M. Phil.
CHEMISTRY
SYLLABUS - 2018

St. JOSEPH'S COLLEGE (Autonomous)

Special Heritage Status Awarded by UGC

Accredited at 'A' Grade (3rd cycle) by NAAC

College with Potential for Excellence Conferred by UGC

DBT-STAR & DST-FIST Sponsored College

TIRUCHIRAPPALLI - 620 002, INDIA

GUIDELINES FOR M.PHIL. PROGRAMME

1. Duration

The programme runs for one year of two semesters. The Semester- I is from August to February and the Semester- II runs from March to August, of the following year.

2. Course Work

Semester-I			Semester-II		
Course	**Title**	**Cr**	**Course**	**Title**	**Cr**
C1	Professional Skills for Teaching - Learning	4	C5	Dissertation (Topic selected should be relevant to the topic of the Guide Paper)	8
C2	Research Methodology	4			
C3	Core Course	4			
C4	Guide Paper	4			
Total		**16**	**Total**		**8**

A) Each Course should contain 5 units, covering the subject requirements of the courses offered. **Marks for CIA and SE are in the ratio 25: 75**.

CIA & SE	Tentatively on
Mid Semester Test	December 2nd week
End Semester Test	February 2nd week
Semester Examinations	February 4th week

A candidate shall be declared to have passed Course I, II, III and IV, if he / she secures not less than 40% of the marks in both CIA and the University Examination and 50% of the marks in the aggregate (i.e. continuous internal assessment and the written Examination taken together.

B) In course C1 on **'Professional Skills for Teaching– Learning'** the first three units are common to all the Departments of the College. The first three unit titles are **Soft Skills, E-teaching, E-learning, Elements of Technology ofTeaching and Learning.** The remaining two units are department specific tomake use of the above mentioned skills & techniques to teach the Core Course.

The C1 Course is (to be) designed to explore the various Teaching – Learning – Research Skills to be imbibed / cultivated to make the research

scholars to be fit for the profession they are likely to acquire in the Education Sector.

Departments will be permitted to offer either paper 2 or paper 3 as Open Online Course to the M.Phil. students. The evaluation method will be the same for both C2 and C3 Courses.

C) **Evaluation:**

C.1:

For CIA and SE there will be a 2 hour test only from the first THREE units. The CIA components are Mid Semester Test (35), End Semester Test(35) and Assignment (15) and Practical Component(15). The total mark 100 will be converted into **25** marks.

C.2, C.3 & C.4:

The CIA components for C-2, C-3 and C-4 are Mid Semester Test (25), End Semester Test (25), Seminar (30), Objective Type test /Assignment (20). *(The marks of Mid semester test (75), End semester test (75) will be converted into 25 each.)*

The total mark 100 will be converted into 25 marks. The tests and Semester Examination are centrally conducted by COE for 3 hours.

a) Question papers for C1, C2 & C3 are set by External Examiners.
b) Question paper for C4 will be set and valued by the Research Advisor only.
c) The evaluation method will be the same for both C2 and C3 Courses.

3. Credits

	Courses	Title		Contact hours	Library hours	Total hours	Credit	CIA marks	SE marks	Total marks
Semester-I	C1	Professional Skills for Teaching-Learning	T	3	2	5	3	25	50	100
			P	2	2	4	1		25	
	C2	Research Methodology		5	4	9	4	25	75	100
	C3	Core Paper		5	5	10	4	25	75	100
	C4	Guide Paper		5	5	10	4	25	75	100
Total				**20**	**18**	**38**	**16**	**100**	**300**	**400**

		Internal	Cr	Mk	External	Cr	Mk
Semester-II	C5	Seminar & Review of Related Literature	1	15	Dissertation Evaluation	6	75
		Mid-term Review Presentation	1	15	Viva-voce	2	25
		Dissertation Work	4	50			
		Publication of Research Articles	1	10			
		Viva-voce	1	10			
Total			**8**	**100**		**8**	**100**

4. Question Pattern

Course	Mid & End Semester Tests		
	SCIENCE		
C1	Section A: Short Answers Section B: Either/Or - Essay Type	7/9 3	7×2 = 14 3×7 = 21
C2	Section A: Short Answers Section B: Either/Or - Essay Type	10 5	10×3 = 30 5×9 = 45
C3	Section A: Short Answers Section B: Either/Or - Essay Type	10 5	10×3 = 30 5×9 = 45
C4	Open Choice: Comprehensive Type	5/8	5×15 = 75
	ARTS		
C1	Section A: Short Answers Section B: Either/Or - Essay Type	7/9 3	7×2 = 14 3×7 = 21
C2	Open Choice: Comprehensive Type	5/8	5×15 = 75
C3	Open Choice: Comprehensive Type	5/8	5×15 = 75
C4	Open Choice: Comprehensive Type	5/8	5×15 = 75

Course	Semester Examination		
	SCIENCE		
C1	Section A: Short Answers Section B: Either/Or - Essay Type	7/9 3	7×2 = 14 3×12 = 36
C2	Section A: Short Answers Section B: Either/Or - Essay Type	10 5	10×3 = 30 5×9 = 45
C3	Section A: Short Answers Section B: Either/Or - Essay Type	10 5	10×3 = 30 5×9 = 45
C4	Open Choice: Comprehensive Type	5/8	5×15 = 75
	ARTS		
C1	Section A: Short Answers Section B: Either/Or - Essay Type	7/9 3	7×2 = 14 3×12 = 36
C2	Open Choice: Comprehensive Type	5/8	5×15 = 75
C3	Open Choice: Comprehensive Type	5/8	5×15 = 75
C4	Open Choice: Comprehensive Type	5/8	5×15 = 75

5. Dissertation

For carrying out the dissertation, it is mandatory to strictly adhering to the rules of the college as given below:

5.1 Requirement

Every student is expected to give two seminars one concerning Review of Related Literature within the four weeks from the beginning of the second semester and the other on Data Analysis/Result/Mid Term Review just before the submission of the final draft of the dissertation

5.2 Submission

Candidates shall submit the Dissertations to the Controller of Examinations **not earlier than five months but within six months** from the date of the start of theSemester –II. The above said time limit shall start from the 1st of the month which follows the month in which Semester - I examinations are conducted. If a candidate is not able to submit his/ her Dissertation within the period stated above, he/she shall be given an extension time of **four** months in the first instance and another **four** months in the second instance with penalty fees. If a candidate does not submit his/her Dissertation even after the two extensions, his/her registration shall be treated as cancelled and he/she has to re-register

for the course subject to the discretion of the Principal. However the candidate need not write once again the theory papers if he/she has already passed these papers.

At the time of Submission of Dissertation, the guide concerned should forward the marks to the CoE through HOD in a sealed cover

5.3 Publications

All the M.Phil. Scholars should publish atleast one Research article in the reputed Journals before the submission of their dissertation. Publication of research article will be considered as CIA component. According to the type of Journals marks will be distributed to each article as follows.

UGC approved Journals	-	10 marks
Other Journals with ISSN number	-	8 marks
ReTeLL or Seminar /Conference Proceedings	-	6 marks

5.4 Requirement

For the valuation of dissertation it is mandatory to have passed in all the four courses. One external examiner and the Research Adviser shall value the Dissertation. The external examiner should be selected only from outside the college and shall be within the colleges affiliated to Bharathidasan University. In case of non-availability, the panel can include examiners from the other university/colleges in Tamil Nadu. The external examiner shall be selected from a panel of 3 experts suggested by the Research Adviser. However, the Controller of Examination may ask for another panel if he deems it necessary. Both the internal and external examiner will evaluate the Dissertation and allot the marks separately. However the *viva-voce* will be done by both of them. The average marks will be considered.

5.5 Curbing Plagiarism

According to The draft of University Grants Commission (Promotion of Academic Integrity and Prevention of Plagiarism in Higher Education Institutions) Regulations, 2017. Before submitting the thesis every students should submit the draft and get the certificate from the college library which will be issued after the verification of plagiarism. The certificate should be enclosed along with the thesis.

Plagiarism would be quantified into following levels in ascending order of severity for the purpose of its definition:

Level-0: Similarities upto 10% Excluded
Level-1: Similarities above 10% to 40%
Level-2: Similarities above 40% to 60%
Level-3: Similarities above 60%

Penalties for Students Plagiarism Disciplinary Authority (PDA) of the HEI, based onrecommendations of the Academic Misconduct Panel (AMP), shall impose penalty considering the severity of the Plagiarism.

i. Level 0: Similarities upto 10% - Minor Similarities, no penalty.
ii. Level 1: Similarities above 10% to 40% - Such student shall be asked to submit a revised script within a stipulated time period not exceeding 6 months.
iii. Level 2: Similarities above 40% to 60% - Such student shall be debarred from submitting a revised script for a period of one year.
iv. Level 3: Similarities above 60% -Such student registration for that programme shall be cancelled.

