Core Lab	4	2
7.	CHM-470	Organic Chemistry Laboratory II	Core Lab	4	2
8.	CHM-480	Physical Chemistry Laboratory II	Core Lab	4	2
			Total Semester Credits		**21**

Semester III

S. No.	Course Code	Title of Course	Type of course	h/week	Credits
1.	CHM-501	Organometallic Chemistry	Core	3	3
2.	CHM-502	Pericyclic Reactions and Photochemistry	Core	3	3
3.	CHM-503	Solid State & Material Chemistry	Core	3	3
4.	CHM-504	Basic Bioinorganic Chemistry	Core	3	3
5.		**Elective-III**	**DSE**	**3**	**3**
6.		**OPEN ELECTIVE-1**	**OE**	**4**	**4**
7.	CHM-530	Inorganic Chemistry Laboratory III	Core Lab	4	2
8.	CHM-540	Organic Chemistry Laboratory III	Core Lab	4	2
9.	CHM-550	Physical Chemistry Laboratory III	Core Lab	4	2
			Total Semester Credits		**25**

Semester IV

S. No.	Course Code	Title of Course	Type of course	h/week	Credits
1.	CHM-500	Research Project	Dissertation	24	12
2.		**Elective - IV**	**DSE**	**3**	**3**
3.		**OPEN ELECTIVE-2**	**OE**	**3**	**4**
			Total Semester Credits		**19**
				Total Credits	**86**

The following are to be implemented by the University for each program:

Credits for Fitness	**2**
Credits for Societal course / work	**2**
Proposed Total Credits of the Program	**90**

DSE = Discipline Specific Elective; OE = Open Elective

<u>Percentage-wise distribution of the courses</u>:

Type of Course	**No. of Courses (A)**	**Credits (B)**	**Total Credits (C = A × B)**	**Percentage w.r.t. Total Credits of the Program (P = C/90 × 100) (%)**
Core	12	3	36	**40**
Laboratory	9	2	18	**20**
D-Electives	4	3	12	**22.22**
Open Electives	2	4	8	
Dissertation	1	12	12	**13.33**
Fitness	1	2	2	**2.22**
Societal	1	2	2	**2.22**
	TOTAL CREDITS		**90**	**100%**

Elective courses:

S. No	Course Code	Title of the Course	h/week	Credits
1.	CHM-610	Analytical Chemistry and Inorganic Spectroscopy	3	3
2.	CHM-612	Natural Products	3	3
3.	CHM-614	Medicinal Chemistry	3	3

4.	CHM-615	Supramolecular Chemistry	3	3
5.	CHM-616	Topics in Heterocyclic Chemistry	3	3
6.	CHM-629	Chemical Binding	3	3
7.	CHM-630	Chemical Binding and Computational Chemistry	4	4

CHM-401 Chemistry of Main Group Elements 3 Credits

Course level: Introductory/Reinforce
Pre-requisite: Undergraduate level in Inorganic Chemistry

Course Description:

To acquire the knowledge in the principle of main group element chemistry (s and p block) with an emphasis on synthesis, structure, and bonding.

Course Content:
Stereochemistry and Bonding in main group compounds: VSEPR Theory, Walsh diagram, Hybridization including energetics of hybridization. Bents rule, dπ-pπ bond. Some simple reactions of covalently bonded molecules: (i) Atomic inversion (ii) Berry-pseudo rotation (iii) Nucleophilic displacement (iv) Free radical mechanism.

Hydrogen, alkali and alkaline earth metals: Classification of hydrides - e-deficient, e-precise & e-rich hydrides. Application of crown ethers in extraction of alkali and alkaline earth metals.

Noble gases: Isolation and properties. Preparation and structure of noble gas compounds.

Boron compounds: Preparation, structure, bonding, reactions and applications of boranes, carboranes, metalloboranes, metallocarboranes, borazines.

Compounds of carbon and silicon: Fullerenes and their compounds, Intercalation compounds of graphite, carbon nano-tubes: Synthesis, structure, properties, and applications. Carbides, fluorocarbons, silanes, silicates, zeolites and silicones.

Compounds of oxygen group elements: Metal selenides and tellurides, oxyacids and oxoanions of S & N.

Compounds of nitrogen group elements: Nitrogen activation. Oxidation states of nitrogen and their interconversion. BN, PN and SN compounds - preparation, structure and bonding.

Compounds of halogen group elements: Synthesis, properties, bonding, and applications of interhalogens, pseudohalogens, polyhalides, oxyacids and oxoanions of halogens.

Reaction in non-aqueous solvents: Classification of solvents, Characteristic properties of an ionizing solvent, Reaction in liquid ammonia, liquid sulphur dioxide, dimethyl formamide (DMF), dimethyl sulphoxide (DMSO) and dioxane. Chemistry of fused salt systems.

Course Outcome:

1) Familiar to understand the reactivity of main group compounds
2) Get stimulate for designing new ligands/materials by proper choice of main group reagents in organic synthesis
3) Gain knowledge about structure-property relationship

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	3			3	3	2
CO2	3	2			2	3	
CO3	3	2	2		2	3	

Reference Books:

1. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson (2007), 6th Edition, John Wiley.
2. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter and R. L. Keiter (1997), 4th Edition, Prentice Hall.
3. Chemistry of the Elements, N. N. Greenwood and A. Earnshow (1997), 2nd Edition, Butterworth-Heinemann.
4. Inorganic Chemistry: A unified Approach, W. W. Porterfield, (2013), 2nd Edition, Academic Press.
5. Inorganic Chemistry, C. E. Housecroft, A. G. Sharpe (2018), 5th Edition, Pearson.
6. Shriver & Atkins' Inorganic Chemistry, P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, M. Hagerman, (2010), 5th Edition, W. H. Freeman and Company, New York.
7. Inorganic Chemistry, G. L. Miessler, P. J. Fischer, D. A. Tarr, (2013), 5th Edition, Pearson.
8. Inorganic Chemistry, G. Wulfsberg, (2018), Viva Books.

Assessment method: Written (and if necessary - Seminar/Assignment/Viva).

CHM-402 Stereochemistry & Reaction Mechanism 3 Credits

Course Description:

This course can be broadly divided into two parts one part as stereochemistry and another as reaction mechanisms. Topics in stereochemistry introduce the concepts of axis of chirality, plane of chirality, and helicity with the help of appropriate examples. Chirality of molecules possessing nitrogen, phosphorous, sulphur atoms will be discussed. This course also introduces advantages of NMR spectroscopy in identifying heterotropic ligands. Merits of Crams rule, Felkin's model, Prelogs rule in the asymmetric synthesis will be demonstrated. This course also deals with conformational analysis of cycloalkanes such as substituted cyclohexanes, Decalins, and sugars. As in the second part, a detailed procedure about proposing a reaction mechanism is introduced as well. This course also covers the effect of stereoelectronics in addition, substitution, and elimination reactions.

Course Content:

UNIT – I Stereochemistry 20 L

Chirality: Stereogenic unit: Center of chirality, axis of chirality, plane of chirality and helicity. Stereochemistry of - allenes, spirans, biphenyls, cyclophanes, ansa compounds, trans-cyclooctene, helicenes, benzphenanthrenes. Configurational nomenclature; Stereochemistry of compounds containing nitrogen, sulphur and phosphorus.

Topicity and Prochirality: Topicity of ligands and faces. Diastereotopic ligands and NMR spectroscopy. Chemical reactivity of heterotropic ligands and faces with chiral and achiral reagents. Resolution of racemates.

Stereoselectivity and stereospecificity: Kinetic and thermodynamic controls, asymmetric induction, chiral auxilliary, diastereotopic induction, Principles of asymmetric synthesis, Cram's rule, Felkin's model, Prelog's rule.

Conformational analysis of cycloalkanes: Cyclohexane, mono-substituted cyclohexanes; disubstituted cyclohexanes, effect of conformation on reactivity. Decalins. Conformational analysis of sugars. Anomeric effect.

UNIT – II Reaction Mechanism 25 L

Structure and reactivity: Ambident electrophiles and nucleophiles; Hard and soft concept. Acidity and basicity: Different concepts. Controlling structural factors, Methods of determining reaction mechanism: Kinetic and non-kinetic methods. Hammet and Taft equations.

Reactive intermediates: Nonclassical carbocations; Carbenes, nitrenes, – Generation, structure, reactions

Nucleophilic substitution reactions: Recapitulation of SN1, SN2 ,SNi reactions with stereochemistry. SNcA and SN' reactions, Nucleophilic substitutions at sp2 hybridized carbon and aromatic ring, including vicarious substitution. Factors affecting reactivity.

Neighbouring group participation

Elimination reactions: E1, E2 and E1cB mechanisms. Orientation in elimination reactions; Reactivity: Effect of substrate, base, leaving group, medium. Pyrolytic elimination reactions.
Addition to carbon–carbon multiple bonds: Additions involving electrophiles and free radicals: Mechanism, reactivity, orientation and stereochemistry, regio- and chemo-selectivity.

Course outcome:

1) To be able to predict, identify and distinguish between various types of stereogenic units present in the molecules.
2) Gains preliminary knowledge of NMR spectroscopic technique.
3) To be able to predict major/minor stereoisomers in a given asymmetric reaction.
4) At the end of the course, the student should be able to propose/write a mechanism for a given organic reaction.
5) To be able to design experiments to determine reaction intermediates/mechanisms.
6) Knowledge of reactive intermediates

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	3				3	1	
CO2	2		1		1	1	
CO3	3	2			2	1	
CO4	2	1	2	2	2		
CO5	3	1	2	2	2	1	
CO6	3	1			3		

Reference Books

1. Organic stereochemistry, Robinson M.J. T., Oxford University Press, 2005.
2. Stereochemistry of Carbon compounds, Eliel E. L., Wilen S. H. and Manden L. N., Wiley, 1995.
3. Stereochemistry: Conformation & Mechanism, Kalsi P. S., Wiley Eastern Ltd., New Delhi, 1993.
4. Stereochemistry of Organic compounds, Nasipuri D., Wiley Eastern, 1991.
5. Advanced Organic Chemistry, Carey F.A. and Sundberg R.J., Plenum
6. A Guide book to mechanism in Organic chemistry, Sykes Peter, Prentice Hall.
7. Organic reaction mechanism (Benjamin) Breslow R.
8. Advanced Organic Chemistry: Reactions, Mechanism, and Structure, Smith M. B. and March J., John Wiley.
9. Reactive Intermediates in Organic chemistry Issacs N. S, John Wiley.
10. Organic Reaction Mechanisms: Ahluwalia V. K., Parashar R. K.
11. Reaction mechanism in Organic Chemistry, Mukherji S.M. and Singh S.P., Mcmillan.
12. Understanding Organic Reaction Mechanisms, Adam Jacobs, Cambridge University Press.
13. Advanced organic chemistry: Reaction mechanism, Reinhard Bruckener, Elsevier, 2008.
14. Advanced organic chemistry: Reactions and mechanism, M.S. Singh, Pearson Education, 2007

Assessment method: Written (and if necessary – Seminar/Assignment/Viva)

CHM-403 **Quantum Chemistry** **3 Credits**

Course level: Advance/Mastery

Pre-requisite: High school mathematics

Course Description:

This course aims to introduce concept of energy quantization to understand the failure of classical mechanics and analysis of microscopic particles/systems. It offers learning of mathematical formulations through wave function to characterise atomics systems.

