

### **DEPARTMENT OF CHEMISTRY**

Name of the programme and specialization	M.Sc. (Chemistry)				
Course Title	Coordination Chemis	Coordination Chemistry: Bonding, Reactions and Spectra			
Course Code	CH 603	No. of Credits	3		
Course Code of Pre- requisite subject(s)	Nil				
Session	Section July 2022 Section (if, applicable		NA		
Name of Faculty	of Faculty Dr. R. Karvembu Department		Chemistry		
Official Email	kar@nitt.edu	Telephone No.	0431-2503636		
Name of Course Coordinator(s) (if, applicable)	Dr. R. Karvembu				
Official E-mail	kar@nitt.edu	Telephone No.	0431-2503636		
Course Type (please tick appropriately)	Core course	Elective co	urse		

### Syllabus (approved in BoS)

Theories of coordination compounds: VB theory - CFT - splitting of d orbitals in ligand fields and different symmetries - CFSE - factors affecting the magnitude of 10 Dq - evidence for crystal field stabilization - spectrochemical series - site selection in spinels - tetragonal distortion from octahedral symmetry - Jahn-Teller distortion - Nephelauxetic effect - MO theory - octahedral - tetrahedral and square planar complexes -  $\pi$ -bonding and molecular orbital theory - experimental evidence for  $\pi$ -bonding.

Reactions: Substitution reactions in square planar complexes - the rate law for nucleophilic substitution in a square planar complex - the trans effect - theories of trans effect - mechanism of nucleophilic substitution in square planar complexes - kinetics of octahedral substitution - ligand field effects and reaction rates — stereochemical outcome in octahedral substitution - mechanism of substitution in octahedral complexes - reaction rates influenced by acid and bases - racemization and isomerization - mechanisms of redox reactions - outer sphere mechanism - excited state outer sphere electron transfer reactions - inner sphere mechanism - mixed valence complexes.

Electronic spectra and magnetism: Microstates, terms and energy levels for  $d^1$  – $d^9$  ions in cubic and square fields - selection rules - band intensities and band widths - Orgel and Tanabe Sugano diagrams - evaluation of 10 Dq and  $\beta$  for octahedral complexes of cobalt and nickel - charge transfer spectra - magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent paramagnetism - spin cross over phenomena -



Magnetic anisotropy and magnetism of dinuclear complexes. Van Vleck equation and its consequence to magnetic properties of transition metal complexes.

Structure: Structure of coordination compounds with reference to the existence of various coordination numbers (2, 3, 4, 5 & 6) - site preferences - isomerism - trigonal prism - absolute configuration of complexes - stereo selectivity and conformation of chelate rings - coordination number seven and eight. Spectral and magnetic properties of lanthanide and actinide complexes.

Solid state chemistry: Close packing of atoms and ions - bcc, fcc and hcp voids - structures of rock salt - caesium chloride - wurtzite - zinc blende - rutile - fluorite - antifluorite - diamond and graphite - spinels (normal and inverse) — perovskite - band theory of solids - dislocation in solids - Schottky and Frenkel defects - electrical properties - insulators, semiconductors and conductors - super conductors.

### **COURSE OBJECTIVES**

To introduce the students to the theory, bonding, reactions, structure and spectra of coordination compounds.

To provide them a brief idea on solid state chemistry and properties of lanthanides and actinides.

#### **MAPPING OF COs with POs**

Course Outcomes	Programme Outcomes (PO) (Enter Numbers only)
<ol> <li>learn about the theories, bonding an compounds</li> </ol>	d structure of coordination PO1, PO2, PO4, PO6, PO8, PO9, PO10
2. learn about the reactions of coordinate	PO1, PO2, PO3, PO4, PO6, PO8, PO9, PO10
learn about the electronic spectra an compounds	d magnetism of coordination PO1, PO2, PO4, PO5, PO6, PO8, PO9, PO10
4. learn about the basics of solid-state of	PO1, PO2, PO4, PO5, PO6, PO8, PO9, PO10

COURSE PLAN - PART II	

### **COURSE OVERVIEW**

This is a 3 credit core course offered to I M.Sc. students in I semester.

### **COURSE TEACHING AND LEARNING ACTIVITIES**

S.No.	Week/Contact Hours	Topic	Mode of Delivery
1	IV week of August	VB theory - CFT - splitting of d orbitals in ligand fields and different symmetries - CFSE - factors affecting the magnitude of 10 Dq - evidence for crystal field stabilization	