5.6 Viva-Voce

An open Viva-Voce examination shall be conducted by both the external examiner and the supervisor **and shall be attended by members of Department Research Committee members, all faculty members of the departments, other research scholars and other interested experts / researchers** and evaluated jointly by the Examiner and the Supervisor. The valuation of M.Phil. Dissertations and the viva-voce examination shall be carried out on the same day at the place of the Research Supervisor (viva is to be conducted only if the student passes in the valuation of the dissertation). The mark should be sent to the Controller of Examinations by the Research supervisor. A candidate shall be declared to have passed Part-II Examination if he secures not less than **55%** of the marks both in internal and external.

6. Classification of Final Results

i. The classification of final results shall be based on the CGPA, as indicated in Table 2.
ii. For the purpose of Classification of Final Results, the candidates who earn the CGPA 9.00 and above shall be declared to have qualified for the Degree as “Outstanding”. Similarly, the candidates who earn the CGPA between 8.00 and 8.99, 7.00 and 7.99, 6.00 and 6.99, and 5.00 and 5.99 shall be declared to have qualified for their Degree in the respective Programmes as “Excellent”, “Very Good”, “Good”, and “Above Average” respectively..
iii. Absence from an examination shall not be taken as an attempt.

Table-1: Grading of the Courses

Marks Range	Grade Point	Corresponding Grade
90 and above	10	O
80 and above but below 90	9	A+
70 and above but below 80	8	A
60 and above but below 70	7	B+
50 and above but below 60	6	B
Below 50	NA	RA

Table-2: Final Result

CGPA	Corresponding Grade	Classification of Final Results
9.00 and above	O	Outstanding
8.00 to 8.99	A+	Excellent
7.00 to 7.99	A	Very Good
6.00 to 6.99	B+	Good
5.00 to 5.99	B	Above Average
Below 5.00	RA	Re-Appearance

6.1 Credit based weighted Mark System is to be adopted for individual semesters and cumulative semesters in the column 'Marks Secured' (for 100).

6.2 Candidates who have failed in the courses may take the supplementary exams conducted by the CoE immediately. Even then, if they could not complete the course(s), they will be given two more chances only to appear for those courses along with the next batch scholars. The maximum duration for the completion of the M.Phil.Programme is 2 Years.

7. **Attendance**: Daily attendance for 90 working days should be enforced for the students. Periodical report of a student to the guide concerned should be recorded in the register kept by the guide.

8. **The Scholar must obtain 80% of attendance per semester in order to appear for the Semester Examinations/*Viva-Voce.***

M. Phil. CHEMISTRY

Programme Outcomes (POs)

1. Scholars are to be adopted with a new paradigm of self-learning in the form of review of earlier knowledge acquired.
2. Scholars are brought to light from the previous investigation completed to the newer thrusts of knowledge and implementation in research.
3. Scholars are trained to design, implement and evaluate secured information (hard and soft) systems with assured quality and efficiency.
4. Scholars are to be oriented towards becoming globally competent.

Programme Specific Outcomes (PSOs)

1. Scholars learn the techniques of teaching and research in chemistry.
2. Scholars explore and expedite the recent avenues in chemistry research
3. Scholars experience the synthetic strategies and analytical instrumentation skills by doing active research.
4. Scholars become globally competent to publish their research articles.

Course Pattern - 2018 Set

Sem	Code	Title of the Paper
I	18MCH101	Course-C1: Professional Skills for Teaching – Learning
	18MCH102	Course-C2: Research Methodology
	18MCH103	Course-C3: Advanced Topics in Chemistry
	18MCH104A	Course-C4: Advanced Studies of Macrocyclic Complexes
	18MCH104B	Course-C4: Synthesis and Characterization Coordination Complexes
	18MCH104C	Course-C4: Corrosion Inhibition on Metals
	18MCH104D	Course-C4: Kinetics and Catalysis
	18MCH104E	Course-C4: Natural Products Chemistry
	18MCH104F	Course-C4: Organometallic Compounds
	18MCH104G	Course-C4: Modern Trends in Coordination Chemistry
	18MCH104H	Course-C4: Recent Advances in Coordination Chemistry
	18MCH104I	Course-C4: Thermodynamics of Liquid Solutions
	18MCH104J	Course-C4: Supramolecular Chemistry
	18MCH104K	Course-C4: Electro-organic Synthesis
	18MCH104L	Course-C4: Principles and Applications of Coordination Complexes
	18MCH104M	Course-C4: Physical Methods in Coordination Chemistry
	18MCH104N	Course-C4: Surface Chemistry
	18MCH104O	Course-C4: Heterocyclic Compounds
II	18MCH205	Course-C5: Dissertation

18MCH101

PROFESSIONAL SKILLS FOR TEACHING-LEARNING

Programme Outcomes

1. To empower scholars with soft skills.
2. To introduce the teaching and dynamics of teaching-learning
3. To facilitate e- learning / e-teaching with the ICT tools
4. To acquire practical skills (in subject) aiming at gaining confidence to handle practical classes.
5. To develop teaching skills and gain confidence in teaching.
6. To acquire knowledge on the preparation of teaching aids

Unit I: Soft Skills

1. Introduction to Soft Skills, Soft Skills Vs Hard Skills, types of Soft Skills
2. Communication skills- Basics in communication, structure of written and oral sentences, Verbal, non-verbal, body language, JOHARI Window, Intrapersonal and Interpersonal Communications, Activities in Effective Communication
3. Behavioral Skills- Leadership skills, Time Management, Creativity and Lateral thinking
4. Interview Skills- Resume Writing, Different types of interviews, Etiquettes in interviews, Mock interviews
5. Team Building and Group Discussion- Progressive stages of Team Building, Parameters of GD (special reference to attending, listening, responding skills), Mock Group GDs

Unit II: Techniques and Dynamics of Teaching- Learning

1. Emerging trends in Educational Psychology- Meaning, Scope and Methods
2. Learning- Different Theories of learning, Approaches to learning (Classical Conditioning- Ivan Pavlov; Operant conditioning- B.F.Skinner); kinds of learning, factors affecting learning
3. Motivation: Intrinsic and extrinsic motivation, Development of memory and intelligence

Unit III: e-Learning and e-Teaching

An overview of Microsoft office-2007: MS WORDS-2007- MS Excel-2007- MS Powerpoint-2007, Concepts in e-Resources and e-design: World Wide Web Concepts - Making use of Web Resources- Web site creation concepts – Creating Web Page Editors- Creating Web graphics – Creating Web Audio files.

Unit IV: Experimental Techniques

Acetate and Phosphate buffer preparation. Preparation of standard curves-glycine, glucose and absorption spectra of plant pigments – Electrophoresis: PAGE – Chromatography: Separation and identification of amino acids. Double staining and permanent slide preparation – submission of 10 slides for evaluation. Biostatistics: Random Sampling (50 samples) using Random number table, Data collection, classification and presentation. Measures of central values and dispersion to the classified data, t-test and chi-square test. Bibliometry.

Unit V: Teaching Methods

Preparation of teaching aids – preparation of Power point, animated and text lecture materials for teaching the lessons – Teaching 18 hours theory both for UG & PG .classes and assisting 18 hours practical classes both for UG & PG

References

Unit I

1. JASS (2013). Winners in the making. Introduction to soft skills. St. Joseph's college, Trichy
2. Murphy, Raymond. (1998). Essential English grammer. 2nd ed. Cambridge university press
3. Trishna (2004). Knowledge system how to do well in GDs and interviews. Reprographic and printing services, secunderabad

Unit II

1. Covey, Stephen. (2004). 7 habits of highly effective people, free press
2. Driscoll, M P (1994). Psychology of learning for instruction, needham, ma: allyn and bacon
3. Gardner, Howard (1983; 1993). Frames of mind: the theory of multiple intelligences, new York; basic books

Unit III

1. Joyce cox, curtisfrye etc (2007), step by 2007 microsoft office system, prentice hall of india pvt Ltd, new delhi

Unit IV & V

1. Jayaraman J., 1972, Techniques in Biology, Higginbothoms Pvt.Ltd., Chennai.
2. Ralph R., 1975, Methods in Experimental Biology, Blackie Publ., London.
3. Educational Psychology in class room – Lindaren Henry – Asia Publishing Home.
4. Psychology of class room learning – Holt Richard.
5. Gupta,S.C. 2013. Fundamentals of statistics, Himalaya Publishers, Mumbai.