Course Contents:

Quantum Chemistry: Historical background of quantum mechanics, Elementary classical mechanics, linear harmonic oscillator, Blackbody Radiation, Photoelectric effect, Planck's Hypothesis, Classical wave equation, Plane-wave solutions, De Broglie matter waves. Uncertainty principle.Time dependent and independent Schrödinger equation. Particle in one dimensional box with infinite and finite walls. Tunneling. Particle in three dimensional box, Separation of variables, Degeneracy.

Postulates of quantum mechanics and their analysis. Operators, Eigenfunctions and Eigenvalues, Expectation values, Dirac Delta function, Step function. Harmonic Oscillator wave function and operator methods. Angular momentum: Angular momentum in quantum mechanics in terms of ladder operators.

Applications of Quantum Chemistry: Electron spin; Pauli spin matrices. Spin and magnetic field Exchange; Slater determinant.Spin-orbit coupling. Spectral term symbols. Time dependent and time independent Schrodinger equation and applications to H, H2+ and He+ systems. Perturbation theory, Variational theorem and its application. Valence bond theory, MO theory, Hybridization, Hückel MO theory and its application to conjugated systems

Course outcome:

1) Knowledge of Schrodinger wave equation and its application to one electron system.
2) Adapt in quantum mechanics principles to apply for rotational and vibrational energy analysis of molecules.
3) Enhancement in understating of molecular orbitals and the basis of orbital shape, size and energy.
4) Advancement in learning of variation and perturbation methods to perform quantum calculation of simple atomic/molecular systems.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	1	1	1	1	3	1
CO2	3	2	1	1	1	3	1
CO3	3	2	2	1	1	3	1
CO4	3	3	2	1	1	3	1

Reference Books:

1. Mathematics for physical chemists, Mortimer R.G. (2005) 3rd edition, Elsevier.
2. Mathematical Methods for Physicist by Arfken & Weber (1995) Academic Press.
3. Mathematical Methods for Scientists and Engineers, McQuarrie (2003) 1st edition, Univ Science Books.
4. Valency, Coulson C.A. (1979) 3rd edition, ELBS.
5. Physical Chemistry, Atkins P.W. (1987) 3rd edition, ELBS.
6. Introduction to Quantum Mechanics with applications to Chemistry by Pauling L. &Wilson E.B. (1985) 3134th edition, Dover Publications.
7. Introduction to quantum chemistry., Chandra A.K. (1998) Tata McGraw Hill
8. Quantum Chemistry, Levine I. N. (2000) Prentice Hall.
9. Molecular Quantum Mechanics, Atkins P.W. and Friedmann R.S. (2010) Oxford University Press.
10. Elementary Quantum Chemistry, F. L. Pilar (1968) McGraw-Hill.
11. Quantum Chemistry, D.A. McQuarrie (2003) Viva books.
12. Quantum chemistry, Lowe J.P. and Peterson K.Q.C. (2005) Academic press.
13. Orbitals in chemistry, Gil V. (2000) Cambridge University Press.

Assessment method: Written (and if necessary - Seminar/Assignment/Viva)

CHM-404 Group Theory and Spectroscopy 3 Credits

Course level: Advance/Mastery

Pre-requisite: CHM-504 (Molecular Structure and basic knowledge of Spectroscopy)

Course Description:

This course render a broad over view of various physical aspects (e.g. dipole moment, molecular orbital, hybridization, different mode of motion etc.) of an object/molecule by considering its symmetry elements with the help of mathematical approaches. This algebraic approach illustrate the construction of “Character Table” (main theme of this course) and its utility towards the application. Moreover, this topic imparts comprehensive understanding of vibration, rotational, electronic and other spectroscopy. Above all, this course would be very useful to get in-depth knowledge of spectroscopy and its application in advance level.

Course Contents:

Group theory: Groups, subgroups & classes, Symmetry elements, operations & associated algebra, Elements of group theory: Dipole moment & optical isomerism, Symmetry point groups, symmetry classification of molecules with examples, Representation of point groups, reducible & irreducible representations, Great orthogonality theorem, construction of character table, reduction formula, direct product, projection operator, symmetry adapted linear combinations.

Spectroscopy: Rotational & vibrational spectroscopy: Intensity & width of a spectral line, Electromagnetic spectrum, Einstein’s coefficient of spontaneous emission, transition moments & selection rules, Types of rotors, pure rotational spectra & energy levels, Stark effect, Rotational

Raman spectra, Selection rules for vibrational spectrum, anharmonicity, vibration-rotation spectra & spectral branches, Normal modes and vibrations of polyatomic molecules, exclusion principle, Electronic spectroscopy: Nature of transition, Franck-Condon factor, Quantum yield and radiative processes, Fluorescence & Phosphorescence, Elementary ideas of laser and laser action, Applications in chemistry, Symmetry aspects of molecular orbital theory with examples. Hybrid orbitals & molecular orbitals. Symmetry of normal modes, normal mode analysis, selection rule for IR & Raman transitions.

Course outcome:

1) Knowledge of various symmetry elements and their mathematical application
2) Extensive idea of various spectroscopy which includes Microwave, IR, Raman, Electronic Transition
3) Develop critical concept to sort out the ambiguous problem of molecular structure.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	2				3	
CO2	3	2				3	
CO3	3	3		1		3	

Reference Books:

1. Group theory in chemistry, Bishop (1993) Dover Publications.
2. Chemical applications of group theory, Cotton (1990) 3rd edition, John Wiley.
3. Introduction to molecular spectroscopy, G.M. Barrow (1962), McGraw-Hill Inc.
4. Symmetry in molecules, Hollas; J.M. (1972) Chapman and Hall.
5. Symmetry in chemistry, Jaffe H.H. and Orchin M. (2002) Dover Publications
6. Chemical applications of group theory, Cotton F.A. (1990) Wiley International.
7. Symmetry and spectroscopy: An introduction to vibrational and electronic spectroscopy, Harris D.C. and Bertolucchi M.D. (1990) Dover Publications.
8. Molecular spectroscopy, Machale J. (1999) Prentice Hall
9. Molecular spectroscopy, Hollas, J.M. (2004), 4th edition, John Wiley & Sons, New York
10. Fundamentals of molecular spectroscopy by C. W. Banwell and McCash, E. (1999) Tata McGraw Hill.
11. Physical methods for chemists by R S Drago (2016) 2nd edition, Saunders College Publication

Assessment method: Written (and if necessary – Seminar/Assignment/Viva)

CHM-430 Inorganic Chemistry Laboratory-I 2 Credits

Course level: Reinforce

Pre-requisite:

UG Level Chemistry Knowledge and practical chemistry basic knowledge

Objectives:

- To expose students to conduct the basic experiments that includes purification, estimation etc.
- To know the estimation of various metal ions in solution by gravimetric analysis

Course Outcomes:

- Know to use various analytical methods for metal complexes purifications.
- Able to determine the metal ion concentration using gravimetric analysis.
- Able to determine the hardness of water using titration techniques.

Course Content:

1. Gravimetry: Determination of unknown concentration of Barium, Lead, Copper, Nickel and Aluminium by gravimetric technique.
2. Paper Chromatography: Separation of metal complexes using paper chromatography.
3. Separation of colored and non-colored compounds by TLC.
4. Synthesis and purification of acetyl ferrocene by column chromatography and recording their absorption spectrum.
5. Determination of KCl concentration by ion exchange column chromatography.
6. Chemistry of Blue printing.
7. Compare the Δ^0 (cm^{-1}) value for three different ligands (H_2O, EDTA, en) of copper complex.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3			2	2	3	
CO2	3	3				3	
CO3	3					3	

Books and Reading References

1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge University Press, 1970.
2. Vogel‘s Textbook of Quantitative Analysis, revised J. Bassett, R. C. Denney, G.H. Jeffery and J. Mendham, ELBS.
3. Advanced Experimental Inorganic Chemistry by V. K. Ahluwalia and Sunita Dhingra, Manakin Press, New Delhi.

Assessment method: Based on experimental skill, Quiz and Viva.

CHM-440 (ORGANIC CHEMISTRY LABORATORY-I) 2 credits

Course level: Master
Pre-requisite: Chemistry Laboratory skills at UG level

Course Description:

To acquire the skills in purifying the mixture of compounds. To provide comprehensive knowledge in identifying constituents present in the molecule. This course will also provide acquaintance in performing few important named reactions.

Course Outcomes:

1) Gain profound skills of separation and purification techniques.
2) Able to identify the functional group and exact structure of the small organic molecules.

Course Content:

1. Purification of compounds: By crystallization, fractional crystallization, distillation, fractional distillation, vacuum distillation, and steam distillation.
2. Use of TLC for separation of organic compounds.
3. Separation of binary mixture containing monofunctional compounds and identification of both constituents, using microscale techniques, and preparation of a suitable derivative of any one component.
4. Single Step Preparation (Any Three)
    a) Acetylation – Preparation of Acetyl salicylic acid (Aspirin) from salicylic acid, Preparation of Acetanilide from aniline
    b) Aldol condensation – Preparation of chalcone from benzaldehyde
    c) Schotten-Baumann Benzoylation
    d) Reduction–Preparation of m-nitroaniline from m-dinitrobenzene: Preparation of ethyl benzene from acetophenone by Wolff-Kishner method
    e) Claisen Condensation – Preparation of ethyl acetoacetate from ethyl acetate
    f) Cannizaro reaction
    g) Nitration – Preparation of m-dinitrobenzene from nitrobenzene

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	1				3	1	
CO2	1				3	1	

Reference books:

1. Vogel's book of Practical Organic Chemistry, Longman Scientific & Technical, 5th Edition, 2006.
2. Organic chemistry experiments: Microscales and semimicroscales, Campbell, B. N. and Ali M, McCarty M, Books/Cole, 1994.
3. Techniques and experiments for organic chemistry, Ault A., University Science Books, 1998.
4. Multiscale Operational Organic Chemistry: A problem solving approach to laboratory course, Lehman,Prentice Hall, 2002.
5. Practical Organic Chemistry, F. G. Mann and B. C. Saunders, ELBS, Longmann, London, 1978.

6. The Systematic Identification of Organic Compounds, Shriner, R. L., Hermann, C. K. F., Morrill, D. Y., Curtin, D. Y. and Fuson, R. C. 8th Edition, 2004.
7. Systematic Qualitative Organic Analysis, H Middleton, Edward Arnold and Co., 1939.
8. A handbook of Organic Analysis: Qualitative and Quantitative, H. C. Clarke, CBS Publishers, 2007.

Assessment method: Written, Viva, Practical

CHM-450 Physical Chemistry Laboratory-I 2 Credits

Course level: Introductory

Pre-requisite: CHM-330 (UG Level Chemistry Knowledge and hands-on computer)

Course Objectives:
The aim of this course is to provide the basic concept of computer knowledge and an introduction to basic practical skills including safe working practices (risk, hazard and control measures), laboratory report writing (written and verbal communication of results), error and accuracy.

Learning Outcomes

1) Program writing skills for various chemistry concept.
2) Enhancement in data extraction and analysis skills.
3) Knowledge of various aspect of the critical miceller concentration.
4) Skill development to conduct experiments in Physical Chemistry individually.

Course Structure

Computer in Chemistry -Theory and Usage
Programming Language: Fortran -Basic knowledge of Fortran 90: Data statements, logical and arithmetic expressions, operators, I-O statements, implementation of loops, control statements, functions & subroutines, array, strings and character processing, format specifications, file processing and data structure.

Wet-Lab Physical Chemistry
Spectroscopy
1. Determination of composition of KMnO4 + K2Cr2O7 solution.
2. Determination of pKa of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar media.
3. Nickel/ molybdenum/ tungsten/ vanadium/ uranium by extractive spectrophotometric method.

