Semester II
Coordination Chemistry (Core IV)
Subject Code: PG2021

No. of hours per week	Credit	Total no. of hours	Marks
6	6	90	100

Objectives:

- To understand the thermodynamic and stereochemical aspects of complexes
- To learn about the various mechanisms of substitution and electron transfer reactions.

Course Outcomes (COs)

CO No.	*Upon completion of this course, the students will be able to:*	PSO Addressed	Cognitive Level
CO-1	understand the various theories and reaction mechanisms related to coordination compounds	PSO-1	U
CO-2	apply the theories and reaction mechanisms to determine the properties of complexes	PSO-2	A
CO-3	analyze the reaction mechanism of coordination compounds	PSO-2,3	Y
CO-4	evaluate the magnetic and spectral properties of complexes	PSO-2,3	E
CO-5	create novel complexes and catalyst	PSO-4,5	C

Unit I Stability of Complexes **(18 Hours)**

Stability of complexes - factors affecting stability of complexes - thermodynamicaspects of complex formation - stepwise and overall formation constants - stability correlations - statistical factors and chelate effect. Determination of stability constant and composition of the complexes - spectrophotometric method - ion exchange method - polarographic method and continuous variation method (Job's method).

Stereochemical aspects - stereoisomerism in inorganic complexes - isomerism arising out of ligand distribution and ligand conformation. Chirality - nomenclature of chiral complexes - application of ORD and CD in the identification of complexes.

Unit II Metal Ligand Bonding **(18 Hours)**

Crystal field theory - Splitting of d orbitals under various geometries - factors affecting splitting - CFSE - evidences for CFSE (structural and thermodynamic effects) - spectrochemical series - Jorgensen relation - site preferences - Jahn-Teller distortion - dynamic and static Jahn-Teller - Jahn-Teller effect and chelation. Application of CFT - magnetic properties - spectral properties and kinetic properties - limitations of CFT- evidences for M-L overlap.

Molecular Orbital Theory - energy level diagrams concept of weak and strong fields - sigma and pi bonding - octahedral - square planar and tetrahedral complexes. Nephelauxetic effect. Magnetic properties of complexes. Comparison of CFT and MOT of bonding in octahedral complexes.

Unit III Electronic Spectra of Complexes (18 Hours)

Spectroscopic term symbols for d^n ions - derivation of term symbols and ground state term symbol - Hund's rule - selection rules - breakdown of selection rules - spin orbit coupling - band intensities - weak and strong field limits - correlation diagram - energy level diagrams. Orgel diagram for weak field Oh and Td complexes - splitting of energy level due to Jahn-Teller distortion. Modified orgel diagram - limitations of orgel diagram. Tanabe- Sugano (T-S) diagrams - evaluation of Dq and B values for d^2- d^8 complexes charge transfer spectra. Complications in band classification between LF (d-d) and CT bands. Comparison between d-d bands and CT bands - numerical problems. Lanthanides and Actinides- spectralproperties.

Unit IV Inorganic Reaction Mechanism (18 Hours)

Electron transfer reactions - Inner sphere (ISET) and outer sphere (OSET) electron transfer processes. Reaction mechanism of coordination compounds - Types of ligand substitution reactions- mechanism- Dissociative mechanism (D) - Associative mechanism (A) interchange mechanism (I) - labile and inert complexes. Substitution reaction in octahedral complexes - general mechanism - general rate law for A - D and I - distinction between D – ID - IA pathways - replacement of coordinated water - mechanism of acid hydrolysis - base hydrolysis – DCB mechanism - direct and indirect evidences in favour of the mechanism. Ligand substitution reactions without cleavage of M-L Bond. Anation Reactions - substituion in square planar complexes - general mechanism - trans effect- influences of entering and leaving groups - application of trans effect – synthesis of isomers of Pt(II) complexes – theories of trans effect and cis-trans isomerisation reaction. Application of substitution reactions in the synthesis of platinum and cobalt complexes.

Unit V Catalysis **(18 Hours)**

General principles of catalysis - basic reactions involved in the catalysis by organometallic compounds. Hydrogenation of olefins (Wilkinson's catalyst) - Hydro formylation of olefins using cobalt or rhodium catalysts (OXO process) - oxidation of olefins to aldehydes and ketones (wacker process) - Monsanto acetic acid synthesis from methanol. Cyclo oligomerisation of acetylene using Ni catalyst (Reppe's catalyst) - synthetic gasoline by using ZSM-5 catalyst (Fisher-Tropsch and mobil process) - polymerization of olefins (Zeigler-Natta Catalyst) - polymer bound catalyst.

Text Books:

1. Lee, J.D. (2008). Concise Inorganic Chemistry. (5th ed.). India: Wiley India.
2. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. (2011). Inorganic Chemistry: Principles of Structure and Reactivity. (4th ed.).India: Pearson Education.
3. Puri B.R., Sharma, L.R. & Kalia, K.C. (2012). Principles of Inorganic Chemistry. (4th ed.). India: Milestone publishers.
4. Malik, W.U., Tuli, G.D. & Madan, R.D. (2012). Selected topics Inorganic Chemistry. (5th ed.). New Delhi: S. Chand Company Ltd.

Reference Books:

1. Cotton, F.A. & Wilkinson, G. (1988). Advance Inorganic Chemistry. (2nd ed.). India: Wiley Eastern Private Ltd.
2. Miessler, G.L. (2004). Inorganic Chemistry. (3rd ed.), India: Pearson Education.
3. Purcell, K.F. &Kotz, J.C. (2012). Inorganic Chemistry. (2nd ed.). India: Cengage Learning India Pvt. Ltd.
4. Kettle, S.F.A, (1996).Coordination Chemistry-Ari Approach. USA: Spectrum Academic publishers Oxford.
5. Mehrotra, R. C. & Singh, A. (2014). Organometallic Chemistry. (2nd ed.) New Delhi: New Age International Ltd.
6. Parkins, A. W. &Poller, R. C. (1987). An Introduction to Organometallic Chemistry. Chennai: Oxford University Press.

Teaching Module

Credit: 6 ***Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Stability of Complexes**					
	1	Stability of complexes - factors affecting stability of complexes- thermodynamic aspects of complex formation	3	Understand the factors affecting the stability of complexes	Lecture and group discussion	Evaluation through class test, online quiz and group discussion Formative assessment I
	2	Stepwise and overall formation constants - stability correlations - statistical factors and chelate effect	3	Apply the theories to determine stepwise and overall formation constants	Lecture	
	3	Determination of stability constant and composition of the complexes - spectrophotometric method - ion exchange method - polarographic method and continuous variation method (Job's method)	5	Apply various methods to determine the stability constants of complexes	Lecture and Seminar	
	4	Stereochemical aspects - stereoisomerism in inorganic complexes - isomerism arising out of ligand distribution and ligand conformation	4	Understand the stereoisomerism in inorganic complexes	Lecture and group discussion	
	5	Chirality - nomenclature of chiral complexes - application of ORD and CD in the identification of complexes	3	Apply ORD and CD in the identification of complexes	Lecture and Seminar	
II	**Metal Ligand Bonding**					
	1	Crystal field theory - Splitting of d orbitals under various geometries - factors affecting splitting - CFSE - evidences for CFSE (structural and thermodynamic effects)	4	Understand crystal field theory and splitting of d-orbitals under various geometries	Lecture with ppt	Evaluation through class test, online quiz and group discussion

	2	Spectrochemical series - Jorgensen relation - site preferences - Jahn-Teller distortion - dynamic and static Jahn-Teller- Jahn-Teller effect and chelation	4	Analyse dynamic and static Jahn-Teller distortion	Lecture and group discussion	Formative assessment I
	3	Application of CFT - magnetic properties - spectral properties and kinetic properties - limitations of CFT- evidences for M-L overlap.	3	Apply CFT to determine the magnetic, spectral and kinetic properties of coordination compounds	Lecture	
	4	Molecular Orbital Theory - energy level diagrams concept of weak and strong fields - sigma and pi bonding - octahedral - square planar and tetrahedral complexes	4	Apply Molecular Orbital Theory to octahedral,square planar and tetrahedral complexes	Lecture with ppt	
	5	Nephelauxetic effect. Magnetic properties of complexes. Comparison of CFT and MOT of bonding in octahedral complexes	3	Analyse CFT and MOT of bonding in octahedral complexes	Lecture	
III	**Electronic Spectra of Complexes**					
	1	Spectroscopic term symbols for d^n ions - derivation of term symbols and ground state term symbol	3	Understand spectroscopic term symbols	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Hund's rule - selection rules - breakdown of selection rules - spin orbit coupling - band intensities - weak and strong field limits - correlation diagram - energy level diagrams	4	Apply Hund's rule and selection rules to spin orbit coupling	Lecture and group discussion	
	3	Orgel diagram for weak field Oh and Td complexes - splitting of energy level due to Jahn-Tellerdistortion. Modified orgel diagram - limitations of orgel diagram	4	Analyse splitting of energy level due to Jahn Teller distortion in weak O_h and T_d com-lexes using Orgel diagram	Lecture with ppt	
	4	Tanabe-Sugano (T-S) diagrams - evaluation of Dq and B values for d^2- d^8 complexes	4	Evaluate Dq and B values for d^2- d^8 complexes	Lecture	