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes

Semester I	Code 18MCH101		Title of the Paper PROFESSIONAL SKILLS FOR TEACHING-LEARNING						Hours 5	Credits 4
Course Outcomes (COs)	Programme Outcomes (POs)				Programme Specific Outcomes (PSOs)				Mean Score of COs	
	PO1	PO2	PO3	PO4	PSO1	PSO2	PSO3	PSO4		
CO1	2	4	4	5	2	5	1	3	3.3	
CO2	5	2	2	2	1	3	5	2	2.8	
CO3	3	4	3	3	3	4	3	3	3.3	
CO4	4	3	2	4	3	4	5	3	3.5	
CO5	5	2	2	2	1	3	5	2	2.8	
CO6	4	3	3	1	4	1	3	5	3.0	
						Overall Mean Score for COs			**3.1**	

Result: The Score for this Course is 3.1 (High Relationship)

Note:

Mapping	**1-20%**	**21-40%**	**41-60%**	**61-80%**	**81-100%**
Scale	**1**	**2**	**3**	**4**	**5**
Relation	**0.0-1.0**	**1.1-2.0**	**2.1-3.0**	**3.1-4.0**	**4.1-5.0**
Quality	**Very poor**	**Poor**	**Moderate**	**High**	**Very High**

Values Scaling:

Mean Score of COs = $\frac{\text{Total of Values}}{\text{Total No. of POs \& PSOs}}$

Mean Overall Score for COs = $\frac{\text{Total of Mean Scores}}{\text{Total No. of COs}}$

18MCH102

RESEARCH METHODOLOGY

Programme Outcomes:

1. To know the information about research journals for publication and writing the thesis
2. To introduce the students to C-language and enable him to solve simple programs in C
3. To understand the methods to minimize errors and correlation analysis
4. To learn functional group inter conversion and stereochemical aspect
5. To apply the retrosynthetic analysis approach to synthesis new target molecules
6. To know the difference between separation and purification

Unit I: Information Retrieval & Documentation

Sources of information -Primary, secondary, tertiary Sources-Journals-Abstracts-Current Titles-Reviews-Monographs-Dictionaries-Information retrievals using internet and other electronic medias [Preparing a review Article related to the problem of Research of the student]. Reports of Research Work - Laboratory Observation- Preparation of Records Manuscripts-Research Paper formats in *Indian J.Chem., J.Indian Chem.Soc., J.Am.Chem.Soc. Tetrahedron, J. Chem.Soc-Dalton Trans, J.Chem. Education* Writing the project report or thesis.

Unit II: Statistical Tools of research

Significant figures - Rounding off the values using significant figures - Precision, accuracy, Error analysis, types of errors – Methods of minimization of errors. Mean, median, measures of spread – range, standard deviation and variance – F test, t test – Types of correlation, correlation coefficient, Regression analysis – binomial distribution, normal distribution – hypothesis generation and testing of hypothesis

Unit III: Computers in Chemistry

C Language: About C – Basics of writing a C program - Constants, variables and Data Types - Operators – Arithmetic, Assignment, Arithmetic-Assignment - Increment – Decrement Relational and Logical operators - Statements – IF and ELSE statements. LOOPS - Simple programming examples from chemistry - Temperature conversion, Calculation of frequency of electromagnetic Radiation, C_v of Solid, Activity coefficient of Electrolytes, Rate constants of I and II order reactions, $t_{1/2}$ of I, II and III order reactions, Calculation of Arrhenius Parameters, Calculation of Modes of vibration – Methods to draw and design structures – Chem Sketch.

Unit IV: Methods of organic synthesis

Applications of Oxidizing agents – DDQ, PCC, SeO_2, $KMnO_4$, $Pb(OAc)_4$, OsO_4, Ag_2CO_3, TEMPO, NBS, Lemieux-Johnson reagent, Prevost and Woodward reagent.

Applications of Reducing agents – LAH, Borohydrides, Dissolving metal reduction, $NaNH_2$, R_3SnH, Me_3SnCl and Wilkinson's Catalyst.

Synthon, Synthetic equivalent – Disconnection – FGI – Umpolung - Retrosynthetic analysis of simple organic compounds – mono and bi-functional open chain target molecules – mono and bicyclic target molecules. Protection of some functional groups – Regioselective, Regiospecific and Stereoselective alkylation of cyclic ketones, enones and 1,3-dicarbonyl compounds – enamines and selective alkylation – Olefination of carbonyl compounds – Wittig reaction.

Unit V: Methods of separation

Distinction between separation and purification – basic principles of separation techniques – solvent extraction, distillation. Chromatography-Paper, Column, Ion-exchange, GC and HPLC techniques and applications

References

Unit-I:

1. Kothari, C.R., Research methodology: Methods and techniques, New age International, 2004.
2. Anderson, Assignment and Thesis writing.

Unit-II:

1. Eckschlager K., Errors, Measurement and results in chemical analysis, London, Van Nostrant Reinhold Company,1969.

Unit-III:

1. E. Balagurusamy, *C*++ I Ed., New Delhi, Tata McGraw Hill,1995.
2. Puneet Nayyar, Sputi Trehan, Samrat Sharma, C-Adventure – Beginners Guide to C-Programming, Diamond Jubilee Publication, NISCOM, New Delhi, 2002.

Unit-IV:

1. Warren S, Designing Organic Synthesis: The Disconnection Approach, Wiley, New Delhi,1984.
2. Mackie R K, and Smith D M, Guide Book of Organic Synthesis, London, ELBS. 1982.

Unit-V:

1. Budhiraja, Separation Chemistry, 2nd Ed., New Age International (P) Ltd, New Delhi, 2007.
2. Willard H H, Dean M W and Settle, Instrumental Methods of Analysis, 6th Ed., New York, CBS Publishers and distributors, 1986.

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes

Semester I	Code 18MCH102	Title of the Paper RESEARCH METHODOLOGY							Hours 5	Credits 4
Course Outcomes (COs)	Programme Outcomes (POs)				Programme Specific Outcomes (PSOs)				Mean Score of COs	
	PO1	PO2	PO3	PO4	PSO1	PSO2	PSO3	PSO4		
CO1	2	4	4	5	2	4	2	3	3.3	
CO2	4	3	1	2	2	3	5	2	2.8	
CO3	2	5	2	2	2	4	2	3	2.8	
CO4	2	4	4	5	2	4	2	3	3.3	
CO5	2	1	2	4	3	5	2	4	2.9	
CO6	4	3	3	1	4	2	3	5	3.1	
							Overall Mean Score for COs		3.0	

Result: The Score for this Course is 3.0 (High Relationship)

Note:

Mapping	1-20%	21-40%	41-60%	61-80%	81-100%
Scale	1	2	3	4	5
Relation	0.0-1.0	1.1-2.0	2.1-3.0	3.1-4.0	4.1-5.0
Quality	Very poor	Poor	Moderate	High	Very High

Values Scaling:

$$\text{Mean Score of COs} = \frac{\text{Total of Values}}{\text{Total No. of POs \& PSOs}} \qquad \text{Mean Overall Score for COs} = \frac{\text{Total of Mean Scores}}{\text{Total No. of COs}}$$

18MCH103

ADVANCED TOPICS IN CHEMISTRY
(Open Online Course)

Programme Outcomes:

1. The applications of UV-Visible, IR spectroscopy and Mossbauer spectroscopy in the study of coordination compounds are learned
2. Students learn the nuclear magnetic resonance techniques
3. Students understand the basic concepts of ultrasonic's techniques
4. Students learn microwave assisted reactions and chemistry of macrocyclic complexes.
5. Students understand the fundamentals of cheminformatics
6. Students understand the concepts of drug designing

Unit I:

UV Visible spectroscopy. Microstates Terms Term symbols Free ion terms for d^1-d^9 systems and their splitting in octahedral and tetrahedral ligand fields – Selection rules and intensity of bands – Electronic spectra of transition metal complexes (from d^1 to d^9 configurations) – Effect of Jahn-Teller distortion on the electronic spectra – Determination of Δ_0 from spectra – Charge transfer spectra.

IR and Raman spectroscopy. Applications of IR spectroscopy in the structural analysis of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide – IR spectra of metal carbonyls with reference to the nature of bonding and geometry

Mossbauer Spectroscopy. Principle – isomer shift – electric and magnetic quadrupole splitting – applications to iron and its compounds

Unit II: NMR and MS

PMR spectroscopy. Introduction – Continuous Wave (CW) NMR spectrometry – Relaxation

– Pulsed FT spectrometry – Instrumentation and Sample handling - chemical shift –Spin coupling constants - AMX, ABX, and ABC rigid systems with three coupling constants – vicinal and germinal coupling – long-range coupling – spin decoupling – NMR shift reagents

13C NMR spectroscopy. Peak assignments – chemical classes and chemical shifts -^{13}C-^{1}H spin coupling (J values)- DEPT- Correlation spectrometry – ^{1}H-^{1}H COSY- Double quantum filtered ^{1}H-^{1}H COSY- HETCOR- Proton detected HETCOR: HMQC and HMBC – INADEQUATE – TOCSY - Gradient field NMR

Mass spectrometry. Instrumentation - Magnetic Field only – Double focusing - Quadrupole Mass filter- Quadrupole ion storage - Time of Flight (TOF) – FC-ICR – MS/MS (Tandem MS)- Mass spectrum- Determination of MF – Ionization techniques - CI, FD, FAB, ESI and MALDI – Fragmetnation – Rearrangements - Determination of structure of organic compounds using UV-Vis, NMR and Mass spectra

Unit III

Nanochemistry: Introduction – nanotechnology and nano machines – molecular nanotechnology – methods of synthesis of nano materials – plasma arching, sol-gel method – electro deposition, ball milling – analytical tools to study nano materials (SEM, TEM & SPM) – applications of nano chemistry – CNT and its applications – molecular switches – rotaxanes – catenanes – lithography – nano biometrics – metal nano clusters – nano crystals – quantum wells, dots, wires, etc – biological materials – future applications