Conductometry

1. To determine the critical miceller concentration (CMC) of sodium dodecylsulphate (SDS) and cetyltrimethylammonium bromide (CTAB) using conductivity method.
2. Precipitation titration and determination of solubility of sparingly soluble salts (Lead sulphate) by conductometry.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

Books & Reading References

1. Computers in Chemistry, Raman K.V., Tata McGraw Hill
2. Computer programming, Rajaraman V., Prentice Hall.
3. Experiments in Physical chemistry, Shoemaker D.P., Garland C.W. and Nibler J.W., McGraw Hill.

Assessment method: Experiment need to be performed (and if necessary - Seminar/Assignment/Viva/lab quiz)

CHM-405 COORDINATION CHEMISTRY 3 Credits

Course Level: Reinforce
Pre-requisite: Students who have studied the basic chemistry courses at UG level

Course Description: The course is designed to make students familiar with bonding theories of transition metal complexes like VBT, CFT and MOT. Advanced topics like structure, spectra and magnetic properties of transition metal complexes with examples will be discussed. In addition, course will make students familiar with fundamental reaction mechanism of transition metals.

Course Contents:
Metal-Ligand bonding theories: Werner's work, Valence Bond Theory (VBT), Crystal field theory (CFT) and its applications. Jahn-Teller effect. Molecular orbital theory of octahedral, tetrahedral and square planar complexes. Pi bonding in bonding in octahedral complexes.

Metal ligand equilibria in solution: Stepwise and overall formation constants and their interaction, trends in stepwise constants. Factors affecting stability of metal complexes with reference to the nature of metal ion and ligand chelate effect and its thermodynamic origin.

Electronic spectra of transition metal complexes: Types of electronic transition, selection rules for d-d transitions. Spectroscopic ground states, Orgel and Tanabe-Sugano diagrams for transition metal complexes. Calculation of Racah parameters, Charge transfer spectra.
Magnetic properties of transition metals: Different types of magnetic behaviour. Factors affecting observed magnetic moments. Origin of magnetic moment, spin contribution, spin only formulas, orbital contribution, spin-spin coupling. Methods for magnetic

CO/PO	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1			2	3	1		1
CO2			2	3	1		1
CO3				3	1		1
CO4			1	3	1		1

susceptibility measurement, Ferro- and antiferromagnetism, mechanism of anti-ferromagnetic interaction, spin cross over and anomalous magnetic moments.

Reaction mechanism of transition metal complexes: Energy profile of a reaction, reactivity of metal complex, inert and labile complexes, kinetics of octahedral substitution, acid & base hydrolysis, conjugate base mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution reaction. Mechanism of redox reactions.

Course Outcome: After successfully completing this course, students will be able to:

1) Understand the metal-ligand bonding and related theories in details.
2) Apply the principles of coordination chemistry in other fields.
3) Explain the basic structure and bonding in transition metal complexes
4) Understand the spectra and magnetic properties like subjects in depth
5) Apply these concepts in understanding the role of metal ions in metallobiomolecules.

Mapping of Course Outcomes (COs) with Program Outcomes (POs)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3					3	
CO2	3	3				3	
CO3	3					3	
CO4	3					3	
CO5	2		3				2

Text Books and Reference Books:

1) Advanced Inorganic Chemistry, Cotton F.A., Wilkinson G., Murollo C.A. and Bochmann M., John Wiley.
2) Inorganic Chemistry, Huheey J.E., Harper & Row.
3) Chemistry of the Elements. Greenwood N.N. and Earnshaw A., Pergamon.
4) Inorganic Electronic Spectroscopy, Lever A.B.P., Elsevier.
5) Magnetochemistry, Carlin R.I., Springer Verlag.
6) Inorganic Chemistry, Wilysberg G, University Science Books.
7) Physical Methods in Inorganic Chemistry, Drago R. S.
8) Inorganic chemistry, Shriver D. F., Atkins P. W. and Langford C. H., ELBS with Oxford University Press
9) Mechanisms of Inorganic Reactions: Study of metal complexes in solution by Pearson R G, Basolo F., John Wiley & Sons.

Assessment method: Written, assignments, seminars + Viva & Quizzes

CHM-406 Synthetic Methods in Organic Chemistry 3 Credits

Course level: Introductory / Reinforce
Pre-requisite: CHM-402 (Stereochemistry and Reaction Mechanism)

Course Description: This course deals with various strategies involved in organic synthesis, comprising transformations, reagents, protection-deprotection concepts and disconnections. Various functional group interconversions, and strategies related to carbon-carbon bond formation will be discussed to provide students a clear understanding and importance of organic synthesis. This course would serve as a stepping stone for other courses on more advanced synthetic concepts and methodologies.

Course Contents:
Metal and non-metal mediated oxidation-reductions:
Oxidation: Oxidation of alcohols; epoxidation and dihydroxylation, including asymmetric versions (Sharpless); oxidative cleavage of C-C double bonds; allylic oxidation; oxidation of ketones and aldehydes; single electron oxidation.

Reduction: Metal hydride reductions; single electron (dissolving metal) reductions; chiral borane reagents including CBS catalyst; asymmetric C-C bond reduction (Noyori's method including dynamic kinetic resolution); Shapiro reaction; catalytic hydrogenation (using Pd, Pt and Ni catalysts); transfer hydrogenation.

Hydroboration: Mechanism, regio- & stereoselectivity; asymmetric hydroboration.

Advances in Carbon–Carbon bond formation:
Enolate chemistry: Asymmetric Aldol reaction (Evans, Mukaiyama & Shibasaki aldol versions); Morita-Baylis-Hillman reaction – importance and applications.

Enamines & Iminiums: Preparation & synthetic applications, Mannich reaction and importance, SAMP & RAMP hydrazones, introduction to organocatalysis – asymmetric enamine and iminium catalysis.

Ylides: Phosphorus ylides; Wittig reaction and its modifications; comparison with other olefination methods; Sulphur ylides - anions derived from sulfoxides and sulfones – Corey-Chaykovsky reaction.

Rearrangements: Important rearrangements in C-C and C-X bond formation.

Designing Synthesis:

Disconnection approach and Retrosynthetic analysis: Idea of synthons, reagents; one group C-X and C-C disconnections; two group disconnections – 1,3 and 1,5-difunctionalized compounds; introduction to ring synthesis – general methods, rules and conventions.

Protection-deprotection of functional groups: Carbonyl, hydroxyl, amino, carboxyl – reagents and methods for protection and deprotection; selectivity aspects.

Umpolung of reactivity: Concept of Umpolung, generation of acyl anion equivalent; N-heterocyclic carbenes (NHC's) and Umpolung of reactivity.

Course outcomes:

1) Knowledge of reagents and methods for various functional group interconversions in synthesis
2) Sound grasp of the concepts of various types of carbon-carbon bond formation, including asymmetric methods
3) Understanding of disconnection strategies and significance of protecting groups
4) Equipped to take up advanced courses in synthetic chemistry and natural products

Mapping of Course Outcomes (COs) with Program Outcomes (POs)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	1			2	3	
CO2	2	2	1		2	2	
CO3	3	1	1		2	2	
CO4	3	2	2		2		1

Reference books

1) Advanced Organic Chemistry: Part B: F.A. Carey and R.J. Sundberg (2007) 5th edition, Springer.
2) Organic Chemistry: J. Clayden, N. Greeves, S. Warren and P. Wothers (2000) 1st edition, Oxford Univ Press
3) Modern methods of Organic synthesis, Carruthers W. (2004), 4th edition, Cambridge University Press
4) Catalytic Asymmetric Synthesis, Iwao Ojima (2010) 3rd edition, Wiley
5) Principles of Asymmetric Synthesis, R. E. Gawley and J. Aube (2012) 2nd edition, Elsevier
6) Organic synthesis: The disconnection approach, S. Warren, P. Wyatt (2008), 2nd edition, Wiley
7) Greene's protective groups in organic synthesis, P. G. M. Wuts (2014), 5th edition, Wiley

Assessment method: Written (and if necessary - Seminar/Assignment/Viva)

CHM-407 **Thermodynamics** **3 Credits**

Course level: Advance/Mastery

Pre-requisite: CHM-201, CHM-303, CHM-403

Course Description: This course deals with computing the change in macroscopic properties (e.g. Pressure, Volume, Temperature etc.) in different ideal and non-ideal systems under perturbation. Moreover, description of statistical part exhibit the theoretical interpretation in correlation between the macroscopic to microscopic properties during the course of changing of a system. Strategically, one can simulate the system subjected to transforming from one physical state to another with the help of various assumption. Above all, this course would impart the knowledge of mathematical description of various indecisive systems.

Course Contents:

Laws of thermodynamics: Statistical interpretation of entropy, thermodynamic potentials, chemical potential; thermodynamic properties of ideal gases and mixtures of ideal gases; thermodynamic treatment of non ideal gases.

Reaction equilibrium: Reactions involving gases. Reactions involving pure condensed phases and a gaseous phase; Ellingham diagrams.

Single component phase diagram: Gibbs energies of pure phases and allotropes; Gibbs energy vs. Temperature and pressure; vapour pressure-temperature relation at equilibrium (Clausius - Clapeyron equation).

Binary solutions: Raoultian and Henrian solutions; Thermodynamic properties of ideal solutions; Non-ideal solutions, activity, activity coefficient, Gibbs-Duhem equation, interaction parameters; Regular solution model, concepts of positive and negative deviation, alpha – function.

Partial molar properties & their significance, fugacity: Concepts and determination, properties of ideal solution, non-ideal systems, excess functions for non-ideal solutions, partial molar quantities, determination of partial molar volume and enthalpy.

Statistical thermodynamics: Concept of distribution. Thermodynamic probability, Ensemble averaging, Canonical, grand canonical and micro canonical ensembles, Statistical mechanics for systems of independent particles and its importance in chemistry. Types of statistics: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Idea of microstates and macro states. Thermodynamic probability (W) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance. Assembly partition function.

Course outcome:

1. Knowledge of theoretical concept of various thermodynamics parameters.
2. Comprehensive understanding of mathematical derivation of different name's expression.
3. Develop critical concept to sort out the problem of various system transformation.

Mapping of Course Outcomes (COs) with Program Outcomes (POs)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3					3	1
CO2	3			2	2	3	1
CO3	3			2	2	3	1

Reference Books:

1) Physical Chemistry, Atkins P.W. (1987) 3rd edition, Oxford University Press ELBS
2) Physical Chemistry: A molecular Approach, McQuarria D.A. and Simon J.D. (1997) 1st edition, University Science Books.
3) Thermodynamics & Introduction to Thermostastics, Callen H B. (2006) Wiley.
4) Physical Chemistry, Levine Ira N. (2007) Tata McGraw Hill,
5) Physical Chemistry, Atkins P.W and Paula J. De, W.H. Freeman (2002) 7th edition, Oxford; New York: Oxford University Press.
6) Thermodynamics for Chemists, Glasstone S. (2008) Ewp,
7) Principles of Equilibrium Thermodynamics, Denbigh K. G. (1981) Cambridge University Press
8) Statistical Mechanics McQuarrie, D. A. (2008) Viva Books Pvt. Ltd.: New Delhi.
9) An introduction to Statistical Thermodynamics, Hill T.L. (1987) Dover Publications.

Assessment method: Written (and if necessary – Seminar/Assignment/Viva)

CHM-408 Spectroscopic Methods of Structure Determination Credits: 3

Course Level: Introductory to Advance
Pre-requisite: Basic Knowledge of Organic Chemistry

Course Description: The course shall cover basic concepts of spectroscopy, viz. UV, IR, NMR, Mass and their combined applications. It will enable students to solve structures of known and unknown molecules and drugs.

