DAV UNIVERSITY JALANDHAR

Course Scheme & Syllabus

For

DOCTOR OF PHILOSOPHY
(CHEMISTRY)
(Program ID-236)

2019-2020

Total minimum credits required for PhD Course Work are 14

Scheme of Courses

S.No	Paper Code	Course Type	Course Title	L	T	P	Cr
1	PHD800	Core	Research Methodology	4	0	0	4
2	PHD801	Core	Seminar-1	0	0	0	2
3	CHE806A	Core	Advance Instrumentation Techniques	4	0	0	4
4		Elective	Departmental Elective*	4	0	0	4
Total							14

Department Elective*							
1	CHE801	Elective	Advanced Organic Chemistry	4	0	0	4
2	CHE802	Elective	Advanced Inorganic Chemistry	4	0	0	4
3	CHE805	Elective	Advanced Physical Chemistry	4	0	0	4

L: Lectures T: Tutorial P: Practical Cr: Credits

Course Title: Advanced Organic Chemistry

Course Code: CHE801

L	T	P	Credits	Marks	Pass Marks
4	0	0	4	100	55

Time: 04 Hours

Course Objectives:

This course is intended to learn advanced organic chemistry. The present syllabus has been framed as per the recent research trends in the subject.

Expected Prospective:

This course will equip the research scholars with the necessary chemical knowledge concerning the advanced organic chemistry that will be useful in their research work.

PART A

MODERN ORGANIC SYNTHESIS: AN INTRODUCTION

SYNTHETIC DESIGN

Retrosynthetic Analysis, Umpolung, Steps in Planning a synthesis, Choice of Synthetic Method, Domino Reactions.

STEREOCHEMICAL CONSIDERATIONS IN PLANNING SYNTHESES

Conformational Analysis, Evaluation of Nonbonded Interactions, Six-Member Heterocyclic Systems, polycyclic Ring Systems, Cyclohexyl Systems with sp2-Hybridized Atoms, Significant Energy difference.

THE CONCEPT OF PROTECTING FUNCTIONAL GROUPS

Protection of NH Groups, Protection of OH Croups of Alcohols, Protection of Diols as Acetals, protection of Carbonyl Groups in Aldehydes and Ketones, Protection of the Carboxyl Group, protection of Double Bonds, Protection of Triple Bonds.

PART B

CATALYSIS IN ORGANIC SYNTHESIS

PHOTO CATALYSIS

Photo induced reductive reaction, Photo induced oxidative reaction, Redox neutral reaction (photo induced electron transfer reaction), Photo induced energy transfer reaction, Photo induced hydrogen transfer reaction.

ORGANO CATALYSIS

Proline based organocatalysts: enamine and iminium ion mechanism.

PART C

Cross Coupling Reactions

Transition metal catalysis: C-H activation, Coupling reactions. Negishi coupling Heck reaction, Suzuki reaction , Stille reaction , Hiyama coupling, Sonogashira coupling, Buchwald-Hartwig amination , Kumada coupling,Cross dehydrogenative coupling, metal catalyzed and metal free reactions. Green approach towards cross coupling.

PART D

APPLICATIONS

Applications in synthetic dyes, synthetic polymers and synthetic drugs: Antimalarials, Sulpha Drugs, Metallic Therapeutics**,** Sweetening Agents.

REFERENCES

1. *Moderan Organic Synthesis: An Introduction*, George S. Zweifel and Michael H. Nantz, W. H. Freeman and Company, New York **2007**.
2. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure 7ed, M. B. Smith, Wiley, 2015
3. *Visible Light Photoredox Catalysis with Transition Metal Complexes: Applications in Organic Synthesis,* Christopher K. Prier, Danica A. Rankic, and David W. C. MacMillan, Chem. Rev. **2013**, 113, 5322−5363, Merck Center for Catalysis at Princeton University,

Princeton, New Jersey, United States.

