Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur

SYLLABUS for M. Sc. CHEMISTRY

Choice Based Credit System (Semester Pattern)

With effect from 2023-24 as per NEP 2020

Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur

SYLLABUS for M. Sc. CHEMISTRY

As per National Education Policy (NEP)-2020

With effect from 2023-24

Pre-requisites to enrol for the M. Sc. Chemistry Programme:

The student who has completed the three-year B. Sc. course with Chemistry (or allied subject) as the major subject with not less than 50% of aggregate marks (45% in case of student from reserved category) or equivalent CGPA from any of the recognised university is eligible to enrol for M. Sc. (Chemistry) course. However, the student who has completed four-year B. Sc. course [B. Sc. (Honours) as per NEP- 2020] with Chemistry (or allied subject) as the major subject with not less than 50% of aggregate marks (45% in case of student from reserved category) or equivalent CGPA from any of the recognised university is eligible to enrol directly in semester III of M. Sc. (Chemistry) course.

Credit distribution structure for two years Post Graduate Programme in Chemistry*

Year (2 Yr PG)	Level	Sem. (2 Yr)	Major		RM	OJT/FP	RP	Cum. Cr.	Degree
			Mandatory	Electives					
I	6.0	Sem. I	14 (2 theory + 2 practical)	4	4			22	PG Diploma (after 3 Yr Degree)
		Sem. II	14 (2 theory + 2 practical)	4		4		22	
Cum. Cr. For PG Diploma/ I year of PG			28	8	4	4	-	44	
Exit option: PG Diploma 44 credits after three-year degree									
II	6.5	Sem. III	14 (3 theory + 1 practical)	4			4	22	PG Degree After 3 Yr UG or PG degree after 4-Yrs UG
		Sem. IV	14 (3 theory)	4			6	22	
Cum. Cr. For II year of PG			26	8			10	44	
Cum. Cr. For 2 year of PG degree			54	16	4	4	10	88	

*Source: शासन निर्णय क्रमांक :एनईपी-२०२२/प्र.क्र.०९/विशि-३ शिक्षण विभाग दिनांक १६ मे ,२०२३

Scheme of teaching and examination for M. Sc. CHEMISTRY (CBCS) As per NEP 2020

Structure and Credit Distribution of PG Degree Program for Two years

Choice Based Credit System (Semester Pattern)

With Effect from 2023-2024

M. Sc. CHEMISTRY Semester I												
Course Category	Code	Theory / Practical	Teaching scheme (Hours / Week)			Credits	Examination Scheme					
			Theory	Practical	Total		Duration in hrs.	Max. Marks		Total Marks	Minimum Passing Marks	
								SEE	CIE		Theory	Practical
DSC	MCH1T01	Paper 1: Inorganic Chemistry	4	-	4	4	3	80	20	100	40	-
DSC	MCH1T02	Paper 2: Physical Chemistry	4	-	4	4	3	80	20	100	40	-
DSE	MCH1T03	Paper 3: Electives (Choose any one) (a) Bioinorganic Chemistry (b) Biomolecules (c) Foundations of Thermodynamics and Electrochemistry (d) Analytical Separation Techniques (e) Equivalent MOOC course	4	-	4	4	3	80	20	100	40	-
RM	MCH1T04	Paper 4: Research Methodology	4	-	4	4	3	80	20	100	40	-
DSC	MCH1P01	Practical 1: Inorganic Chemistry	-	6	6	3	3-8	50	50	100	-	50
DSC	MCH1P02	Practical 2: Physical Chemistry (Including Research Methodology)	-	6	6	3	3-8	50	50	100	-	50
		TOTAL	**16**	**12**	**28**	**22**	--	**420**	**180**	**600**	**160**	**100**

CIE = Continuous Internal Evaluation and SEE = Semester End Examination

M. Sc. CHEMISTRY Semester II												
Course Category	Code	Theory / Practical	Teaching scheme (Hours / Week)			Credits	Examination Scheme					
			Theory	Practical	Total		Duration in hrs.	Max. Marks		Total Marks	Minimum Passing Marks	
								SEE	CIE		Theory	Practical
DSC	MCH2T05	Paper 5: Organic Chemistry	4	-	4	4	3	80	20	100	40	-
DSC	MCH2T06	Paper 6: Analytical Chemistry	4	-	4	4	3	80	20	100	40	-
DSE	MCH2T07	Paper 7: Electives (Choose any one) (a) Solid state and organometallic chemistry (b) Organic Reaction Mechanism (c) Quantum, Statistical and Nuclear Chemistry (d) Instrumental Methods of Analysis (e) Equivalent MOOC course	4	-	4	4	3	80	20	100	40	-
OJT	MCH2P03	Practical 3: On Job Training/ Field Project	-	8	8	4	3-8	50	50	100	-	50
DSC	MCH2P04	Practical 4: Organic Chemistry	-	6	6	3	3-8	50	50	100	-	50
DSC	MCH2P05	Practical 5: Analytical Chemistry	-	6	6	3	3-8	50	50	100	-	50
		TOTAL	**12**	**20**	**32**	**22**	-	**390**	**210**	**600**	**120**	**150**

M. Sc. CHEMISTRY Semester III												
Course Category	Code	Theory / Practical	Teaching scheme (Hours / Week)			Credits	Examination Scheme					
			Theory	Practical	Total		Duration in hrs.	Max. Marks		Total Marks	Minimum Passing Marks	
								SEE	CIE		Theory	Practical
DSC	MCH3T08	Paper 8:Spectroscopy-I	4	-	4	4	3	80	20	100	40	-
DSC	MCH3T09	Paper 9: Advanced Organic Chemistry-I	4	-	4	4	3	80	20	100	40	-
DSC	MCH3T10	Paper 10: Advanced Inorganic Chemistry	4	-	4	4	3	80	20	100	40	-
DSE	MCH3T11	Paper 11: Elective (Choose any one) (a) Inorganic Chemistry Special I (b) Organic Chemistry Special I (c) Physical Chemistry Special I (d) Analytical Chemistry Special I (e) Equivalent MOOC course	4	-	4	4	3	80	20	100	40	-
DSE	MCH3P06	Practical 6: Based on Elective subject	-	4	4	2	3-8	50	50	100	-	50
RP	MCH3P07	Research Project (RP)	-	8	8	4	3-8	50	50	100	-	50
		TOTAL	**16**	**12**	**28**	**22**	-	**420**	**180**	**600**	**160**	**100**