Course Contents:
Electromagnetic spectrum, basic laws of absorption, electronic transitions, Woodward Fieser Rules for conjugated dienes and α, β-unsaturated carbonyl compounds, UV spectra of aromatic compounds. IR region and IR absorption, types of molecular absorptions, origin of vibrational spectra, number of fundamental vibrations, vibrational coupling, the finger print region, instrumentation, Group frequencies and application to simple problems.

Nuclear spin, resonance condition chemical shift and factors affecting it, coupling constants and factors affecting it, complex coupling patterns, NOE, NMR shift reagents, .13C NMR, 2D NMR, COSY, HETCOR, NOESY, APT, DEPT, INEPT.

Molecular ion peak, methods of ionisation – EI, CI, FAB, ESI, Maldi-TOF; HRMS, accurate mass measurement, resolution, mass fragmentation patterns and mass spectra of representative class of compounds, Structure elucidation using combined spectroscopic techniques.

Course outcome:

1) Complete knowledge of basic spectroscopic techniques
2) Shall be able to handle simple and complex research problems
3) Design spectroscopic experiments to solve unknown R & D problems in industry and advanced research laboratories.

Mapping of Course Outcomes (COs) with Program Outcomes (POs)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3					3	
CO2	3	2				3	
CO3	3	1				3	

Reference Books:

1. Spectroscopic Methods in Organic Chemistry, Williams & Fleming, 6th Edition, McGraw Hill, 2011.
2. Spectrometric Identification of Organic Compounds, Siverstein, Bassler & Morrill, 7th Edition, 2008.
3. Organic Chemistry, T. W. Graham Solomons and Craig B. Fryhle, 7th Edn., John Wiley & Sons, New York, 2000.
4. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George A. Kriz and James R. Vyvyan, 5th Edition, Cengage Leaning, USA, 2015.
5. Carbon-13 NMR Spectroscopy, J. B. Stothers, AP, NY, 1972.
6. Topics in ^{13}C NMR Spectroscopy Vol. 1-3, Ed. G.C. Levy John Wiley & Sons, NY 1979.
7. NMR – Basic Principles, Atta-ur-Rahman, Springer-Verlag, NY, 1986
8. Spectroscopic Methods in Organic Chemistry, M. Hesse, H. Meier and B. Zeeh, 2nd Edn, Thieme, 2007.
9. Mass Spectrometry – A Text Book, Jürgen Gross, Springer-Verlag Berlin, Heidelberg, 2002.
10. Mass Spectrometry – Principles and Applications, Wiley, Hoffman & Strobent, 2007.

Assessment method: Written, assignments & Quizzes.

CHM-460 Inorganic Chemistry Laboratory-II 2 Credits

Course level: Reinforce

Pre-requisite: UG Level Chemistry Knowledge and practical chemistry basic knowledge

Objectives:

- To expose students to conduct the basic experiments that includes estimation of different metal ions etc.
- To know how to determine the stoichiometry for metal complexes with chelating ligands.
- To know the estimation of ions in solution by gravimetric analysis.

Learning Outcomes:

1) Able to use various analytical methods for determining the metal complexes purifications
2) Able to determine the metal ion concentration using gravimetric analysis
3) Able to determine the hardness of water using titration techniques.

Course Content:

1 Fluorimetry: Emission and excitation spectra of a fluorescent compound.
2 Determination of concentration of a given sample of potassium permanganate by Colorimetry.
3 Determination of concentration of a given sample of Iron(II) by Colorimetry.
4 Solvent extraction methods using metal ions using suitable ligands.
5 Determination of stoichiometry of Iron-Phenanthroline complex: Job's method of continuous variations.
6 Simultaneous determination of two metal ions by spectrophotometry.
7 Determination of stoichiometry of Iron-Phenanthroline complex: Mole ratio.
8 Determination of stoichiometry of Iron-Phenanthroline complex: Slope ratio.
9 Determination of unknown concentration zinc by complexometric titration.
10 Determination of hardness of water by complexometric titration.

Mapping of Course Outcomes (COs) with Program Outcomes (POs)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	2	3	1	3		
CO2	3		3	1	3		
CO3	3		3	1	3		

Books and Reading References

1 Experimental Inorganic Chemistry by W.G. Palmer, Cambridge University Press, 1970.
2 Vogel's Textbook of Quantitative Analysis, revised J. Bassett, R. C. Denney, G.H. Jeffery and J. Mendham, ELBS.
3 Advanced Experimental Inorganic Chemistry by V. K. Ahluwalia and Sunita Dhingra, Manakin Press, New Delhi.

Assessment method: Based on experimental skill, Quiz and Viva.

CHM-470 Organic Chemistry Laboratory-II 2 credits

Course level: Master

Pre-requisite: CHM-440

Course Description:

This course deals with laboratory experiments of ternary mixture separations using techniques like filtration, distillation etc. followed by identification of compounds through functional group identification. Some advance experiments like determination of optical purity of chiral compounds using polarimeter, separation of (chiral) compounds on HPLC and /or GC. Two step preparations of compounds using well known organic reactions learned by the students in their theory classes.

Course Outcome:

1) Gain the skills in basic techniques required for separation of organic compounds in complex mixture.
2) To be able to handle the instruments like GC, HPLC and Polarimeter.
3) Become trained in the art of multistep synthesis.

Course Content:

Estimation of the amount of aniline/phenol in the given unknown solution; determination of the strength of the given glucose solution by Fehling solution method; separation of ternary mixture; determination of optical purity of a given compound using Polarimeter; separation of a given mixture using GC; separation of a given mixture including stereoisomers using HPLC; two-step preparation (e.g. preparation of EOSIN from Fluorescence using phthalic anhydride; preparation of chalcone followed by olefin epoxidation.

Mapping of Course Outcomes (COs) with Program Outcomes (POs)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	1				3	1	
CO2	1				3	1	
CO3	1				3	1	

Reference Books:

1) Vogel's book of Practical Organic Chemistry (2006), 5th Edition, Longman Scientific & Technical.
2) Organic Chemistry A Lab Manual, Pavia, Lampman, Kriz and Engel (2009), Cengage Learning.
3) The Systematic Identification of Organic Compounds, R. L. Shriner, C. K. F. Hermann, T. C. Morrill, D. Y. Curtin, and R. C. Fuson (2004), 8th Edition, John Wiley & Sons.
4) Techniques and Experiments for Organic Chemistry, A. Ault (1998), 6th Edition, University Science Books.
5) Organic Chemistry Experiments: Microscale and Semi-Microscale, Campbell, B. N. and McCarthy, M.(1994), Pacific Grove, CA.
6) Practical Organic Chemistry, Mann & Saunders (2009), 4th Edition, Pearson.

Assessment method: Experimental and Viva

CHM-480 **Physical Chemistry Laboratory-II** **2 Credits**

Course level: Advance/Mastery

Pre-requisite: UG Level Chemistry Knowledge

Course Objectives:

An introduction to basic practical skills including safe working practices (risk, hazard and control measures), laboratory report writing (written and verbal communication of results), error and accuracy

Learning Outcomes:

1) Explain the effect of (i) temperature (ii) change of concentration of reactants and catalyst (iii) ionic strength of the media and be able to determine the energy of activation.
2) Calculate the equilibrium constant, standard Gibbs free energy.
3) Extract the model from experimental data.
4) Define the term and determine the enthalpy and entropy change associated with a reaction.
5) Setup glassware and apparatus to conduct experiments in Physical Chemistry.

Course structure:

Kinetics:

1. Determination of the effect of (i) Change of temperature (ii) Charge of concentration of reactant and catalyst and (iii) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reaction. And determine energy of activation.
2. Determination of the velocity constant of ionic reaction in micellar media.
3. Polarimeter: Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter. Enzyme kinetics-inversion of sucrose.
4. Oscillatory reaction.

Thermodynamics:

5. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
6. Study the influence of ionic strength on the solubility of CaSO4 and hence determine its thermodynamic solubility product and mean ionic activity.

Phase Equilibria:

7. Partition coefficient of Iodine in water and carbon tetrachloride.
8. Distribution coefficient of succinic acid in water and ether.

Electrochemistry:

9. Determination of diffusion co-efficient and hydrodynamic radius of K3Fe(CN)6 by cyclic voltammetry (CV).

10. Cyclic voltammetry of fullerene (C60)/ferrocene.
11. Verification of Kouhlrasch's Law (Determination of eq. conductivity of a weak electrolyte at infinite dilution).
12. Verification of Debye-Huckle-Onsager equation.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1			1	3	1		1
CO2			1	3	1		1
CO3			1	3	1		1
CO4			1	3	1		1
CO5			1	3	1		1

Books & Reading References

1. Experiments in Physical chemistry, Shoemaker D.P., Garland C.W. and Nibler J.W., McGraw Hill.
2. Systematic Experimental Physical Chemistry by S.W. Rajbhoj and T.K. Chondhekar, Anjali Publication.
3. Experimental Physical Chemistry by V.D. Athawale and Parul Mathur, New Age International (P) Ltd. Publishers.

Assessment method: Experiment need to be performed (and if necessary – Seminar/ Assignment/ Viva/ lab quiz)

CHM-501 Organometallic Chemistry 3 Credits

Course level: Introductory/Reinforce
Pre-requisite: Students who have studied the basic chemistry courses at UG level

Course content:

UNIT̃ I

4 Introduction: Types of transition metal to carbon bonds. Classification of organometallic compounds based on hapticity and polarity of M-C bond. Nomenclature and general characters. Synthesis, stability and decomposition pathways. Electron counting and 16 and 18 electron rules - applications and exceptions. 6L

5 Alkyl and aryl complexes of transition metals: Synthesis, stability and decomposition pathways, organocopper compounds in organic synthesis. 2L

6 Transition metal π-complexes: Transition metal π- complexes with unsaturated organic molecules, CO, alkenes, alkynes, allyl, diene, cyclopentadienyl, arene complexes: preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis. 7L

UNIT̃II

7 Compounds with Metal-carbon multiple bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bonds, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis. 7L

8 Bimetallic and cluster complexes: Structure and applications in catalysis. 2L

9 Fluxional organometallic compounds: Fluxionality and dynamic equilibria in organometallic compounds – (i) Compounds with acyclic alkenes (ii) Compounds with σ-bonded cyclic alkenes (iii) Compounds with one or more cyclopolyenes π-bonded or σ and π-bonded to several metal atom (iv) Compounds involving rotation of ligands on metals (v) Compounds involving ligands scrambling on metals. 6L

UNIT̃ III

10 Basic organometallic reactions: Ligand substitution, oxidative reactions, migratory reactions, migratory insertion, extrusion, oxidative addition, reductive elimination, reductive elimination –mechanism and stereochemistry. 4L

11 Organometallic Chemistry: Selected Synthetic Applications 10L

Organopalladium Chemistry – Wacker process, Heck reaction, Cross Coupling reactions – Suzuki, Sonogashira, Negishi, Stille, Kumada coupling; -allyl palladium chemistry; Carbonylation, hydroformylation, aryl aminations - Buchwald-Hartwig amination & Organo-Cu modification.

Other transition metal complexes: Cr carbonyls – regioselective alkylation & acylation of aromatics & nucleophilic substitution; Co carbonyls in Hydroformylation, carboxylation and application in the Pauson-Khand reaction; reactions of Fe carbonyls; Organo-Ti chemistry – Tebbe's and Petasis reagents.