Sonochemistry: Fundamentals of sound and ultrasound – cavitation and its principle – instrumentation – homogeneous and heterogeneous processes – sonoluminescence – uses in chemistry, material science, medicine and life – synthetic applications – esterification, saponification, hydrolysis, substitution, cannizaro reaction, Strecker's synthesis

Unit IV: Microwave assisted synthesis and Macrocyclic Chemistry

Microwave assisted synthesis: Instrumentation – microwave assisted reactions in water (Hoffmann elimination, hydrolysis, oxidation of toluene) and in organic solvents (esterification, Fries rearrangement, Claisen rearrangement, Diels Alder reaction) – Solvent free microwave reactions: deacylation, deprotonation and saponification of esters

Macrocyclic Chemistry: Design and synthesis of macro cyclic ligands (1+1 and 2+2) – Direct macro cyclic synthesis – template synthesis – kinetic and thermodynamic effects on synthesis – binucleating macrocycles – compartmental ligands – natural macrocyclic systems– Host-Guest chemistry – sequestration

Unit V: Cheminformatics

Definition – scope – use of cheminformatics – evolution – history – applications of cheminformatics – CHUCKLES (monomer level of molecules) – CHORTLES (regular mixtures) – CHARTS (Searchins) – contour of drugs – drug dynamics and kinetics – drug action – drug interaction – drug abuse – drug administration, distribution and elimination – pharmacodynamics – development of new drugs – economics of drug discovery – drug design

with the help of computer tools – use of silica chips to find lead molecules – chemical parameters in drug design – physic-chemical parameters in drug design – structure based drug design

References:

http://www.sjctni.edu/Department/CH/OOC/unit1.jsp
http://www.sjctni.edu/Department/CH/OOC/unit2.jsp
http://www.sjctni.edu/Department/CH/OOC/unit3.jsp
http://www.sjctni.edu/Department/CH/OOC/unit4.jsp
http://www.sjctni.edu/Department/CH/OOC/unit5.jsp

Unit-I

S. No.	Topics	Type of Contents	Location
1.	UV-Visible Spectroscopy, IR and Raman Spectroscopy	PPT	http://www.sjctni.edu/department/CH/ooc/uvvis.ppt http://www.sjctni.edu/department/CH/ooc/IR.ppt http://www.sjctni.edu/department/CH/ooc/Raman.ppt
2.	IR and Raman	Web Content	YouTube videos on IR and Raman Spectroscopy

Unit-II

S. No.	Topics	Type of Contents	Location
1.	PMR and ^{13}C-NMR Spectroscopy	PPT	http://www.sjctni.edu/department/CH/ooc/PMR.ppt http://www.sjctni.edu/department/CH/ooc/NMR.ppt
2.	PMR and ^{13}C-NMR Spectroscopy	Web Content	www.youtube.com/watch?v=k0eR8YqcA8c www.youtube.com/watch?v=ROfzVAUb5ls www.youtube.com/watch?v=BeBcPQ9zGAA www.youtube.com/watch?v=8hL3GXCttuo https://www.khanacademy.org https://www.youtube.com/watch?v=biH065y1I4

Unit-III

S. No.	Topics	Type of Contents	Location
1.	Nano Biometrics Nano-Preparation Sonochemistry Uses of Nanotube	PPT	http://www.sjctni.edu/department/CH/ooc/biometrics.ppt http://www.sjctni.edu/department/CH/ooc/nano preparation.ppt http://www.sjctni.edu/department/CH/ooc/sonochemistry.ppt http://www.sjctni.edu/department/CH/ooc/nanotube.ppt

Unit-III

2.	Nano Biometrics Nano preparation Sonochemistry Uses of Nanotube	Web Content	YouTube videos- sonochemical reactions sonochemistry - wikipedia www.unc.edu/depts/mtcgroup/litmeetings/sonochemistry.pdf https://uqu.edu.sa/files2/tiny_mce/plugins/.../files/.../nanochemistry.pdf

Unit-IV

S. No.	Topics	Type of Contents	Location
1.	Microwave Chemistry 1 Microwave Chemistry 2	PPT	http://www.sjctni.edu/department/CH/ooc/microwavechemistry1.ppt http://www.sjctni.edu/department/CH/ooc/microwavechemistry2.ppt
2.	Microwave Chemistry 1 Microwave Chemistry 2	Web Content	YouTube videos on macrocyclic compounds

Unit-V

S. No.	Topics	Type of Contents	Location
1.	Cheminformatics	PPT	http://www.sjctni.edu/department/CH/ooc/cheminformatics.ppt
2.	Cheminformatics	Web Content	YouTube videos on cheminformatics

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes

Semester I	Code 18MCH103	Title of the Paper ADVANCED TOPICS IN CHEMISTRY					Hours 5	Credits 4
Course Outcomes (COs)	Programme Outcomes (POs)				Programme Specific Outcomes (PSOs)				Mean Score of COs
	PO1	PO2	PO3	PO4	PSO1	PSO2	PSO3	PSO4	
CO1	4	4	4	4	2	4	2	3	3.4
CO2	3	2	3	4	3	4	2	4	3.1
CO3	4	4	4	4	2	4	2	3	3.4
CO4	3	2	3	4	3	4	2	4	3.1
CO5	3	4	2	2	2	4	2	3	2.8
CO6	4	3	3	3	4	2	3	4	3.3
							Overall Mean Score for COs		3.2

Result: The Score for this Course is 3.2 (High Relationship)

Note:

Mapping	1-20%	21-40%	41-60%	61-80%	81-100%
Scale	1	2	3	4	5
Relation	0.0-1.0	1.1-2.0	2.1-3.0	3.1-4.0	4.1-5.0
Quality	Very poor	Poor	Moderate	High	Very High

***Values Scaling*:**

Mean Score of COs = $\frac{\text{Total of Values}}{\text{Total No. of POs \& PSOs}}$	**Mean Overall Score for COs** = $\frac{\text{Total of Mean Scores}}{\text{Total No. of COs}}$

18MCH104A

ADVANCED STUDIES OF MACROCYCLIC COMPLEXES

Programme Outcomes:

1. To study the methods and characterization of macrocyclic complexes.
2. To know about the theories of coordination chemistry
3. To prepare and characterize different Macrocyclic ligands and their metal complexes.
4. To study the application of spectral techniques in studying coordination complexes
5. To know about the application of coordination complexes.

Unit I:

Methods of preparation of coordination compounds - Analysis and determination of molecular formula - Volumetric, gravimetric and colorimetric methods - Conductance and magnetic measurements of complexes

Unit II:

Theories of coordination - CF, MO, LF Theories - Merits and demerits - Macrocycles and their classifications - Synthesis of Macrocycles - Properties and applications

Unit III:

Special application to the study of coordination compounds - Electronic spectra - IR spectra - NMR spectra - ESR spectra - Mossbauer spectra – PES

Unit IV:

Kinetics and reaction mechanism in coordination compounds - SN1, SN2, SN1CB mechanisms - Trans effect - Electron transfer and electron exchange reactions - Catalysis by organometallic compounds

Unit V:

Transition metal ions in biology - Iron enzymes - structure and their functions - Model system for molecular activation and corresponding biochemical system.

References:

1. Lee J.D., *Concise Inorganic Chemistry,* 6th Ed., London, ELBS,1998.
2. Huheey JE., *Inorganic Chemistry: Principle, Structure and Reactivity*, 2nd Ed., New York, Harper & Row publishers,1972.
3. Drago RS., *Physical methods in inorganic chemistry*, London, Saunders Golden Sunburst Series, W.B.Saunders Company,1977.
4. Cotton FA and Wilkinson G., *Advanced Inorganic Chemistry, 3rd Ed.*, London, John Wiley & Sons, 1988.

18MCH104B

SYNTHESIS AND CHARACTERIZATION COORDINATION COMPLEXES

Programme Outcomes:

1. To study the methods of preparing different coordination complexes
2. To characterize coordination complexes based on spectral and instrumental techniques
3. To know about the theories of coordination chemistry
4. To study the application of spectral techniques in studying coordination complexes
5. To know about the application of coordination complexes.

Unit I:

Methods of preparation of coordination compounds – design and synthesis of macrocyclic complexes – template effect – Conductance studies - magnetic measurements of complexes – Gouy method

Unit II:

Theories of coordination - CF, MO, LF Theories - Merits and demerits - donor and acceptor ligands - Carbonyls - Nitrosyls - Cyanides - Triphenyl phosphine complexes - Organo metallic compounds - Allene, alkyne and allyl complexes

Unit III:

Special application to the study of coordination compounds - Electronic spectra – Racah parameters- IR spectra - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide- - NMR spectra of fluxional molecules- ESR spectra -Factors affecting the magnitude of g and A tensors in metal complexes - Mossbauer spectra of Fe complexes – Photoelectron spectroscopy

Unit IV:

Kinetics and reaction mechanism in coordination compounds – acid hydrolysis and base hydrolysis mechanisms - Trans effect and its theories - Electron transfer and electron exchange reactions - Catalysis by organometallic compounds

Unit V:

Transition metal ion in biology - Iron enzymes - structure and their functions - Model system for molecular activation and corresponding biochemical system.