4. *Dual Catalysis Strategies in Photochemical Synthesis,* Kazimer L. Skubi, Travis R. Blum, and Tehshik P. Yoon, **2016,** DOI: 10.1021/acs.chemrev.6b00018, Department of Chemistry, University of Wisconsin−Madison.
5. *Stereoselective Organocatalysis: Bond Formation Methodologies and Activation modes*, Ramon Rios Torres, Wiley; 1 edition, **2013.**
6. *Asymmetric Organocatalysis*, Benjamin, Topics in Current Chemistry, **2009**, ISBN 978-3-642-02815-1, Springer.
7. *C-H Activation*, Jin-Quan Yu and Zhangjie Shi, Topics in Current Chemistry, **2010**, ISBN 978-3-642-12356-6, Springer.
8. *Complete Field Guide to Asymmetric BINOL-Phosphate Derived Brønsted Acid and Metal Catalysis: History and Classification by Mode of Activation; Brønsted Acidity, Hydrogen Bonding, Ion Pairing, and Metal Phosphates*, Dixit Parmar, Erli Sugiono, Sadiya Raja, and Magnus Rueping, **2014**, dx.doi.org/10.1021/cr5001496, Institute of Organic Chemistry, RWTH Aachen University, Landoltweg 1, 52074 Aachen, Germany.
9. *Modern Carbon−Fluorine Bond Forming Reactions for Aryl Fluoride Synthesis,* Michael G. Campbell and Tobias Ritter, **2014**, dx.doi.org/10.1021/cr500366b, Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, Massachusetts 02138, United States.
10. *Advances in Catalytic Enantioselective Fluorination, Mono-, Di-, and Trifluoromethylation, and Trifluoromethylthiolation Reactions*, **2014**, dx.doi.org/10.1021/cr500277b, Xiaoyu Yang, Tao Wu, Robert J. Phipps, and F. Dean Toste, Department of Chemistry, University of California, Berkeley, California 94720, United States.

Course Title: Advanced Inorganic Chemistry

Course Code: CHE802

Time: 04 Hours

L	T	P	Credits	Marks	Pass Marks
4	0	0	4	100	55

Course Objectives:

This course is intended to learn advanced inorganic chemistry. The present syllabus has been framed as per the recent research trends in the subject.

Expected Prospective:

This course will equip the research scholars with the necessary chemical knowledge concerning the advanced inorganic chemistry that will be useful in their research work.

PART A

Coordination Chemistry: Coordination number and structures of coordination complexes. Crystal field and molecule orbital theory. JT distortion Electronic Spectra of coordination compounds. Tanabe-Sugano diagrams, Thermodynamic aspects of coordination complexes: lrving William Series. Kinetic aspects: reactions and reaction rates, electron transfer reactions. Reaction mechanism in inorganic reactions.

PART B

Organometallic Chemistry: Structure, Bonding, and Reactivity studies of metal carbonyls, metal alkyls, carbenes and carbynes. Metallocenes and related chemistry. Homogeneous and heterogeneous catalysis. Organometallic complexes with metal-metal bonds.

PART C

Supramolecular Chemistry: Crown ether, Cram's principle of preorganization, Cryptands. Covalent and non-covalent forces. Principle of self-assembly. Host guest chemistry and molecular receptors. Supramolecular inorganic architectures, Zeolites, MOFs, Supramolecular gel.

PART D

Bioinorganic Chemistry: Energy sources for life, metalloprophyrins, dioxygen binding, transport, utilization, electron transfer, photosynthesis, nitrogen fixation, essential and trace elements in biological systems.

Inorganic compounds in medicine and materials: Metal complexes in organic reactions, cisplatin, gold complexes, metal nano-particles in heterogeneous catalysis, functional materials, metal complexes in display technologies, DNA cleavage by transition metal complexes, anti-cancer drugs, and therapeutic drugs.

REFERENCES:

1. *Inorganic Chemistry – Principles of Structure and Reactivity. 4th Edn*. J.E. Huheey, E. A. Keiter and R.L. Keiter Harper-Collins, NY, **1993**.
2. *Inorganic Chemistry 4th edition D. F. Shriver and P. W. Atkins, Oxford University, Oxford,* **2006**.
3. *Concepts and Models of Inorganic Chemistry. 3rd Edn*. B. Douglas, D. Mc Daniel, and J. Alexander, John Wiley, New York. **1993.**
4. *Modern Inorganic Chemistry. 2nd Edn*. W.L. Jolly, McGraw-Hill, Singapore, **1991**.
5. *Supramolecular Chemsitry*. J. M. Lehn, VCH, Weinheim, **1995.**
6. Advanced Inorganic Chemistry, 6ed, F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Wiley, 2007.