Organo-Si chemistry – -silicon effect; Peterson olefination; Brook's rearrangement and applications. Olefin metathesis – Cross metathesis, RCM, ROM, ROMP, kinetic resolution in metathesis, Grubb's and Schrock's catalysts.

12 Importance of organometallic compounds in biological systems 1L

Course outcome:

1. Have a good overview of the fundamental concept of organometallic chemistry: Synthesis, structure, bonding, properties and reactivity of organometallic compounds.
2. Know important applications of organometallic compounds as catalysts in organic synthesis.
3. Able to explain and rationalize the industrial important catalytic process using organometallic complexes based catalysts.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3					3	
CO2	3	2				3	

CO3	3			2		3	

Reference Books

1. Principles and applications of organotransition metal chemistry, Collman J.P., Hegsdus L.S.,. Nortan J.R. and Finke R.G., University Science Books.
2. The Organometallic chemistry of the transition metals, R.H. Crabtree, John Wiley.
3. Metallo-organic chemistry, Pearson A.J., Wiley.
4. Organometallic Chemistry: A unified approach, R.C. Mehrotra & A. Singh, New Age International.
5. Organometallic Chemistry and Catalysis, Didier Astruc, Springer Science & Business Media.
6. Organometallics, Christoph Elschenbroich, Wiley VCH, Weinheim.
7. Handbook of reagents in organic synthesis, P. Wipf, John Wiley & Sons.
8. Organic Chemistry, Jonathan Clayden, Nick Greeeves, Stuart Warren, Oxford University Press, 2nd Edition.
9. Basic Organometallic Chemistry: Concepts, Syntheses and Applications, B. D. Gupta and Anil J. Elias, Universities Press & CRC Press.
10. Organotransition metal chemistry, Anthony F. Hill, RSC.

Assessment method: Written, assignments & Quizzes.

CHM-502 **Pericyclic Reactions and Photochemistry** **3 Credits**

Course level: Introductory / Reinforce / Mastery
Pre-requisite: CHM-402 (Stereochemistry and Reaction Mechanism)

Course Description: This course introduces the students to the domain of pericyclic reactions – concerted reactions that are mediated by heat / light and are characterised by a cyclic transition state. The course also explores the photochemistry of organic compounds and their applications in synthesis. The course also sheds light on the chemistry of free radicals and associated synthetic transformations.

Course Contents:
Pericyclic reactions:
General: Classification, MO's of simple acyclic and cyclic polyenes; FMO and role of FMO in organic reactions.

Electrocyclic reactions: Conrotatory and disrotatory motions, 4n and 4n+2 π electron systems; analysis using different approaches; important examples; torquoselectivity and applications; Nazarov cyclisation.

Cycloaddition: analysis of cycloadditions – suprafacial and antarafacial interaction; Diels-Alder reaction – regioselectivity & stereoselectivity; Alder’s endo rule; normal and inverse electron demand Diels-Alder reactions; retro-cycloadditions; cheletropic reactions; 1,3-Dipolar cycloadditions; [2+2] cycloadditions.

Sigmatropic rearrangements: H-migration and Carbon-migration, analysis – supra and antarafacial migrations – retention & inversion of configuration; Cope and Claisen rearrangements; [2,3]-sigmatropic shifts.

Ene & retro-ene reactions and applications.

Photochemistry:
Introduction: Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule.; life times of reactive intermediates; types of photochemical reactions; concept of photo-sensitisation and quenching.

Photochemistry of alkenes: cis-trans isomerisation & photostationary state; optical pumping.

Photochemistry of carbonyl compounds: Paterno-Buchi reaction; Norrish Type I & Type II reactions; photoreduction; intramolecular reactions.

Photochemical rearrangements – di-π-methane and oxa- di-π-methane rearrangements, dienone phenol rearrangement; Photo-Fries reaction of anilides and Photo-Fries rearrangement.

Photochemistry of aromatic compounds: Isomerisations, additions and substitutions.

Free Radicals in organic synthesis:
General aspects & Reactivity: Generation, stability, electrophilic & nucleophilic radicals and their reactivity.

Chain reactions and non-chain reactions: Mechanisms and important examples of each; addition, fragmentation & polymerisation reactions; radical rearrangements

Radical cyclisations: Baldwin's rules; applications in synthesis.

Miscellaneous reactions: 1e- oxidations and reductions; triplet carbenes & applications

Course outcomes:

1) Sound grasp of concepts related to pericyclic reactions and their applications in synthesis
2) Knowledge of various organic photochemical reactions and rearrangements, and synthetic applications
3) Understanding of various types of radical reactions and a good grasp of the mechanisms involved.
4) Equipped to take up advanced courses in synthetic chemistry and natural products

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	2	1	1	2	3	
CO2	2	1	2	1	1	2	
CO3	3	2		1	1	3	
CO4	2	1	3		2		1

Reference books:

1. Pericyclic reactions, Ian Fleming, Oxford Chemistry Primers, 2nd Edition
2. Pericyclic reaction, G. Gill, Chapman & Hall Chemistry Textbook Series
3. Pericyclic reactions, Mukherji S.M., MacMillan
4. The art of writing reasonable organic reaction mechanisms, Robert B. Grossman, Springer, 2nd Edition
5. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy and J. C. Scaiano, University Science Books
6. Advanced organic chemistry, F. A. Carey and R. J. Sundberg, Springer, 5th Edition
7. Organic Photochemistry, Coxon J. and Halton B., Cambridge University Press.

Assessment method: Written (and if necessary - Seminar/Assignment/Viva)

CHM-503 Solid State and Material Chemistry 3 Credits

Course level: Advance/Mastery

Pre-requisite: CHM-412 (fundamental knowledge of Solid state stuctures)

Course Description:

This course communicates mathematical comprehension of various category of solid states and its physical aspects which includes crystal structure, crystal defects, electronic properties, band structure, magnetic and optical property etc. In addition, it provides more insight towards the chemical properties, featuring various kind of doping process, alloy formation, surface chemistry and catalytic activity etc. Moreover, this topic impart the understanding of mechanism in various kind of modernised instrumentation. Nonetheless, foundational concept of nanoscience and its various applications in current field of research are acquainted. Above all, this course would be very useful to get catholic knowledge of material science and its advancement in application field.

Course Contents:

Solid state chemistry: Crystal structure, crystal types, crystal defects. Electronic structure of solids– Band theory.Superconductivity.Theory of insulators, semiconductors and metals.Optical and magnetic properties.Alloys. Solid state reactions

Surface Chemistry: Surface excess properties and thermodynamics. Surface tension, capillary action

Adsorption: Thermodynamics and kinetics. Estimation of surface area (BET). Surface films on liquids.Catalytic activity at surface.Surface active agents and various aggregations of them in aqueous solutions, CMC and factors affecting CMC. Thermodynamics of micellization. Microemulsions.

Surface characterization: Surface area, surface acidity and basicity, XPS, UPS, AES, EXAFS, XANES, XRD TPD SEM TEM etc.

Catalysis: Types of catalysis: Heterogeneous and Homogeneous catalysis, advantages and disadvantages. Catalytic cycles. Heterogeneous catalysis: Preparation methods, characterization and quantification of surface active sites, kinetics of heterogeneous catalytic reactions. Structure of adsorbed species.Supported catalysts and metal-support interaction. Catalyst deactivation and regeneration.

Nanomaterial: Elements of nanoscience and nanotechnology, introduction of nanoscale materials: fullerenes, nanotubes, nanoparticles, nanorods/ nanowires, and nanofibers. Synthesis and fabrication of nanomaterials: Top-down approaches (mechanical process, nanolithography, thermal evaporation), and bottom-up approaches (chemical synthesis, sol-gel processes). Properties of nanomaterials: melting point and phase-transition, quantum size effects, size-induced metal-insulator transition, optical properties, chemical reactivity.

Course outcome:

1. Knowledge of various kind of solid state and its crystal structure and its physical and chemical properties.
2. Comprehensive understanding of ultramodern instruments for characterization.
3. Develop critical concept in order to implement in different application based research.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	1				3	
CO2	3	1	2			3	
CO3	3	3	3	1		3	

Reference Books:

1. Solid state chemistry and its applications, West A.R. (2014), Student Edition, Wiley.
2. Principles of solid state, Keer H.V (1994), Wiley-Blackwell
3. Solid state chemistry: An introduction, Moore E., and Smart L. (1996) Chapman Hall
4. X-ray diffraction, Warren B. (1990) Dover Publications.
5. Introduction to crystallography, Sands, D.E. (2012) Dover Publications.
6. Homogeneous transition metal catalysis, Masters C. (1980) Springer.
7. Principles and practice of heterogenous catalysis, Thomas J.M. and Thomas M.J., John (2015) 2nd edition, Wiley.
8. Concepts of modern catalysis and kinetics, Chorkendoff I. B. and Niemantsverdriet J. M.

(2017) 3rd edition, Wiley
9. The Physics and Chemistry of Nanosolids; Frank J. Owens, & Charles P. Poole, Jr. (2008) Wiley.
10. Introduction to Nanoscience & Nanotechnology; G. L. Hornyak, H. F. Tibbals, J. Dutta and J. J. (2008) 1st edition, CRC Press
11. Nano: The Essentials, T. Pradeep (2017) 1st edition Tata McGraw-Hill.

Assessment method: Written (and if necessary – Seminar/Assignment/Viva)

CHM-504 Basic Bioinorganic Chemistry 3 Credits

Course Level: Advance/Mastery

Pre-requisite: Students who have studied the transition metal chemistry at UG & PG level

Course Description: Metalloenzymes and metalloproteins are the important component of biological system. They carry out the functions like transporting biochemical, catalysing biochemical transformations; almost every important reaction in biology requires presence of a metal centre. In order to understand these processes knowledge of specific functions carried out by these metals are necessary. This course will be helpful to understand the fundamental properties of the metals present in biological system and mechanism of their action.

Course Contents:

Overview of Bioinorganic Chemistry: Classification and scope of inorganic elements in biology. Metal Function of metal ions in Metalloproteins and Metalloenzyme, Principles of coordination chemistry pertinent to bioinorganic research. Storage and transport of metal ions

Transport and Storage Proteins: Metalloporphyrins, Oxygen Carrier, Hemoglobin and Myoglobin, Physiology of blood (O2 affinity, cooperativity and Bohr effect). Non-heme proteins: hemerythrin and hemocyanin, model inorganic systems

Dioxygen reactions: Chemistry of dioxygen, dioxygen toxicity and biological defense and repair systems: Superoxide dismutase and catalases, Cytochromes c oxidase, Monooxygenases: Cytochrome-P450, tyrosinase and methane monooxygenase, Dioxygenases.

Biological Redox Processes: Blue copper proteins, mitochondrial electron-transfer chain, Iron-sulfur proteins, and cytochromes

Metalloenzymes: Molybdenum enzyme - xanthine oxidase; Zinc enzymes - carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase, phosphatases, lipases and other hydrolases; Vitamin B12 and B12 coenzymes

Mn in Photosynthesis/O2 production (water oxidation): Photosystem I and II – Chlorophyll, Oxygen evolving complex (OEC), 4Mn –Cluster and O2 evolution

Medicinal Inorganic Chemistry: Metal deficiency - excess and disease; chelation therapy; metals used for chemotherapy, platinum complexes as anticancer drugs, Pt-DNA binding, other metal complexes as drug, side effects. Metal complexes in Radioimaging techniques: PET and SPECT imaging, MRI basic principle.

