Name of the Programme: M.Sc. Part-I (Inorganic Chemistry)

Course Code: CHI-501 **Title of the course:** Chemistry of Coordination & Organometallic Compounds

Number of Credits: 04

Effective from AY: 2022-23

Prerequisites for the course:	Students should have studied Inorganic chemistry courses at M.Sc. Chemistry in semester I	
Course Objective:	1. To make understand fundamentals of coordination and organometallic chemistry. 2. To gain the knowledge on structural aspects of compounds. 3. To make understand bonding using various models. 4. To correlate spectroscopic and magnetic properties with bonding models. 5. To develop a skill of interpretation of magnetic and spectroscopic properties. 6. To understand fundamental concepts of inorganic chemistry reaction mechanisms. 7. To provide knowledge on applications of organometallic compounds in homogenous catalysis.	
Content:	**1. Electronic structure of coordination compounds** Basic introduction to bonding theories: a. Valence Bond theory & its utility, limitations of VBT. b. Crystal field theory and its uses in: i) Octahedral compounds; ii) tetrahedral compounds; iii) square-planar compounds and other geometries; iv) tetragonally distorted compounds (Jahn-Teller Effect); v) octahedral vs tetrahedral; vi) Evidences showing covalency to the M-L bonds. c. Molecular orbital theory (MOT): σ & π-bonding in octahedral, tetrahedral, square planar compounds.	No of hours 12
	2. Spectra and magnetic studies of coordination compounds a.(i) Electronic spectra of atoms, (ii) Electronic spectra of complexes; Orgel diagrams, correlation diagrams, T-S diagrams examples and problem solving, (iii) Charge-transfer bands; (iv) Selection rules and intensities, (v) Luminescence. b. Vibrational spectra of coordination compounds. c. Magnetic studies: cooperative magnetism, basic concepts of magnetic properties: diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism, temperature dependent magnetism, Curie law, Curie Weiss Law; spin cross over phenomenon.	12
	3. Inorganic reaction mechanisms	12

	a. The thermodynamics of complex formation: Formation constants; Trends in successive formation constants; The chelate and macrocyclic effects; Steric effects and electron delocalization. b. Ligand substitution reactions and mechanisms: Rates of ligand substitution; The classification of mechanisms; Ligand substitution in square-planar complexes: The nucleophilicity of the entering group; The shape of the transition state. Ligand substitution in octahedral complexes: Rate laws and their interpretation; The activation of octahedral complexes; Base hydrolysis; Stereochemistry; Isomerization reactions. C. Redox reactions: The classification of redox reactions; The inner-sphere mechanism; The outer-sphere mechanism. d. Photochemical reactions: Prompt and delayed reactions; d–d and charge-transfer reactions; Transitions in metal–metal bonded systems.	
	4. Organometallic chemistry of d-block elements a. Stable electron configurations; Electron count preference; Electron counting and oxidation states. b. Ligands: Carbon monoxide, Phosphines, Hydrides and dihydrogen complexes, η^1-Alkyl, -alkenyl, -alkynyl, and -aryl ligands, η^2-Alkene and -alkyne ligands, Nonconjugated diene and polyene ligands, Butadiene, cyclobutadiene, and cyclooctatetraene, Benzene and other arenes, The allyl ligand, Cyclopentadiene and cycloheptatriene, Carbenes, Alkanes, agostic hydrogens, and noble gases, Dinitrogen and nitrogen monoxide. c. Compounds: *d*-Block carbonyls, Metallocenes, Metal–metal bonding and metal clusters. d. Reactions: Ligand substitution, Oxidative addition and reductive elimination, σ-Bond metathesis, 1,1-Migratory insertion reactions, 1,2-Insertions and β-hydride elimination, α-, β-, and δ-Hydride eliminations and cyclometallations. e. Catalysis: general concepts, catalytic cycle for isomerization of prop-2-en-l-ol to prop-1-en-l-ol, Alkene metathesis, hydrogenation of alkenes, hydroformylation, Wacker oxidation of alkenes, Asymmetric oxidations, Palladium catalyzed C-C bond forming reactions, methanol carbonylation (Monsanto acetic acid process).	24
Pedagogy:	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	

References / Readings:	1. P. W. Atkins, T. L. Overton, J. P. Rourke, M. T. Weller & F. A. Armstrong 2010, Shriver & Atkins' Inorganic Chemistry, 5th Ed., Oxford University Press, 2010. 2. J. E. Huheey, E. A. Keiter& R. L. Keiter, Inorganic Chemistry:Principles of structure and reactivity, 4th Ed.;Pearson, 2014. 3. J. D. Lee, Concise Inorganic Chemistry, 5thEd, Chapman and Hall, 1996. 4. F. A. Cotton, G. Wilkinson & P. L. Gaus, Basic Inorganic Chemistry, 3rd Ed.; John Wiley, 1995. 5. F. A. Cotton & G. Wilkinson, Advanced Inorganic Chemistry, 3rd Ed. (4th & 5th Eds. preferred);Wiley Eastern, New-Delhi, 1984. 6. D. Banerjee, Coordination Chemistry, 1st Ed.;Tata McGraw–Hill, New Delhi, 1994. 7. N. N. Greenwood & A. Earnshaw, Chemistry of the Elements, Pergamon Press, Exeter, 1984. 8. G. Rodgers, Introduction to coordination, solid state, and descriptiveInorganic chemistry, 1st Ed.; McGraw–Hill,1994. 9. R. S. Drago, Physical Methods in Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 2017 10. G. C. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd Ed.; Pearson, 2004
Course outcomes:	1. Students will be able to understand the electronic structure of coordination and organometallic compounds. 2. Students will be well equipped with knowledge of CFT and MOT 3. Students will be in position to understand the magnetic and electronic properties. 4. Students will be able to acquire skill on interpretation of electronic and IR spectra of inorganic compounds 5. Students will be able understand concepts of inorganic reactions & mechanisms. 6. Students will be aware of applications of organometallic compounds in industrial processes.