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 - thermodynamic aspects 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- spectral properties.

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 double and triple bonds. Nucleophilic addition to carbon-carbon multiple bonds	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 - Shapiro reaction - 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 the relation for cyclic polyene 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 - properties types 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 - rates of 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 **Core IX**

Name of the Course: Organic Chemistry IV

Subject Code: PG1741

Teaching Plan

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Retrosynthetic Analysis**					
	1	Planning – relay, linear and convergent approach, protecting groups and activating groups. Target molecule containing one functional group requiring a single disconnection.	4	Understand the concept of reterosynthesis	Lecture	Evaluation through class test Formative assessment I
	2	Synthons and synthetic equivalents. Latent polarity. Target molecules with two functional groups - 1,3-, 1,5- and 1,4-dicarbonyl compounds.	5	Analyse the reterosynthetic approach of target molecules with two functional groups	Lecture	
	3	Functional group interconversions. Umploung synthesis.	3	Generalize functional group interconversions and Umploungsynthesis	Lecture	
	4	Retrosynthetic analysis of bisabolene, cis-Jasmone and longifolene.	3	Explain the retrosynthesis of bisabolene, cis-Jasmone and longifolene	Lecture	
II	**Alkaloids**					
	1	Alkaloids, Extraction, general properties and classification.	4	Discuss the chemistry of alkaloids	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Alkaloids -general methods for determining structure.	3	Know about the general methods for determining the structure of alkaloids	Lecture	
	3	Structural elucidation of morphine, atropine and cocaine.	5	Elucidate the structure of morphine, atropine and cocaine	Lecture and group discussion	
	4	Structural elucidation of quinine and papaverine.	3	Elucidate the structure of quinine and papaverine	Lecture and group discussion	
III	**Molecular rearrangements**					

	1	Classification - electrophilic, nucleophilicand free radical rearrangements. Mechanisms of Di- π- methane rearrangement.	2	Classify the types of rearrangements and understand the mechanism of Di- π- methane rearrangement	Lecture	Evaluation through class test Formative assessment III
	2	Mechanisms of Tiffenev-Demyanov, Dienone- Phenol and von-Richter rearrangements.	3	Explain the mechanism of Tiffenev-Demyanov, Dienone- Phenol and von-Richter rearrangements	Lecture	
	3	Mechanisms of Favorskii, Fries, Baeyer-Villager rearrangements.	4	Explain the mechanism of Favorskii, Fries and Baeyer-Villager rearrangements	Lecture	
	4	Mechanisms of Stevens, Neber and Sommelet-Hauser rearrangements.	3	Explain the mechanism of Stevens, Neber and Sommelet-Hauser rearrangements	Lecture	
	5	Mechanisms of Baker-Venkatraman,Wagner Meerwin and Ullmann rearrangements.	3	Explain the mechanism of Baker-Venkatraman,Wagner Meerwinand Ullmann rearrangements	Lecture	
IV	**Organic Photochemistry**					
	1	General introduction. Thermal versus photochemical reactions. Jablonski diagram.	3	Differentiate thermal and photochemical reactions	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Photochemical reactions of ketones– photosensitization, Norrish type - I and Norrish type - II reactions and mechanisms.	3	Know the photochemical reactions of ketones	Lecture and group discussion	
	3	Paterno–Buchi reaction, photooxidation and photoreduction of ketones,.	3	Identify photooxidation and photoreduction of ketones	Lecture	
	4	Photochemistry of arenes. Photodimerisation and photoisomerisation.	3	Understand the mechanism of photochemical reactions in ketonesandarenes	Lecture	
	5	Reactions involving free radicals – Barton, Huns-diecker, Pschorr and Gomberg-Bauchman reactions.	3	Know the mechanism of photochemical reactions in free radicals	Lecture	
V	**Pericyclic Reactions**					

	1	Characteristics and classifications of pericyclic reactions - electrocyclic, cycloaddition and sigmatropic reactions.	4	Identify the reactions involving in pericyclic reaction	Lecture	Evaluation through class test, group discussion and quiz Formative assessment I
	2	Woodward Hofmann rule. 2+2, 2+4 – reactions, Retro-Diels Alder reaction and Diels Alder reaction.	4	Understand the mechanism of photochemical reactions	Lecture	
	3	Cope rearrangements and Claisen rearrangements. Conservation of orbital symmetry. Prediction of reaction conditions using FMO.	4	Know about FMO diagram	Lecture and group discussion	
	4	Correlation diagrams and Zimmerman (Mobius-Huckel analysis) approaches.	3	Correlate pericyclic reactions	Lecture	