Course Outcome: After successfully completing this course, students will be able to:

1) Understand the role of metal ions in biology and how metal ions interact with biological environments.
2) Apply the principles of coordination chemistry in explaining how nature tailors properties of metal centres for specific applications.
3) Understand the role of metalloenzymes in bio-catalysis. Develop the scientific temperament to appreciate the powerful catalytic systems designed by nature and hence be capable to propose new bio-inspired model system for mimicking similar chemistry.
4) Learn the various aspects of medicinal inorganic chemistry including application of coordination complexes in diagnosis and treatment of different diseases.
5) Develop the ability to grasp current problems in bioinorganic chemistry and answer specific scientific questions using the knowledge provided during the course.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	3	3			2	
CO2	3						
CO3	3		3			3	
CO4	3			3			
CO5	3					3	3

Text Books and Reference Books:

1. Bertini, H. B. Gray, S. J. Lippard & J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd. (2004).
2. S. J. Lippard & J. M. Berg. *Principles of Bioorganic Chemistry*, Panima Publ. Corpn.
3. Robert R. Crichton, *Biological Inorganic Chemistry An Introduction*, Elsevier (2008)
4. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi. *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education, Inc 1993.
5. Shriver and Atkins *Inorganic Chemistry*, Fifth Edition, Publisher: Oxford University Press (2009).

Assessment method: Written, assignments, seminars + Viva & Quizzes

CHM-530 Inorganic Chemistry Laboratory-III 2 Credits

Course level: Reinforce

Pre-requisite: UG Level Chemistry Knowledge and practical chemistry basic knowledge

Objectives

- To expose students to conduct the basic experiments that includes synthesis and purification of inorganic complexes.
- To know the different analytical methods for purification and separation of metal complexes

Course Outcome

1. Able to synthesize various metal precursors.
2. Able to use various analytical methods for metal complexes purifications.
3. Able to analyze the IR, UV-Vis and NMR data.

Course Content

Synthesis and Characterization of transition metal complexes:

1. [Mn(acac)3]
2. [Fe(acac)3]
3. [VO(acac)2]
4. [Ni(NH3)6]Cl2
5. K3[Fe(C2O4)3]
6. [Cu(NH3)4]SO4.H2O
7. Cis& trans-K[Cr(C2O4)2(H2O)2].2H2O
8. Hg[Co(SCN)4]
9. [Co(NH3)6][Co(NO2)6]
10. Cis-[Co(trien)(NO2)2]Cl.H2O
11. Na[Cr(NH3)2(SCN)4]
12. Cu(PPh3)3]Cl

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	2			3	1	
CO2	3	2			2	1	
CO3	3	3	1	1	3	3	

Books and Reading References

1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge University Press, 1970.
2. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
3. Inorganic Preparations: a systematic course of experiments by Alexander King, Allen & Unwin Edition, London.

Assessment method: Based on experimental skill, Quiz and Viva.

CHM-540 **Organic Chemistry Laboratory-III** **2 Credits**

Course level: Advance/Mastery
Prerequisite: UG Level Chemistry Knowledge and practical chemistry basic knowledge ; **Preferable:** CHM-440 (Organic Chemistry Laboratory-I) and CHM-470 (Organic Chemistry Laboratory-II)
Course Description:
The course provides to the students the skills in handling of multi-step organic reactions. This course also emphasises the importance of yield and purity, while also introducing the students to real-time analysis using instrumentation techniques such IR, NMR, etc. for the characterization of compounds. Another objective of the course is the extraction of active ingredients from their natural sources.
Course Contents:

1 Multi-step Preparation (Any Two):
  - Synthesis of Organic Compounds through a sequence of three steps, involving important named reactions, new reagents, and green principles
  - Aspects such as conversion, overall yield, selectivity, atom economy etc. should be paid attention to.
  - TLC should be used to monitor the reaction and finding out the purity of the product.
    - ➢ Preparation of dibenzoylmethane from chalcone (prepared from benzaldehyde and acetophenone) via dibromochalcone
    - ➢ Benzaldehyde to Benzoin using N-heterocyclic carbene catalysis, followed by oxidation to benzyl and rearrangement to benzilic acid
    - ➢ Synthesis of chalcone from benzaldehyde, followed by Michael addition of ethyl acetoacetate and intramolecular aldol condensation

2 Extraction of natural products (any one):
  a. Caffeine from Tea leaves
  b. Active component from common drugs – paracetamol or aspirin
  c. Nicotindipicrate from Tobacco
  d. Casein from milk

3 Use of instrumental methods for identification/characterization of compounds (UV, IR, NMR and Mass spectral techniques based on availability)

4 Advanced Synthesis Experiments (any two):
  a. Photochemistry experiment – photoreduction of benzophenone to benzpinacol
  b. Stereoselective and non-stereoselective reactions – example using reduction of unsymmetrical ketones
  c. Synthesis of cycloadducts using the Diels-Alder reaction
  d. Grignard reaction

Learning Outcomes:
Students going through this laboratory course would be expected to:

1. Become trained in the art of multi-step synthesis
2. Gain profound skills related to the isolation of products and charecterisation techniques.
3. Possess deeper knowledge related to calculation of reaction stoichiometries and overall yield of products.
4. Become aware of the techniques for extraction of natural products from available sources.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	3	1	3	3	2	2

CO2	2	1		2	3	1	2
CO3	3	1			2		1
CO4	2	2	2		2	1	1

Reference books:

1 Organic Chemistry: A Lab Manual, Pavia, Lampman, Kriz & Engel, Cengage Learning
2 Vogel's book of Practical Organic Chemistry, Longman Scientific & Technical, 5th Edition, 2006
3 Multiscale Operational Organic Chemistry: A problem solving approach to laboratory course, Lehman, Prentice Hall, 2002.
4 Practical Organic Chemistry, F. G. Mann and B. C. Saunders, ELBS, Longmann, London, 1978.

Assessment method: Written, Viva, Practical

CHM-550 **Physical Chemistry Laboratory-III** **2 Credits**

Course level: Advance/Mastery

Pre-requisite: UG Level Chemistry Knowledge and practical chemistry basic knowledge

Course Objectives

The objective of the course is to apply the principles of spectroscopy, pH metry, conductometry, potentiometry and surface chemistry in contemporary experiments. It will help students to understand the basic concept of physico-chemical measurements and limitations of experiments in practical applications.

Learning Outcomes

1. Determination of the concentration of analytes and dissociation constant of indicators using spectroscopy and pH metry.
2. Calculation of critical miceller concentration (CMC) of surfactants using conductometry.
3. Determination of the degree of hydrolysis of a compound by pH and potentiometry.
4. Evaluation of thermodynamic properties (ΔG, ΔH, and ΔS) using electrochemical techniques.
5. Construction of the ternary phase diagram for microemulsion of TX-100 / water / cyclohexane.

Course structure

Potentiometry

1. Determination of activity and activity coefficient of electrolytes.
2. Potentiometric titration of a mixture of KCl + KBr + KI to determine the composition of each component in the mixture.
3. Determination of thermodynamic properties (G, H, and S) using electrochemical techniques.

4. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.

pH Metry

5. Determination of the acid and base dissociation constant of an amino acid (glycine/histidine/cysteine) and hence the iso-electric point of the acid.
6. Determine the degree of hydrolysis and the hydrolysis constant of aniline hydrochloride by pH/potentiometry.

Surface Chemistry

7. Determine and compare surface tension values of detergents of different trade mark.
8. Determine for the system: acetic acid charcoal the adsorption isotherm and constants ‘a and ‘b for a modified Freundlich equation.
9. Construct the ternary phase diagram for microemulsion of TX-100 / water / cyclohexane.
10. Investigation of the solubility of a three-component system and hence draw a tie line on a bi-nodal curve. System; acetic acid / water / butanol.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1			1	3	2		1
CO2			1	3	2		1
CO3			1	3	2		1
CO4			1	3	2		1
CO5			1	3	2		1

Books & Reading References

1. Experiments in Physical chemistry, Shoemaker D.P., Garland C.W. and Nibler J.W., McGraw Hill.
2. Systematic Experimental Physical Chemistry by S.W. Rajbhoj and T.K. Chondhekar, Anjali Publication.
3. Experimental Physical Chemistry by V.D. Athawale and Parul Mathur, New Age International (P) Ltd. Publishers.

Assessment method: Written, Viva, Practical

CHM–610 Analytical Chemistry and Inorganic Spectroscopy 3 Credits

Course level: Reinforce
Pre-requisite: UG level analytical chemistry knowledge

Course Description:

To study and use the specific methods to separate, purify, identify and quantify the mixture of unknown/known substance by various sophisticated instrumental (chromatographic or spectroscopic methods) techniques. Further, the students will acquire the knowledge in principle, instrumentation and applications of advanced techniques such as atomic spectroscopy (AAS, AES, AFS), Photoelectron spectroscopy (XPS, UPS and Auger), EPR, Mössbauer and radioanalytical method (NAA, Isotope dilution analysis).

Course Contents:

UNIT I

1. Data analysis and Fingerprint: Accuracy, precision, sensitivity and specificity. Significant figures. Determinate and indeterminate errors and minimization of errors, standard deviation. Fingerprint: Types, characterize and application.

2. Solvent extraction: Classification, distribution law, separation factor, extraction equilibria and extraction systems - Chelation, solvation and ion-pair formation. Application in metal ion separation. Batch, continuous and counter current extractions. Membrane separation.

3. Radioanalytical methods: Radioactivity as analytical tool. Neutron activation analysis - Instrumentation and application for trace and ultra trace analysis, isotope dilution analysis.

UNIT II

4. Chromatography: Types. Ion exchange chromatography, planar chromatography - paper and TLC. Stationary and mobile phases. GC – Theory, instrumentation and applications. Liquid-liquid partition chromatography. HPLC. Reverse phase chromatography. Size exclusion and Affinity chromatography.

5. Spectral methods: Basic Principles, Bear-Lambert Law. UV-Visible spectrophotometry - Instrumentation and application. AAS - Hollow cathode lamp, graphite furnace, interferences. AES. Flame photometry, ICP - AES. Fluorescence spectrophotometry - Principle and instrumentation. Basic principles of UPS, XPS and Auger Spectroscopy.

UNIT III

6. Mossbauer spectroscopy: Principle, isomer shift, isotropic and anisotropic electronic fields for iron and tin complex, effects of nuclear quadrupole on Mossbauer spectra.

7. ESR spectroscopy: ESR spectra of metal complexes: Zeeman interaction and energy levels, g factor, Ligand field effects, dipolar coupling, Hyperfine coupling and A parameter, super-hyperfine coupling. Orbital moment quenching and g values, Anisotropy in g and A values. ESR spectra of multielectronic ion complexes. Zero field splitting and Kramer's degeneracy, ESR spectra of d1 to d9 metal ions.

Course outcome:

Having successfully completed this course, students can find application in forensic science and also analyse inorganic, biological, environmental, and material samples even in trace amount.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3	3	2	2	3	3	1

Reference Books:

1. Analytical Chemistry, G. D. Christian, P. K. Dasgupta, K. A. Schug, (2004), 7th edition, John Wiley.
2. Fundamentals of Analytical Chemistry. D. A. Skoog. F. J. Holler, (1995), 7th edition, Brooks Cole.
3. Analytical Chemistry: Principles, J. H. Kennedy, (2011), 2nd edition, Cengage.
4. Analytical Chemistry: Principles and Techniques, L. G. Hargis, (1988), Englewood Cliffs (N.J.): Prentice-Hall.
5. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler, S. R. Crouch, (2006), 6th edition, Cengage Learning.
6. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler, T. A. Nieman, (1998), 5th edition, Harcourt Asia PTE Ltd.
7. Basic Concepts of Analysis Chemistry, S. M. Khopkar, (2008), 3rd edition, New Age Science.
8. Vogel’s Textbook of Quantitative Chemical Analysis, D. J. Barnes, J. Mendham, R. C. Denney, M. J. K. Thomas (2008), 6th edition, Pearson Education.
9. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, (2004), 7th edition, CBS Publishers & distributors.
10. Mossbauer Effect and its Applications, V. G. Bhide, (1973), Tata McGraw Hill.
11. Physical Methods for Chemists, R. S. Drago, (2016), 2nd edition, Affiliated East West Press Pvt. Ltd.

