Department of Chemistry

Ph.D. Course work

Semester	Paper Code	Course Title	Credits	Total
Core Courses				
I	17CHER0101 17CHER0102 17CHER0103 17CHER0104	Advances in Inorganic Chemistry Advances in Organic Chemistry Advances in Physical Chemistry Research Methodology	4 4 4 4	
II	17CHER0205 17CHER02SX	Analytical Techniques Specific course to be prescribed by the Doctoral Committee	4 4	24
	Seminar (3) Term paper/Topical Research			
III Semester onwards	Research Credits a)Project planning including literature collection, finalization of objectives and methodology b) Field/ Lab Studies, Data collection, compilation of results, statistical analysis, results and final conclusion.		4 32	
End of Program	Synopsis and thesis submission, final viva		6	

List of courses that are candidate centric (17CHER02SX)

17CHER02S1	Synthetic Organic Chemistry
17CHER02S2	Natural Products Chemistry
17CHER02S3	Surface science
17CHER02S4	Environmental chemistry
17CHER02S5	Coordination chemistry
17CHER02S6	Electrochemistry
17CHER02S7	Polymer chemistry
17CHER02S8	Photovoltaics
17CHER02S9	Supramolecular chemistry

17CHER0101 Advances in Inorganic Chemistry Credits: 4

Learning Objectives: The objective of the course is to impart knowledge in bonding, reaction mechanisms and electronic spectra of coordination compounds and to develop an understanding of organometallic chemistry and bio-inorganic chemistry.

Specific learning outcomes: At the end of the course, students will be able to:

- Explain crystal field theory, crystal field splitting in complexes, its limitations, and constructing MO diagrams of complexes
- Deduce the mechanisticpathway of reactions of inorganic complexes
- Analyze and interpret the electronic spectra of coordination complexes.
- Understand the catalytic activities of organometallic complexes.
- Revealthe magnetic properties of inorganic complexes
- Outline and evaluate the functions, mechanism of photosynthesis, enzymes and oxygen transport in biological systems.

Unit I :Coordination Chemistry

Crystal field and molecular orbital theories in formation of Coordination Compounds, splitting of d-orbitals in different geometries, factors influencing crystal field splitting, Jahn–Teller Effect; Stability constants of Transition metal complexes and their determination by spectrophotometric and Job's Method.

Electronic states and term symbols, Spin–orbit Coupling, Selection rules (Laporte and spin selection rule), Interpretation of electronic spectra of Transition metal complexes, Orgel and Tanabe-Sugano diagrams - Charge Transfer spectra.

Unit II : Reaction Mechanisms

Substitution reactions in octahedral complexes, associative and dissociative mechanisms, base catalysis. Substitution reaction in square planar complexes, trans-effect and its applications.

Electron transfer reactions in coordination complexes, outer sphere and inner sphere mechanisms, factors influencing rate of electron transfer reactions, electron transfer reactions in biological systems – Cytochrome-C oxidase and blue copper proteins (plastocyanin).

Unit III :Organometallic Chemistry

The 18 Valence Electron Rule, Structure and bonding in metal carbonyls, oxidative addition and reductive elimination reactions, C-H activation, migratory Insertion.

Organometallic catalysis: Mechanism of hydrogenation of olefins, isomerization of olefins, oxo-process, Wacker process, Monsantoacetic acid process. Water gas shift reaction, carbonylation, alkene hydrosilation, Fischer-Tropsch reaction and Ziegler-Natta catalysis.

Unit IV : Magnetic Properties of Inorganic Compounds

Definition of Magnetic Properties, Types of magneticbodies,Diamagnetism and Pascal's Constant, Russell-Saunders or LS Coupling,Stereo chemical applications of Magnetic Properties of the First Transition Series,Lanthanides and actinides, Determination of magnetic susceptibility by Gouy's Method, Derivation of Van Vleck formula for Susceptibility.

Unit-V :Bio-inorganic Chemistry

Metal ions in biology, structure and function of metallo-proteins and enzymes, heme and non-heme systems with one-, two- or multi-metal, photosynthesis and photosystem I and II; O_2-binding, nitrogen fixation, water-oxidation reactions. Synthetic models, Correlation with structure and function of the natural enzymes,Metal based drugs, Porphyrins and Corrins.