References:

1. Drago R.S., *Physical Methods in Inorganic Chemistry*, London, Saunders Golden Sunburst Series, W.B.Saunders Company1977.
2. Lee JD, *Concise Inorganic Chemistry,* 6th Ed., London, ELBS,1988.
3. Huheey JE., *Inorganic Chemistry Principle Structure and Reactivity*, 2nd Ed., New York, Harper & Row publishers,1972.
4. Cotton F.A. and Wilkinson G., *Advanced Inorganic Chemistry,3rd* Ed., London, John Wiley & Sons,1988.

18MCH104C

CORROSION INHIBITION ON METALS

Programme Outcomes:

1. To understand the concept and types of corrosion
2. To understand the factors influencing corrosion
3. To study how to control corrosion
4. To know the theories of inhibiting corrosion
5. To use different types of inhibitors in preventing corrosion

Unit I: Corrosion - definition- costs of corrosion - economic losses - Human life and safety – Types of corrosion: dry corrosion - wet corrosion - mechanisms - galvanic corrosion, concentration cell corrosion, atmospheric corrosion, soil corrosion, pitting corrosion, inter granular corrosion, waterline corrosion, stress corrosion, microbial corrosion

Unit II: Factors influencing corrosion: Nature of metals: Position in galvanic series - over voltage - relative areas of anodic and cathodic parts - purity of metals - physical state of metal – nature of surface film - solubility of corrosion products. Nature of corroding environment temperature - Humidity - presence of impurities in atmosphere - influence of pH - nature of ions present conduction of the corroding medium - formation of oxygen concentration cell.

Unit III: Corrosion control: Proper designing - use of pure metals - using metal alloys – cathodic protection -sacrificial anodic protection method - impressed current cathodic protection - Use of inhibitors: inhibitors - definition - classification - due to Putilova - due to Deano - anodic - cathodic – mixed

Unit IV: Theories of inhibition of corrosion: Adsorption theory and molecular structure - hydrogen over potential theory, film formation theory - synergistic effect - example - corrosion inhibition in neutral gaseous environments - chromate, molybdates, nitrite, phosphate, silicate, cations, organic inhibitors carboxylate and tannins.

Unit V: Phosphates as inhibitors: Phosphonates: definition - reasons for using Phosphonates as inhibitors - Use of HEDP, ATMP, ethyl phosphonic acid, 2-carboxyethyl phosphonic acid as corrosion inhibitors.

References:

1. Antropov.L., *Theoretical electro chemistry*, Moscow, Mir Publishers, 1972.
2. Bockris.J.O.M. and Reddy A.K.N, *Modern Electro chemistry* Volume I and II, New York, Plenum Press,1970.

18MCH104D

KINETICS AND CATALYSIS

Programme Outcomes:

1. To study rate of a reaction and influence of various factors on rate of a reaction
2. To understand types of kinetic reactions and their theories
3. To study and apply different types of kinetic reactions
4. To understand the concept and applications of surface reactions.

Unit-I:

Factors influencing the rate of a reaction. Methods of determining order of a reaction. Mechanism of complex reactions –Equilibrium approximation – Steady state approximation- Product study –stoichiometry- Isokinetic relation –Isokinetic temperature-Exner plot-Nature of reaction series and selectivity.

Unit-II:

Arrhenius equation –Activated complex theory- Chain reaction(Photo Chemical and thermal reaction)-Chain initiation process-Hydrogen-halogen reaction-Branching chain reaction-Gas
phase combustion H2O2 reaction-Explosive reaction

Unit-III:

Application of ARRT in solution kinetics –Factors affecting reaction rate in solution Influence of internal pressure – influence of solvent dielectric constant-influence of ionic strength ion dipole and dipole –dipole reactions - influence of hydrostatic pressure – Vant Hoff equation and volume of activation Kinetic isotope effect-Primary and Secondary isotope effect

Unit-IV:

Acid-base catalysis - Mechanism of acid base catalysis – Vant Hoff intermediate, Arrhenius intermediate protolytic and prototropic mechanism - Catalysis law. Acidity functions – Hammet Zucker hypothesis –catalysis in biological systems –Enzyme catalysis – Michaelis Menten equation-Line -Weaver Burk and Eadie Hofster Plots - influence of substrate concentration - influence of pH - influence of temperature-influence of substituents on reaction rates –Hammet and Taft equations-Linear free energy relationships-kinetics of biological oxidation reaction and mechanism

Unit-V:

Surface phenomena-Adsorption and free energy relations at interface - Gibbs adsorption isotherm-physical and chemical adsorption - Langmuir adsorption

isotherm - BET isotherm- Measurement of surface area - Heterogenous catalysis - Role of surface in catalysis- Mechanism of Heterogenous catalysis-Langmuir-Hinshelwood mechanism of bimolecular reaction - Langmuir Rideal mechanism of bimolecular reaction

References:

1. Laidler K J, *Chemical Kinetics*, 3rd Ed., New Delhi TATA McGraw Hill Co. 1984.
2. Investigations of Rates and mechanism of Reaction PartI-Edword.S.Lewis
3. Kinetics and Mechanism-Frost.A and Pearson.R.C
4. Laidler K J, *Chemical Kinetics*, 3rd Ed., New Delhi TATA McGraw Hill Co. 1984.
5. Radiation Chemistry - Hughes.G.

18MCH104E

NATURAL PRODUCTS CHEMISTRY

Programme Outcomes:

1. To understand how plants are classified and techniques of extraction process
2. To apply the instrumental concepts in separating plant extracts
3. To analyze plant extracts and characterizing them using UV,IR, and NMR spectral techniques.
4. To study the different separation and characterization methods for phenolic and terpinoid compounds
5. To understand the charecterisation of nitrogen compounds and carbohydrates etc.

Unit I: Plants and Plant Products

Classification of Plants - Nomenclature - Cells - Tissues - Structures and Functions of Cells and tissues - Primary Metabolites - Secondary Metabolites - Microorganism- Types - Microbes and Man - Biological Activities - Microbial Studies - Techniques - Interpretation of Results

Unit II: Methods of Plant Analysis I

Methods of Extraction - Cold Percolation Method - Soxhlet Method - Methods of Isolation - Methods of Separation- Chromatography - Paper Chromatography - Column Chromatography - Thin layer Chromatography - Gas Chromatography - High performance Liquid Chromatography Electrophoresis - Paper and Gel Electrophoresis - Distillations - Steam Distillation - Fractional Distillation - Vacuum Distillation - Crystallization Techniques

Unit III: Methods of Plant Analysis II

UV-VIS spectroscopy - IR Spectroscopy - Proton and Carbon-13 NMR Spectroscopy – Mass Spectroscopy - X-ray and Neutron Diffraction studies - Optical studies - Qualitative and Quantitative Analyses - Interpretation of Results

Unit IV: Phenolic Compounds and Terpenoids

Methods of separation, isolation and identification - Phenolics - Phenyl propanoids - Anthocyanins - Flavonoids - Xanthones - Stilbenes - Chemical conversions of these compounds - Structure Elucidation of Quercetin, Vitexin and Naringin Methods of separation, isolation and identification - Monoterpenes - Sesquiterpenes - Diterpenes - Triterpenoids - Steroids -

Carotenoids - Chemical conversions of these compounds - Structure Elucidation of Menthol and Carotol.

Unit V: Nitogen Compounds, Sugars, Lipids and other related Compounds

Methods of separation, isolation and identification - Amino acids - Proteins - Peptides - Amines - Alkaloids - Cyanogenic glycosides - Purines - Pyrimidines - Cytokinins - Chlorophylls - Chemical conversions of these compounds - Structure Elucidation of Nicotine and Cytisin. Methods of separation, isolation and identification - Monosaccharide - Disaccharide - Polysaccharides - Shikimic acids - Quinic acid - Fatty acids - Polyacetylenes – Sulfur compounds - Chemical conversions of these compounds - Structure Elucidation of Shikimic acid and Rhanmonse.

References:

1. Peach K and Tracey MV , *Moderne der pfranzenanalyse*, Berlin, Spingerverlag, 1956- 1964,.
2. Krishnasamy N.R, *Chemistry of Natural Products,* Hyderabad, University Press,1999.
3. Boyer RF, *Modern Experimental Biochemistry,* II Ed., California, The Benjamin Cummings publishing company Inc., 1993.
4. Furniss BS, Hannaford AJ, Smith PWG and Tatchell AR, Vogel's *Text book of Practical Organic Chemistry*, V Ed., Essex, England, ELBS with Longman, 1989.
5. Harborne JB, Phytochemical Methods: *A Guide to Modern Techniques of Plant Analysis,* II Ed., London and New York, Chapman and Hall,1988.
6. Finar I.L. *Organic Chemistry*, Vol. 2. ELBS London.
7. Raphael Ikan, *Natural Products: A Laboratory Guide*, Jerusalem, Israel University Press,1969.
8. Jeffrey C, *An Introduction Plant Taxonomy*, II Ed., Cambridge, Cambridge University Press,1982.
9. William J and Sham M, *Microorganisms*, London, Mills and Boon Limited,1976.
10. Ari Koskinen, *Asymmetric Synthesis of Natural Products,* Chichester, New York, Brisbane, Toronto, Singapore, John Wiley and Sons,1993.