	5	Charge transfer spectra. Complications in band classification between LF (d-d) and CT bands. Comparison between d-d bands and CT bands - numerical problems. Lanthanides and Actinides- spectral properties	3	Evaluate the spectral properties of lanthanides and actinides	Lecture	
IV	**Inorganic Reaction Mechanism**					
	1	Electron transfer reactions - Inner sphere (ISET) and outer sphere (OSET) electron transfer processes	4	Understand the reaction mechanisms of electron transfer processes	Lecture with ppt	Evaluation through class test, online quiz and group discussion Formative assessment II
	2	Reaction mechanism of coordination compounds - Types of ligand substitution reactions- mechanism- Dissociative mechanism (D) - Associative mechanism (A) interchange mechanism (I) - labile and inert complexes	3	Analyse the types of substitution mechanisms in coordination compounds	Lecture and group discussion	
	3	Substitution reaction in octahedral complexes - general mechanism - general rate law for A - D and I - distinction between D – ID - IA pathways - replacement of coordinated water - mechanism of acid hydrolysis - base hydrolysis – DCB mechanism - direct and indirect evidences in favour of the mechanism	5	Understand the mechanism of substitution reaction in octahedral complexes	Lecture	
	4	Ligand substitution reactions without cleavage of M-L Bond. Anation Reactions - substituion in square planar complexes - general mechanism	3	Apply the mechanism of substitution reaction to square planar complexes	Lecture with ppt	

	5	Trans effect- influences of entering and leaving groups - application of trans effect – synthesis of isomers of Pt(II) complexes – theories of trans effect and cis-trans isomerisation reaction. Application of substitution reactions in the synthesis of platinum and cobalt complexes	3	Apply Trans effect and substitution reactions to synthesise Pt and Co complexes	Lecture	
V	**Catalysis**					
	1	General principles of catalysis - basic reactions involved in the catalysis by organometallic compounds	4	Understand the general principles and basic reactions involved in the catalysis by organometallic compounds	Lecture	Evaluation through class test, group discussion and quiz Formative assessment II
	2	Hydrogenation of olefins (Wilkinson's catalyst) - Hydro formylation of olefins using cobalt or rhodium catalysts (OXO process)	3	Understand the mechanism of hydrogenation and hydroformylation of olefins using Co or Rh catalysts	Lecture with ppt	
	3	Oxidation of olefins to aldehydes and ketones (wacker process) - Monsanto acetic acid synthesis from methanol	4	Apply Wackers process to the oxidation of olefins	Lecture and group discussion	
	4	Cyclooligomerisation of acetylene using Ni catalyst (Reppe's catalyst) - synthetic gasoline by using ZSM-5 catalyst (Fisher-Tropsch and mobil process)	4	Apply Reppe's catalyst ans ZSM-5 catalyst to the cyclooligomerisation of acetylene and synthetic gasoline	Lecture	
	5	Polymerization of olefins (Zeigler-Natta Catalyst) - polymer bound catalyst	3	Create new polymer catalyst	Lecture	

Course Instructor: Dr. S. Lizy Roselet HOD: Dr. G. Leema Rose

Semester II
Reaction Mechanism and Molecular Rearrangements (Core V)
Subject Code: PG2022

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

Objectives:

- To understand the mechanism of organic reactions.
- To get an in-depth knowledge on the various types of oxidation and reduction reactions along with their synthetic utility.

Course Outcomes (COs)

CO No.	*Upon completion of this course, the students will be able to:*	PSO Addressed	Cognitive Level
CO-1	understand the mechanisms of organic reactions	PSO-1	U
CO-2	apply the reaction mechanisms to synthesize organic compounds	PSO-2,3	A
CO-3	analyze the type of reactions in organic compounds	PSO-2,3	Y
CO-4	evaluate nucleophilic, electrophilic substitution and elimination reactions in aromatic and aliphatic compounds	PSO-2	E
CO-5	create novel organic compounds	PSO-3,4	C

Unit I Addition to Carbon-Carbon Multiple Bond (18 Hours)

Electrophilic addition to carbon-carbon double and triple bonds. Nucleophilic addition to carbon-carbon multiple bonds. Mechanism and stereochemical factors in reactions - addition of hydrogen halides, hypohalous acids and hydroboration. Hydroxylation of olefinic double bonds - OsO_4 - $KMnO_4$ - Woodward and Prevost hydroxylation. Epoxidation using peracids - Sharpless epoxidation and ozonolysis.

Mechanism and applications of Michael addition - Robinson annulation sequence - Diels' Alder - Knoevenagal - Mannich - Stork-enamine - Grignard - Darzen's and Reformatsky reactions.

Unit II Addition to Carbon-Oxygen Multiple Bond (18 Hours)

Nucleophilic addition to carbon-oxygen double bond - Mannich, benzoin - Darzen's glycidic ester - Stobbe and Knovenagel condensation reactions. Wittig - Wittig-Horner

olefination reactions. Reactions of sulphur and sulphoniumylides. Julia olefination and Peterson alkene synthesis. Asymmetric reduction of carbonyl functions (Corey's procedure).

Unit III Elimination Reactions (18 Hours)

Elimination reactions - E_1 - E_2 - E_{1cb} and E_i elimination. Effect of solvent - substrate and leaving group in elimination reactions. Hofmann - Saytzeff and Bredt's rule. Saytzeff's Vs Hoffman elimination. Stereochemistry of E_2 elimination. Mechanism of pyrolytic elimination - Chugaev and Cope elimination reactions. Hoffmann exhaustive methylation and pyrolysis of esters.

Unit IV Molecular Rearrangments and Name Reactions (18 Hours)

Molecular rearrangements - classification - electrophilic - nucleophilic and free radical rearrangements. Mechanisms of Wagner Meerwin - Tiffenev-Demyanov - Dienone-Phenol - Favorskii - Fries - Baeyer-Villager - Stevens - Neber - Sommelet-Hauser - Baker-Venkatraman - von-Richter - Ullmann - Pummerer and di- π methane rearrangements.

Name reactions - Dieckmann cyclization - Hofmann-Loffler Freytag reaction - Mitsunobu reaction - Shapiro reaction - Eschenmoser-Tanabe and Ramburg-Backlund reactions.

Unit V Oxidation and Reduction Reactions (18 Hours)

Oxidation with Cr - PCC - PDC and Jones. Oxidation with Mn - MnO_2 and $BaMnO_4$ reagents. Oxidation with LTA - DDQ and SeO_2. Oxidation using DMSO - DCC - acetic anhydride and oxaloyl chloride. Oxidation using IBX and Dess-Martin Periodinane (DMP) reagent.

Reduction with $NaBH_4$ - $NaCNBH_3$ - $Zn(BH_4)_2$ - $LiAlH_4$ - $Li(BuO)_3AlH$ - DIBAL-H - Red-Al - Et_3SiH and Bu_3SnH. Reduction using selectrides - Birch reduction.

Text Books:

1. March, J. (2006). Advanced organic chemistry. (4th ed.).New York: John Wiley and Sons.
2. Ahluwalia, V.K. & Parshar, R.K. (2005). Organic Reaction Mechanism. (2nd ed.). India: Narosa, publishing House.
3. Norman, R.O.C. & Coxon, J.M. (1993). Principles of Organic Synthesis, (3rded.). New York: CRC press, Taylor and Francis Group.
4. Morrison, R.T. & Boyd, R.N. (1997). Organic Chemistry. (6th ed.). New Jersey: Prentice Hall.
5. Jain, M.K. & Sharma, S.C. (2014). Modern Principles of Organic Chemistry. India: Vishal publication.

6. Chatwal, G.R. (2016). Reaction Mechanism and Reagents in Organic Chemistry. (5th ed.). India: Himalaya Publishing House.

Reference books:

1. Carey, F. & Sundberg, R.J. (2007). Advanced Organic Chemistry-Part A and B. (5^{th}ed.). USA: Springer.
2. Smith, M.B. & March, J. (2001). Advanced Organic Chemistry. (5^{th}ed.). New York: John Wiley and Sons.
3. Bansal, R.K. (2005). Reaction Mechanism in Organic Chemistry. (3^{rd} ed.). Tata McGraw Hill.
4. Clayden, J. Greeves, N & Warren, S. (2012). Organic Chemistry. (2^{nd} Ed.). Oxford University Press.
5. Tewari, K.S., Vishnol, N.K. & Mehrotra, S.N. (2002). A text book of organic chemistry. India: Vikas publishing House Ltd.
6. Kalsi, P.S. (1996). Organic Reactions and Mechanism. (1^{st} ed.). India: New Age International Ltd.