M. Sc. CHEMISTRY Semester IV

Course Category	Code	Theory / Practical	Teaching scheme (Hours / Week)			Credits	Examination Scheme					
			Theory	Practical	Total		Duration in hrs.	Max. Marks		Total Marks	Minimum Passing Marks	
								SEE	CIE		Theory	Practical
DSC	MCH 4T12	Paper 12: Spectroscopy-II	4	-	4	4	3	80	20	100	40	-
DSC	MCH 4T13	Paper 13: Advanced Organic Chemistry-II	4	-	4	4	3	80	20	100	40	-
DSC	MCH 4T14	Paper 14: Advanced Physical Chemistry	4	-	4	4	3	80	20	100	40	-
DSE	MCH 4T15	Paper 15: Elective (Choose any one) (a) Inorganic Chemistry Special II (b) Organic Chemistry Special II (c) Physical Chemistry Special II (d) Analytical Chemistry Special II (e) Equivalent MOOC course	4	-	4	4	3	80	20	100	40	-
RP	MCH 4P08	Research Project (RP)	-	12	12	6		100	100	200	-	100
		TOTAL	**16**	**12**	**28**	**22**	**-**	**420**	**180**	**600**	**160**	**100**

Elective papers:

In addition to the mandatory papers, the student has to opt for ONE elective paper in each semester from the basket of elective papers mentioned in the following table.

Basket for Elective Courses (4 Credits each)

Semester	Course Category	Name of the course	Course Code
I	Elective	(a) Bioinorganic Chemistry (b) Biomolecules (c) Foundations of Thermodynamics and Electrochemistry (d) Analytical Separation Techniques (e) Equivalent MOOC course	MCH1T03 (Paper 3)
II	Elective	(a) Solid state and organometallic chemistry (b) Organic Reaction Mechanism (c) Quantum, Statistical and Nuclear Chemistry (d) Instrumental Methods of Analysis (e) Equivalent MOOC course	MCH2T07 (Paper 7)
III	Elective	(a) Inorganic Chemistry Special I (b) Organic Chemistry Special I (c) Physical Chemistry Special I (d) Analytical Chemistry Special I (e) Equivalent MOOC course	MCH3T11 (Paper 11)
IV	Elective	(a) Inorganic Chemistry Special II (b) Organic Chemistry Special II (c) Physical Chemistry Special II (d) Analytical Chemistry Special II (e) Equivalent MOOC course	MCH4T15 (Paper 15)

The students can opt either the elective paper taught in the college in offline mode or any other equivalent online course of at least 4 credits offered by MOOC or any other such platform. The equivalence of such courses will be decided by the college committee comprising of the faculty members of the department and chaired by the Head, Dept. of Chemistry in that College.

EVALUATION and DISTRIBUTION OF MARKS

(1) Continuous Internal Evaluation (CIE): Twenty (20) marks in theory based on overall participation (Such as, Attendance in theory and practical classes, seminar, assignment, quiz, participation in field tours, conferences, workshops, and the general behaviour in the department.)

(2) Semester End Examination (SEE)

Theory Paper: Maximum Marks: 80, Duration of Examination-Three Hours, The paper will be set so as to cover all units/sections of the syllabus as below:

Type of questions	Total Number of questions	No. of questions to be answered	Marks for Each Question	Total maximum marks
• Short answer questions • Long answer questions • Numerical questions • Analytical questions	4 + 1 = 5 one question from each unit (4) + one question on all the units (1)	5	16	80

(3) General Scheme for Distribution of Marks in Practical Examination in Chemistry

Time: 6-8 h (One day Examination) Marks:100

Exercise-1	15 Marks	- Evaluated jointly by Internal and External Examiner
Exercise-2	15 Marks	- Evaluated jointly by Internal and External Examiner
Record	10 Marks	- Evaluated by Internal
Viva-Voce	10 Marks	- Evaluated by External
SEE	**50 Marks**	
CIE	**50 Marks**	
Total	**100 marks**	

(4) General Scheme for Distribution of Marks in Project Examination in Chemistry

The project work will be evaluated by both external and internal examiners. The examiners will evaluate the project work considering the coverage of subject matter, presentation, literature etc.

Written Project work	-	Evaluated jointly by External and Internal
For Presentation	-	Evaluated jointly by External and Internal
ForViva-Voce	-	Evaluated by External Examiner
Internal Assessment	-	Evaluated by Internal Examiner

Sem-III: Total 100 Marks (50 CIE and 50 SEE)

Sem-IV: Total 200 marks (100 CIE and 100 SEE)

Teacher and research project supervisor:

The regular full-time subject teacher of the College / Approved Contractual teacher / Approved Adhoc faculty / Approved Contributory teacher /scientist of government or private research laboratory appointed by university as a contributory teacher and having M. Phil. or Ph. D. degree in Chemistry can supervise the research project of the student.

SEMESTER I

Paper 1

MCH1T01: Inorganic Chemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course students would be able to

1. *predict the nature of bond and its properties through various electronic structural methods; bonding models*
2. *design new coordination compounds based on a fundamental understanding of their electronic properties*
3. *develop the possible catalytic pathways leading to desired products*
4. *apply the principles of transition metal coordination complexes to derive reaction mechanisms.*

Unit I

Electronic spectra and MO theory of Transition Metal complexes

Determining the Energy terms, Spin-orbit (L-S) coupling scheme, Hund's rule, Hole formalism, Determination of the term symbol (ground and excited states) for d^1 to d^9 configurations, Electronic spectra of transition metal complexes, Laporte 'orbital' selection rule, spin selection rule. Orgel diagrams for octahedral metal complexes. Charge transfer spectra, Racah parameters, calculations of 10Dq, B, β parameters. Tanabe- Sugano Diagrams of octahedral complexes with d^2 and d^8 configuration. M.O. Theory for octahedral, tetrahedral and square planar complexes with and without π-bonding.

Unit II

A) Boron hydrides: Classification, nomenclature, structure, bonding and topology of boranes, 4-digit coding (s, t, y, x) numbers for higher boranes and their utilities. Chemistry of diboranes: Study of Carboranes and Metallocarboranes with reference to preparations and structures.

B) Metal-Metal bonds: Occurrence of metal-metal bond, Classification of metal clusters, Binuclear, trinuclear, tetranuclear, pentanuclear and hexanuclear with reference to halide, oxide, alkoxide and acetate clusters.