18MCH104F

ORGANOMETALLIC COMPOUNDS

Programme Outcomes:

1. To study about organo metallic compounds
2. To understand the reactions and mechanisms involving Organometallic reagents
3. To study the theory , instrumentation and applications of UV, IR and NMR spectra
4. To study the applications of different C-NMR spectra and thermal analysis
5. To study the applications of different spectral techniques in characterizing different organic compounds

Unit I:

Organometalic compounds-Olefin complexes, and cyclopentadienyl complexes, Bonding in ferrocene compounds, Arene metal complexes, Alkyne complexes fluxional organometallic compounds and its identifications

Unit II:

Reactions of organometallic compounds-Homogeneous Catalytic reactions, Stereochemistryand mechanism of addition reactions, hydrogenation of alkenes, formylation and polymerization reactions.

Unit III:

Organometallic reagents- Lead tetraacetate, sodium ethoxide, Aluminiumiso-propoxide, Dess-Martine reagent, silver, palladium and platinum compounds, Role of organometallic compounds in organic synthesis.

Unit IV:

Theory, instrumentation and applications of UV-spectroscopy, Instrumentation and Applications of IR spectroscopy with reference to organometallic compounds, NMR applications.

Unit V:

Applications of 2D-NMR techniques like COSY, HMQC, HMBC and NOESY. Applications of C -13 NMR spectroscopy, Mass spectral technique and its applications.Theory instrumentation and applications of Thermal experiments-TG, DTA, and DSC

References:

1. V.K.Ahluvalia, Renu Aggarval, *Organic synthesis*, 2nd Ed., Narosa Publications.
2. Cotton F.A. and Wilkinson G., *Advanced Inorganic Chemistry,* 3rd Ed., John Wiley & Sons, London,,1988.
3. Robert M Silvberstein and Francis X Webster, *Spectrometric identification of organic compounds*, 6th Ed., John Willey and Sons.

18MCH104G

MODERN TRENDS IN COORDINATION CHEMISTRY

Programme Outcomes:

1. To study the methods of preparation of coordination complexes
2. To understand the concept of characterization of coordination complexes
3. To know about the theories of coordination chemistry
4. To study the application of spectral techniques in studying coordination complexes
5. To know about the application of coordination complexes.

Unit I:

Preparation methods of complexes-physical methods of determination of molecular formula- conductance, magnetic measurement – faraday method – Gouy method

Unit II:

Theories of coordination compounds-VBT, CFT, MOT, LFT-merits and demerits. Sigma donor and pi-acceptor ligands- preparation, structure and reactivity of organometallic complexes

Unit III:

Applications of spectroscopic methods in the study of coordination complexes

NMR – fluxional complexes - IR-Effect of coordination on ligand vibrations – Metal-ligand vibrations - Mossbauer spectroscopy of iron complexes – Electron paramagnetic resonance – theory and applications

Unit IV:

Kinetics and reaction mechanism in coordination complexes-SN1, SN2, SN1CB. Theories and applications of trans effect-inner sphere and outer sphere electron transfer reactions-two electron transfer reactions-catalysis by organometallic compounds – hydrogenation, hydroformylation, oxidation and polymerization

Unit V:

Bioinorganic chemistry-structure and functions of chlorophyll, haemoglobin, myoglobin, cyctochromes and iron enzymes

References:

1. Drago R.S., *Physical methods in inorganic chemistry*, London, Saunders Golden Sunburst Series, W.B.Saunders Company,1977.
2. Huheey JE., *Inorganic chemistry Principle structure and reactivity*, 2nd Ed., New York, Harper & Row publishers,1972.
3. Cotton F.A. and Wilkinson G., *Advanced inorganic chemistry,* 3rd Ed., John Wiley & sons, London,1988.
4. Peter Atkins**,** Fraser Armstrong**,** Jonathan Rourke**,** Mark Weller and Tina Overton, 2010, Shriver and Atkins' Inorganic Chemistry, 5th Ed., Oxford University Press, New Delhi.

18MCH104H

RECENT ADVANCES IN COORDINATION CHEMISTRY

Programme Outcomes:

1. To Synthesis Novel Coordination Compounds
2. To study the Theories of Coordination Compounds and their Mechanisms
3. To study the Determination of Electronic Structure and Geometry of Coordination Compounds
4. To study the Magnetic Behaviour and Electroanalytical techniques involving coordination compounds
5. To understand Catalysis of Organometallic compounds and their Bio-inorganics

Unit I: Synthesis of Novel Coordination Compound

Macrocyclic Ligands - Design and Synthesis of macrocyclic Ligands - Synthetic Procedures - Direct Macrocyclic synthesis, Microwave assisted synthesis - Metal ion template synthesis – Macrocyclic systems - Macrocycles with pendant arm functional group - Catenands, Cage macrocycles, Cryptands and Crown Polyethers – Binucleating macrocycles - Compartmental Ligands. Natural macrocycles - Host-guest chemistry-macrocyclic host and non-metallic guests.

Unit-II: Theories of Coordination Compounds and Mechanisms

Crystal Field, Ligand Field, Molecular Orbital Theories and Angular Overlap – Model Mechanism of Electron Transfer Reactions – Inner sphere and Outer sphere electron transfer mechanisms - Substitution reaction in square planar complexes, trans effect -Oxidative addition and insertion reactions.

Unit-III: Determination of Electronic Structure and Geometry of Coordination Compounds-I

Electronic spectroscopy: Electronic states and spectra of Td and Oh complexes, charge transfer spectra LMCT, MLCT, crystal field spectra. Evaluation of values in Co(III) Oh and Ni(II) Oh complexes Dqxy and Dqz in tetragonally distorted cobalt(II) octahedral complexes. Infrared and Raman spectroscopy: Structural diagnosis: IR spectral assignment of coordinated ligands in metal complexes and differentiation of isomers (CN/NC, OCN/NCO, SCN/NCS, CNO/ONC, NO2/ONO NMR Spectroscopy - Application of spin-spin coupling to structure determination. NMR of paramagnetic transition metal ion complexes, scalar shift and covalency. Lanthanide shift

reagents. ESR anisotropy in the g-value, hyperfine and zerofield effect on the spectrum, Survey of the EPR spectrum of first row transition metals.

Unit-IV: Determination of Magnetic Behaviour and Electroanalytical techniques

Magnetic Behaviour of Coordination Compounds. Methods of determining magnetic susceptibility and electron states - Electrochemical methods of studying coordination compounds.Electrochemical and electrochemical reversibility. Pulse polarography, AC Polarography - Cyclic voltammetry - Coupled chemical reactions - EC, CE and ECE mechanisms. Photoelectron spectroscopy and X-PES - Mass Spectroscopy - CIMS, EIMS and FAB-MS.

Unit-V: Catalysis of Organometallic compounds and Bio-inorganics

Ziegler - Natta polymerization, Cyclooligomerization, Olefin isomerization, Metathesis and Polymer bound catalysis. The oxygen carriers- hemoglobin and myoglobin and synthetic oxygen carriers. Electron transfer agents - Cytochromes, iron-sulphur proteins. Mechanism of electron transfer reactions. Nitrogen Fixation. Essential and trace elements in biological systems. Chelate therapy and its applications.

References

1. Lindoy, L. F, The Chemistry of Macrocyclic Ligand Complexes, Cambridge University Press, N.Y,1989.
2. Huheey J.E., *Inorganic Chemistry*, 4th Ed., Harper and Row, NY, 1988.
3. Cotton.F.A and Wilkinson.G *Advanced Inorganic Chemistry*, 6th Ed., Wiley Interscience, NY,2001.
4. Purcell.K.F and Kotz. J.C. *Inorganic Chemistry*, Saunders,1976.
5. Lever.A.B.P, Inorganic Electronic Spctroscopy, 2nd Ed., Elsevier Publishing Company, Amsterdam, 1984.
6. Nakamoto. K, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, 4th Ed., Wiley interscience,1986.
7. Basolo F and Pearson .R.G, *Mechanism of Inorganic reactions*, 2nd Ed., Wiley Eastern. New Delhi,1967.
8. Kissinger.P.T, and Heineman.W.B, *Laboratory Techniques in Electroanalytical Chemistry*, Editors, Marcel Dekker, Inc., New York, 1984.
9. Drago R.S., *Physical Methods in Inorganic Chemistry*, Saunders, Amsterdam,1977. 10. J. Chem. Educn., 1983, 60, 252-308.
11. J. Chem. Educn., 1983, 60, 687-706.
12. Eichhorn G.L., Ed., *Inorganic Biochemistry*, Elsevier, Amsterdam,1976

18MCH104I

THERMODYNAMICS OF LIQUID SOLUTIONS

Programme Outcomes:

1. To study the Chemistry of Solutions
2. To study the various Theories of Liquid Mixtures
3. To understand the Thermodynamic Properties of liquid mixtures
4. To understand the concept of Ultrasonic Studies in Liquid Mixtures
5. To study the Applications of Ultrasonic Sound Waves and ionic liquids

Unit I: Chemistry of Solutions

Concentration units- molarity, molality, mole fraction, volume fraction, percentage by weight and volume. Ideal and non-ideal solutions-Raoult's law, Henry's law, models in ideal and non-ideal solutions, their miscibility's, thermal properties, Binary and ternary liquid mixtures.