Teaching Module

Credit: 5 ***Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Unit I Addition to Carbon-Carbon Multiple Bond**					
	1	Electrophilic addition to carbon-carbon doubleand triple bonds.Nucleophilic addition tocarbon-carbon multiplebonds	4	Understand electrophilic addition and nucleophilic addition to carbon-carbon multiple bonds	Lecture	Evaluation through online quiz Formative assessment I
	2	Mechanism and stereochemical factors in reactions - addition of hydrogen halides, hypohalous acids and hydroboration	4	Understand the mechanisms stereochemical factors in organic reactions	Lecture and Group discussion	
	3	Hydroxylation of olefinic double bonds - OsO_4 - $KMnO_4$ - Woodward and Prevost hydroxylation	3	Synthesize the organic compounds using hydroxylating agents	Lecture and Seminar	
	4	Epoxidation using peracids - Sharpless epoxidation and ozonolysis	3	Understand the Epoxidation reactions	Lecture	
	5	Mechanism and applications of Michael addition - Robinson annulation sequence - Diels' Alder - Knoevenagal - Mannich - Stork-enamine - Grignard - Darzen's and Reformatsky reactions	4	Apply the name reactions to synthesize organic compounds	Lecture	
II	**Addition to Carbon-Oxygen Multiple Bond**					
	1	Nucleophilic addition to carbon-oxygen double bond - Mannich, benzoin - Darzen'sglycidic ester - Stobbe and Knovenagel condensation reactions	5	Understand the nucleophilic addition to carbon-oxygen double bond	Lecture with models	Evaluation through class test, online quiz and group discussion

	2	Wittig - Wittig-Horner olefination reactions	3	Infer the mechanism of Wittig - Wittig-Horner olefination reactions	Lecture	Formative assessment I
	3	Reactions of sulphur and sulphoniumylides. Julia olefination and Peterson alkene synthesis	5	Know the reactions of sulphur and sulphoniumylides	Lecture and group discussion	
	4	Asymmetric reduction of carbonyl functions (Corey's procedure)	5	Illustrate asymmetric reduction of carbonyl functions	Lecture	
III	**Aromatic Electrophilic and Nucleophilic Substitutions**					
	1	Elimination reactions - E_1 - E_2 - E_{1cb} and $E_i$elimination. Effect of solvent - substrate and leaving group in elimination reactions	5	Understand the concept of elimination reaction	Lecture	Evaluation through class test, online quiz and group discussion Formative assessment II
	2	Hofmann - Saytzeff and Bredt's rule. Saytzeff's Vs Hoffman elimination	4	Compare saytzeff's Vs Hoffman elimination	Lecture	
	3	Stereochemistry of E_2 elimination. Mechanism of pyrolytic elimination - Chugaev and Cope elimination reactions	4	Infer the mechanism of pyrolytic elimination reaction.	Lecture and group discussion	
	4	Hoffmann exhaustive methylation and pyrolysis of esters	5	Understand the concept of Hoffmann exhaustive methylation	Lecture	
IV	**Molecular Rearrangements and Name Reactions**					
	1	Molecular rearrangements - classification - electrophilic - nucleophilic and free radical rearrangements	4	Classify molecular rearrangements	Lecture	Evaluation through class test and group discussion
	2	Mechanisms of Wagner Meerwin - Tiffenev-Demyanov - Dienone-Phenol - Favorskii - Fries - Baeyer-Villager - Stevens and Neber rearrangements	5	Infer the mechanism of molecular rearrangements	Lecture and group discussion	Formative assessment II

	3	Sommelet-Hauser - Baker-Venkatraman - von-Richter - Ullmann - Pummerer and di- π methane rearrangements	5	Infer the mechanism of rearrangements	Lecture	
	4	Name reactions - Dieckmann cyclization - Hofmann-Loffler Freytag reaction - Mitsunobu reaction - Shapiroreaction - Eschenmoser- Tanabe and Ramburg- Backlund reactions	4	Understand the mechanism of name reactions	Lecture	
V	**Oxidation and Reduction Reactions**					
	1	Oxidation with Cr - PCC - PDC and Jones. Oxidation with Mn - MnO_2 and $BaMnO_4$ reagents	5	Understand and apply oxidising agents in organic synthesis	Lecture with videos	Evaluation through class test, group discussion and quiz Formative assessment I
	2	Oxidation with LTA - DDQ and SeO_2	4	Understand the application of LTA - DDQ and SeO_2	Lecture	
	3	Oxidation using DMSO - DCC - acetic anhydride and oxaloyl chloride	4	Understand the application of DMSO - DCC - acetic anhydride and oxaloyl chloride	Lecture	Evaluation through class test, group discussion and quiz Formative assessment II
	4	Oxidation using IBX and Dess-Martin Periodinane (DMP) reagent	5	Apply oxidising agents in organic synthesis	Lecture and Group Discussion	

Course Instructor: Dr. Y. Christabel Shaji HOD: Dr. G. Leema Rose

Semester II
Quantum Chemistry and Spectroscopy (Core VI)
Subject Code: PG2023

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

Objectives:

- To learn the principle of quantum mechanics of simple systems.
- To understand the principle, instrumentation, interpretation and applications of various spectroscopic and analytical techniques.

Course Outcomes (COs)

CO No.	*Upon completion of this course, the students will be able to:*	PSO Addressed	Cognitive Level
CO-1	understand the concepts of quantum chemistry, spectroscopy and surface chemistry	PSO-1	U
CO-2	apply the principles of quantum mechanics to simple systems, spectroscopy to characterize compounds and surface chemistry to determine the surface area of surface films and liquids	PSO-2	A
CO-3	analyse molecules using quantum mechanics and spectroscopic techniques	PSO-2,3	Y
CO-4	evaluate eigen values, bond angles, electron density and surface area of simple molecules	PSO-2,3	E

Unit I Quantum Chemistry-I **(18 Hours)**

Black body radiation - Planck's quantum theory - wave particle duality - uncertainty principle. Operators - linear - commutation - Hermitian and Hamiltonian operators. Eigen functions and eigen values. Postulates of quantum mechanics. Derivation of Schrodinger's time-independent wave equation - application - one dimensional box - particle in a three dimensional box - harmonic oscillator and hydrogen atom.

Unit II Quantum Chemistry - II **(18 Hours)**

Born-Oppenheimer approximation - Hydrogen molecule ion. LCAO-MO and VB treatments of the hydrogen molecule. Anti-symmetry and Pauli's exclusion principle. Slater detrimental wave function - term symbols and spectroscopic states - Russell Saunders coupling. The variation theorem and perturbation theory - applications of variation method and perturbation theory to the helium atom. Hybridization-determination of bond angles of sp

- sp^2 and sp^3 hybridizations. Huckel pi electron (HMO) theory and its applications to ethylene - butadiene and benzene.

Unit III Molecular Spectroscopy - I **(18 Hours)**

Electronic Spectroscopy - principle - laws of light absorption - Born-Oppenheimer approximation. Franck-Condon principle - wave-mechanical formulation - dissociation energy - dissociation products and predissociation. Microwave spectroscopy - rotation of molecules - rotational spectra of diatomic molecules - intensity of spectral lines - effects of isotopic substitution - non-rigid rotator. Rotational spectra of polyatomic molecules - chemical analysis by microwave spectroscopy.

Unit IV Molecular Spectroscopy - II **(18 Hours)**

ESR - theory - hyperfine interactions in ESR - double resonance (ENDOR, ELDOR) - Mc Connell's relation - verification of the relation for cyclic polyene radical - calculation of electron density and experimental techniques.

Laser Raman Spectroscopy - Einstein treatment of absorption and emission phenomena- Einstein's coefficients - probability of induced emission - applications to lasers- conditions for laser action - properties - types of lasers - advantages of lasers in Raman spectroscopy and experimental techniques.

Unit V Surface chemistry **(18 Hours)**

Electrical aspects of surface chemistry - electrical double layer - zeta potential. BET and Gibbs adsorption isotherms - derivation – applications - determination of surface area (BET equation) - surface films and liquids. Membrane equilibria and dialysis.

Surface active reagents - classification of surface agents - micellization - hydrophilic interactions - critical micellar concentration - factors affecting the CMC of surfaces. Transition state theory of surface reactions - rates of chemisorptions - Hertz-Knudson equation.

Text Books:

1. Chandra. A.K. (2001). Introductory Quantum Chemistry. (4^{th}ed.). India: Tata McGraw-Hill.
2. Prasad, R.K. (2014). Quantum Chemistry. (4^{th} ed.). New Delhi: New Age International Publishers.
3. Atkins, P. & Atkins, J.P. (2002). Physical Chemistry. (7^{th}ed.).USA: Oxford university press.
4. BanWell, C.N. & Mccash, E.M. (1997). Fundamentals of Molecular Spectroscopy. New Delhi: Tata Mc Grow Hill.

Reference Books:

1. Mcquarrie, D.A. (2008). Quantum Chemistry. Sausalito: University Science Books.
2. Puri, B.R., Sharma, L.R. & Pathania, M.S. (2016). Principles of Physical Chemistry (47^{th}ed.). India: Vishal Publications.
3. Aruldhas, G. (2011). Molecular Structure and Spectroscopy. (2^{nd} ed.), India: PHI Learning Pvt. Ltd.