Unit III

A) Metal – Ligand Equilibria in Solution: Stepwise and overall formation constants; trends in stepwise formation constants; factors affecting stability of metal complexes with reference to nature of metal ion, ligand, chelate effect and thermodynamic origin. Determination of formation constant by:

(1) spectrophotometric method (Job's and Mole ratio method)

(2) Potentiometric method (Irving-Rossotti Method)

B) Reaction Mechanism of Transition metal complexes-I: Energy Profile of a reaction, reactivity of metal complexes, Inert and Labile complexes, Kinetics of Octahedral substitution: Acid hydrolysis, factors affecting acid hydrolysis, Stereochemistry of intermediates in S_N1 and S_N2, Base

hydrolysis, Conjugate base mechanism, Direct and indirect evidences in favour of conjugate mechanism, Annation reaction, reaction without metal-ligand bond breaking.

Unit IV

A) Metal carbonyls: EAN concept and 18-electron rule for metal carbonyls, Structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls. Metal carbonyl clusters with reference to classification, synthesis and structures.

B) Metal nitrosyls: Nitrosylating agents for synthesis of metal nitrosyls, vibrational spectra and X-ray diffraction studies of transition metal nitrosyls for bonding and structure elucidation, important reactions of transition metal nitrosyls, structure and bonding. Dinitrogen and dioxygen complexes.

References

1. S. F. A. Kettle, J. N. Murral and S. T. Teddler: Valency Theory
2. C. A. Coulson: Valency
3. J. E. Huheey: Inorganic Chemistry
4. F.A. Cotton and G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5thand 6th Editions.
5. A. F. Willims: Theoretical Approach in inorganic chemistry.
6. A. Mannas Chanda: Atomic Structure and chemical Bonding
7. L. E. Orgel: An Introduction To transition metal chemistry, Ligand field theory, 2nd Edition.
8. J. J. Logowski: Modern Inorganic Chemistry
9. B.Durrant and P.J.Durrant: Advanced Inorganic Chemistry
10. J. C. Bailar: Chemistry of coordination compounds.
11. W. L. Jolly: Modern Inorganic Chemistry
12. R. S. Drago: Physical methods in inorganic chemistry.
13. Waddington: Nonaqueous solvents.
14. Sisler: Chemistry of nonaqueous solvents.
15. A. K. Barnard: Therotical Inorganic Chemistry
16. Emeleus and Sharpe: Modern Aspect of Inorganic Chemistry.
17. F. A. Cotton: Chemical Applications of Group theory.
18. Jones: Elementary Coordination chemistry.
19. B. N. Figgis: Introduction to Ligand field.
20. S. F. A. Kettle: Coordination chemistry.
21. M.C.Day and J.Selbin: Theoretical Inorganic Chemistry.
22. J. Lewin and Wilkins: Modern Coordination Chemistry.
23. Gowarikar, Vishwanathan and Sheedar: Polymer science.
24. H. H. Jattey and M. Orchin: Symmetry in chemistry.
25. D. Schonaland: Molecular Symmetry in chemistry.
26. L. H. Hall: Group theory and Symmetry in chemistry
27. H. H. Jattey and M. Orchin: Symmetry in chemistry
28. R.L.Dutta and A.Symal: Elements of magneto chemistry
29. Inorganic Chemistry 4th Edition, P.Atkins, Oxford University Press.
30. Essential Trends in Inorganic Chemistry, D.M.P.Mingos, Oxford University Press.
31. Purcell and Kotz: Inorganic Chemistry, Cengage Publishers.
32. Puri, Sharma, Kalia: Principles of Inorganic Chemistry, Milestone Publishing.
33. Madan, Malik, Tuli, Selected topics in Inorganic Chemistry.
34. Agarwal and Kimtilal: Advanced Inorganic Chemistry, Pragati Prakashan.

SEMESTER I

Paper 2

MCH1T02: Physical Chemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Understand, analyze and exercise the principles of classical thermodynamics in various applications*
2. *Understand and execute the quantum mechanical problems and their applications*
3. *Understand the concept of adsorption and its application in surface chemistry*
4. *Analyze and understand the characterization techniques for polymer*
5. *Understand the principles of chemical kinetics and their applications in chemical dynamics*

UNIT I :CLASSICAL THEMODYNAMICS

A) Recapitulation of Laws of thermodynamics, Exact and inexact differentials, condition of exactness, Ptaff differential expression and equations, Applications of Ptaff differential equations to first and second law of thermodynamics, Carathéodory's principle and its equivalence to the Kelvin Plank and Clausius statement of the Second law of Thermodynamics, Homogeneous functions of degree 0 and 1, extensive and intensive properties, derivation of thermodynamic equations of state, Maxwell's relations .Third law of thermodynamics, Nernst Heat Theorem, unattainability of absolute zero, calculation of entropy based on third law of thermodynamics, residual entropy and its application, Numerical.

UNIT II :FORMULATION OF QUANTUM MECHANICS

A) Introduction of Quantum Mechanics, Wave Function, Acceptability of Wave Functions, Normalized and Orthogonal Wave Functions, Operators, Operator Algebra, Eigen Functions and Eigen Values of Quantum Mechanical Properties)e.g .Linear, Angular momentum, etc(., Hermitian Operators, Orbital and generalized Angular Momentum, Postulates of Quantum Mechanics, Problems on Operator algebra, Eigen Values and Average Values of quantities.

B) Application of Schrödinger Wave Equation to Simple Systems :Particle in a 3-Dimensional Box, Concept of degeneracy and breakdown in degeneracy, Rigid Rotor, Potential Well of Finite Depth)Tunneling Effect(, Simple Harmonic Oscillator, The Hydrogen Atom.

UNIT III :SURFACE CHEMISTRY AND MACROMOLECULES

A) Recapitulation of Surface tension, Adsorption :Freundlich adsorption isotherm, Langmuir theory, Gibbs adsorption isotherm, BET theory and estimation of surface area, enthalpy and entropy of adsorption .Surface film on liquids and catalytic activity, Electro-kinetic phenomena, Surface active agents, hydrophobic interactions, micellization, Critical Micelle Concentration)CMC(, mass action model and phase separation model of micelle formation, shape and structure of micelles, factors affecting CMC, micro-emulsion and reverse micelles.

