ACADEMIC AFFAIRS OFFICE
INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

No. Acd./ 459 /IAPC-97 Dated: January 15, 2021

Head, Department of Chemistry

The IAPC in its 97th meeting held on 11.01.2021 vide Item No. 97.2.3 considered and approved the proposal of Department of Chemistry about the reorganization of following courses of Inorganic Chemistry:

1. CYN-502: Advanced Organometallic Chemistry
2. CYN-509: Advanced Coordination Chemistry
3. CYN-516: Chemistry of Main Group and Transition Elements

The syllabi of approved courses are attached as **Appendix-A**.

Reeti

Assistant Registrar (Curriculum)

Encl: as above

Copy to (through e mail):-

1. All faculty
2. All Heads of Departments/ Centres
3. Dean, Academic Affairs
4. Associate Dean of Academic Affairs (Curriculum)
5. Channel I/ Acad portal/ Academic webpage of iitr.ac.in

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE: Department of Chemistry

1. **Subject Code:** CYN-502 **Course Title:** Advanced Organometallic Chemistry
2. **Contact Hours:** **L:** 3 **T:** 0 **P:** 0
3. **Examination Duration (Hrs.):** **Theory:** 3 **Practical:** 0
4. **Relative Weightage:** **CWS:** 20-35 **PRS:** 0 **MTE:** 20-30 **ETE:** 40-50 **PRE:** 0
5. **Credits:** 3 **6. Semester:** Spring **7. Subject Area:** PCC
8. **Pre-requisite:** Nil
9. **Objective:** To impart advanced concepts in organometallic chemistry.
10. **Details of the Course**

S.No.	Contents	Contact hours
1.	**Structure and bonding in organometallics:** 18 electron rule and its application to π-acceptor ligands, limitations of 18 electron rule, description of bonding models for π-acceptor ligands including CO, alkenes (Dewar-Chatt-Duncanson model) and tertiary phosphines, physical evidences and consequences of bonding. Main group organometallics: Introduction, review of comparative aspects of synthetic methods, reactivity and bonding in ionic, covalent, electron deficient and electron rich organometallic compounds. Kinetics and mechanism of ligand substitution (associative and dissociative), oxidative addition and reductive elimination, transmetallation, migratory insertions, reactivity at metal-bound ligands.	14
2.	**Organotransition metal chemistry:** σ-Bonded transition metal-alkyls, -aryls, -alkenyls (vinyls), -alkynyls (acetylides), reactions in σ–organyls: homolytic cleavage, reductive elimination, electrophilic cleavage, insertion, β-metal hydrogen elimination, α-abstraction or α-elimination and γ- and δ-remote C-H functionlization.	**7**
3.	**Organotransition compounds with multiple metal-carbon bonding:** Transition metal-carbenes/-carbynes, -bridging carbenes/carbynes, reactions of carbene/carbyne complexes such as ligand substitution, nucleophilic, electrophilic attack, dismutation, and ligand coupling reactions.	**7**
4.	**Organotransition compounds with multicenter bonds:** Concept of hapticity, transition metal complexes of alkenes, Ziese salt, alkynes, allyls, acyclic conjugated dienes; π-metal complexes of cyclobutadienes, cyclopentadienyls, arenes, cycloheptatrienyls and cyclooctatetraenes, reactions and bonding in ferrocene; stereochemical non-rigidity in organometallic compounds and fluxionality, bimetallic complexes and clusters.	**7**
5.	**Applications of organometallics and clusters in catalysis:** Alkene metathesis, Cativa and Monsanto processes for production of acetic acid, carbonylation and decarbonylation reactions, Wacker process, cyclooligomerisation of acetylene using Ni/Cr catalysts, Mobil and Fischer-Tropsch processes, polymer-bound catalysts, metal carbonyl clusters in catalysis.	7
Total		**42**

11. Suggested Books:

S.No.	Name of Authors/Book/Publisher	Year of Publication / Reprint
1.	Huheey, J.E., Keiter, E.A. and Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education Inc.	**2003**
2.	Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons.	**1999**
3.	Hill, A.F., "Organotransition Chemistry", The Royal Society of Chemistry, Cambridge.	**2002**
4.	Crabtree, R. H., "The Organometallic Chemistry of the Transition Metals", 6th Edition, Wiley.	**2014**
5.	Gupta, B.D. and Elias A.J., "Basic Organometallic Chemistry", 2nd Ed., Univ. Press (India) Pvt. Ltd.	**2013**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE: Department of Chemistry