Teaching Module

Credit: 5 ***Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Quantum Chemistry-I**					
	1	Black body radiation- Planck's quantum theory- wave particle duality- uncertainty principle	4	Explain the principle of black body radiation	Lecture	Evaluation through class test and quiz Formative assessment I
	2	Operators-linear - commutation - Hermitian and Hamiltonian operators	3	Gain knowledge about operators	Lecture	
	3	Eigen functions and eigen values. Postulates of quantum mechanics	3	Understand the postulates of quantum mechanics	Lecture and Seminar	
	4	Derivation of Schrodinger's time-independent wave equation	3	Derive Schrodinger's wave equation	Lecture	
	5	Application - one dimensional box -particle in a three dimensional box -harmonic oscillator and hydrogen atom	5	Apply Schrodinger's wave equation to hydrogen atom	Lecture	
II	**Quantum Chemistry - II**					
	1	Born-Oppenheimer approximation-Hydrogen molecule ion. LCAO-MO and VB treatments of the hydrogen molecule	4	Compare LCAO-MO and VB treatments of the hydrogen molecule	Lecture	Evaluation through class test, group discussion and online quiz Formative assessment I
	2	Anti-symmetry and Pauli's exclusion principle. Slater detrimental wave function	4	Apply Slater determinant to construct anti-symmetric wave function	Lecture and group discussion	
	3	Term symbols and spectroscopic states-Russell Saunders coupling	4	Gain knowledge about term symbols	Lecture	

	4	The variation theorem and perturbation theory - applications of variation method and perturbation theory to the helium atom.	3	Apply variation method and perturbation theory to the helium atom	Lecture	
	5	Hybridization- determination of bond angles of sp - $sp^2$and sp^3hybridizations.Huckel pi electron (HMO) theory and its applications to ethylene - butadiene and benzene	3	Determine hybridization and bond angles	Lecture	
III	**Molecular Spectroscopy – I**					
	1	Electronic Spectroscopy - principle - laws of light absorption - Born-Oppenheimer approximation	4	Understand the principle of electronic spectroscopy	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Franck-Condon principle - wave-mechanical formulation - dissociation energy - dissociation products and predissociation	4	Apply Franck-Condon principle to dissociation.	Lecture and seminar	
	3	Microwave spectroscopy - rotation of molecules - rotational spectra of diatomic molecules	3	Gain knowledge about microwave spectroscopy	Lecture and group discussion	
	4	Intensity of spectral lines - effects of isotopic substitution - non-rigid rotator	4	Know about the effects of isotopic substitution.	Lecture	
	5	Rotational spectra of polyatomic molecules - chemical analysis by microwave spectroscopy	3	Apply the principle of microwave spectroscopy in chemical analysis	Lecture and seminar	
IV	**Molecular Spectroscopy – II**					
	1	ESR - theory - hyperfine interactions in ESR - double resonance (ENDOR, ELDOR)	4	Know about hyperfine interactions in ESR	Lecture	Evaluation through class test, group discussion and online quiz Formative
	2	Mc Connell's relation - verification of therelation for cyclicpolyene radical	3	Verify Mc Connell's relation for cyclic polyene radical	Lecture and group discussion	

	3	Calculation of electron density and experimental techniques in solution	3	Calculate electron density	Lecture	assessment II
	4	Laser Raman Spectroscopy - Einstein treatment of absorption and emission phenomena- Einstein's coefficients - probability of induced emission - applications to lasers	4	Derive Einstein coefficient	Lecture	
	5	Conditions for laser action - propertiestypes of lasers - advantages of lasers in Raman spectroscopy and experimental techniques	4	Understand different types of lasers	Lecture	
V	**Surface chemistry**					
	1	Electrical aspects of surface chemistry - electrical double layer - zeta potential.	4	Understand the concepts of surface chemistry	Lecture	Evaluation through class test, group discussion and quiz Formative assessment II
	2	BET and Gibbs adsorption isotherms - derivation	3	Compare BET and Gibbs adsorption isotherms		
	3	Applications - determination of surface area (BET equation) - surface films and liquids. Membrane equilibria and dialysis	4	Apply BET equation in determination of surface area	Lecture	
	4	Surface active reagents - classification of surface agents - micellization - hydrophilic interactions - critical micellar concentration - factors affecting the CMC of surfaces	4	Gain knowledge about CMC	Lecture with videos	
	5	Transition state theory of surface reactions - ratesof chemisorptions - Hertz-Knudson equation	3	Derive Hertz-Knudson equation	Lecture	

Course Instructor: Dr. M. Shirley Treasa HOD: Dr. G. Leema Rose

Semester II
Research Methodology (Elective II)
Subject Code: PG2024

No. of hours per week	Credit	Total no. of hours	Marks
4	3	60	100

Objectives

- To understand the importance of research for future development.
- To get information about computation techniques in research

Course Outcomes (COs)

CO No.	*Upon completion of this course, the students will be able to:*	PSO Addressed	Cognitive Level
CO-1	understand the sources of literature survey and analytical techniques for documentation of research and cheminformatics for molecular representation	PSO-1	U
CO-2	apply the features of literature survey in research and analytical techniques to characterize compounds	PSO-2,3	A
CO-3	analyse the sources of research information and chemical compounds	PSO-2,3	Y
CO-4	evaluate the results using analytical techniques	PSO-2,3	E
CO-5	create a journal article	PSO-3	C

Unit I Literature Survey **(12 Hours)**

Source of chemical information - primary - secondary and tertiary sources. Literature survey - indexes and abstracts in science and technology. Applied science and technology index - chemical abstracts - chemical titles - current chemical reactions - current contents and science citation index. Classical and comprehensive reference works in chemistry- synthetic methods and techniques - treatises - reviews - patents and monographs.

Unit II Chemical Abstracts **(12 Hours)**

Current awareness searching - CA weekly issues and CA issue indexes. Retrospective searching - CA volume indexes- general subject index - chemical substance index- formula index - index of ring systems - author index and patent index. CA collective indexes - collective index (CI) and decennial index (DI). Access points for searching CA indexes- index guide - general subject - terms - chemical substance names - molecular formulas - ring

systems - author names - patent numbers. Locating the reference - finding the abstract - finding the original document chemical abstract and service source index.

Unit III Research Problem and Scientific Writing (12 Hours)

Identification of research problem - assessing the status of the problem - guidance from the supervisor - actual investigation and analysis of experimental results - conclusions. Scientific writing - research reports - thesis - journal articles and books. Steps to publishing a scientific article in a journal. Types of publications - communications - articles and reviews. Documenting - Abstracts indicative - descriptive abstracts - informative abstract - footnotes - end notes - referencing styles - bibliography - journal abbreviations - abbreviation used in scientific writing.

Unit IV Instrumental Analysis (12 Hours)

Principle - instrumentation and applications - AFM - SEM - STM - TEM and XRD. Determination of surface morphology and particle size. Sample preparations and applications of UV - IR - NMR and mass spectroscopy.

Unit V Cheminformatics (12 Hours)

Cheminformatics - history and applications. Representing molecules - connection tables and line notation - Inchi - SMILES and WLN canonicalization. Line notation versus connection tables. Query languages - SMARTS. Molecular similarity. 2D topology and 3D configuration. Chemistry softwares - Chemdraw - writing chemical equations and schemes - editing - transporting picture to word and image document. Origin -importing and exporting data - scientific graphing and data analysis - curve fitting and peak analysis - transporting graph to tag image file format.

Text Books:

1. Berg, B.L. (2009). Qualitative Research Methods for the Social Sciences. (7th ed.). India: Pearson Education.
2. Patton, M.Q. (2002). Qualitative research and evaluation methods. (3rd ed.). India: Sage Publications.
3. Alexis, L. & Mathews, L. (1999). Fundamentals of Information Technology. Chennai: Leon Vikas.
4. Mohan, J. (2001). Organic Spectroscopy Principles and Applications. India: Narosa publishing house.
5. Kemp, W. (1994). Organic Spectroscopy. (3rd ed.). New York: Macmillan.
6. Polanski, J. (2009). Cheminformatics. Poland: Elsevier Publications.

Reference Books:

1. Silverman, D. (2011). Qualitative Research: Issues of Theory, Method and Practice. (3rd ed.). India: Sage Publications.
2. Marczyk, G. Dematteo, D. & Festinger, D. (2005). Essential of Research Design and Methodology. New York: John Wiley and Sons.
3. Silverstein, S.M., Bassler, G.V. &Morril, T.C. (2004). Spectrometric identification of organic compounds. (6th ed.). New York: Wiley.
4. Dyer, J.R. (1987). Applications of Absorption spectroscopy of Organic Compounds. New York: Prientice Hall.
5. Dani, V.R. (1995). Organic spectroscopy. India: Tata McGraw Hill.
6. Gasteiger, J. & Engel, T. (2003). Chemoinformatics. New York: John Wiley and Sons.