B) Definition of macromolecule (Polymer), types of polymers, Number average and mass average molecular mass, molecular mass determination by Osmometery, Viscometry, Ultracentrifugation, light scattering and size-exclusion chromatography method, Numericals.

UNIT IV :CHEMICAL KINETICS

A(Temperature dependence of chemical reaction rates, Arrhenius equation, Energy of activation, pre-exponential factor and its limitations, Collision theory and its limitations, steric factors, Transition State theory of gas and liquid phase bimolecular reactions, comparison of three theories of reaction rates.

B(Bodeinstein steady state approximation and its application in consecutive reactions, Dynamics of unimolecular reactions :Lindeman-Hinshelwood mechanism, RRKM theory, Thermodynamic formulation of transition state theory, Enthalpy, Gibbs free energy and enthalpy of activation.

References

1. R .P .Rastogi and R .R .Mishra, An Introduction to Chemical Thermodynamics, Vikas Publication, Gorakhpur, 2010.
2. P .W . Atkins and D .Paula, Physical Chemistry, 8th Edition, Oxford University Press, 2010.
3. E .N . Yenemin, Fundamentals of Chemical Thermodynamics, MIR, Publications.
4. G .K .Vemulapalli, Physical Chemistry, Prentice –Hall of India, 1997.
5. S . Glasstone and De Van No Strand, Thermodynamics for Chemists, 1965.
6. S .M .Blinder, Advanced Physical Chemistry,
7. D .Mcquarie and J .Simon, Physical Chemistry –A Molecular Approach, University Press, 2000
8. Ira N .Levine, Quantum Chemistry, 5th edition)2000(, Pearson educ., Inc.New Delhi
9. A.K.Chandra, Introductory Quantum Chemistry, 4th edition)1994(, Tata Mcgraw Hill, New Delhi.
10. M.W.Hanna, "Quantum Mechanics in Chemistry", Benjamin
11. L .Pualing and E .B .Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York)1935.(
12. R .K .Prasad, Quantum Chemistry, New Age International, Delhi .
13. R .K .Prasad, Quantum Chemistry through problems and solutions, New Age International, New Delhi, 2009.
14. B .C .Reed, Quantum Mechanics, Jones and Bartlett, New Delhi, 2010.
15. G .M .Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.
16. H .K .Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
17. G. M. Panchenkov and V.P. Labadev, "Chemical Kinetics and catalysis", MIR Publishing
18. E.A .Moelwyn -Hughes, "Chemical Kinetics and Kinetics of Solutions", Academic
19. K. J .Laidler, Chemical Kinetics, Third Edition)1987(, Harper and Row, New York.
20. J. Raja Ram and J.C.Kuriacose, Kinetics and Mechanism of Chemical Transformations MacMilllan Indian Ltd., New Delhi)1993(

21. C .H .Bamford and C .F .H .Tipper, Comprehensive Chemical Kinetics, **Vol 1**., Elsevier Publications, New York, 1969.
22. C .H .Bamford and C .F .H .Tipper, Comprehensive Chemical Kinetics, **Vol 2**., Elsevier Publications, New York, 1969.
23. S .Glasstone, K .J .Laidler and H .Eyring, The Theory of Rate Processes, Mc-Graw Hill, New York, 1941.
24. A .Findley, The Phase Rule and its Applications, Longmans Green and Co., Mumbai.
25. K .S .Birdi, Surface Chemistry Essentials, CRC Press, New York, 2014.
26. Eric KeightleyRideal, An Introduction to Surface Chemistry, Cambridge University Press, 1926.
27. D .M .Ruthven, Principles of Adsorption and Adsorption Processes, John Wiley and Sons, NewYork, 1984.
28. A .W .Adamson, A .P .Gasi, Physical Chemistry of Surfaces, Wiley, 2007.
29. P .C .Hiemenz and R .Rajagopalan, Principles of Colloid and Surface Chemistry, CRC Taylor and Fransis, 2007.
30. P .D .Hede and S .P .Beier, Inorganic and Applied Chemistry, e-Book, 2007.
31. Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
32. E.M .Mc Cash, Surface Chemistry, Oxford University Press, Oxford)2001.(
33. G .K .Agrawal, Basic Chemical Kinetics, Tata-Mc-Graw Hill, 1990.
34. N .B .Singh, N .S .Gajbhiye, S .S .Das, Comprehensive Physical Chemistry, New Age International, 2014.
35. K .L .Kapoor, Text Book of Physical Chemistry, Vol –I to Vol-VI, 2011.
36. Spectroscopic identification of organic compound-RM Silverstein,GCBassler and TC Morril, John Wally
37. Application of Spectroscopy to Organic Compound-J .R .Dyer, Printice Hall
38. Organic Spectroscopy-William Kemp, ELBS with McMillan
39. Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
40. Organic Spectroscopy-RT Morrison and RN Boyd
41. Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
42. Fundamentals of Molecular Spectroscopy-CN Banwell

NPTEL sources weblinks

For Quantum Chemistry Introduction:

- https://archive.nptel.ac.in/courses/104/108/104108057/
- https://onlinecourses.nptel.ac.in/noc20_cy27/preview
- https://nptel.ac.in/courses/104106083
- https://nptel.ac.in/courses/104108057
- https://www.digimat.in/nptel/courses/video/104108057/L11.html

For Chemical Kinetics

- https://archive.nptel.ac.in/courses/104/101/104101128/
- https://www.youtube.com/watch?v=uep2XeLCGkc

SEMESTER I

Paper 3 (Elective)

MCH1T03: (a) Bioinorganic Chemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student would be able to

1. *apply the principles of transition metal coordination complexes in understanding functions of biological systems*
2. *identify the medicinal applications of inorganic compounds*
3. *understand mechanism of energy transfer processes in biological systems*
4. *develop the possible enzymatic pathways in biosystems*
5. *explain oxygen transport mechanisms in biosystems*

Unit I

A) Essential and trace metals in biological systems: Biological functions of inorganic elements, biological ligands for metal ions. Coordination by proteins, Tetrapyrrole ligands and other macrocycle. Influence of excess and deficiency of V, Cr, Mn, Fe, Co, Cu and Zn. Genetic defects in the absorption of trace elements. Regulation and storage of trace elements. Role of minerals. Toxic effects of metals.

B) Metal storage, transport and biomineralization with respect to Ferritin, Transferrin and Siderophores, Na+ /K+ pump. Role of Ca in transport and regulation in living cells.