Unit II: Theories of Liquid Mixtures

Cell theory, Hole theory, lattice model, Prigogine's model, Flory theory, scaled particle theory, free length theory, Kharare equation, Kalidoss-Jacobson theory. Types of interactions in solutions.

Unit III: Review on Thermodynamic Properties

Review of thermodynamic properties of solutions. Liquid solutions of non-electrolytes and electrolytes- activity coefficient- Deby- Huckel theory and its implications- thermodynamics of mixing. Measurement of density, viscosity, heat of solution, heat of mixing and vapour pressure.

Unit IV: Ultrasonic Studies in Liquid Mixtures

Ultrasonic interferometer- principle, instrumentation, generation of ultrasonic waves, measurement of velocity, ultrasonic transducers. Calculation of excess volume, internal pressure, isentropic compressibility and its deviation, free volume, free length, relative association, acoustic impedance, molar sound speed, isothermal compressibility, thermal expansion coefficient, partial and apparent molar volume, excess viscosity, excess molar Gibbs free energy of activation, stability constants of complexes. Relation of ultrasonic velocity with hydrogen bonding, phases, boiling points, molecular interactions and electrolytes.

Unit V Applications of Ultrasonic Sound Waves

Ultrasonic testing - Laser ultrasonic - ultrasonics in medicine, biology and industry. Sonochemistry - ionic liquids.

References:

1. Gupta MC, *Statistical Thermodynamics*, Madras, Wiley Eastern Ltd, 1990.
2. Glasstone S, *Thermodynamics for Chemists*, New Delhi, East-West Press Ltd., 2002.
3. Rowlinson JS, *Liquids and liquid mixtures*, London, Butterworth, 1971.
4. Alexander Findlay and Kitchener J A, *Practical Physical chemistry*, 8th edition, Longmans Green and Co. Ltd., 1959.
5. Srivastava KC, *Hand book of Ultrasonic testing*, International Inspection services, 2001.
6. Kinsler LE and Frey AR, *Fundamentals of Acoustics*, 2nd Ed., Wiley Eastern Ltd.,1991.
7. Bhaldev Raj, Rajendran V and Palanichamy, *Science and Technology of Ultrasonics*, Narosa Publishing House, Chennai. 2004.

18MCH104J

SUPRAMOLECULAR CHEMISTRY

Programme Outcomes:

1. To understand the concepts of Supramolecular Assemblies and Architectures.
2. To study the Synthesis of Supramolecular Assemblies and Templates
3. To study about Dendrimers and metallodendrimers.
4. To study Supramolecular Medicinal Chemistry.
5. To study about Nonlinear optical Materials.

Unit1: Supramolecular Assemblies and Architectures

Nature of supramolecular interactions, homo- and heteropolymetallic polypyridyl systems; supramolecular host- guest compounds. Terpyridine and bipyridine-appended spacers, phenazene based spacers. Different kinds of supramolecular assemblies constructed by covalent-, coordination-, and hydrogen bonding. Templates and self assembly: biochemical self-assembly, self-assembly in synthetic systems, self-assembling coordination compounds, catenanes and rotaxanes. Supramolecular devices: photoinduced elelctron and energy transfer, photo- and electrochemical sensors, light conversion and energy transfer devices, molecular electronic devices (molecular switches, wires, and rectifiers), molecular machines.

Unit 2: Synthesis of Supramolecular Assemblies

Templates and self-assembly: synthesis of Schiff base macrocycles and macrocyclic binucleating ligands by coordination template effects, self-assembling coordination compounds-design principles, molecular cubes, squares and boxes; self-assembly ofmetal arrays; catenanes and rotaxanes. Design of Robson-type compartmental Schiff base macrocycles derived from dialdehydes and diamines. Methods of self-assembling coordination compounds. Polyaza macrocycles and macrocycles with pendant arms. Construction of polynuclear supramolecular assemblies and nanostructures.

Unit 3: Dendrimers and metallodendrimers.

Synthetic methodology-divergent andconvergent methodologies; types of metallodendrimers, characterization techniques. Dendrimer encapsulated metal nanoclusters: silver and gold nanoclusters andnanoparticles, quantum dots, quantum size related photochemical properties, dendrimerencapsulated catalysis. Light harvesting dendrimers and multiporphyrin arrays); Rhodopsin (a supramolecular photonic device); biochemical self-assembly.

Antenna effect and funneling of electronic energy in supramolecular assemblies. Generation of 99mTc chelates.

Unit 4: Supramolecular Medicinal Chemistry

Contrast enhancing agents for medical diagnostics: thoeory of MRI imaging, Gdbased contrast agents-synthesis and structural features; optical contrast agents-Agand AuNPs; metal complexes as photosensitizers.Metal complexes for radiotherapy: diagnostic radiopharmaceuticals, non-technitium for diagnostic imaging, Tc-labelled small molecules and peptides as diagnostic radiopharmaceuticals. Targeted cancer nanotherapy: magnetic nanoparticles and cancer therapy; goldnanoparticles- tunable optical properties and in vivo cancer detection and therapy.

Unit 5: NonlinearopticalMaterials

Principle and supramolecular originof NLO behavior.Structural and electronicorigin ofNLO properties.Experimentaltechniques for the measurement of SHG: Kurtz and Powder method, EFISH and THG. Computational methods in design and screening of NLO materials. Dipole moment, polarizability, hyperpolarizability calculations, the energetics of FMOs, and MEP models, Mulliken electronegativites by the RHF and DFT computational methods.

References

1. J. W. Steed, J. L. Atwood, *Supramolecular Chemistry*, John Wiley & Sons Ltd.: NewYork; 2000.
2. J. M. Lehn, *Supramolecular Chemistry, Concepts and Prespectives*, VCH: Weinheim; 1995.
3. Izatt, R. M.; Christensen, J. J. Eds. *Synthesis of Macrocycles: The Design of Selective Complexing Agents, Progress in Macrocyclic Chemistry*, Vol. 3; Wiley-Interscience: NY, 1987.
4. Lindoy, L. F. *The Chemistry of Macrocyclic Ligand Complexes*; Cambridge University Press: Cambridge; 1989.
5. Caravan, P.; Ellison, J. J.; McMurry, T. J.; Lauffer, R. B. *Chem. Rev*. 1999, *99*,2293.
6. Bosman, A. W.; Janssen, H. M.; Meijer, E. W. "About Dendrimers: Structure, Physical Properties, and Applications"; *Chem. Rev.* 1999, *99*, 1665.
7. Newkome, G. R.; He, E.; Moorefield, C. N. "Suprasupermolecules with Novel Properties: Metallodendrimers"; *Chem. Rev.* 1999, *99*, 1689.
8. Majoral, J. N.; Caminade, A.-M. "Dendrimers Containing Heteroatoms", *Chem. Rev.* 1999, *99*, 845.

9. Bunzli, J. C. G; Piguet, C. "Lanthanide-Containing Molecular and Supramolecular Polymetallic Functional Assemblies", *Chem. Rev*. 2002, *102*, 1897.
10. Kuriki, K.; Koike, Y. "Plastic Optical Fiber Lasers and Amplifiers Containing Lanthanide Complexes", *Chem. Rev*. 2002, *102*, 2347.
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18MCH104K

ELECTROORGANIC SYNTHESIS

Programme Outcomes:

1. To understand the basic concepts of electro organic chemistry.
2. To study the concept of electrochemical oxidation and reduction of organic compounds
3. To understand the concept of aromatic substitution
4. To study separation techniques in organic chemistry
5. To study the application of spectral techniques in identifying organic compounds

Unit I: Basic concepts of electroorganic chemistry

The contents of an electrolytic cell, electrode materials, anodes, cathodes.Electrolytic media- aqueous and non-aqueous media, Reference electrodes, salt bridges, Liquid-Junction potentials.Application of reference electrodes, diaphragms, permeable membranes and semi- permeable membranes.Designing of simple special cells.

Unit II: Electrochemical oxidation of some organic compounds

Oxidation of phenols, alcohols and glycols. Kolbe reaction, oxidation of carbonyl compounds - aldehydes, ketones, esters and lactones.

Unit III: Electrochemical reduction of some organic compounds

Carbon-Carbon bond formation reactions- acid and base catalyzed condensations. Carbon heteroatom bond formation reactions-Pericyclic reactions

Unit IV: Aromatic substitution reactions

Concepts of aromaticity, electrophilic substitution of aromatic compounds (like chlorination, bromination and sulphonation). Substituent effects on aromatic electrophilic substitution.