Course Title: Advanced Physical Chemistry

Course Code: CHE805

Time: 04 Hours

L	T	P	Credits	Marks	Pass Marks
4	0	0	4	100	55

Course Objectives:

This course is intended to learn advanced solution thermodynamics. The present syllabus has been framed as per the recent research trends in the subject.

Expected Prospective:

This course will equip the research scholars with the necessary chemical knowledge concerning the advanced thermodynamics that will be useful in their research work.

PART A

Ideal and non-ideal solutions, activity and activity coefficients, mixing and excess properties of liquid-liquid mixtures. Theories of solutions of electrolyte and non-electrolyte liquids: van Laar theory, van der Waals theory, Scatchard-Hildebrand theory, Lattice theory, Prigogine Cell theory, Flory equation of state theory, Prigogine-Flory-Patterson theory, Extended Real Associated Solution model and Kirkwood-Buff theory.

PART B

Modern experimental techniques: determination of vapour-liquid equilibrium by static and dynamic methods, heat capacity and heat of mixing by calorimeters, and determination of volumetric, transport, acoustic and optical properties of liquid-liquid mixtures. Thermodynamic relations of excess Gibbs energy, excess entropy, excess enthalpy, excess volume, viscosity deviation, excess heat capacity and excess compressibility.

PART C

Partial molar properties, their physical significance and methods of their determination. Study of non-ideal behaviour of various types of solutions: nonpolar + nonpolar, polar + nonpolar, polar + polar, and mixtures with hydrogen-bond formation and charge transfer complexes; interpretation in terms of molecular interactions.

Empirical and semi-empirical formulas, theoretical expressions, correlations, group contribution methods and computational models for the prediction of thermodynamic properties of liquids and liquid mixtures.

PART D

Surface active agents, Critical micelle concentration (CMC) and factor affecting cmc, thermodynamics of micellization, phase separation and mass atom models, micellar catalysis, Gemini surfactants and Reverse micelles.

Methods preparation of colloidal dispersion, size and shape of colloidal particles, pharmaceutical applications. Types of colloidal systems, stability of colloidal systems. Sensitization of protective colloidal action.

REFERENCES

1. Prausnitz J. M., Lichtenthaler R.N., Azevedo E.G., Molecular Thermodynamic of Fluid-Phase Equilibria, (Prentice Hall, 3rd edition, 1998).
2. Rowlinson J.S., Liquid and Liquid Mixtures, (Springer; 1st edition, 1995).
3. Acree W.E., Thermodynamic Properties of Nonelectrolyte Solutions, (Academic Press, 1984).
4. J. Bevan Ott, Juliana Boerio-Goates, Chemical Thermodynamics: Advanced Applications, (Academic Press, 1st edition, 2000).
5. Prigogine, The Molecular Theory of Solutions, (North Holland Publishing Co. Amsterdam 1957).
6. Arieh Ben-Naim, Molecular Theory of Solutions, (Oxford University Press, USA, 2006).
7. P. Atkins, J. De Paula, Physical Chemistry, Oxford, 10th Ed. 2014.

Course Title: Advance Instrumentation Techniques

Course Code: CHE806A

L	T	P	Credits	Marks	Pass Marks
4	0	0	4	100	55

Time: 04 Hours

Course Objectives:

This course is intended to learn advance spectroscopy. The present syllabus has been framed as per the recent research trends in the subject.

Expected Prospective:

This course will equip the research scholars with the necessary chemical knowledge concerning the advance spectroscopy and its applications that will be useful in their research work.