C) Medicinal use of metal complexes as antibacterial, anticancer, use of cis-platin as antitumor drug, antibiotics and related compounds. Metal used for diagnosis and chemotherapy with particular reference to anti-cancer drugs.

Unit II

A) Bio-energetics and ATP cycle: DNA polymerization, metal complexes in transmission of energy, chlorophylls, photosystem I and photosystem II in cleavage of water, Model systems.

B) Electron transfer in Biology: Structure and functions of metalloproteins in electron transfer proteins, cytochromes and Fe-S proteins, Non-heme iron proteins; Rubredoxins, Synthetic models. Biological Nitrogen fixation (in vitro and in vivo)

Unit III

Transport and Storage of Dioxygen: Heme proteins and oxygen uptake, structure and functions of haemoglobin, myoglobin, hemocyanins and hemerythrin. Perutz mechanism showing structural changes in porphyrin ring system. Oxygenation and deoxygenation. Model compounds. Cyanide poisoning and treatment. Vanadium storage and transport.

Unit IV

Metallo-enzymes: Apoenzymes, Haloenzyme and Coenzyme. The principle involved and role of various metals in i) Zn-enzyme: Carboxyl peptidase and Carbonic anhydrase. ii) Fe-enzyme: Catalase Peroxidase and Cytochrome P-450 iii) Cu-enzyme: Super Oxide dismutase iv) Molybdenum: Oxatransferase enzymes, Xanthine oxidase, Co-enzyme Vit.B_{12}, Structure of vitamin B_{12}, Co-C bond

cleavage, Mutase activity of coenzyme B-12, Alkylation reactions of Methyl Cobalamin. Synthetic model of enzyme action, stability and ageing of enzyme.

References

1) Akhmetov, N.: General and Inorganic Chemistry
2) Aylett, B. and Smith, B.: Problems in Inorganic Chemistry, (English University Press)
3) Bertini, et al: Bioinorganic Chemistry
4) Charlot, G and Bezier, D.: Quantitative Inorganic Analysis (John Wiley).
5) Douglas, B. E. McDanirl, D. H. et al: Concept and Models of Inorganic Chemistry (4th edt.) J. Wiley
6) Dutt P. K.: General and Inorganic Chemistry.(Sarat Books House)
7) Fenton, David E.: Biocoordination chemistry, Oxford
8) Jolly, W. L. Inorganic Chemistry (4th edn) Addison-Wesley
9) Katakis, D. and Gordon, G.: Mechanism of Inorganic Reactions (J.Wiley)

SEMESTER I

Paper 3 (Elective)

MCH1T03: (b) Biomolecules

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Draw the structures of essential biomolecules*
2. *Understand the role of biomolecules in various life processes*
3. *Understand the way how drug can be administrated, absorbed, distributed and metabolized*
4. *Understand the relation of drug with different types of receptors, chemical messengers, binding site and DNA.*

Unit I:

Carbohydrate: Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, methyl ethers and acid derivatives of sugars, configurations of aldoses and ketoses, general methods of structure and ring size determination with reference to maltose, lactose, sucrose, Structural features and applications of inositol, starch, cellulose, chitin and heparin

Unit II:

Amino acids, protein and peptides: Amino acids, structural characteristics, acid base property, stereochemistry of amino acids, optical resolution, Stecker synthesis, peptide and proteins structure of peptide and protein, primary, secondary, tertiary and quaternary structure. Reaction of polypeptide, structure determination of polypeptide, end group analysis, strategy of peptide bond synthesis: *N*-Protection and *C*-Activation, Solid phase peptide synthesis

Unit III:

Nucleic Acids: Primary, secondary and tertiary structure of DNA; DNA replication and heredity; Structure and function of mRNA, tRNA and rRNA. Purines and pyrimidine bases of nucleic acids and their preparation, Biosynthesis of DNA and RNA, Polymerase Chain Reaction (PCR) and RTPCR

Lipids: Fatty acids, essential fatty acids, structures and functions of triglycerols, glycerophospholipids, spingolipids, lipoproteins, composition and function, role in atherosclerosis Properties of lipid aggregates, micells, bilayers, liposomes and their biological functions, biological membranes, fluid mosaic model of membrane structure, Lipid metabolism, β-Oxidation of fatty acids

Unit IV: Enzyme chemistry

A) **Enzymes:** Introduction, chemical and biological catalysis, remarkable properties of enzymes likecatalytic power, specificity and regulation. Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Nomenclature and classification, Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Baker's yeast catalysed reactions

B) **Mechanism of Enzyme Action:** Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A

C) Vitamins and Co-Enzyme Chemistry: Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, biotin as CO_2 carrier. Mechanisms of reactions catalyzed by the above cofactors

References

1) Bioorganic Chemistry :A Chemical Approach to Enzyme Action, Hermann Dugas and C .Penny, Springer-Verlag
2) Understanding Enzymes, Trevor Palmer, Prentice Hall
3) Enzyme Chemistry :Impact and Applications, Ed .Collin J .Suckling, Chapman and Hall
4) Enzyme Structure and Mechanism, A .Fersht, W .H .Freeman
5) Introduction to Medicinal Chemistry, A .Gringuage, Wiley-VCH
6) Wilson and Gisvold's Text Book of Organic Medical and Pharmaceutical Chemistry, Ed Robert F .Dorge
7) Strategies for Organic Drug Synthesis and Design, D .Lednicer, John Wiley

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Weblink to Equivalent MOOC on NPTEL/SWAYAM if relevant:

- Essentials of Biomolecules: Nucleic Acids and Peptides https://nptel.ac.in/courses/104/103/104103121/
- Biocatalysis in Organic Synthesis https://archive.nptel.ac.in/courses/104/105/104105032/
- Biochemistry https://archive.nptel.ac.in/courses/104/105/102105034/
- Organic Chemistry in Biology and Drug Development https://archive.nptel.ac.in/courses/104/105/104105120/

SEMESTER I

Paper 3 (Elective)

MCH1T03: (c) Foundations of Thermodynamics and Electrochemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Understand, the mathematical concepts used in chemistry*
2. *Understand the principle involved in fundamental physical chemistry*
3. *Understand the concept of ideal and non-ideal solutions*
4. *Understand the theories of electrolytes*

Unit-I: Mathematical concepts

Equation of a straight line and calculation of slope and intercepts, Differentiation, Derivative function, various differential formulas, Chain rule, finding minima and maxima, partial differentiation. Integration, methods of integration, integration by parts, integration formulas, permutation combination fundamentals, Vectors, Matrices, Determinants, Complex numbers, series expansions, Stirling approximation, Practice numerical based on these concepts.