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

Semester: IV **Core X**

Name of the Course: Inorganic Chemistry III

Sub Code: PG1742

Teaching Plan

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Application of spectroscopy to the study of Inorganic compounds – III**					
	1	NMR Spectroscopy: Principle, ^{31}P, ^{19}F, ^{15}N, applications in structural problems. Monitoring the course of reaction.	4	Know the principle and applications of NMR spectroscopy in structural determination	Lecture	Evaluation through class test Formative assessment I
	2	NMR of fluxional molecules. NMR of paramagnetic molecules - contact shift and shift reagents.	3	Analyse the NMR spectrum of various molecules	Lecture	
	3	NQR Spectroscopy: Principle, comparison with NMR, electric field gradient, quadrupolar splitting of energy levels in symmetric and asymmetric fields, quadrupolar coupling in atoms and molecules, asymmetry parameter.	5	Compare and understand NQR and NMR spectroscopy	Lecture	
	4	Application - hydrogen bonding, phase transition, substituent effect and structural information.	3	Know the applications of NQR spectroscopy	Lecture and Seminar	
II	**Applications of spectroscopy to the study of inorganic compounds – IV**					
	1	ESR spectroscopy - Introduction and Principle. Presentation of the spectrum and hyperfine splitting. Factors affecting the magnitude of g values	3	Understand the concept of ESR spectroscopy	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Zero-field splitting and Kramer's degeneracy. Anisotropy in the hyperfine coupling constant	3	Know about zero-field splitting, Kramer's degeneracy and anisotropy	Lecture	

	3	Covalency of M-L bonding by ESR.Jahn- Teller distortion in Cu (II) complexes from ESR studies.	3	Determine the ESR spectrum of Cu complexes	Lecture and group discussion	
	4	Mossbauer Spectroscopy: Principle, Doppler Effect, recoil energy, minimizing recoil energy, Doppler broadening.	3	Understand the principle and concept of Mossbauer spectroscopy	Lecture and group discussion	
	5	Isomer shift in Fe and Sn compounds. Electro negativity and chemical shift. Quadrupole interaction - quadrupole splitting in the MB spectra of Fe complexes.	3	Differentiate the MB spectrum of Fe^{2+} and Fe^{3+} complexes	Lecture	
III	**Non- aqueous solvents**					
	1	Non- aqueous solvents- Introduction General properties and classification of solvents	2	Classify solvents	Lecture	Evaluation through class test and group discussion Formative assessment III
	2	Self-ionization and leveling effect. Reactions in non- aqueous solvents. Solute- solvent interaction.	2	Understand the reactions in non-aqueous solvents and solute-solvent interaction	Lecture and seminar	
	3	Solution of metals in liquid ammonia. Reaction in liquid HF, liquid halogens, interhalogens and liquid H_2SO_4.	3	Identify the reactions in non-aqueous solvents	Lecture and group discussion	
	4	Molten salts as non-aqueous solvents. Titration in non-aqueous solvents.	3	Know about molten salts and titrations in non-aqueous solvents	Lecture and seminar	
	5	HSAB theory and solvent system definitions.	2	Define HSAB theory and solvent systems	Lecture	
	6	Acid base concepts - Arrhenius, Lux flood, Usanovich, Lowry-Bronsted and Lewis concept.	3	Infer acids and bases using various concepts	Lecture	
IV	**Electrical and magnetic properties of solids**					
	1	Conductivity of pure metals and Electrical conductivity	2	Explain the conductivity of metals	Lecture	Evaluation through class test and