Teaching Module

Credit: 3 ***Total Hours: 60 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Literature Survey**					
	1	Source of chemical information - primary - secondary and tertiary sources	2	Understand and identify the sources of information's	Lecture and group discussion	Evaluation through periodic test, class test and group discussion Formative assessment I
	2	Literature survey - indexes and abstracts in science and technology	2	Apply the features of literature survey in research	Lecture and seminar	
	3	Applied science and technology index - chemical abstracts - chemical titles - current chemical reactions - current contents and science citation index	3	Understand the terms chemical abstracts and citation index	Lecture with group discussion and seminar	
	4	Classical and comprehensive reference works in chemistry-synthetic methods and techniques	2	Understand classical and comprehensive reference works in chemistry	Lecture and seminar	
	5	Treatises - reviews - patents and monographs	3	Understand patents and monographs	Lecture with videos	
II	**Chemical Abstracts**					
	1	Current awareness searching - CA weekly issues and CA issue indexes. Retrospective searching - CA volume indexes and general subject index	2	Understand the importance of current awareness and retrospective searching in research	Lecture and seminar	Evaluation through periodic test, class test, online quiz and class assignment Formative assessment II
	2	Chemical substance index- formula index - index of ring systems - author index and patent index	2	Analyzevarious indexes in chemical abstracts	Lecture and seminar	
	3	CA collective indexes collective index (CI) and decennial index (DI)	2	Differentiate CI and DI	Lecture and seminar	

	4	Access points for searching CA indexes- index guide - general subject - terms - chemical substance names - molecular formulas - ring systems - author names and patent numbers	3	Know how to search CA indexes	Lecture and seminar	
	5	Locating the reference - finding the abstract - finding the original document chemical abstract and service source index	3	Pinpoint chemical abstract and service source index	Lecture and seminar	
III	**Research Problem and Scientific Writing**					
	1	Identification of research problem - assessing the status of the problem, guidance from the supervisor, actual investigation and analysis of experimental results and conclusions	3	Identify and solve research problems	Lecture with videos and group discussion	Evaluation through periodic test, class test and group discussionFormative assessment II
	2	Scientific writing - research reports, thesis, journal articles and books	2	Know the art of scientific writing in research	Lecture with ppt and seminar	
	3	Steps to publishing a scientific article in a journal. Types of publications - communications, articles and reviews	3	Create journal articles, communication and reviews	Lecture and group discussion	
	4	Documenting - Abstracts indicative - descriptive abstracts and informative abstracts	2	Analyze descriptive and informative abstracts	Lecture and seminar	
	5	Documenting - footnotes, end notes, referencing styles,bibliography, journal abbreviations, abbreviation used in scientific writing	2	Identifythe format for documentation of research	Lecture with ppt	

IV	**Instrumental Analysis**					
	1	Principle, instrumentation and applications of AFM - SEM and STM	4	Understandthe principle and applications of AFM, SEM andSTM	Lecture with videos	Evaluation through periodic test, class test, online quiz and group discussion Formative assessment I
	2	Principle, instrumentation and applications of TEM and XRD	2	Understandthe principle and applications of TEM and XRD	Lecture with videos	
	3	Determination of surface morphology and particle size	2	Determine the surface morphology and particle size of compounds	Seminar and group discussion	Evaluation through periodic test, class test, online quiz and class assignment Formative assessment II
	4	Sample preparations and applications of UV and IR spectroscopy	2	Apply UV and IR spectroscopy for structural elucidation of compounds	Lecture with ppt and videos	
	5	Sample preparations and applications of NMR and mass spectroscopy	5	Apply NMR and mass spectroscopy for structural elucidation of compounds	Seminar	
V	**Cheminformatics**					
	1	Cheminformatics - history and applications. Representing molecules - line notation - Inchi - SMILES and WLN canonicalization	2	Understand cheminformatics and line notations	Lecture with ppt	Evaluation through periodic test, class test and online quiz and problem solving Formative assessment I
	2	Connection table and line notation versus connection table. SMARTS	2	Relate line notation and connection tables. Know about the query language SMARTS	Lecture with ppt	
	3	Molecular similarity - 2D topology and 3D configuration	2	Understand the importance of molecular similarity, 2D topology and 3D configuration in cheminformatics	Lecture	

	4	Chemistry softwares - Chemdraw - writing chemical equations and schemes - editing - transporting picture to word and image document	3	Apply Chemdraw software to draw chemical equations and schemes	Lecture with demo using Chemdraw software	
	5	Origin -importing and exporting data - scientific graphing and data analysis - curve fitting and peak analysis - transporting graph to tag image file format	3	Apply Origin software to sketch graph and data analysis	Lecture with demo using Origin software	

Course Instructor: Dr. Sheeba Daniel HOD: Dr. G. Leema Rose

Semester IV
Inorganic Spectroscopy, Photochemistry and Organometallics (Core IX)
Subject Code: PG2041

Hours per week	Credits	Total Hours	Marks

6	6	90	100

Objectives:

- To understand the principle, interpretation and applications of various spectroscopic techniques to inorganic compounds
- To know the applications of photochemistry, organometallics and bio-inorganic chemistry

Course Outcomes (COs)

CO	***Upon completion of this course, the students will be able to*:**	**PSO Addressed**	**CL**
CO-1	understand the principles and concepts of inorganic spectroscopy, photochemistry and organometallics.	PSO-1	U
CO-2	apply the principles of spectroscopy, photochemistry and organometallic chemistry to inorganic compounds.	PSO-2	A
CO-3	analyse the structure, reactions and functions of inorganic compounds.	PSO-2	Y
CO-4	evaluate the spectral data and properties of inorganic compounds	PSO-3	E

Unit I **(18 Hours)**

IR, Raman and NMR Spectroscopy

IR spectroscopy: introduction - selection rules - stretching frequency of some inorganic ions - effect of coordination on the stretching frequency of sulphato - carbonato - sulphito - aqua - nitro - thiocyanato - cyano - thiourea and DMSO complexes.

Raman spectroscopy: introduction - combined applications of IR and Raman spectroscopy in the structural elucidation of N_2O - ClF_3 - NO_3^- - ClO_4 and metal carbonyls.

NMR spectroscopy: introduction - structural assessment of simple inorganic compounds - applications of ^{1}H - ^{15}N - ^{19}F and ^{31}P NMR spectroscopy in structural problems. Fluxional molecules and effect of quadrupolar nuclei in NMR spectroscopy.

Unit II **(18 Hours)**

Mössbauer and Photoelectron Spectroscopy

Mössbauer (MB) spectroscopy: introduction - principle - recoil energy - doppler effect - number of MB signals - isomer shift - quadrupole splitting and magnetic hyperfine splitting. Applications of MB spectroscopy to ^{57}Fe - ^{119}Sn and ^{129}I compounds.

Photoelectron Spectroscopy (PES): theory - types - origin of fine structures - shapes of vibrational fine structures - adiabatic and vertical transitions. PES and evaluation of

vibrational constants of homonuclear diatomic molecules - N_2 and O_2 - heteronuclear diatomic molecules - CO and HCl - polyatomic molecules H_2O - CO_2 - CH_4 and NH_3. Koopman's theorem- applications and limitations.

Unit III **(18 Hours)**

Inorganic Photochemistry: Importance of photochemistry. Photochemistry of Co(III) complexes - photosubstitution - photooxidation - photoreduction and photoanation reactions. Photochemistry of Cr(III) complexes - Adamson's rule - photoaquation - photoisomerization - photoracemization - photoanation - photosubstitution in non-aqueous solvents and photoredox reactions. Photochemistry of ruthenium polypyridyls - preparation and characteristics of $[Ru(bpy)_3]^{2+}$ complex. Ground state and excited state properties of $[Ru(bpy)_3]^{2+}$ complex. Reactions of $[Ru(bpy)_3]^{2+}$ complex - photosubstitution - photoredox and reductive quenching reactions.

Unit IV **(18 Hours)**

Organometallic Chemistry: Organometallic compounds - types. EAN rule - 18e- and 16e- rules - determination of oxidation state - configuration - coordination number of the metal centre - types and application 18e- / 16e- rules. Carbonyls - isolated concept - structure of simple and polynuclear carbonlys. Nitrosyls - bridging and terminal nitrosyls - bent and linear nitorsyls. Synthesis, properties and structural features of metal complexes with carbene - alkene - alkyne and arene. Hapticity. Metallocenes - synthesis - properties and bonding in ferrocene. Covalent versus ionic bonding in beryllocene. Reactions of organometallic compounds - substitution - oxidative addition and reductive elimination - insertion and deinsertion (elimination) reactions.

Unit V **(18 Hours)**

Bio Inorganic Chemistry: Photosynthesis - photosystem I and II. Photosynthetic reaction center. Metallo enzymes - Zinc enzymes - structure and functions of carbonic anhydrase and carboxy peptidase. Iron enzymes - catalase and peroxidase. Super oxide dismutase (SOD) - superoxide toxicity - structure and function of Cu,Zn-SOD. Trace elements in biological system. Metal ion toxicity - classes of toxic metal compounds and detoxification. Metals in medicine - anti-arthritis drugs - Au and Cu in rheumatoid arthritis - Li in psychiatry - Pt, Au and metallocenes in anti-cancer drugs. Metals in radiodiagnosis and magnetic resonance imaging.

Text Books

5. Roundhill, D.M. (1994). Photochemistry and Photophysics of Metal Complexes. (1st ed.). New York: Plenum Press.
6. Kaur, H. (2006). Spectroscopy. (3rded.).Meerut: Pragati Prakasan Publications.
7. BanWell, C.N. & Mccash, E.M. (1997). Fundamentals of Molecular Spectroscopy. New Delhi: Tata Mc Grow Hill.
8. Malik, W.U., Tuli, G.D. & Madan, R.D. (2012). Selected topics Inorganic Chemistry. (5th ed.). New Delhi: S. Chand Company Ltd.