Unit II :Thermodynamics and Phase Equilibria

Concept of fugacity, determination of fugacity, The Le-Chatelier's Principle and its quantitative treatment. Ideal solutions and Roult's law, non-ideal solutions (Henry's Law), Deviation from ideal behavior, Chemical potential in Non-ideal solutions, excess functions for non-ideal solutions, Partial molar quantities **:**Determination of partial molar quantities, chemical potential, partial molar volume, Gibbs- Duhem equation, Gibbs Duhem Mergules equation Entropy of mixing, Enthalpy of mixing, Fractional Distillation, Distillation of Azeotropic Mixtures.

Unit-III: The Phase Rule

Recapitulation of Gibbs Phase rule (Without Derivation), degrees of freedom, reduced phase rule, construction of phase diagram, one component systems **)**Water, Sulphur, carbon**(**, 1st and 2nd order phase transition, lambda line, Helium,system, Eutectic systems, two component systems forming solid solutions having congruent and incongruent melting point, Construction of a phase diagram, partially miscible solid phase, three component systems, graphical presentation, related Numerical

Unit-IV: Electrochemistry - I

Electrolytic conductance (Specific, Equivalent and molar), Variation of Eq./molar conductance with dilution, Transport number and its determination using Hittorf's method and Moving boundary method, Kohlrausch's law, calculation of molar ionic conductance, conductometric titrations, High frequency titrations, Ostwald dilution law, Determination of ionic mobility, numerical. Principle of potentiometry, Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode and glass electrode. Reference electrodes: Calomel electrode and Ag/AgCl electrode. potentiometric titrations, Nernst equation, standard electrode potential, Determination of cell potential, n, Kf and Ksp. pH titrations.

References

1. R .P .Rastogi and R .R .Mishra, An Introduction to Chemical Thermodynamics, Vikas Publication, Gorakhpur, 2010.
2. P .W .Atkins and D .Paula, Physical Chemistry, 8th Edition, Oxford University Press, 2010.
3. E .N .Yenemin, Fundamentals of Chemical Thermodynamics, MIR, Publications.
4. G .K .Vemulapalli, Physical Chemistry, Prentice –Hall of India, 1997.
5. S .GlasstoneandDe Van No Strand, Thermodynamics for Chemists, 1965.
6. S .M .Blinder, Advanced Physical Chemistry,
7. D .Mcquarie and J .Simon, Physical Chemistry –A Molecular Approach, University Press, 2000
8. Ira N .Levine, Quantum Chemistry, 5th edition)2000(, Pearson educ., Inc.New Delhi
9. G .M .Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.

A. Findley, The Phase Rule and its Applications, Longmans Green and Co., Mumbai.

10. N .B .Singh, N .S .Gajbhiye, S .S .Das, Comprehensive Physical Chemistry, New Age International, 2014.
11. K .L .Kapoor, Text Book of Physical Chemistry, Vol –I to Vol-VI, 2011.
12. Spectroscopic identification of organic compound-RM Silverstein, GCBassler and TC Morril, John Wally
13. Application of Spectroscopy to Organic Compound-J .R .Dyer, Printice Hall

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NPTEL sources Weblinks

For Classical Thermodynamics:

- https://archive.nptel.ac.in/courses/104/103/104103112/
- https://digimat.in/nptel/courses/video/104106094/L18.html

For Phase rule:

- https://www.youtube.com/watch?v=2LywAiZBQW4
- https://archive.nptel.ac.in/courses/113/104/113104068/
- https://archive.nptel.ac.in/courses/104/103/104103112/

For electrochemistry

- https://onlinecourses.nptel.ac.in/noc23_cy19/preview
- https://www.youtube.com/watch?v=XTt3gXB0a84

SEMESTER I

Paper 3 (Elective)

MCH1T03: (d) Analytical Separation Techniques

60 h (4 h per week): 15 h per unit *100 Marks*

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

1. *Understand various separation technique based on sample and target analyte*
2. *Elaborate the working principles of various separation techniques.*
3. *Apply logic behind working and applicability of each technique.*
4. *Identify most suitable separation tool resolution of mixtures.*
5. *Develop separation methods for multicomponent analysis.*
6. *Evaluate efficiency of separation of mixture based on analysis parameters.*

Unit I: Column, paper and thin layer chromatography

Definition and general classification of chromatographic techniques**.** Normal and reverse phase chromatography. Terminology used in separation techniques.

Column chromatography: Basic principle, technique and applications in qualitative and quantitative analysis. Properties of good column adsorbents.

Paper chromatography: Basic principle, techniques and applications in qualitative and quantitative analysis. Calculations involving R_f values.

Paper electrophoresis: Principle and technique. Factors affecting migration of ions. Applications.

Thin layer chromatography: Principle and technique. Advantages over paper and column chromatography. Applications.

Unit II: Ion exchange and solvent extraction

Ion exchange: Principle and technique**.** Types of ion exchangers and their structures**.** Ion exchange equilibria and action of cation and anion exchange resins**.** Factors affecting ion exchange efficiency. Ion exchange capacity**.** Experimental determination of ion exchange capacities of cation and anion exchange resins. Effect of complexing ions**.** Zeolites as ion-exchangers**.** Applications of ion exchange.

Solvent extraction: Principle and techniques**.** Distribution ratio and distribution coefficient**.** Factors affecting extraction efficiency**:** Ion association complexes, chelation, synergistic extraction, pH**.** Numericals based on multiple extractions**.** Role of chelating ligands, crown ethers, calixarenes and cryptands in solvent extraction**.** Introduction to Solid phase extraction **(**SPE**)** and Microwave assisted extraction **(**MAE**)**, Applications**.**

Unit III: Gas Chromatography

Principle including concept of theoretical plates. Calculations involving number of theoretical plates and height equivalent of theoretical plates. Column resolution, retention factor and selectivity factor. van-Deemter equation. Factors affecting retention, peak resolution and peak broadening**.** Instrumental set up**-** carrier gas, sampling system, column and detector**.** Types of columns in GC: Packed and open tubular, their advantages and limitations**.** Detectors in GC analysis**.** Characteristics of ideal detectors.