	2	Photoconductivity, photoconductive device. Solar cell and solar energy conversion.	3	Describe solar cells and solar energy conversion	Lecture and group discussion	group discussion Formative assessment II
	3	Dielectric properties - permittivity, dielectric constant, electric susceptibility, electronic polarization, ionic polarization, orientation, dielectric loss and dielectric break down, ferro electricity.	4	Define the electrical proprieties of metals	Lecture	
	4	Applications of magnetic properties of solids - dia, para, ferro, antiferro and ferrimagnetism.	3	Describe the magnetic properties of metals	Lecture	
	5	Effect of temperature on magnetism - Curie and Weiss law. Calculation of magnetic moments.	3	State Curie and Weiss law and determine the magnetic moment of metals	Lecture	
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 assessment I
	2	Metalloenzymes - enzymes in di-oxygen management.	2	Describemetalloenzymes	Lecture	
	3	Super oxide dismutase, superoxide toxicity, structure of Cu, Zn-SOD, enzymatic activity and mechanism.	3	Know about superoxide dismutase	Lecture and group discussio n	
	4	Peroxidases, catalases, oxidases and mono oxygeneases.	2	Explain peroxidases, catalases, oxidases and mono oxygeneases	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 inzinc enzymes	Lecture	
	6	Metal complexes as probes of nucleic acids. Gold compounds and anti-arthritic agents.	2	Express the role of metal complexes and its applications	Lecture and group discussio n	

Course Instructor: A.K. Shermila HOD: G. Leema Rose

Semester: IV **Core XI**

Name of the Course: Physical Chemistry IV

Sub Code: PG1743

Teaching Plan

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Advanced topics in electrochemistry**					
	1	Photo-electrochemistry - Introduction, band bending at the semiconductor/solution interface.	3	Understand photo-electro chemistry	Lecture	Evaluation through class test Formative assessment I
	2	Photo-excitation of electrons by absorption of light, surface effects in photo-electrochemistry.	2	Explain photo-excitation of electrons	Lecture and Seminar	
	3	Photo-electro catalysis, photo-electrochemical splitting of water, photo-electrochemical reduction of CO_2.	3	Generalize photo-electrochemical reactions	Lecture and Seminar	
	4	Bio-electrochemistry – bio-electrodes, membrane potentials. Electrochemical communication in biological organisms	3	Know about bio-electrochemistry	Lecture with PPT	
	5	Enzymes as electrodes, electron transfer in p450 enzymes	2	Understand the role of enzymes as electrodes	Lecture	
	6	Electrochemical sensors, electrochemical biosensors, gas sensors and sensor arrays.	3	Describe various sensors	Lecture with ppt	
II	**Nanomaterials for catalysis**					
	1	Nanocatalyst: fundamentals, homogeneous vs heterogeneous catalysis	3	Differentiate homogeneous and heterogeneous nano-catalysis	Lecture and seminar	Evaluation through class test and group discussion Formative assessment II
	2	Effect of surface area, shape, morphology, particle size and composition on catalysis.	3	Know the effect of surface area, shape, morphology, particle size and composition on catalysis	Lecture with ppt	
	3	Nano-materials for photo-catalysis - dye degradation, water splitting, organic transformations.	4	Apply nano-materials for photo-catalysis	Lecture and group discussion	

	4	Plasmon assisted photo-catalysis and band gap tuning	3	Understand the concept of plasmon assisted photo-catalysis and band gap tuning	Lecture and group discussion	
	5	Nanomaterials for CO_2 capture and conversion.	2	Explain nanomaterials for CO_2 capture and conversion	Lecture	
III	**Molecular Spectroscopy - II**					
	1	Electronic Spectroscopy: Principle, laws of light absorption, Born-Oppenheimer approximation	3	Know the principle of electronic spectroscopy and Born-Oppenheimer approximation	Lecture	Evaluation through class test and group discussion Formative assessment III
	2	Franck-Condon principle, Wave-mechanical formulation, dissociation energy and dissociation products.	3	Understand Franck-Condon principle, dissociation energy and dissociation products	Lecture and seminar	
	3	Pre-dissociation, fluorescence and phosphorescence - principle and theory.	2	Generalize the principle and theory of fluorescence and phosphorescence	Lecture and group discussion	
	4	Nuclear magnetic resonance spectroscopy: Principle, Nuclear spin and nuclear moment, chemical shift and its measurements.	2	Explain the principle and concept of NMR spectroscopy	Lecture and seminar	
	5	Factors influencing chemical shift, shielding and deshielding effects, spin-spin interactions,	2	Discuss the factors affecting chemical shift and sipn-spin interactions	Lecture	
	6	NMR of simple AMX type molecules, coupling constant, FTNMR, NMR of ^{19}F, ^{31}P and ^{13}C .	5	Interpret the concept of FTNMR, ^{19}F, ^{31}P and ^{13}C NMR spectroscopy	Lecture	
IV	**Molecular Spectroscopy - III**					
	1	ESR: Theory, hyperfine interactions in ESR. Double resonance (ENDOR, ELDOR), Mc Connell's relation.	4	Understand the theory of ESR spectroscopy, double resonance and Mc Connell's relation	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Verification of the relation for cyclic polyene radical and calculation of electron density. Experimental techniques.	3	Explain the ESR spectroscopy of cyclic polyene radical and calculation of electron density	Lecture and group discussion	