1. **Subject Code:** CYN-509 **Course Title:** Advanced Coordination Chemistry
2. **Contact Hours:** **L:** 3 **T:** 0 **P:** 0
3. **Examination Duration (Hrs.):** **Theory:** 3 **Practical:** 0
4. **Relative Weightage:** **CWS:** 20-35 **PRS:** 0 **MTE:** 20-30 **ETE:** 40-50 **PRE:** 0
5. **Credits:** 3 **6. Semester:** Autumn **7. Subject Area:** PCC
8. **Pre-requisite:** Nil
9. **Objective:** To impart advanced concepts of coordination chemistry.
10. **Details of the Course**

S.No.	Contents	Contact hours
1.	**Stability and stereochemistry of coordination compounds:** Studies of coordination compounds in solution, detection of complex formation in solution, thermodynamic stability and kinetic lability, successive (*K*) and overall stability (β) constants, trend in *K* values, factors affecting stability of the complexes, determination of stoichiometry (Job's method) and stability constants by spectrophotometric, potentiometric and polarographic methods, chelate and macrocyclic effect. Optical isomerism in metal complexes, chirality and nomenclature of chiral complexes, optical rotatory dispersion (ORD) and circular dichroism (CD).	**7**
2.	**Metal-ligand bonding:** Overview of crystal field and ligand field theories of 4-, 5- and 6-coordinated complexes, d-orbitals splitting in linear, trigonal, octahedral, square planar, tetrahedral, square pyramidal, trigonal-bipyramidal and cubic complexes, measurement of CFSE (d^1 to d^{10}) in weak and strong ligand fields, Jahn-Teller distortion, nephelauxetic series, variation of lattice energy, ionic radii and heat of hydration across 1^{st} row transition metal ions.	**7**
3.	**Molecular orbital theory (MOT) of coordination compounds:** Composition of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes including both σ- and π-bonding, angular overlap model.	**7**
4.	**Electronic spectra of coordination compounds:** Energy states from spectral terms of d^n configurations, selection rules for ligand-field and charge transfer transitions in metal complexes, band intensities, factors influencing band widths, splitting of various terms, Orgel and Tanabe-Sugano diagrams of octahedral and tetrahedral d^n complexes, calculation of ligand field parameters, luminescence, phosphorescent complexes.	**7**
5.	**Magnetic properties of coordination compounds:** Fundamental equations in molecular magnetism, magnetic susceptibility and magnetic moment, diamagnetic and paramagnetic behavior of transition metal complexes, spin-orbit coupling effects (L-S coupling and j-j coupling), orbital angular moment and its quenching in octahedral and tetrahedral complexes, temperature independent paramagnetism (TIP) of complexes, spin cross over phenomenon, spin admixed states, metal-metal direct spin interaction and super exchange spin-spin interaction through bridging	**10**

6.	**Transition Metal Clusters**: Di-, tri-, tetra- and hexanuclear clusters, concept of δ-bonding and its effect in electronic transition.	**4**
Total		**42**

11. Suggested Books:

S.No.	Name of Authors/Book/Publisher	Year of Publication / Reprint
1.	Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons.	**1999**
2.	Douglas, B.E., McDaniel, D.H. and Alexander, J.J., "Concepts and Models in Inorganic Chemistry", 3rd Ed., John Wiley & Sons.	**2001**
3.	Figgis, B.N., and Hitchman, M.A "Ligand Field Theory and Its Applications", Wiley Eastern Ltd.	**1999**
4.	Huheey, J.E., Keiter, E.A. and Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education, Inc.	**2003**
5.	Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., "Shriver and Atkins' Inorganic Chemistry", 4th Ed, Oxford university press.	**2009**
6.	Greenwood, N.N. and Earnshaw, A., "Chemistry of the Elements", 2nd Ed, Elsevier.	**2005**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE: Department of Chemistry