Unit V: Separation and characterization techniques

Chromatographic techniques. TLC, column chromatography, paper chromatography, high performance liquid chromatography (HPLC)-principle, methods and applications of ^{1}H-NMR, ^{13}C NMR, FT-IR and UV spectra.

References

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18MCH104L

PRINCIPLES AND APPICATIONS OF COORDINATION COMPLEXES

Programme Outcomes:

1. To study the methods of preparation of coordination complexes
2. To study the concept of characterization of coordination complexes.
3. To know about the theories of coordination chemistry
4. To study the application of spectral techniques in studying coordination complexes
5. To study the application of coordination complexes.

Unit I: Preparation and characterization of complexes

Methods of preparation of coordination compounds –Detection of complex formation – colorimetric methods- Job's method- stability constants of complexes - Conductance and magnetic measurements of complexes – electrochemical studies of coordination complexes

Unit II : Bonding in coordination compounds

Theories of coordination compounds- Crystal field theory, MOT and LFT- donor and acceptor ligands –Structure and bonding in metal carbonyls, nitrosyls and cyanides - Organo metallic compounds - Allene, alkyne and allyl complexes

Unit III: Applications of spectral methods

Electronic spectra –selection rules – electronic spectra of complexes in cubic and square N, fields-charge transfer spectra -IR spectra - NMR spectra ^{15}N ^{19}F and ^{31}P- ESR spectra hyperfine splitting – zero field splitting - Spectra of Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes - Mossbaur spectroscopy – basic principles and applications

Unit IV: Homogeneous catalytic reactions by complexes

Wilkinson's catalyst - Ziegler-Natta polymerization – Fischer-Tropsch process – oxidation of alknes - metathesis

Unit V: Bioinorganic chemistry

Oxygen carriers and oxygen transport proteins-Hemoglobin and myoglobin - Cytochromes and peroxidases -Vitamin B12. Medicinal applications of coordination complexes – detoxification by chelation therapy

References:

1. Drago R.S., *Physical methods in inorganic chemistry*, London, Saunders Golden Sunburst Series, W.B.Saunders Company, 1977.

2. Huheey JE., 1972, *Inorganic chemistry Principle structure and reactivity*, 2nd Ed., New York, Harper & Row publishers,1977.
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18MCH104M

PHYSICAL METHODS IN COORDINATION CHEMISTRY

Programme Outcomes:

1. To study the techniques of preparing coordination compounds
2. To understand the concepts of analyzing coordination compounds
3. To understand the theories of coordination chemistry
4. To study the spectral characterization techniques in coordination compounds
5. To study the kinetics and applications of coordination compounds.

Unit I:

Methods of preparation of coordination compounds - Analysis and determination of molecular formula - Volumetric, gravimetric and colorimetric methods - Conductance and magnetic measurements of complexes

Unit II:

Theories of coordination - CF, MO, LF Theories - Merits and demerits - Macrocycles and their classifications - Synthesis of Macrocycles - Properties and applications

Unit III:

Special application to the study of coordination compounds - Electronic spectra - IR spectra - NMR spectra - ESR spectra - Mossbauer spectra – PES

Unit IV:

Kinetics and reaction mechanism in coordination compounds - SN1, SN2, SN1CB mechanisms - Trans effect - Electron transfer and electron exchange reactions - Catalysis by organometallic compounds

Unit V:

Transition metal ions in biology - Iron enzymes - structure and their functions - Model system for molecular activation and corresponding biochemical system.

References

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2. Huheey JE., *Inorganic chemistry: Principle, structure and reactivity*, 2nd Ed., New York, Harper & Row publishers, 1972.
3. Drago RS., *Physical methods in inorganic chemistry*, London, Saunders Golden Sunburst Series, W.B.Saunders Company,1977.
4. Cotton FA and Wilkinson G., *Advanced inorganic chemistry,* 3rd Ed., London, John Wiley & Sons. 1988.

18MCH104N

SURFACE CHEMISTRY

Programme Outcomes:

1. To understand the concept of adsorption on diffeternt surfaces
2. To study about the concept of surface phenomena
3. To study about emulsion and their applications
4. To study the nature and properties of interfaces between gases, liquids and solids
5. To understand the basic concepts of thermodynamics and its application in surface phenomena

Unit-I: Adsorption and surface phenomenon

Physisorption and chemisorption , adsorption isotherms, Langmuir and B. E. T. equation and significance in surface area determination, surface films, states of insoluble films, L. B. films and their application, adsorption from solution, adsorption types, surface excess concentration , Gibb's adsorption equation : derivation , significance and experimental verification , catalytic activity of surfaces.

Unit-II: Emulsion

Types of emulsion, theories of emulsion and emulsion stability, identification of emulsion types, inversion emulsion, microemulsion : theory and application.

Unit-III: Liquid gas and liquid interfaces

Surface tension, capillary action, methods of determination of surface tension, surface tension across curved surfaces, vapor pressure of droplet (Kelvin equation) , surface spreading , spreading coefficient, cohesion and adhesion energy, contact angle, constant angle hysteresis, wetting and detergency.

Unit-IV: Solid - Solid interfaces and Chemical Kinetics

Surface energy of solids, adhesion and adsorption, sintering mechanism, Tammann temperature and its importance, surface structure and surface composition.Experimental methods of following kinetics of a reaction, chemical and physical (measurement of pressure, volume, EMF, conductance, diffusion current and absorbance) methods and examples. Order and methods of determination (Initial rate, Integration, graphical and half life methods), rate determining step, steady state approximation.

Unit-V: Thermodynamics

Thermodynamic scale of temperature – Entropy as a state function – Entropy as a function of P, V and T - Entropy change in phase change – Entropy of mixing – Entropy as a criterion of spontaneous and equilibrium processes in isolated systems – Gibbs function(G) – Hemholtz function(A) as thermodynamic quantities - Equilibrium constant and free energy change - Thermodynamic interpretation of Le Chatelier principle (concentration, Temperature, Pressure) - addition on inert gases – Reaction isotherm – Van't Hoff equation.

References:

1. A. W. Adamson, *Physical chemistry of surfaces*,Wiley-Interscience; 6th Ed., 1997.
2. Alfred Clark, *Theory of adsorption and catalysis*, Academic Press, 1970.
3. B. M. W. Trapnell and H.O. Hayward, *Chemisorption*, Interscience Publishers, New York, 1963.
4. D. J. Shaw, *Introduction to colloid and surface chemistry*, 4th Ed., D. J. Shaw. Butter- worth/Heinemann, Oxford, 1992.
5. A. J. K , *Theories of chemical reaction rates,* McGrew Hill, New York,1969 .
6. J.J. Bikermann, *Surface chemistry*, 2nd Ed., Academic Press, New York, 1958.
7. Samuel H. Maron and Carl F. Prutton, *Principles of Physical Chemistry*, Hardcover Publisher,6th Ed., 1965 .
8. G. M. Barrow, *Physical Chemistry* , Tata-McGraw Hill, 5th Ed., 2003.

18MCH104O

HETEROCYCLIC COMPOUNDS

Programme Outcomes:

1. To know about heteroatom and Aromaticity of heterocycles
2. To study the Synthesis of heterocycles
3. To understand the Properties of heterocycles
4. To study the applications of Heterocycles in medicine
5. To study the uses of penicillins and sulpha drugs in medicine

Unit 1: Introduction

Definition of heteroatom – examples of heterocycles and their structures (alkaloids, purine and pyrimidine bases) — Nomenclature of four, five and six membered nitrogen heterocylces – Aromaticity of heterocycles

Unit 2: Synthesis of heterocycles

Paal-Knor Synthesis of pyrrole, furan and thiophene – Fischer indole synthesis – Hantzsch pyridine synthesis – Skraup quinoline synthesis – Pomeranz-Fritsch isoquinoline synthesis – Hofmann-Loffler-Freytag pyrrolidine synthesis – Von Richter Cinnoline synthesis

Unit 3: Properties of heterocycles I

Physical properties and structures of 5-membered heterocycles (pyrrole, furan, thiophene and indole), 6-membered heterocycles (pyridine, quinoline and isoquinoline), diazins (pyrazine and Pyrimidine), azines (oxazine and azepine) – Acidity and basicity of heterocycles (pyrrole, furan, thiophene, pyridine, indole, piperidine and pyrrolidine)

Unit 4: Properties of heterocycles-2

Oxidation and reductions in heterocyclic chemistry - Electrophilic and nucleophilic substitutions in pyrrole, thiophene, furan, pyridine, quinoline and isoquinoline

Unit 5: Heterocycles in medicine

Structure - synthesis - medicinal uses of chromone, flavanones, flavones, flavonols, isoflavones, anthocyanins, purines, pyrimidines, uric acid, penicillins and sulpha drugs

References:

1. Final I L, *Organic Chemistry* Volume I and II, 6th Ed., ELBS with Longmann, Singapore, 1997.

2. Clayden, Greaver,Warren and Wothers, *Organic Chemistry,* Oxford UniversityPress,New York, 2006.
3. Bansal and Raj K, Heterocyclic Chemistry, 5th Ed., New Age International Publishers, New Delhi, 2010.