PART A

X-ray Fluorescence Spectroscopy (XRF)

Introduction to fluorescence, fluorescence lifetime and quantum yields, fluorescence anisotropy, instrumentation for fluorescence spectroscopy, fluorescence polarization, effects of solvents on fluorescence, emission spectra, mechanism and dynamics of solvent relaxation, quenching of fluorescence, energy transfer

Circular Dichroism Spectroscopy (CD)

Introduction to Circular Dichroism spectroscopy, the basics of polarization, the origin of optical activity, Circular birefringence and optical rotation, Circular dichroism, Circular dichroism and the study of biological molecules

Surface Enhanced Raman (SERS)

Raman effect, Limitataions of Raman Spectroscopy, Introduction to Surface-Enhanced Raman Spectroscopy, applications of SERS

PART B

Microscopy

Scanning Electron Microscopy (SEM), Scanning Tunneling Microscopy (STM), Transmission Electron Microscopy (TEM) Atomic Force Microscopy (AFM) : Introduction, instrumentation and applications

X-ray Absorption Spectroscopy (XAS)

The basic physical process in XAS, characteristic excitation energies of various elements, X-ray absorption in condensed matter, XAS and valence state, XAS and local atomic structure, applications

X-ray Photoelectron Spectroscopy (XPS)

Introduction, photoelectric effect, binding energies, instrumentation, qualitative analysis

PART C

X-ray diffraction methods of analysis

Production of X-rays, solid state symmetry, reciprocal lattice, Bragg's law in reciprocal space, the powder method, interpretation of powder pattern of a cubic system, particle size determination by powder method, qualitative and quantitative analysis using powder method. X-ray fluorescence spectroscopy, X-rays emission method, applications (qualitative and quantitative).

Energy Dispersive X-ray Spectroscopy (EDS/EDX)

Introduction and applications (qualitative and quantitative)

Gamma Ray Spectroscopy

Basic gamma-ray properties, observables, methods of producing the nuclei of interest (not an exhaustive list), gamma-ray interactions in matter, detector types, detector arrays, measurement techniques: angular correlation, angular distribution, linear polarization, lifetime measurements: doppler shift attenuation method, recoil distance method, electronic timing.

PART D

Electron Paramagnetic Resonance (EPR)

Introduction to EPR spectroscopy, Electron-Nuclear Hyperfine Interaction, Instumentation and applications

Scattering Methods

Basic scattering theory, basic principles of the scattering from a dispersion of spherical colloidal particles, small angle neutron scattering (SANS), small angle X-ray scattering (SAXS), and static and dynamic light scattering (SLS and DLS)

Inductively Coupled Plasma MS (ICP-MS), Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES)

Introduction, principle, instrumentation, interferences, matrix effects, applications

Chromatography

Ion-exchange chromatography, Size Exclusion Chromatography, Affinity Chromatography, GC-MS: Introduction, instrumentation and applications

REFERENCES

1. Drago, R.S. *Physical Methods in Chemistry,* Reinhold Publishing Corporation, 1965.

2. Silverstein, R.M. Bassler, G.C. and Morrill, T.C. *Spectrometric Identification of Organic Compounds,* Wiley, 1991.

3. Kemp, W. *Organic Spectroscopy,* Macmillan, 1987.

4. Dyer, J. R. *Application of Absorption Spectroscopy of Organic Compounds,* Prentice Hall, 1965.

5. Williams, D. H. and Fleming, I. *Spectroscopic Problems in Organic Chemistry,* McGraw Hill, 1967.

6. Barrow, G.M. *Introduction to Molecular Spectroscopy*, McGraw Hill, 1962

7. Banwell, C.N. *Fundamentals of Molecular Spectroscopy*, McGraw Hill, 1966.

8. Pavia, D.L., Lampan, G.M. and Kriz, G. S. *Introduction to Spectroscopy*, Hartcourt College Publishers, 2001.

9. Lakowicz, J. R. *Principles of fluorescence spectroscopy*, Springer, 1983.

10. Egerton, R.F. *Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM*, Springer, 2008.

11. Lundanes, E., Greibrokk, T., Reubsaet, L. *Chromatography: Basic Principles, Sample Preparations and Related Methods*, WILEY-VCH, 2013