Construction and working of thermal conductivity, flame ionization, electron capture and mass spectrometric detectors. Temperature programmed GC and its advantages**.**

Unit IV: Liquid Chromatography

HPLC**:** Principle of HPLC. Instrumentation including mobile phase injection system, sample injection system, column and detector. Types of columns and packing materials. Normal and reverse phase systems. Detectors in HPLC: Construction and working of UV detector, fluorescence detector, photodiode array detector**.** Principle and applications of size exclusion, gel permeation and ion retardation chromatography**.** Comparison of HPLC with GC

Supercritical fluid chromatography**:** Principle, advantages and applications.

References

1. Quantitative analysis**:** Day and Underwood **(**Prentice**-**Hall of India**)**
2. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3. Analytical Chemistry**:** Gary D**.** Christian **(**Wiley, India**).**
4. Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West
5. Instrumental Methods of Analysis**:** Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
6. Introduction to Instrumental analysis: Robert Braun (Tata McGraw-Hill)
7. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
8. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
9. Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
10. Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
11. Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
12. An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
13. Instrumental Methods of Chemical Analysis: G. W. Ewing

Web link for related NPTEL courses

Analytical Chemistry: https://nptel.ac.in/courses/104105084

SEMESTER I

Paper 4

MCH1T04: Research Methodology

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *understand what research is and what is not.*
2. *raise awareness of crucial aspect of the nature of Knowledge and the value of scientific method.*
3. *Introduce the concept at the heart of every research project – the research problem - and to discuss what a researchable problem is.*
4. *evaluate literature, form a variety of sources, pertinent to the research objectives.*
5. *identify and justify the basic components of the research framework, relevant to the tackled research problem.*
6. *explain and justify how researchers will collect research data.*
7. *discuss how to cite sources, and justify this choice.*
8. *put forward a credible research proposal, and*
9. *warn the common mistakes in the field of research methodology.*

Unit – I: Foundations of Research

Meaning, Objectives, Motivation, Utility. Concept of theory, empiricism, deductive and inductive theory. Characteristics of scientific, method - Understanding the language of Research - Concept, Construct, Definition, Variable. Research Process. Problem Identification and Formulation - Research Question – Investigation, Question - Measurement Issues - Hypothesis - Qualities of a good Hypothesis Null Hypothesis and Alternative Hypothesis. Hypothesis Testing - Logic and Importance. Research Design: Concept and Importance in Research - Features of a good research design - Exploratory Research Design - concept, types and uses, Descriptive Research Designs - concept, types and uses. Experimental Design: Concept of Independent and Dependent variables. Qualitative and Quantitative Research: Qualitative research – Quantitative research - Concept of measurement, causality, generalization, replication. Merging the two approaches.

Unit – II: Statistical analysis for Chemists

Errors in chemical analysis. Classification of errors- systematic and random, additive and proportional, absolute and relative. Accuracy and precision. Mean, median, average deviation and standard deviation. Significant figures and rules to determine significant figures. Calculations involving significant figures. Confidence limit, correlation coefficient and regression analysis. Comparison of methods: F-test and T-test. Rejection of data based on Q-test. Least squares method for deriving calibration graph. Application of Microsoft Excel in statistical analysis (statistical functions and spreadsheets in MS-Excel). Validation of newly developed analytical method. Certified reference materials (CRMs). Numerical problems.

Unit – III:

A] Scientific Writing and Presentation

Scientific writing. Basics in Scientific grammar. Importance of abbreviations and acronyms. Types of scientific publications- magazines, journals, reviews, news-letters, structure of scientific paper. Various reference styles.

Report Writing, Significance of report writing, different steps in report writing, types of Journals and reports, layout of research paper.

Research Ethics (Issues relating to referencing and documentation, copyrights, plagiarism), Impact Factor, CiteScore, *h*-Index, i10-Index, Citation Index, references/bibliography, structuring the thesis, use of software in thesis writing.

B] Intellectual Property Rights (IPR)

Introduction to IPR (Patents, Trademarks, Geographical indicators, Copyright and neighbouring rights), Concept and theories, kinds of IPR, Economic analysis of IPR, Need for private rights versus public interests, Advantages and disadvantages of IPR.

Unit – IV: Use of tools / techniques for Research

Methods to search required information effectively, Reference Management Software like Zotero/Mendeley, Software for paper formatting like LaTeX, Beamer presentation, preparation of bibliography database, MS Word, MS Excel, Graph and chart preparation, MS Power Point, Microcal Origin, ChemSketch, ChemDraw, Other computational software like Guassian, Mathematica, Software for detection of Plagiarism.

References

1. Research Methodology- C. R. Kothari
2. Best and Kahn, Research Methodology, PHI Limited
3. Design of Experience: Statistical Principles of Research Design and Analysis, by Robert O. Kuehl Brooks/cole.
4. Patrick Carey, Katherine T. Pinard, Ann Shaffer, Mark Shellman, New Perspectives Microsoft Office 365 and Office 2019 Introductory, 2020.

SEMESTER I

Practical 1

MCH1P01: Inorganic Chemistry

6 h per week *100 Marks*

I. Preparation of Inorganic Complexes and their characterization by:

Elemental analysis and physico-chemical methods (Electronic and IR Spectra, magnetic susceptibility measurements, Thermal analysis and Molar conductance studies).

1. K_3 [Al $(C_2O_4)_3$]$(H_2O)_3$ 2. [VO (acac) $_2$] 3. Na [Cr $(NH_3)_2(SCN)_4$]

4. $K_3[Cr(SCN)_6]$. 5. [Mn (acac) $_3$] 6. K_3 [Fe $(C_2O_4)_3$]

7. Hg [Co (SCN) $_4$] 8. [Co (Py) $_2$ Cl_2] 9.$[Ni(NH_3)_6]Cl_2$ 10. [Ni (DMG) $_2$]

11. $[Cu_2 (CH_3COO)_4(H_2O)_2]$ 12. $[Cu(NH_3)_4(H_2O)_2]SO_4$

II. Quantitative Analysis:

Separation and determination of two metal ions from the following alloys involving:

Volumetric, Gravimetric and Spectrophotometric methods

i) Copper (II) and Nickel (II)

ii) Copper (II) and Zinc (II)

iii) Nickel (II)—Zinc (II) and

iv) Copper (II)—Iron (III)

