ASSAM DON BOSCO UNIVERSITY
SCHOOL OF FUNDAMENTAL AND APPLIED SCIENCES
DEPARTMENT OF CHEMISTRY

Modified Course Structure/Syllabus in SPRING 2019

MASTER OF SCIENCE – CHEMISTRY

Semester	Category	Course Name	Course Code	Credits
IV	One Elective Course (of the five offered) and one of the three Specialisation Courses (Physical/ Organic/ Inorganic Chemistry) to be selected			
	Electives			
	DE	Materials Chemistry	CHMC0018	3
	DE	Computational Chemistry	CHCC0019	
	DE	Food Chemistry	CHFC0020	
	DE	Industrial Chemistry	CHIC0021	
	DE	Medicinal Chemistry	CHMD0022	
	Specialisation I - Physical Chemistry			
	DE	Recent Advances in Catalysis	CHRC0023	3
	DE	Biophysical Chemistry	CHBC0024	
	Specialisation II - Organic Chemistry			
	DE	Heterocyclic Chemistry	CHHC0025	3
	DE	Natural Products Chemistry	CHNP0026	
	Specialisation III - Inorganic Chemistry			
	DE	**Organometallic Chemistry**	**CHOC0027**	3
	DE	**Inorganic Rings, Clusters and Polymers**	**CHIP0028**	
	DC	Research Project	CHRP6005	9
Total Credits				**18**

CHAP0009: ADVANCED PHYSICAL CHEMISTRY I

(4 Credits - 60 hours)

Objective: *This course is intended to give students a deep understanding of the kinetics and reaction dynamics of chemical reactions as well as an insight into the principles of electrochemistry*

Module I Chemical Kinetics (15 hours)

Theories of unimolecular reactions: Lindemann theory, drawbacks of Lindemann theory-Hinshelwood modification, RRK theory, Slaters treatment, RRKM theory. Steady state approximation and its applications, oscillating reactions, chemical chaos, Belousov-Zhabotinski reaction, straight chain reactions - hydrogen-halogen reactions, alkane pyrolysis, Branching-chain reactions - the hydrogen- oxygen reaction, explosion limits, Enzyme catalyzed reactions, Michaelis-Menten mechanism- Lineweaver-Burk and Eadie plots, enzyme inhibition.

Module II Study of Fast Reactions (5 hours)

Stopped flow technique, temperature and pressure jump methods, NMR studies in fast reactions, shock tube kinetics, relaxation kinetics, Linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time.

Module III Molecular Reaction Dynamics (15 hours)

Collisions of real molecules- trajectory calculations, Laser techniques, reactions in molecular beam, reaction dynamics, estimation of activation energy and calculation of potential energy surface- the transition state theory (TST) of bimolecular gaseous reactions, statistical and thermodynamic formulations. Comparison between TST and hard sphere collision theory, theory of unimolecular reactions- Lindemann theory and its limitations, kinetics of reactions in solution-diffusion controlled and chemically controlled reactions, TST of reactions in solution- Bronsted and Bjerrum equation, effect of ionic strength, kinetic salt effect.

Module IV Electrochemistry - I (10 hours)

a) Ion-solvent interaction- the Born model, Thermodynamic parameters of ion solvent interactions-structural treatment, the ion-dipole model-its modifications, ion-quadrupole and ion-induced dipole interactions.

b) Primary solution- determination of hydration number, compressibility method and viscosity-mobility method, Debye-Huckel theory of ion-ion interactions, derivation, validity and limitations, extended Debye-Huckel-Onsager equation, random walk model of ionic diffusion-Einstein Smoluchowski reaction.

Module V Electrochemistry - II (15 hours)

a) Theories of Electrical Interface: Electrocapillary phenomena - Lippmann equation, electron transfer at interfaces, polarizable and, non polarizable interfaces, Butler-Volmer equation, Tafel plot

b) Electro-analytical Techniques: Potential step methods, potential sweep methods, Polarography and Pulse voltammetry, controlled current techniques, techniques based on impedance.

c) Systems for Electro-chemical Energy Storage and Conversion: Types of Batteries, Lead- acid batteries, Nickel-cadmium batteries and Li-ion batteries, electrical double layer capacitor, pseudo-capacitor, fuel cells.