Assessment method: Written, Viva, Practical

CHM-612 **Natural Products** **3 credits**

Course level: Master
Pre-requisite: Undergraduate Chemistry

Course Description: This course introduces the students to the vast world of natural products and natural product synthesis. The initial part of the course focuses on biosynthesis of natural products pertaining to various classes such as terpenes, fatty acids, steroids, polyketides and alkaloids. The second part of the course pertains to advanced concepts of retrosynthesis and the laboratory synthesis of natural products, where the students shall be exposed to the concept of total synthesis with the help of classical and contemporary examples from literature.

UNIT – I Biogenesis and Biosynthetic Pathways in Natural System **15L**

Isoprene rule, mevalonic acid-isopentylpyrophosphate pathway; biosynthesis of monoterpenes, sesquiterpenes and diterpenes, triterpenes, squalene and cholesterol

Biosynthesis of fatty acids and polyketides

Shikimic acid/shikimate biosynthesis and mechanistic pathway; biosynthesis of aromatic amino acids; biosynthesis of quinolone, isoquinoline, indole and pyrrolidine alkaloids

UNIT – II Essential Concepts for Natural Product Synthesis 10L

Advanced disconnection strategies and techniques two-group disconnections involving 1,2-, 1,4- and 1,6-difunctionalized compounds; disconnections based on rearrangements.

Recent advancements in the use of protecting groups and deprotection methods

UNIT – III Total Synthesis of Natural Products 20L

Classics in Total Synthesis Specific examples of reserpine, strychnine & prostaglandin by Woodward / Corey; contemporary /modern examples of total synthesis of biologically active natural products (by the groups of Nicolaou, Danishefsky, Overman, etc.)

Total Synthesis Perspectives one or two important natural products, eg. Strychnine, taxol, etc., synthesised by various practitioners - comparison of strategies

Enhanced learning through Total Synthesis puzzles; using total synthesis as a tool for the recapitulation fundamental concepts & reaction mechanisms and illustration of modern concepts of bond formation such as organocatalysis and C-H activation

Course outcome:

1. This course opens up the students to the importance of total synthesis
2. Arms the students with the knowledge of contemporary methods of synthesis
3. The course also serves to assist the students in recapitulating the concepts learnt over previous semesters, such as mechanism, asymmetric synthesis, spectroscopy, etc., through examples of multi-step synthesis of natural products
4. Students going through this course are thus expected to be more rounded in their knowledge of various aspects of synthetic organic chemistry

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3				3	1	
CO2	2		1		1	1	
CO3	3	2			2	1	

Reference Books

1 Organic stereochemistry, Robinson M.J. T., Oxford University Press, 2005.

2 Stereochemistry of Carbon compounds, Eliel E. L., Wilen S. H. and Manden L. N., Wiley, 1995.
3 Stereochemistry: Conformation & Mechanism, Kalsi P. S., Wiley Eastern Ltd., New Delhi, 1993.
4 Stereochemistry of Organic compounds, Nasipuri D., Wiley Eastern, 1991.
5 Advanced Organic Chemistry, Carey F.A. and Sundberg R.J., Plenum
6 A Guide book to mechanism in Organic chemistry, Sykes Peter, Prentice Hall.
7 Organic reaction mechanism (Benjamin) Breslow R.
8 Advanced Organic Chemistry: Reactions, Mechanism, and Structure, Smith M. B. and March J., John Wiley.
9 Reactive Intermediates in Organic chemistry Issacs N. S, John Wiley.
10 Organic Reaction Mechanisms: Ahluwalia V. K., Parashar R. K.
11 Reaction mechanism in Organic Chemistry, Mukherji S.M. and Singh S.P., Mcmillan.
12 Understanding Organic Reaction Mechanisms, Adam Jacobs, Cambridge University Press.
13 Advanced organic chemistry: Reaction mechanism, Reinhard Bruckener, Elsevier, 2008.
14 Advanced organic chemistry: Reactions and mechanism, M.S. Singh, Pearson Education, 2007

Assessment method: Written (and if necessary - Seminar/Assignment/Viva)

CHM614 Medicinal Chemistry 3 Credits

Course Description:
The main objective of this course is to familiarize students with the fundamental concepts of drug discovery and development. To train students in various aspects of new drug design, development, drug screening, target identification, lead discovery, optimization and the molecular basis of drug design and drug action.

Course Content:
Unit-1
Introduction to Medicinal Chemistry
General Introduction, History, Objectives of the course, Brief summary of the course. Introduction to the Principles of Drug Discovery

Role of medicinal chemistry in drug discovery, clinical trials, drug discovery without lead
Lead Discovery Approaches: Random Screening, non-random screening, drug metabolism studies, clinical observations

Lead Modification identification of the pharmacophore, functional group modification, Structure-activity relationship, privileged structures and drug-like molecules

Receptors

Basic ligand concepts agonist, antagonist, partial agonist, inverse agonist, efficiency and potency

Interactions (Forces) involved in drug-receptor complexes

Receptor theories occupancy theory, rate theory and activation theory

Topographical and stereochemical considerations in drug receptor interactions

Unit-2
Enzyme Kinetics and Mechanism
Introduction: Scope, Enzyme kinetics in drug action
Mechanisms of enzyme catalysis; Electrostatic catalysis and desolvation; Covalent catalysis, acid-base catalysis, strain / distortion in enzyme catalysis
Coenzyme catalysis: Pyridoxal 5-phosphate (PLP), Tetrahydrofolate and Pyridine Nucleotides, Flavin coenzyme, Heme, ATP
Enzyme Inhibition Enzyme inhibition and inactivation
Kinetics of Enzyme inhibition
Theories of enzyme inhibition and inactivation, Enzyme activation of drugs-prodrugs Nucleic acids (NA) as targets for drug action
Chemical structure of DNA, Hydrogen bonding among base pairs
NA-interactive agents; Classes of drugs that interact with nucleic acids
Intercalation, NA-alkylation, NA-strand breaking and their importance in drug action.

Unit-3
Drug likeness
Drug like molecules and theories associated with the recognition of drug like properties. The concept of Chemical space Lipinski rule of five, Veber rules
Applications in drug design
Drug action after Metabolism
Basic concept of Metabolism: Phase I and phase II transformations
Prodrug: Basic concept and its utility in drug discovery, Mechanism of activation of prodrug, Classifications of prodrug

QSAR
Historical Aspects
Electronic Effects- the Hammett equation, lipophilic effects, experimental measurement of lipophilicity, logP and logD, effect of ionization on logP, calculation of logP and logD, Steric effects- the Taft equation
Hansch Analysis, Free-Wilson method, Topliss operational scheme

Course Outcome:

1 Students could be able to understand the drug action in the living system.
2 Able to design new drug candidates.
3 Able to integrate the role of enzymes and drugs.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3				3	1	
CO2	2		1		1	1	
CO3	3	2			2	1	

Books & Reading References

1. The Organic Chemistry of Drug Design and Drug Action, Silverman R. B., Academic Press.
2. Textbook of Drug Design and Discovery, Eds. Krogsgaard-Larsen P., Liljefors T., Madsen U., Taylor & Francis.
3. Drug Discovery A History, Sneader W., Wiley.
4. Medicinal Chemistry: An Introduction, Thomas G, Wiley.
5. Drug Discovery A History, Sneader W, John Wiley & Sons, Ltd
6. Comprehensive Medicinal Chemistry, Series Ed., Hansch C., Pergamon Press.
7. Burgers Medicinal Chemistry, Drug Discovery and Development, Wiley.
8. An Introduction to Medicinal Chemistry, Fourth Edition, Graham L. Patrick, Oxford Press

Assessment method: Written (and if necessary – Seminar/Assignment/Viva)

CHM-615 **Supramolecular Chemistry** **3 Credits**

Course level: Reinforce

Pre-requisite: Undergraduate level in General Chemistry

Course Description:
This course makes familiar in the topics of non-covalent bonding, molecular recognition, host-guest chemistry and self-assembly with artificial system of fascinating molecule such as crown ethers, cucurbiturils, spherands, cryptands, calixarene and cyclophanes.

Course Contents:
Introduction to Supramolecular Chemistry

- General Introduction, History, Objectives of the course, Brief summary of the course.

Introduction to the Principles of Molecular Recognition

- Non-covalent interactions: Ion pairing, Ion-Dipole Interactions, Dipole-Dipole interactions, Dipole-Induced Dipole and Ion-Induced Dipole interactions, vander Waals or Dispersion Interactions, Hydrogen bonding, Cation-π interactions, Anion– π interactions, π–π interactions, Closed shell interactions, Aromatic-Aromatic Interactions: Benzene Crystals, Edge-toface vs. π-π Stacking Interactions, N-H—π interactions, Sulfur-aromatic interactions, Benzene-Hexafluorobenzene π– stacking.
- Solvation and Binding: Hydrophobic Interactions, The Hansch Equation: Estimating the Hydrophobic Character of Small Functional Groups.

Principles of Cation Complexation

- Crown Ether Complexation: Structures, Nomenclature, Solvent dependence, Role of the Counterion, Cavity Size and Ion Radii, Complexation Enthalpy and Entropy, Nature of the Donor Atoms in the Crown, Complexation Kinetics.
- Cation Complexation by Cryptands: Structures of Cryptands and Their Complexes, X-Ray Crystal Structures of Cryptandes and Their Complexes, Stability in Solution, Kinetics of Cation Complexation by Cryptands.
- Cation Complexation by Spherands: Structures and Stabilities of Spherand Complexes. • The Lariat Ethers and Podands
- Complexation of Primary and Secondary Ammonium Ions: Complexes of Primary Ammonium Ions, Complexation of Secondary Ammonium Ions by Crown Ethers, The Ionic N+-HO bond.
- Synthesis: The High Dilution Rule, Templated Cyclizations, Crown Ether Synthesis, Cryptand Synthesis, Spherand and Hemipherand Synthesis

Anion Complexation

- Introduction: Scope, Challenges in Anion Receptor Chemistry,
- Halide Ion Receptors and Complex Stabilities, Protonation and Complexation Properties of Macrocyclic Polyamines and Synthesis
- Anion Receptors
- Applications of anion and cation complexation • Phase Transfer Catalysis and Anion Activation:
- Allosteric Effects

Complexation of neutral molecules in aqueous solution

- Cyclophane Receptors: Electronic Effects in Cyclophane Complexes with Aromatic Substrates, Complexation of Polyaromatic Hydrocarbons , Combination of Apolar Binding and Ion Pairing, Water Soluble Cyclophane Receptors

Hydrogen Bonding

- Hydrogen Bonds: Definition, Structure and Stability, Effect of angle and Bond Distance on Strength Strength

Molecular Self-Assembly

- Examples of Self-assembly in Nature, Biological Self-assembly
- Rotaxanes and Catenanes: From Cyclophanes to Catenanes, Properties of Catenanes, Rotaxanes, Switchable Catenanes and Rotaxanes Molecular Machines and Motors.