9. Chatwal, G.R. & Bhagi, A.K. (2005). Bio-inorganic Chemistry. (2nd ed.). India: Himalaya Publishing House.

Reference Books

1. Rohatgi, K.K. & Mukherjee, K.K. (2014). Fundamentals of Photochemistry. (3rd ed.). India: New Age International.
2. Iggo, J.A. (2000). NMR Spectroscopy in Inorganic Chemistry. USA: Oxford Scientific Publications.
3. Brisdon, A.K. (1998). Inorganic Spectroscopic Methods. USA: Oxford Scientific Publications.
4. Horwood, E. (2010). NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry. (1st ed.). New York: Ellis Horwood Ltd.
5. Puri, B.R., Sharma L.R. & Kalia, K.C. (2012). Principles of Inorganic Chemistry. (4th ed.), India: Milestone publishers.
6. Miessler, G.L. (2004). Inorganic Chemistry. (3rd ed.), India: Pearson Education.
7. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. (2011). Inorganic Chemistry, Principles of Structure and Reactivity. (4th ed.). India: Pearson Education.

Teaching Module

Credits: 6 **Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**IR, Raman and NMR Spectroscopy**					
	1	IR spectroscopy: introduction - selection rules - stretching frequency of some inorganic ions - effect of coordination on the stretching frequency of sulphato - carbonato - sulphito - aqua - nitro - thiocyanato - cyano - thiourea and DMSO complexes.	5	Understand the principle and applications of IR spectroscopy in structural determination	Lecture and PPT	Evaluation through class test Formative assessment I
	2	Raman spectroscopy: introduction - combined applications of IR and Raman spectroscopy in the structural elucidation of N_2O - ClF_3 - NO_3^- - ClO_4 and metal carbonyls.	5	Understand the principles of Raman Spectroscopy and compare IR and Raman Spectroscopy in structure elucidation	Lecture and PPT	
	3	NMR spectroscopy: introduction - structural assessment of simpleinorganic compounds - applications of ^{1}H - ^{15}N - ^{19}F and ^{31}P NMR spectroscopy in structural problems	5	Understand the principles of NMR spectroscopy and apply NMR spectroscopy to solve structural problems	Lecture and PPT	
	4	Fluxional molecules and effect of quadrupolar nucleiin NMR spectroscopy.	3	Analyse the effect of quadrupolar nuclei in NMR spectroscopy	Lecture and Seminar	
II	**Mössbauer and Photoelectron Spectroscopy**					
	1	Mössbauer (MB) spectroscopy: introduction - principle - recoil energy - doppler effect - number of MB signals - isomer shift - quadrupole splitting and magnetic hyperfine splitting. Applications of MB spectroscopy to ^{57}Fe - ^{119}Sn and ^{129}I compounds.	6	Understand the principle of Mössbauer (MB) spectroscopy and apply MB spectroscopy to ^{57}Fe - ^{119}Sn and ^{129}I compounds.	Lecture and PPT	Evaluation through class test and group discussion Formative assessment II

	2	Photoelectron Spectroscopy (PES): theory - types - origin of fine structures - shapes of vibrational fine structures - adiabatic and vertical transitions.	5	Apply Photoelectron Spectroscopy to predict the origin and shapes of vibrational fine structures	Lecture and demonstration	
	3	PES and evaluation of vibrational constants of homonuclear diatomic molecules - N_2 and O_2 - heteronuclear diatomic molecules - CO and HCl -	4	Evaluate the vibrational constants of homonuclear and heteronuclear diatomic molecules	Lecture and group discussion	
	4	Polyatomic molecules H_2O - CO_2 - CH_4 and NH_3. Koopman's theorem- applications and limitations	3	Apply Koopman's theorem	Lecture and group discussion	
III	**Inorganic Photochemistry**					
	1	Importance of photochemistry. Photochemistry of Co(III) complexes - photosubstitution - photooxidation - photoreduction and photoanation reactions	5	Understand the various photochemical reactions of Co(III) complexes	Lecture and PPT	Evaluation through class test and group discussion Formative assessment II
	2	Photochemistry of Cr(III) complexes - Adamson's rule - photoaquation - photoisomerization - photoracemization - photoanation - photosubstitution in non-aqueous solvents and photoredox reactions	5	Compare the types of photochemical reactions in non-aqueous solvents and photoredox reactions	Lecture and seminar	
	3	Photochemistry of ruthenium polypyridyls - preparation and characteristics of $[Ru(bpy)_3]^{2+}$ complex.	4	Understand the preparation and characteristics of $[Ru(bpy)_3]^{2+}$ complex	Lecture and group discussion	
	4	Ground state and excited state properties of $[Ru(bpy)_3]^{2+}$ complex. Reactions of $[Ru(bpy)_3]^{2+}$ complex - photosubstitution - photoredox and reductive quenching reactions.	4	Compare the ground state and excited state properties of $[Ru(bpy)_3]^{2+}$ complex	Lecture and seminar	
IV	**Organometallic Chemistry**					

	1	Organometallic compounds - types. EAN rule - 18e- and 16e- rules - determination of oxidation state - configuration - coordination number of the metal centre - types and application 18e- / 16e- rules	5	Understand the types of Organometallic compounds and apply EAN rule	Lecture and group discussion	Evaluation through class test and group discussion Formative assessment I
	2	Carbonyls - isolated concept - structure of simple and polynuclear carbonlys.	2	Compare the structure of simple and polynuclear carbonlys	Lecture and group discussion	
	3	Nitrosyls - bridging and terminal nitrosyls - bent and linear nitorsyls.	2	Classify bridging and terminal nitrosyls - bent and linear nitorsyls	Lecture and discussion	
	4	Synthesis, properties and structural features of metal complexes with carbene - alkene - alkyne and arene.	4	Correlate the structural features of metal complexes	Lecture and project	
	5	Hapticity . Metallocenes - synthesis - properties and bonding in ferrocene. Covalent versus ionic bonding in beryllocene.	3	Compare Covalent versus ionic bonding in beryllocene	Lecture	
	6	Reactions of organometallic compounds - substitution - oxidative addition and reductive elimination - insertion and deinsertion (elimination) reactions	2	Analyse the various reactions of organometallic compounds	Lecture and Discussion	
V	**Bio Inorganic Chemistry - II**					
	1	Photosynthesis, photosystem I and II and photosynthetic reaction centre.	3	Generalize photosystem I, II and photosynthetic reaction	Lecture	Evaluation through class test, group discussion and quiz Formative
	2	Metalloenzymes - enzymes in di-oxygen management.	3	Explain metalloenzymes	Lecture	

	3	Super oxide dismutase, superoxide toxicity, structure of Cu, Zn-SOD, enzymatic activity and mechanism.	3	Deduce the structure of Cu, Zn-SOD	Lecture and PPT	assessment I
	4	Peroxidases, catalases, oxidases and mono oxygeneases.	3	Explain the functions of enzymes	Lecture	
	5	Zinc enzymes - the structural role of zinc and zinc constellations of carbonic anhydrase, carboxy peptidase and alcohol dehydrogenase.	3	Understand the role of zinc in zinc enzymes	Lecture	
	6	Metal complexes as probes of nucleic acids. Gold compounds and anti-arthritic agents.	3	Explain the role of metal complexes and its applications	Lecture and group discussion	

Course Instructor: Dr. S. Lizy Roselet HOD: Dr. G. Leema Rose

Semester IV
Photochemistry and Natural Products (Core X)
Subject Code: PG2042

Hours per week	Credits	Total Hours	Marks
6	5	90	100

Objectives:

- To understand various organic reactions with their mechanism and synthetic utility.
- To elucidate the structure and synthesise natural products.

Course Outcomes (COs)

CO	*Upon completion of this course, the students will be able to:*	PSO Addressed	CL
CO-1	understand various organic reactions and their mechanism	PSO-1	U
CO-2	apply the reaction mechanism in organic synthesis	PSO-2	A
CO-3	analyze the structure and mechanism of reactions	PSO-2	Y
CO-4	evaluate the synthetic utility of reactions	PSO-2	E

Unit I **(18 Hours)**

Organic Photochemistry: Introduction - Thermal versus photochemical reactions and Jablonski diagram. Photochemical reactions of ketones - photosensitization - Norrish type - I and Norrish type - II reactions and mechanisms - Paterno-Buchi reaction - photooxidation and photoreduction of ketones. Photochemistry of arenes - Photodimerisation - photoisomerisation. Reactions involving free radicals - Barton - Hundsdiecker - Pschorr and Gomberg-Bauchman reactions.

Unit II **(18 Hours)**

Pericyclic Reactions: Characteristics and classifications of pericyclic reactions - electrocyclic - cycloaddition and sigmatropic reactions. Woodward Hofmann rule. Retro- Diels Alder reaction - Diels Alder reaction - 2+2 - 2+4 reactions. Cope rearrangements and Claisen rearrangements. Conservation of orbital symmetry. Prediction of reaction conditions using FMO - correlation diagrams and Zimmerman (Mobius-Huckel) approaches.

Unit III **(18 Hours)**

Retrosynthetic Analysis: Retrosynthetic terminologies - linear and convergent approach - protecting groups - activating groups - synthons and synthetic equivalents. Target molecule - one functional group disconnection - two functional groups disconnection - 1,3- 1,5- and 1,4-dicarbonyl compounds. Functional group addition and interconversions. Umploung synthesis. Latent polarity. Retrosynthetic analysis - bisabolene - cis-jasmone - longifolene and cubane. Synthetic uses of nitrocompounds and alkenes.