COURSE/LEARNING OUTCOMES

At the end of this course students will be able to:

CO1: Recall about kinetics of different types of chemical reaction including unimolecular, bimolecular and chain reactions. They would also able to recall the theories of electrochemistry (Knowledge)
CO2: Understand the application of kinetic theories to different systems, interactions of ionic species with solvent molecules, different electrochemical techniques, different types of batteries (Comprehension)
CO3: Apply the knowledge of kinetic theories to some important types of reactions and to learn the use of different analytical techniques, and batteries (Application)

CO4: Analyse the application of reaction rate theories to different system and to analyse the application of electrochemistry in different fields (Analysis)
CO5: Understanding of kinetics of chemical reaction and application of electrochemistry (Synthesis)
CO6: Calculate rate of different types chemical reactions, compare reaction rate theories, apply the electrochemical techniques to analyse samples, construct different types of batteries (Evaluation)

Suggested Readings

1. Atkins, P. and Paula, J. Physical Chemistry, Oxford University Press, Oxford.
2. Levine, I. R., Physical chemistry, Mcgraw Hill Education.
3. Laidler, K. J., Chemical Kinetics, Pearson.
4. Bockris, J. O., Reddy, A. K. N., Modern Electrochemistry Part 1, 2A and 2B, Springer.
5. Bard, A. J., Faulkner, L. R., Electrochemical Methods Fundamentals and Applications, Wiley India.

CHOC0027: ORGANOMETALLIC CHEMISTRY

(3 Credits - 45 hours)

Objective: *This paper has been developed to enable students specializing in inorganic chemistry to gain a deep insight into the properties and applications of organometallic compounds*

Module I: Introduction to organometallic compounds and reaction mechanisms (7 hours)

History of Organometallic Chemistry, 18 electron rule, Electronic structure, Ligand substitution, oxidative addition, reductive elimination, migratory insertion, hydride elimination, trans-metallation, nucleophilic and electrophilic attack on the ligands coordinated to metals.

Module II: Physical methods in organometallic chemistry (8 hours)

Characterization of organometallic compounds using NMR, EPR, Mössbauer, IR, Mass spectroscopy and X-ray crystallography; Isotope effect; Fluxionality of organometallic complexes.

Module III: Main group organometallic compounds (8 hours)

Synthesis and reactions of main group organometallic compounds including organolithium, organomagnesium, organoboron, organoaluminium, organosilicon and organotin compounds.

Module IV: d-block organometallic compounds (8 hours)

Structure, preparation, and chemistry of transition metal carbene and –carbyne complexes. N-heterocyclic carbene complexes

Transition metal compounds with M-H bonds (classical and non-classical metal-hydrides), agostic interaction

Module V: Organometallic catalysis and application of organometallic chemistry to organic synthesis (14 hours)

Synthetic applications of metathesis reactions, ring opening, ring closing metathesis in organic synthesis, macrocycle synthesis. Asymmetric hydrogenation, Hydrosilylation, Hydrocyanation, Palladium in Homogenous catalysis- Heck coupling, Stille coupling, Suzuki coupling, Negishi coupling, Sonogashira coupling and Buchwald-Hartwig coupling reactions. Synthetic utility of organotitanium, organochromium, organonickel, organocopper, organorhodium compounds.

COURSE/LEARNING OUTCOMES

At the end of the course students will be able to:

CO1: Systematically understand the chemistry of organometallic compounds that includes understanding of bonding, reaction mechanism, physical methods in organometallic chemistry, organometallic catalysis and application of organometallic chemistry to organic synthesis (Knowledge)
CO2: Have a conceptual understanding of the (i) Main group organometallic compounds (ii) d-block organometallic compounds (Comprehension)
CO3: Learn the techniques in physical methods such as NMR, EPR, Mössbauer, IR, Mass spectroscopy and

X-ray crystallography to characterize the organometallic compounds (Application).
CO4: Explain the synthesis process and reactions of main group organometallic compounds including organolithium, organomagnesium, organoboron, organoaluminium, organosilicon and organotin compounds. (Analysis)
CO5: To design organometallic compounds whose properties they can predict (Synthesis)
CO6: Have an overall understanding of organometallic compounds, their synthesis, structure, reaction mechanism, catalysis and applications (Evaluation).