References:

1. Inorganic Chemistry, J.E. Huheey, E.A. Keiter and R.L. Keiter, Harper Collins College Publisher, 4thEdn., New York, 1993.
2. Inorganic Chemistry, G.L. Miessler and D.A. Tarr, Pearson Publishers, 5th edition, Delhi, 2013.
3. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and CH. Langford, ELBS, Oxford UniversityPress, 2000.
4. Physical Inorganic Chemistry: A Coordination Chemistry Approach, S.F.A. Kettle, Oxford University Press, 2000.
5. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard, Valentine, Viva Publishers, 1994.

17CHER0102 Advances in Organic Chemistry Credits: 4

Learning Objectives: The objective of the course is to impart knowledge in bonding, reaction mechanisms and electronic spectra of coordination compounds and to develop an understanding of organometallic chemistry and bio-inorganic chemistry.

Specific learning outcomes: At the end of the course, students will be able to:

- Explain crystal field theory, crystal field splitting in complexes, its limitations, and constructing MO diagrams of complexes
- Deduce the mechanisticpathway of reactions of inorganic complexes
- Analyze and interpret the electronic spectra of coordination complexes.
- Understand the catalytic activities of organometallic complexes.
- Revealthe magnetic properties of inorganic complexes
- Outline and evaluate the functions, mechanism of photosynthesis, enzymes and oxygen transport in biological systems.

Unit I : Reagents in organic synthesis

Reagents for Oxidation: Jones reagent, Pyridine chlorochromate, Collins reagent, Serette's reagent, m-Chloroperbenzoic acid, Swern oxidation. Reagents for Reduction: Catalytic hydrogenation, Pd-C, Lindlar's catalyst, Wilkinson' catalyst, DiBAL-H, Sodium cyanoborohydride.

Synthetic importance of diazomethane, poly phosphoric acid, Gilman reagents, Lithium diisopropylamide (LDA), DABCO, Butyl lithium, Potassium t-butoxide, DCC, EDC, HOBt, Phase Transfer Catalysis, Crown ethers, Baker's yeast, DBU, DDQ and Trifluoroacetic acid.

Unit II : Name reactions

Mechanism and Strategic applications of Suzuki coupling,Heckarylation, Prins reaction, Shapiro reaction, Mitsunobu reaction, Robinson annulation, Junjappa – Ila aromatic and heteroaromatic annulation, Pauson-Khandreaction, Huisgen 1,3-dipolar cycloaddition reaction and Grubb's olefin metathesis.

Unit III : Retro synthetic analysis and protecting groups

Synthons, synthetic equivalents, 1,1-, 1,2- and 1,3-difunctionalized compounds, two group disconnections, Diels-Alder reaction, 1,3-, 1,5-difunctionalized compounds, protection and deprotection of alcohols, carboxylic acids, and amines – Retrosynthesis of camphor and Juvabione.

Unit IV : Stereochemistry

Stereoselective, Enantioselective and Diastereoselective reactions; Asymmetric synthesis-chiral auxiliaries; Catalytic asymmetric synthesis – Asymmetric dihydroxylation, asymmetric hydrogenation, and alkylation - asymmetric amplification and autocatalysis.ORD, CD and their applications in the study of α-hydroxy ketones and steroids.

Unit V : Structure elucidation of organic compounds

Structural assignment of simple organic molecules by employing UV, IR, NMR and Mass spectrometry.

References:

1. Moderns Methods of Organic Synthesis, W. Carruthers, and I. Coldham, Cambridge UniversityPress, UK, 4th edition, 2004.
2. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, M.B. Smith and J. March, Wiley Interscience, 6th edition, 2007.
3. Organic Synthesis: The Disconnection Approach, Stuart Warren, Paul Wyatt, Wiley, 2nd edition, 2008.
4. The Logics of Chemical Synthesis, Part-1, E.J. Corey and Xue-Min Chelg, John Wiley & Sons, 2006.
5. Greene's Protective Groups in Organic Synthesis, Peter G. M. Wuts, JohnWiley& Sons, Inc, 5thedition, 2014.
6. Stereochemistry of Organic Compounds, E.L. Eliel, S.H. Wilen, Wiley Publishers, 2008.
7. Spectrometric Identification of Organic Compounds, R.M. Silverstein, F.X. Webster, D.J. Kiemle, D.L. Bryce, 8th edition, John Wiley & Sons, New Delhi, 2015.
8. Organic Spectroscopy, W. Kemp, ELBS, 2nd edition, 1991.