Unit IV **(18 Hours)**

Alkaloids: Extraction - general properties - classification and general methods for determining structure. Structural elucidation - atropine - cocaine - dictamnine - reserpine - aeronycine and morphine.

Unit V **(18 Hours)**

Heterocyclic Compounds: Synthesis - reactions - structure - carbazole - oxazole - imidazole - thiazole - pyrones - pyrazole - pyrimidine - pyrazine - coumarins and chromone. Structural elucidation - flavones - isoflavone - anthocyanins - caffeine - theobromine and theopylline.

Text Books

1. Singh, J & Singh, J. (2012). Photochemistry and Pericyclic Reactions. (3rd ed.). India: New Age International Pvt. Ltd.
2. Tewari, K. S., Vishnol, N. K. & Mehrotra, S.N. (2002). A Text Book of Organic Chemistry. India: Vikas Publishing House Ltd.
3. Warren, S. (2014). Organic Synthesis: The Disconnection Approach. India: Wiley Pvt. Ltd.
4. Finar, I.L. (2002). Organic Chemistry Volume II. (5th ed.). India: Pearson Education
5. Bansal, R.K. (2014). Heterocyclic Chemistry. (5th ed.). India: New Age International Pvt. Ltd.
6. Clayden, J. Greeves, N& Warren, S. (2012). Organic Chemistry. (2nd ed.). Oxford University Press.

Reference Books

1. Depuy, C.H., & Chapman, O.S. (1988). Molecular Reactions and Photochemistry. India: Prentice Hall Pvt. Ltd.
2. Gill, G.B. & Wills, M.R. (1974). Pericyclic Reactions. London: Chapman and Hall
3. Agarwal, O.P. (1947). Chemistry of Organic Natural Product Vol. I & II India: Goel Publishing House.
4. Joule, J.A. & Mills, K. (2010). Heterocyclic Chemistry. (5th ed.). India: Wiley Pvt. Ltd.
5. Ireland, R.E. (1969). Organic Synthesis. Prentice Hall, Englewood Cliffs, New Jersey, U.S.A.
6. Carruthers, W. (2015). Modern Methods of Organic Synthesis. (4th ed), Cambridge University Press.

Teaching Module

Credit: 5 **Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Organic Photochemistry**					
	1	Introduction - Thermal versus photochemical reactions and Jablonski diagram.	4	Understand the basic concepts of photochemistry	Lecture with ppt	Evaluation through online quiz Formative assessment I
	2	Photochemical reactions of ketones - photosensitization - Norrish type - I and Norrish type - II reactions and mechanisms	4	Analyze the photochemical reaction mechanisms of carbonyl compounds	Lecture and Group discussion	
	3	Paterno-Buchi reaction - photooxidation and photoreduction of ketones.	4	Interpret photoxidation and photoreduction mechanisms in ketones	Lecture and Seminar	
	4	Photochemistry of arenes Photodimerisation - photoisomerisation.	2	Understand the mechanisms of Photodimerisation and photoisomerisation	Lecture	
	5	Reactions involving free radicals - Barton - Hundsdiecker - Pschorr and Gomberg-Bauchman reactions.	4	Understand various name reactions involving free radicals	Lecture with ppt	
II	**Pericyclic Reactions**					
	1	Characteristics and classifications of pericyclic reactions - electrocyclic - cycloaddition and sigmatropic reactions.	4	Classify the types of pericyclic reactions	Lecture and Seminar	Evaluation through class test, online quiz and group discussion Formative assessment I
	2	Woodward Hofmann rule. Retro-Diels Alder reaction - Diels Alder reaction - 2+2 - 2+4 reactions.	5	Differentiate Retro-Diels Alder and Diels Alder reaction	Lecture	
	3	Cope rearrangements and Claisen rearrangements. Conservation of orbital symmetry.	4	Compare Cope and Claisen rearrangements	Lecture and group discussion	

	4	Prediction of reaction conditions using FMO - correlation diagrams and Zimmerman (Mobius-Huckel) approaches.	5	Predict FMO - correlation diagrams and Zimmerman (Mobius-Huckel) approaches	Lecture	
III	**Retrosynthetic Analysis**					
	1	Retrosynthetic terminologies - linear and convergent approach - protecting groups - activating groups - synthons and synthetic equivalents.	4	Understand the basic terminologies of retero synthesis	Lecture with models	Evaluation through class test, online quiz and group discussion Formative assessment II
	2	Target molecule - one functional group disconnection - two functional groups disconnection - 1,3- 1,5- and 1,4- dicarbonyl compounds.	6	Interpret one and two functional groups disconnections	Lecture	
	3	Functional group addition and interconversions. Umploung synthesis. Latent polarity.	5	Illustrate functional interconversions in retro synthesis	Lecture and group discussion	
	4	Retrosynthetic analysis - bisabolene - cis-jasmone - longifolene and cubane.	3	Interpret the retrosynthetic analysis of bisabolene - cis-jasmone - longifolene and cubane.	Lecture	
	5	Synthetic uses of nitrocompounds and alkenes.		Describe the synthetic uses of nitrocompounds		
IV	**Alkaloids**					
	1	Extraction and general properties of alkaloids	3	Understand the general properties of alkaloids	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Classification of Alkaloids	3	Classify the types of alkaloids		
	3	General methods for determining structure of alkaloids	4	Understand the methods for determining structure of alkaloids	Lecture	

	4	Structural elucidation - atropine and cocaine	4	Elucidate the structure of atropine and cocaine	Lecture	
	5	dictamnine - reserpine - aeronycine and morphine.	3	Elucidate the structure of various alkaloids	Lecture	
V	**Heterocyclic Compounds**					
	1	Synthesis - reactions - structure - carbazole - oxazole - imidazole	5	Understand the synthesis and reactions of heterocyclic compounds	Lecture with videos	Evaluation through class test, group discussion and quiz Formative assessment I
	2	Synthesis of thiazole - pyrones - pyrazole - pyrimidine	5	Understand the synthesis and reactions of heterocyclic compounds	Lecture	
	3	Pyrazine - coumarins and chromone	2	Understand the synthesis and reactions of heterocyclic compounds	Lecture	Evaluation through class test, group discussion and quiz Formative assessment II
	4	Structural elucidation - flavones - isoflavone - anthocyanins	3	Elucidate the structure of flavones, isoflavone and anthocyanins	Lecture and Group Discussion	
	5	Caffeine - theobromine and theopylline.	3	Elucidate the structure of caffeine, theobromine and theopylline		

Course Instructor: Dr. Y. Christabel Shaji HOD: Dr. G. Leema Rose

Semester IV
Polymer chemistry (Core XI)
Subject Code: PG2043

Hours per week	Credits	Total Hours	Marks
6	5	90	100

Objectives:

- To gain knowledge about applications of polymers.
- To know the importance of various polymerization techniques.
- To study about synthetic polymers.

Course Outcome (COs)

CO	Upon completion of this course, the students will be able to:	PSO Addressed	CL
CO -1	Understand the concept of polymer chemistry	PSO - 1	U
CO -2	Apply the processing techniques in the manufacture of synthetic polymer	PSO - 5	A
CO -3	Analyze glass transition temperature, crystallinity and degradation in polymers.	PSO - 3	Y
CO -4	Evaluate molecular weight and size of the polymer	PSO - 3	E

Unit I **(18 hours)**

Chemistry of Polymerization: Basic concepts of polymer chemistry - repeat unit - degree of polymerization - classification - chain polymerization - free radical polymerization - ionic polymerisation - coordination polymerisation: Zeigler- Natta catalyst - stereo regulating polymerization - step polymerization - ring opening polymerization - copolymerisation - types - free radical copolymerisation - ionic copolymerization - copolycondensation - block and graft copolymers.

Unit II **(18 hours)**

Polymerisation Techniques Molecular Weight and Size: Polymerisation techniques - bulk - solution - suspension - emulsion - polymerizations -melt polycondensation - solution polycondensation interfacial condensation - solid and gas phase polymerization - molecular weight and size -number average and weight average molecular weights - sedimentation and viscosity average molecular weights -polydispersity and molecular weight distribution in polymers - practical significance of polymer molecular weight.

Unit III **(18 hours)**

Polymer Processing: Processing techniques - calendering - die casting - rotational casting - film casting - compression moulding - injection moulding - blow moulding - extrusion moulding - thermoforming, foaming and reinforcing techniques - hand lay-up technique - filament winding technique - spray-up technique. Fibre spinning - dry spinning - wetspinning - uniaxial orientation - post treatment for fibres.

Unit IV **(18 hours)**

Synthetic Polymers: Synthetic resins - plastics - manufacture - applications - polyethylene - PVC - teflon -polystyrene - polymethylmethacrylate -polyurethane - phenol-formaldehyde resins - urea- formaldehyde and melamine- epoxy polymers. Synthetic fibers - rayon -nylons -polyesters -acrylics – modacrylics. Natural rubber -production -constitution - vulcanization (hot and cold) - fillers and accelerators - antioxidants - synthetic rubber - SBR - butyl rubber - nitrile rubber -neoprene - silicone rubberand polysulphides.