Suggested Readings

1. C. Elschenbroich, Organometallics, Wiley.
2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Blackwell.
3. M. Bochmann, Organometallics and Catalysis: An Introduction, Oxford University Press.
4. Gary O. Spessard and Gary L. Miessler, Organometallic Chemistry, Oxford University Press, New York.
5. F. Mathey, Transition Metal Organometallic Chemistry, Springer.
6. M. B. Smith, Organic Synthesis, McGraw Hill Higher Education.

CHIP0028: INORGANIC RINGS, CLUSTERS AND POLYMERS

(3 Credits - 45 hours)

Objective: *This paper will allow students specializing in inorganic chemistry to understand in detail the chemistry and applications of boranes, heteroboranes, isolobility, metal clusters and inorganic polymers*

Module I: Boranes and Heteroboranes (13 hours)

a) Polyhedral boranes, concept of electron deficiency and sufficiency, types and IUPAC nomenclature of polyhedral boranes. Polyhedral skeleton electron pair theory (PSEPT). W. N. Equivalent and resonance structures. Wade's vs Lipscomb's methods of studying higher boranes.

b) Heteroboranes: types and IUPAC nomenclature, structure and bonding of heteroboranes with special reference to carboranes, metallaboranes, metallacarboranes, metal σ and μ bonded borane/carborane clusters. Resemblance of Metallaboranes/ Metallacarboranes to ferrocene and related compounds. Applications of metallaboranes/metallacarboranes as drug delivery system. Applications of PSEPT over heteroboranes.

Module II: Isolobility (6 hours)

Concept of isolobility and isolobal groups with examples and their applications in the understanding of structure and bonding of heteroboranes.

Module III: Metal Clusters (11 hours)

Metal-metal bonding, quadrupolar bond and its comparison with a C-C bond; Types of metal clusters and multiplicity of M-M bonds. Simple and condensed metal carbonyl clusters. Applications of PSEPT and Wade's-Mingo's and Lauhr's rule over metal carbonyl clusters. Metal halide and metal chalcogenide clusters, polyatomic Zintl ions, Bloomington shuffle.

Module IV: Inorganic Polymers (15 hours)

Inorganic polymers, classification of inorganic polymers, comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, polysilanes, polyphosphazenes, coordination polymers, sulphur-nitrogen, sulphur-nitrogen-fluorine compounds, preceramic inorganic polymers.

COURSE/LEARNING OUTCOMES

At the end of the course students will be able to:

CO1: Acquire detailed knowledge of inorganic rings, clusters and inorganic polymers with special emphasis to their structural diversity. (Knowledge)
CO2: Understand important concepts such as isolobal analogy, polyhedral skeleton electron pair theory

(PSEPT) and metal-metal bonding. (Comprehension)
CO3: Differentiate the properties of inorganic polymers from organic polymers. They will be able to apply the concepts of isolobal analogy, PSEPT, Wade's-Mingo's and Lauhr's rule to predict the structure of metal clusters. (Application)
CO4: Analyze bonding and properties of clusters such as boranes, carboranes, heteroboranes, metal carbonyl clusters, metal chalcogenides, zintl ions and polyoxometalates. In addition to it, they will be able to apply the knowledge of structure and bonding to study properties of various inorganic polymers such as phosphazenes, silicones, polysilanes, B-N containing polymers. (Analysis)
CO5: Have clear understanding of synthesis, structure, bonding and applications of inorganic clusters, chains and polymers. (Synthesis)
CO6: Appreciate the importance of inorganic clusters and polymers and different phenomenon associated with these compounds. (Evaluation).

Suggested Readings

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley & Sons, New York.
2. James E. Huheey, Inorganic Chemistry, Addison Wesley Pub. Co., New York
3. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, Butterworth Heinemann, London.
4. James E. Mark, Harry R. Allcock and Robert West, Inorganic polymers, Oxford University Press, New York