17CHER0103 Advances in Physical Chemistry Credits: 4

Learning Objectives: The objective of the course is to impart knowledge in bonding, reaction mechanisms and electronic spectra of coordination compounds and to develop an understanding of organometallic chemistry and bio-inorganic chemistry.

Specific learning outcomes: At the end of the course, students will be able to:

- Explain crystal field theory, crystal field splitting in complexes, its limitations, and constructing MO diagrams of complexes
- Deduce the mechanisticpathway of reactions of inorganic complexes
- Analyze and interpret the electronic spectra of coordination complexes.
- Understand the catalytic activities of organometallic complexes.
- Revealthe magnetic properties of inorganic complexes
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Unit-I Solid State Chemistry

Crystal Structure: Crystalline and amorphous solids; crystal systems, point groups: methods of characterizing crystal structure - Powder X-ray diffraction, electron and neutron diffraction. Band theory of conductors and semi-conductors.

Methods of Single Crystal Growth: Solution growth; Melt Growth-Bridgeman, Czochralski, Kyropoulus, Verneuil; Chemical Vapour Transport; Fused Salt Electrolysis; Hydrothermal method; Flux Growth.

Unit-II Electrodics

Electrochemistry concepts- kinetics of electron transfer - electrode kinetics- Faradaic vs. capacitive currents - electrochemical techniques, voltammetry - rotating electrodes - equivalent circuits, A.C. voltammetry - adsorption on electrodes- thin layer cells - electrochemistry of polymers and inorganic solids, study of reactions by spectroelectrometry.

Unit-III Surface Chemistry

Contact angle, wetting, Langmuir adsorption isotherm- Temkin isotherm, D-R isotherm, Gibbs-Adsorption equation- BET equation –Estimation of surface area- catalytic activity of surfaces- Principles, instrumentation and applications of X-ray Photoelectron Spectroscopy and AugarElectron Spectroscopy. Determination of Zeta potential using Dynamic Light Scattering (DLS) method.

Unit-IV Nano Chemistry

Synthesis and characterization of low-dimensional structures: Quantum wells, quantum wires, and quantum dots, carbon nanotubes and graphene, nanocomposites. Characterization by transmission electron microscopy. Biomedical applicationsofnanomaterials.

Unit-V Photochemistry

Excited state processes, experimental determination of quantum yields, reasons for low and high quantum yield, photochromism, transient absorption techniques, luminescence emission lifetimes, two- and multiphoton processes, photo-induced energy and electron transfer, Forster resonance energy transfer and Dexter energy transfer, fluorescence polarization, excimers, exciplexes, delayed fluorescence. Photochemistry in organized and confined media.

References:

1. Solid State Chemistry and its Applications, A.R. West, John Wiley & Sons, 2007.
2. L. Smart and E. Moore, Solid State Chemistry - An Introduction, Chapman & Hall, 1992.
3. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, 1993.
4. Electrochemical Methods: Fundamentals and Applications, A.J. Bard, L.R. Faulkner, John Wiley & Sons, 2nd edition, 2004.
5. Modern Electrochemistry, John M. Bockris and Amulya K.N. Reddy, Vol. I & II, 2nd edition, Springer, New Delhi, 2000.
6. Physical Chemistry of Surfaces, A.W. Adamson, A.P. Gast, John Wiley & Sons, 1997.
7. Physical chemistry, P.W. Atkins, ELBS, Edn, 1998.
8. Introduction to Nanoscience and Nanotechnology, G.L. Hornyak, H.F. Tribbals, J. Dutta, J.M. Moore, CRC Press, 2008.
9. Principles of Fluorescence Spectroscopy, J.R. Lokowicz, 3rd edition, Springer, 2010.
10. Fundamentals of Photochemistry, K.K. Rohatgi Mukherjee, New Age International Publishers, New Delhi, 2006.

17CHER0104 **Research Methodology** **Credits: 4**

Learning Objectives: The objective of the course is to impart knowledge in bonding, reaction mechanisms and electronic spectra of coordination compounds and to develop an understanding of organometallic chemistry and bio-inorganic chemistry.

Specific learning outcomes: At the end of the course, students will be able to:

- Explain crystal field theory, crystal field splitting in complexes, its limitations, and constructing MO diagrams of complexes
- Deduce the mechanisticpathway of reactions of inorganic complexes
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- Understand the catalytic activities of organometallic complexes.
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Unit-I Literature Survey

Scope of the problem – choosing a research problem – research design objectives, schedule of work plan- directions for the literature search – chemical abstracts – science citation indices, location of articles & journals.