2	I week of September	Spectrochemical series - site selection in spinels - tetragonal distortion from octahedral symmetry - Jahn-Teller distortion - Nephelauxetic effect	Chalk & Talk
3	II week of September	MO theory - octahedral - tetrahedral and square planar complexes - $\pi$ -bonding and molecular orbital theory - experimental evidence for $\pi$ -bonding	Chalk & Talk
4	III week of September	Substitution reactions in square planar complexes - the rate law for nucleophilic substitution in a square planar complex - the trans effect - theories of trans effect - mechanism of nucleophilic substitution in square planar complexes	Chalk & Talk
5	IV week of September	Kinetics of octahedral substitution - ligand field effects and reaction rates – stereochemical outcome in octahedral substitution - mechanism of substitution in octahedral complexes - reaction rates influenced by acid and bases	Chalk & Talk
6	I week of October	Racemization and isomerization - mechanisms of redox reactions - outer sphere mechanism - excited state outer sphere electron transfer reactions - inner sphere mechanism - mixed valence complexes	Chalk & Talk
7	II week of October	Microstates, terms and energy levels for $d^1-d^9$ ions in cubic and square fields - selection rules - band intensities and band widths - Orgel and Tanabe Sugano diagrams - evaluation of 10 Dq and $\beta$ for octahedral complexes of cobalt and nickel	Chalk & Talk
8	III week of October	Charge transfer spectra - magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent paramagnetism - spin cross over phenomena	Chalk & Talk
9	IV week of October	Magnetic anisotropy and magnetism of dinuclear complexes. Van Vleck equation and its consequence to magnetic properties of transition metal complexes	Chalk & Talk
10	I week of November	Structure of coordination compounds with reference to the existence of various	Chalk & Talk



		coordination numbers (2, 3, 4, 5 & 6) - site preferences - isomerism	
11	II week of November	Absolute configuration of complexes - stereo selectivity and conformation of chelate rings	Chalk & Talk
12	III week of November	Coordination number seven and eight. Spectral and magnetic properties of lanthanide and actinide complexes	Chalk & Talk
13	IV week of November	Close packing of atoms and ions - bcc, fcc and hcp voids - structures of rock salt - caesium chloride - wurtzite - zinc blende - rutile - fluorite - antifluorite	Chalk & Talk
14	I week of December	Diamond and graphite - spinels (normal and inverse) - perovskite - band theory of solids - dislocation in solids	Chalk & Talk
15	II week of December	Schottky and Frenkel defects - electrical properties - insulators, semiconductors and conductors - super conductors	Chalk & Talk

# COURSE ASSESSMENT METHODS (shall range from 4 to 6)

S. No.	Mode of Assessment	Week/Date	Duration	% Weightage
1	Assignment I	III week of September	One week	05
2	Test 1	II week of October	1 h	20
3	Assignment 2	I week of November	One week	05
4	Test 2	III week of November	1 h	20
CPA	Compensation Assessment*	I week of December	1 h	20
5	Final Assessment *	III week of December	3 h	50

<sup>\*</sup>mandatory; refer to guidelines on page 4

COURSE EXIT SURVEY (mention the ways in which the feedback about the course shall be assessed)



Students shall submit feedback through MIS

COURSE POLICY (including compensation assessment to be specified)

Compensation assessment (except for final assessment) will be conducted only for medical

Institute policies on attendance, academic dishonesty and plagiarism are applicable

# ATTENDANCE POLICY (A uniform attendance policy as specified below shall be followed)

- At least 75% attendance in each course is mandatory.
- A maximum of 10% shall be allowed under On Duty (OD) category.
- Students with less than 65% of attendance shall be prevented from writing the final assessment and shall be awarded 'V' grade.

# **ACADEMIC DISHONESTY & PLAGIARISM**

- Possessing a mobile phone, carrying bits of paper, talking to other students, copying from others during an assessment will be treated as punishable dishonesty.
- > Zero mark to be awarded for the offenders. For copying from another student, both students get the same penalty of zero mark.
- > The departmental disciplinary committee including the course faculty member, PAC chairperson and the HoD, as members shall verify the facts of the malpractice and award the punishment if the student is found guilty. The report shall be submitted to the Academic office.
- > The above policy against academic dishonesty shall be applicable for all the programmes.

ADDITIONAL INFORMATION, IF ANY

Nil

FOR APPROVAL

CC- Chairperson

Department of National Institute of Technology

Tiruchirappalli - 620 015, Tamil Nadis



## **Guidelines**

- a) The number of assessments for any theory course shall range from 4 to 6.
- b) Every theory course shall have a final assessment on the entire syllabus with at least 30% weightage.
- c) One compensation assessment for absentees in assessments (other than final assessment) is mandatory. Only genuine cases of absence shall be considered.
- d) The passing minimum shall be as per the regulations.

B.Tech. Admitted in			P.G.	
2018	2017	2016	2015	
35% or (Class	0	(Peak/3) or (Cla whichever is low	The second secon	40%

- e) Attendance policy and the policy on academic dishonesty & plagiarism by students are uniform for all the courses.
- f) Absolute grading policy shall be incorporated if the number of students per course is less than 10.
- g) Necessary care shall be taken to ensure that the course plan is reasonable and is objective.