Course outcome:

1) Students will learn the role of supramolecular chemistry in organic chemistry, chemical biology and material science
2) Understand the concept of self-assembly, molecular recognition and non-covalent interactions
3) Apply these concepts for the preparation of functional materials for wide range of applications.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	2	2	2	1	1	2	
CO2	1	2	2	1	1	2	
CO3	1	2	1				

Reference Books:

1. Supramolecular Chemistry, J. W. Steed, J. L. Atwood (2009), 2nd Edition, John Wiley & Sons Inc.
2. Supramolecular Chemistry, J.–M. Lehn, (1995), 1st Edition, Wiley–VCH.
3. Macrocylic Chemistry, B. Dietrich, P. Viout, J. –M. Lehn, (1993), VCH.
4. The Weak Hydrogen Bond, G. Desiraju, T. Steiner, (2001), Oxford science publications.
5. Principles and Methods in Supramolecular Chemistry, H.–J. Schneider, A. Yatsimirsky, (2000), Wiley.
6. Crystal Engineering: A textbook, G. R. Desiraju, J. J. Vittal and A. Ramanan, (2011), World Scientific Publishing Co. Pte Ltd.

Assessment method: Written (and if necessary – Seminar/Assignment/Viva).

CHM-619 **Green Chemistry** **3 Credits**

UNIT- I

1. Green chemistry: General aspects of Environment, Environmental Toxicology, Renewable energy, Green chemistry and Sustainability: History, need, and goals. Green chemistry and Sustainability. Dimensions of sustainability, Limitations/Obstacles in pursuit of the goals of Green Chemistry. Opportunities for the next generation of materials designers to create a safer future. 5L
2. Basic principles of Green Chemistry and their illustrations with examples. 10L
   - i. Prevention of waste/byproducts.
   - ii. Maximum Incorporation of the materials used in the process into the final product (Atom Economy): Green metrics
   - iii. Prevention/Minimization of hazardous/toxic products.
   - iv. Designing safer chemicals - different basic approaches
   - v. Selection of appropriate auxiliary substances (solvents, separation agents etc.)
   - vi. Energy requirements for reactions—use of microwave, ultrasonic energy
   - vii. Selection of starting materials—use of renewable starting materials.
   - viii. Avoidance of unnecessary derivatization—careful use of blocking/protection groups.
   - ix. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents.
   - x. Designing biodegradable products.
   - xi. Prevention of chemical accidents.

xii. Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

UNIT – II

3. Green solvents and Green Analytical Methods 10L
   i. Aqueous medium: Enhancement of selectivity, efficiency, and industrial applicability
   ii. Ionic liquids
   iii. Supercritical fluids
   iv. Solvent free reactions
   v. Flourous phase reactions
   vi. Green Analytical Methods
4. Green catalysis 5 L
   Heterogeneous catalysis; Biocatalysis.

UNIT - III

5. Future trends in Green Chemistry: Oxidation-reduction reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solvent less reactions; Non-covalent derivatization; Biomass conversion. 10L
6. Selected examples from synthesis world and US Presidential Green Chemistry Challenge Award Winners. 3L
7. Hazard assessment and mitigation in chemical industry. 2L

Course outcome:

1) Rationalize the existing chemical processes , assess their sustainability and propose more sustainable amendments or commercial viable alternatives
2) Shall be able to perform the laboratory experiments by applying the concepts of stoichiometry and green metrics.
3) Able to apply the knowledge of sustainability to new production processes and new research projects.

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	3					3	
CO2	3	2		2		3	
CO3	3			1	2	3	

Reference Books:

1. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press.
2. Green Chemistry: Introductory Text. M. Lancaster Royal Society of Chemistry (London).
3. Introduction to Green Chemistry. M.A. Ryan and M.Tinnesand, American Chemical Society (Washington).

4. Real World Cases in Green Chemistry. M.C. Cann and M.E. Connelly. American Chemical Society
(Washington).
5. Real World Cases in Green Chemistry (Vol. 2). M.C. Cann and T.P.Umile. American Chemical
Society (Washington).
6. Alternative Solvents for Green Chemistry. F.M. Kerton. Royal Society of Chemistry (London).
7. Recoverable and Recyclable Catalysts. M. Benaglia. Wiley.
8. Handbook of Green Chemistry & Technology. J. Clark and D. Macquarrie. Blackwell Publishing.
9. Solid-Phase Organic Synthesis. K. Burgess. Wiley-Interscience.
10. Eco-Friendly Synthesis of Fine Chemicals. R. Ballini. Royal Society of Chemistry (London).

Assessment method: Written, assignments & Quizzes.

CHM- 629 **Chemical binding** **Credits 3**
Course level: Advance/Master
Pre-requisite: CHM-403 (Quantum chemistry)

Course Description:

- In this course, the student applies the techniques learnt in the course CHM-403 (Quantum chemistry) to understand the structure and bonding in molecules.
- Electronic structure methods ranging from ab-initio to molecular mechanics will be introduced.

Course Contents:
Unit-1: Atomic structure
Recapitulation of Quantum chemistry – I results, Hatree-Fock SCF method, Term symbols, Zeeman and Stark effects, L-S and J-J couplings, Condon-Slater rules, Electron configuration and periodic table

Unit-2: Structure of polyatomic molecules (Ab-initio)
Structure of polyatomic molecules: Born-Oppenheimer approximation, Adiabatic and diabatic states, electronic and nuclear Schrodinger equations, Potential energy surface (PES), Ground and excited states of H2+ ion, Molecular orbital and valence bond theories, Hatree-Fock SCF method, Electron correlation and configuration interaction, Basis sets, PES of H2+ and O2, Survey of post Hatree-Fock SCF methods

Unit-3: Structure of polyatomic molecules (Semi-empirical and molecular mechanics)
Semiempirical and molecular mechanics methods, Force fileds, QM/MM methods. Types of calculations (energy, optimization, frequencies, excited states, etc). Calculation of properties (dipole moments, transition dipole moments, polarizabilities, hyper polarizabilities, charges on the atoms,

bond orders, hybridization etc.). Comparison of properties (geometries, frequencies, energies, thermochemistry, dipolemoments, polarizabilities and hyperpolarizabilities etc) obtained with various methods and basis functions. Future of Quantum chemistry

Course outcome:

1 enhanced understanding of structure and bonding in chemistry
2 learn fundamental principles and concepts that leads to different types of chemical bond
3 develop concept of molecular orbitals and their experimental manifestation and concept of electronic state
4 explain the chemical reactivity based on electronic structure of molecules
5 interpret underlying phenomena at a molecular level in all branches of chemistry

Mapping of Course Outcomes (COs) with Program Outcomes (Pos)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	3					3	2
CO2	3			2	2	3	2
CO3	3			2	2	3	2
CO4	3			2	2	3	2
CO5	3			2	2	3	2

Recommended Text Books and reference materials:

1. Quantum Chemistry, Levine I. N. (2000) Prentice Hall.
2. Introduction to Computational Chemistry, Frank Jensen, John Wiley & Sons, 2007.
3. Modern Quantum Chemistry. A. Szabo and N. S. Ostlund.
4. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.
5. Introductory Quantum Chemistry, A. K. Chandra, Tata McGraw-Hill Publishing Company
6. Elementary Quantum Chemistry, F. L. Pilar, Dovar Publications Inc.
7. Exploring Chemistry with Electronic Structure Methods, J. B. Foresman, A. Frisch, Gaussian Inc.

Assessment method: Written, assignments & Quizzes.

CHM- 630 Chemical binding and computational chemistry Credits 3

Course level: Advance/Master
Pre-requisite: CHM-403 (Quantum chemistry)

Course Description:

- In this course, the student applies the techniques learnt in the course CHM-403 (Quantum chemistry) to understand the structure and bonding in molecules.
- Electronic structure methods ranging from ab-initio to molecular mechanics will be introduced.

Course Contents:

Unit-1: Atomic structure

Recapitulation of Quantum chemistry – I results, Hatree-Fock SCF method, Term symbols, Zeeman and Stark effects, L-S and J-J couplings, Condon-Slater rules, Electron configuration and periodic table

Handson: Survey of ab-initio quantum chemistry packages, Introduction to GAMESS and Avogadro packages. Creation of input files and analysis of the output files

Experiment 1: Calculate the 2P fine structure splittings in sodium and potassium at CASSCF level of theory

Unit-2: Structure of polyatomic molecules (Ab-initio)

Structure of polyatomic molecules: Born-Oppenheimer approximation, Adiabatic and diabatic states, electronic and nuclear Schrodinger equations, Potential energy surface (PES), Ground and excited states of H2+ ion, Molecular orbital and valence bond theories, Hatree-Fock SCF method, Electron correlation and configuration interaction, Basis sets, PES of H2+ and O2, Survey of post Hatree-Fock SCF methods

Experiment 2: Calculate the potential energy surface of H2 at RHF/STO-3G level of theory. Identify the attractive, repulsive and dissociative regions on the PES. Plot the molecular orbitals at the most stable geometry of H2O and analyse the bonding, anti-bonding and non-bonding molecular orbitals

Experiment 3: Do HF/6-31G* partial geometry optimizations of n-butane conformations with CCCC dihedral angles fixed at several values. Plot the energy versus dihedral angle. From the plot, estimate the barriers for the conversions gauche —> anti and anti —> gauche, (b) Start from a 60° dihedral angle and do a full geometry optimization to find the predicted dihedral angle for the gauche conformer. Calculate the predicted energy difference between gauche and anti conformers at 0 K, neglecting zero-point energy.

Experiment 4: Consider the reaction HCN —>CNH. (a) Find the HF/6-31G* equilibrium geometries of HCN and HNC. (Recall that 180° is not allowed as a Z-matrix bond angle.) (b) Find the HF/6-31G* transition-state structure for this reaction. We expect the transition-state (TS) structure to be roughly halfway between the reactant and product structures. Thus we expect a triangular TS with the CN distance somewhere between its values in the reactant and product, the HC distance somewhat longer than its values in the reactant, and the HN distance somewhat longer than its value in the product. Start with an initial guess for the TS structure.

Unit-3: Structure of polyatomic molecules (Semi-empirical and molecular mechanics)

Semiempirical and molecular mechanics methods, Force fileds, QM/MM methods. Types of calculations (energy, optimization, frequencies, excited states, etc). Calculation of properties (dipole moments, transition dipole moments, polarizabilities, hyper polarizabilities, charges on the atoms, bond orders, hybridization etc.). Comparison of properties (geometries, frequencies, energies, thermochemistry, dipolemoments, polarizabilities and hyperpolarizabilities etc) obtained with various methods and basis functions. Future of Quantum chemistry

Experiment 5: Use a molecular-mechanics program to find the geometries and the energy difference between (a) cis and trans 1,2-difluoroethylene; (b) cis and trans 1,2-dichloroethylene; (c) cis and trans 1,2-diiodoethylene. Compare your results with available literature data as to which is the more stable isomer of each pair.

Experiment 6: Consider the thermal reaction 1,3,5-hexatriene —> l,3-cyclohexadiene. (a) Use the symmetry of the polyene HOMO to predict whether the reaction path is conrotatory or disrotatory. (b) Do the same as in (a) when the reaction occurs photochemically. (c) State the general rules for the cyclization of the polyene with nπ π electrons.

Course outcome:

1 enhanced understanding of structure and bonding in chemistry
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Mapping of Course Outcomes (COs) with Program Outcomes (POs)

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
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Assessment method: Written, assignments & Quizzes.