Unit V **(18 hours)**

Polymer Degradation and Additives: Polymer degradation - types - thermal degradation - mechanical degradation - photo degradation – degradation by ultrasonic waves - degradation by high energy radiation - hydrolytic and oxidative degradations - additives for polymers - fillers - plasticisers - thermal stabilizers - photo stabilizers - antioxidants and colourants.

Text Books

1. Billmeyer, F. (1971). Textbook of Polymer Science. (2nd ed), New York : John Wiley and Sons.
2. Gowariker, V.R (2009). Polymer Science. (2nd ed), New Age international .). India: New Age International Pvt. Ltd.
3. Braun, D. (1982). Simple Methods for Identification of Plastics. New York : Macmillan Publishing Co.
4. Robert Weast, C. (1985). Handbook of Chemistry and Physics. (65th ed), Boca Raton, FL : CRC Press.
5. Hightstown, N.J. (1990). Modern Plastics, Encyclopedia, Volume 67: McGraw Hill.

Reference Books

1. Odian, G. (2004). Principles of Polymerization. (4th ed): John Wiley and Sons
2. Manas Chanda. (2000). Advanced Polymer Chemistry: Marcel Dekker Inc.
3. Malcolm. P. Stevens. (1999). Polymer Chemistry: An Introduction. (3rd edition) : USA : Oxford University Press
4. Misra .G.S. (1993). Introductory Polymer Chemistry : New York : J. Wiley and Sons.
5. Charles E. Carraher Jr. (2017). Introduction to Polymer Chemistry. (4th ed):CRC Press.
6. Rodriguez, F., Cohen, C., Ober, C.K. & Archer, L. (2015). Principles of Polymer Systems. (6th ed), CRC Press.

Teaching Module

Credit: 5 **Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Chemistry of Polymerization**					
	1	Basic concepts of polymer chemistry - repeat unit - degree of polymerization - classification	4	Understand the basic concepts of polymer chemistry	Lecture and group discussion	Evaluation through class test Formative assessment I
	2	stereochemistry of polymers -nomenclature of stereo regular polymers	3	Discuss the nomenclature of stereo regular polymers	Lecture and group discussion	
	3	chain polymerization - free radical polymerization - ionic polymerisation coordination polymerisation: Zeigler-Natta catalyst - step polymerization - ring openingpolymerization	8	Explain the different types of polymerization	Lecture and ppt	
	4	copolymerisation - block and graft copolymers - preparation.	3	Describe copolymers preparation	Lecture	
II	**Polymerisation Techniques Molecular Weight and Size**					
	1	Polymerisation techniques -bulk - solution -suspension - emulsion – polymerizations	4	Explain various polymerization techniques	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	melt polycondensation - solution polycondensation interfacialcondensation	4	Compare different types of poly condensation processes	Lecture and group discussion	

	3	solid and gas phase polymerization.	4	Analyse solid and gas phase polymerization processes	Lecture	
	4	polydispersity and molecular weight distribution in polymers	3	Evaluate the poly dispersity index and molecular weight of polymers	Lecture	
	5	the practical significance of polymer molecular weight.	3	Explain the practical significance of polymer molecular weight.		
III	**Polymer Processing**					
	1	Processing -Calendering - die casting - rotational casting - film casting	5	Explain the various polymer casting processes	Lecture	Evaluation through class test and group discussion Formative assessment III
	2	compression moulding - injection moulding - blow moulding - extrusion moulding	5	Compare the moulding processes in polymers.	Lecture and field visit	
	3	thermoforming, foaming and reinforcing techniques	2	Explain the techniques of polymer processes.	Lecture	
	4	synthetic resins – plastics- manufacture and applications of polyethylene -PVC - Teflon -polystyrene - polymethylmethacrylate -polyurethane - phenol- formaldehyde resins - urea-formaldehyde and melamine- epoxy polymers.	6	Describe the manufacture and application of synthetic resins	Videos and industrial visit	
IV	**Synthetic Polymers**					

	1	Synthetic fibres -rayon - nylons -polyesters - acrylics -modacrylics	5	Describe the manufacture and application of synthetic fibres	Lecture and video	Evaluation through class test and group discussion Formative assessment II
	2	spinning techniques	2	Explain the spinning techniques of polymer process	Lecture and video	
	3	natural rubber - production -constitution - vulcanization (hot and cold)	3	Discuss the production and vulcanization of rubber	Lecture and field visit	
	4	fillers and accelerators – antioxidants	3	Compare the functions of fillers accelerators and antioxidants	Lecture and group discussion	
	5	Synthetic rubber -SBR - butyl rubber - nitrile rubber -neoprene - silicone rubber and polysulphides.	5	Describe the manufacture and application of synthetic rubber	Lecture	
V	**Polymer Degradation and Additives**					
	1	Polymer degradation	1	Describe polymer degradation	Lecture	Evaluation through class test, group discussion and quiz Formative assessment I
	2	types of degradation - thermal -mechanical photo - hydrolytic and oxidative degradations	7	Classify the types of polymer degradation	Lecture	
	3	additives for polymers - fillers -plasticizers	5	Discuss the role of additives in polymers	Lecture and group discussion	
	4	thermal stabilizers - photo stabilizers - antioxidants and colorants.	5	Differentiate thermal and photo stabilizers	Lecture and group discussion	

Course Instructor: M.Shirly Treasa HOD: G. Leema Rose

Teaching Module

Credits: 3 **Total Hours: 60 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Introduction to Energy Sources**					
	1	Introduction, conventional energy sources like coal, oil, gas, agricultural and organic wastes, water power, thermal power and nuclear power.	3	Recall the sources of conventional energy	Lecture with videos	Evaluation through class test and seminar Formative assessment I
	2	Non-conventional energy sources like solar energy and wind energy.	3	Explain non-conventional energy sources	Lecture and group discussion	
	3	Energy from bio-mass and bio-gas, ocean thermal energy, tidal energy.	3	Understand various sources of energy	Lecture	
	4	Geothermal energy and hydrogen energy. Advantages of renewable energy.	3	Discuss the advantages of renewable energy	Lecture and PPT	
II	**Solar Energy**					
	1	Solar radiation and its measurement - Introduction, solar constant, solar radiation at the earth's surface, solar radiation geometry and solar radiation data.	3	Explain solar radiations and its measurement	Lecture and videos	Evaluation through class test and seminar Formative assessment II
	2	Solar energy collectors - Introduction, physical principles of the conversion of solar radiation into heat, flat plate and concentration collectors.	3	Understand the principle of solar energy conversion and collectors	Lecture and PPT	
	3	Advantages and disadvantages of concentration collectors over flat collectors.	2	Compare the concentration collectors and flat collectors	Lecture	
	4	Energy balance equation and collector efficiency.	4	Determine energy balance and collector efficiency	Lecture	
III	**Wind Energy**					

	1	Introduction, basic principles of wind energy conversion, power of the wing, forces on the blades.	2	Understand the basis of wind energy	Lecture with videos	Evaluation through class test and seminar Formative assessment II
	2	Wind energy conversion, wind data and estimation, site selection.	2	Illustrate wind energy conversion	Lecture with ppt and videos	
	3	Types of wind machines - Horizontal axis and vertical axis machines.	2	Classify the types of wind machine	Lecture and seminar	
	4	Analysis of aerodynamic forces acting on the blade, performance of wind machines.	2	Analyse the forces acting on the blade	Lecture and group discussion	
	5	Generating systems - Introduction, schemes of electric generation, generator control, load control, energy storage. Application of wind energy.	4	Explain generating system and applications of wind energy	Lecture with videos	
IV	**Bio-energy**					
	1	Introduction, biomass conversion techniques - wet processes and dry processes.	2	Explain biomass and its conversion	Lecture and PPT	Evaluation through class test and quiz Formative assessment I
	2	Biogas generation. Classification of biogas plants - floating drum plant and fixed dome type plant. Biogas from plant waste.	3	List out the classification of biogas plants	Lecture and seminar	
	3	Materials used for biogas generation, selection of site for a biogas plant, digester design. Problems related with biogas plants.	3	Describe the biogas generation and identify the problems related to biogas plant	Lecture and seminar	
	4	Fuel properties of biogas and utilization of biogas.	4	Understand the properties of biogas	Lecture and seminar	
V	**Chemical energy sources**					
	1	Fuel cells - Introduction, conversion efficiency of fuel cells, types of electrodes, work output.	2	Understand the basis of fuel cells	Lecture and seminar	Evaluation through class test and quiz

	2	EMF of fuel cells. Applications of fuel cells.	2	Determine the EMF of fuel cells and explain the applications of it	Lecture and seminar	Forma assessr
	3	Hydrogen energy: Hydrogen production – electrolysis, thermo-chemical, fossil fuel and solar energy methods.	3	Explain hydrogen production by various methods	Lecture and Seminar	
	4	Hydrogen storage and hydrogen transportation.	2	Explain the hydrogen storage and hydrogen transportation	Lecture and seminar	
	5	Utilization of hygrogen gas. Hydrogen as an alternative fuel for motor vehicles. Safety and management.	3	Describe the utilization and safety measures of hydrogen gas	Lecture and PPT	

Course Instructor: B.T Delma Leema Rose

HOD: Dr. G.