1. **Subject Code:** CYN-516 **Course Title: Chemistry of Main Group and Transition Elements**
2. **Contact Hours:** **L:** 3 **T:** 0 **P:** 0
3. **Examination Duration (Hrs.):** **Theory:** 3 **Practical:** 0
4. **Relative Weightage:** **CWS:** 20-35 **PRS:** 0 **MTE:** 20-30 **ETE:** 40-50 **PRE:** 0
5. **Credits:** 3 **6. Semester:** Spring **7. Subject Area:** PEC
8. **Pre-requisite:** Basic knowledge of inorganic chemistry.
9. **Objective:** To impart concepts in chemistry of main group and transition elements.
10. **Details of the Course**

S.No.	Contents	Contact hours
1.	**Chemistry of main group elements:** (i) Chemistry of Gr. 1 and 2 metals–solutions of alkali metals in liquid ammonia (reactions, electrical and magnetic properties), metal anions, complexation of Gr. I/II metals with crown ethers, cryptands and calixarenes, anomalous behavior of Li and Be. (ii) Chemistry of *p*-block elements– borides, borates and boran halides, allotropes of carbon (diamond, graphite, fullerene, carbon nanotubes), carbides, chlorofluorocarbons, silicon halides, silanes, silanols. Hydrides, oxides and oxoacids of pnictogens (N, P), chalcogens (S, Se and Te) and halogens. Pseudohalogens, inter-halogens, polyhalide anions, synthesis, structures and reactivity of compounds of xenon, bonding in xenon fluorides. Overall structural and bonding aspects (VBT) of B, Al, Si, N, P and Cl compounds.	**14**
2.	**Non-covalent interactions in main group and transition metal complexes:** Inter- and intramolecular hydrogen bonding interactions and their effects, electrostatic interactions (ion-ion, ion-dipole, dipole-dipole, dipole-induced dipole) and other weak intermolecular forces. Principle of self-assembly, host-guest chemistry and molecular receptors, examples of supramolecular inorganic architectures, and supramolecular photochemistry.	**6**
3.	**Lanthanides and actinides:** Separation and isolation of lanthanides, separation of Np, Pu and Am from U, electronic spectra and magnetic properties of lanthanides and actinides, general comparison of lanthanides and actinides and their applications in technology, lanthanide shift reagents.	**6**
4.	**Bioinorganic and Bioorganometallic chemistry:** Inorganic composition of cells, compartmentalization, classification of biomolecules, biological metal-coordination sites including special ligands like porphyrins and quinone based ligands. Role of metallobiomolecules in oxygen transport, transfer and transcription (preliminary ideas), selective transport and storage of iron. Chemistry of elements in medicine–chelation therapy, cancer treatment, imaging agents, anti-arthritis agents, radioisotopes and contribution of individual elements. Electron transfer proteins - active site structure and functions of ferredoxin, rubridoxin and cytochromes, and their comparisons. Mechanism of nitrogen fixation. Organometallo-therapeutic drugs, enzyme inhibitors, biological importance of Vitamin B_{12} and coenzymes and their biommietic studies.	**10**
5.	**Inorganic chains, rings and clusters:** Chains - catenation and hetero-catenation, one-dimensional conductors: $(SN)_x$ chains, chalcogenide glasses, iso- and hetero-	**6**

	polyanions. Rings - borazines, boron nitride, phosphazenes-structural models, phosphazene polymers, and other homocylic and heterocyclic inorganic ring systems. Cages - Boron cage compounds– structural aspects (boranes-styx number and Wade's rule) of higher boranes, carboranes, metallacarboranes.	
Total		**42**

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2.	Douglas, B.E., McDaniel, D.H. and Alexander, J.J., "Concepts and Models in Inorganic Chemistry", 3rd Ed., John Wiley & Sons.	**2001**
3.	Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons.	**1999**
4.	Greenwood, N.N. and Earnshaw, A., "Chemistry of the Elements", 2nd Ed, Elsevier.	**2005**
5.	Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F. "Shriver and Atkins' Inorganic Chemistry", 4th Ed, Oxford University Press.	**2009**
6.	Elias, A. J. "The Chemistry of the *p*-Block Elements", 1st Edition, University Press (India) Pvt. Ltd.	**2018**