	3	Laser Raman spectroscopy: Einstein treatment of absorption and emission phenomena. Einstein's coefficients.	2	Know about Laser Raman spectroscopy	Lecture	
	4	Probability of induced emission and its applications to lasers. Conditions for laser action.	4	Describe the applications of laser Raman spectroscopy	Lecture	
	5	Properties and types of lasers. Advantages of lasers in Raman spectroscopy. Experimental Techniques.	2	Discuss the properties and advantages of lasers in Raman spectroscopy	Lecture	
V	**Solid State Chemistry**					
	1	Ionic radii - determination. Gold Schmit'srule.	2	Determine the ionic radii of solids	Lecture	Evaluation through class test, group discussion and quiz Formative assessment I
	2	Closed packing in solids. Structure of metallic crystals.	3	Explain the structure of metallic crystals		
	3	Perovskite, CsCl, Zinc blende, Wurtzite, Rutile, fluorite and antifluorite. Covalent crystals. Diamond and graphite.	5	Discuss the structure of covalent crystals, diamond and graphite	Lecture	
	4	Mechanical properties of solids.	2	Understand the mechanical properties of solids	Lecture with videos	

Course Instructor: S. LizyRoselet HOD: G. Leema Rose

Semester: IV **Elective IV**

Name of the Course: Energy for the Future

Subject Code: PG1744

Teaching Plan

Unit	Module	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.	4	Know 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 Seminar	
	3	Energy from bio-mass and bio-gas, ocean thermal energy, tidal energy.	4	Understand various sources of energy	Lecture and Seminar	
	4	Geothermal energy and hydrogen energy. Advantages of renewable energy.	4	Generalize the advantages of renewable energy	Lecture and seminar	
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.	4	Explain solar radiations and its measurement	Lecture and seminar	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.	4	Understand the principle of solar energy conversion and collectors	Seminar	
	3	Advantages and disadvantages of concentration collectors over flat collectors.	3	Know the advantages and disadvantages of different collectors	Lecture	
	4	Energy balance equation and collector efficiency.	4	Determine energy balance and collector efficiency	Lecture and seminar	
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 III
	2	Wind energy conversion, wind data and estimation, site selection.	3	Illustrate wind energy conversion	Lecture with ppt and videos	
	3	Types of wind machines - Horizontal axis and vertical axis machines.	3	Classify the types of wind machine	Lecture and seminar	
	4	Analysis of aerodynamic forces acting on the blade, performance of wind machines.	3	Analyse the forces acting on the blade	Lecture and seminar	
	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.	3	Explain biomass and its conversion	Lecture and seminar	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.	4	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.	4	Generalize biogas generation and identify the problems related to biogas plant	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 Formative assessment II
	2	EMF of fuel cells. Applications of fuel cells.	3	Determine the EMF of fuel cells and explain the applications of it	Lecture and seminar	

	3	Hydrogen energy: Hydrogen production – electrolysis, thermo-chemical, fossil fuel and solar energy methods.	4	Explain hydrogen production by various methods	Seminar	
	4	Hydrogen storage and hydrogen transportation.	2	Know about hydrogen storage and hydrogen transportation	Lecture and seminar	
	5	Utilization of hygrogen gas. Hydrogen as an alternative fuel for motor vehicles. Safety and management.	4	Describe the utilization and safety measures of hydrogen gas	Seminar	

Course Instructor: S. Santhiya HOD: G. Leema Rose