Unit-II Science sources

Primary sources – Journals – patents – Secondary sources – listing of titles abstracts – compendia and tables of information – review – annual review – general treatise – monograph – Importance of text books and other non-text books. Quality metrices – h-index, impact factor, i10-index, citation index.

Unit-III Modern methods of literature survey

Use of computers in the literature survey – Websites, search engines (Scifinder, scopus, web of science, pubmed), internet, e-mail – Scientific information and documentation centers – Recent trends in scientific documents-digital library, e-journals.

Unit-IV Research paper and thesis writing

Preparation of seminar, abstract communication research papers for national and international journals. Tabulation and computation of data- Illustration of graphical data,

compilation of results, presentation, synopsis preparation and thesis writing. Publication of results – ethical issues, ethical committees, commercialization, copyright, intellectual property rights, patent law, reproduction of published materials and plagiarism.

Unit- V Statistical methods of analysis

Error analysis – significant figures – Accuracy and precision – methods of expressing accuracy and precision. Statistical approach for solving problems in chemistry - correlation analysis – simple and multiple regression analysis – Curve fitting.

References:

1. Advanced organic chemistry, Jerry March, John Wiley & Sons, 4th Edition, 2007.
2. A.I.Vogel, Elementary methods practical – Chemistry, CBS publication and distributors, New Delhi 2nd Edition,1987.
3. Principles of instrumental analysis, D.A. Skoog, F.J. Holler, T.A. Nieman, Brookes/Cole, 5th edition, 2005.
4. Research Methodology, Methods and Techniques, C.R. Kothari, New age international publishers, 3rd edition, 2004.
5. Research design: Qualitative and mixed method approaches, J.W. Creswell, 2008, Sage publications, USA.
6. http://edutechwiki.unige.ch/en/Research_methodology_resources
7. http://www.ncrm.ac.uk/

17CHER0205 Analytical Techniques Credits: 4

Learning Objectives: The objective of the course is to impart knowledge in bonding, reaction mechanisms and electronic spectra of coordination compounds and to develop an understanding of organometallic chemistry and bio-inorganic chemistry.

Specific learning outcomes: At the end of the course, students will be able to:

- Explain crystal field theory, crystal field splitting in complexes, its limitations, and constructing MO diagrams of complexes
- Deduce the mechanisticpathway of reactions of inorganic complexes
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Unit:I

Separation methods: Principles, Instrumentation and applications of HPTLC,HPLC, Counter current chromatography.

Size Exclusion chromatography - Principles of LC-MS, LC-TOF, LC-MS-MS, MALDI-TOF

Unit:II

Electro analytical techniques: Principles, Instrumentation and application of cyclic voltammetry, amperometry, coulomentry and electrogravimetry.

Atomic Absorption Spectroscopy and Inductively Coupled Plasma Emission Spectroscopy-Principle and applications.

Unit:III

Principles, Instrumentation and application of scanning electron microscopy, Tunnelling Electron Microscopy, Electron Spectroscopy for Chemical Analysis, X-Ray Diffraction spectroscopy - Atomic fluorescence spectrometry. Thermogravimetric analysis and differential thermal analysis - principles and applications.

Unit: IV

Principles, instrumentation and applications of ^{1}H and ^{13}C-NMR (^{1}H-^{1}H COSY,HETCOR,HMBC and HMQC)to organic molecules.

Unit: V

UV, IR, Raman, ESR and Mossbauer spectroscopy – principle, instrumentation and applications to inorganic compounds.

Reference Books:

1. Instrumental Methods of Analysis by Willard Merit and Dean.
2. Spectrometric Identification of Organic Compounds, R.M. Silverstein, F.X. Webster, D.J. Kiemle, D.L. Bryce, 8th edition, John Wiley & Sons, New Delhi, 2015.
3. Organic Spectroscopy, W. Kemp, ELBS, 2nd edition, 1991.
4. Principles of Instrumental Analysis by S.Skoog, Holler and S.R. Crouch, 6th edition, 2007.
5. http://www.kinetics.nsc.ru/chichinin/books/spectroscopy/Stuart04.pdf
6. http://chemsites.chem.rutgers.edu/~nmurali/nmr_course/Chem_542_Spring2010_Lecture_1.pdf
7. http://courses.chem.indiana.edu/a315/documents/CVhandout_000.pdf