III. Qualitative analysis of radicals:

Semimicro analysis of inorganic mixture containing four cations out of which two will be rare metal ions such as W, Mo,Se,Ti,Zr,Ce,Th,V and U.(Spot Test for individual cations shall be performed)

References

1. Practical Inorganic Chemistry - Pass
2. Practical Inorganic Chemistry - Marr and Rocket
3. Basic Concept Of Analytical Chemistry - Khopkar S. M.
4. Synthesis And Characterisation Of Inorganic Compounds – W. L. Jolly, Prentice Hall
5. Inorganic Experiments – J. Derck Woollins, Vch.
6. Practical Inorganic Chemistry – G. Marrand, B.W. Rockett, Van Nostrand
7. A Text Book Of Quantitative Inorganic Analysis – A.I. Vogel, Longoman.
8. Edta Titration – F. Laschka
9. Instrumental Methods Of Analysis – Willard, Merit And Dean (Cbs, Delhi)
10. Inorganic Synthesis – Jolly
11. Instrumental Methods Of Chemical Analysis – Yelri Lalikov
12. Fundamental Of Analytical Chemistry- Skoog D .A. And West D. M. Holt Rinehart And Winston Inc.
13. Experimental Inorganic Chemistry7 – W.G. Palmer, Cambridge

Practical 2

MCH1P02: Physical Chemistry including RM

6 h per week *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Understand the basic principle involved in physical chemistry.*
2. *Evaluate various physical parameters*
3. *Interprete the experimental results.*
4. *Calculation involved in inpreting results*

Understand the concept of Qualitative analysis

It is expected to perform minimum 14 experiments in a semester.

1. To study the variation of volume contraction with mole fraction of alcohol in alcohol -water system
2. To determine the activation parameters of viscous flow for a given liquid.
3. To Determine the critical micelle concentration)CMC (of a given surfactant /soap /shampoo by surface tension measurements .
4. Determination of molecular mass of a polymer by viscometry method.
5. To determine integral heat of KNO_3, at two different conc .and calculation of heat of dilution.
6. Effect of 1 %NaCl, 1 %succinic acid, 0.5 %naphthalene on CST in phenol-water systems.
7. Distribution of succinic acid in H_2O -benzene, H_2O-ether and comparison of distribution coefficient.
8. To construct the phase diagrams of two components system)phenol -urea, diphenyl aminebenzophenone; a-naphtyl amine-phenol (forming compounds with congruent melting points.
9. To study the mutual solubility of glycerol-m-toluidine and to determine congruent points.
10. To study kinetics of hydrolysis of an ester by NaOH reaction.
11. To determine equilibrium constant of the equation $KI+I_2=KI_3$ by distribution method.
12. To study the kinetics of the reaction between potassium persulphate and potassium iodide.
13. Determination of order of reaction of oxidation of ethyl alcohol by acid dichromate.
14. To titrate conductometrically monobasic and dibasic acids with NaOH and determine the strength of given acid.
15. To determine equivalent conductance of weak electrolyte at infinite dilution by kaulrausch's method.
16. Determination of heat of reaction, entropy change and equilibrium constant of the reaction between metallic zinc and Cu^{+2} ions in solution.
17. Determination of thermodynamic constants ΔG, ΔH, ΔS for $Zn^{+2}+H_2SO_4 \rightarrow ZnSO_4 +2H^+$ by emf measurement.
18. Titration of Ferrous Ammonium Sulphate against ceric sulphate and hence the formal redox potential of $Fe^{2+} \rightleftharpoons Fe^{3+}$ and $Ce^{3+} \rightleftharpoons Ce^{4+}$ systems .
19. To determine the pH of a buffer solutions using a quinhydrone electrode
20. RM-1: Statistical Analysis using MS Excel program (mean, average deviation, standard deviation, variance, F-test, t-test, chi-square test, correlation coefficient, slope, intercept, etc).
21. RM-2: Graph plotting through least square method and

22. RM-3: Molecular designing through Chemsketch and ChemDraw softwares in 2D and 3D formats (simple organic compounds and ions)
23. RM-4: Reference formatting using Mendeley and Zotero.
24. RM-5: Preparation and formulation of questionair for survey
25. RM-6: Sample collection methods

References

1. Vogel A **:** A Textbook Of Quantitative Inorganic Analysis, Longman
2. Das and Behra, Practical Physical Chemistry
3. Carl W. Garland, Joseph W. Nibler and David P. Shoemaker, Experiments in Physical Chemistry, Mc-Graw Hill, 8th Edition, 2009.
4. Farrington Daniels, Joseph Howard Mathews, John Warren Williams, Paul Bender, Robert A**.** Alberty, Experimental Physical Chemistry, Mc**-**Graw Hill, Fifth Edition, 1956**.**
5. John W**.** Shriver and Michael George, Experimental Physical Chemistry, Lab Manual and Data Analysis, The University of Alabama in Huntsville, Fall 2006
6. Day And Underwood **:**Quantitative Analysis
7. Merits And Thomas**:**Advanced Analytical Chemistry
8. Ewing, G**.** W**. :** Instrumental Methods of Chemical Analysis, Mcgraw**-**Hill
9. Drago, R**.**S**:**Physical Methoods In Inorganic Chemistry
10. Christain G**.**D**:**Analytical Chemistry
11. Khopkar S**.**M**.:**Basic Concept Of Analytical Chemistry
12. Koltath And Ligane**:**Polorography
13. Braun**:**Instrumental Methods Of Chemical Analysis
14. Willard, Merritt And Dean**:** Instrumental Methods Of Chemical Analysis ,Van Nostrand
15. Strouts,Crifi;Llan And Wisin**:** Analytiacl Chemistry
16. Skoog S**.**A**.** And West D**.** W**.:**Fundamental of Analytical Chemistry
17. Dilts R**.**V**.:** Analytiacl Chemistry
18. Jahgirdar D**.**V **:**Experiments In Chemistry
19. Chondhekar T**.**K**:** Systematic Experiments In Physical Chemistry, Rajbog S**.**W**.**, Aniali Pubn**.**
20. Wlehov G**.** J**:** Standard Methods Of Chemicalanalysis 6th Ed

SEMESTER II

Paper 5

MCH2T05: Organic Chemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Implement rules of aromaticity to organic molecules*
2. *Sketch organic molecules in different projection formula and assign its configuration.*
3. *Apply their understanding about the organic reactions of industrial significance with respect to the chemo- selectivity, regioselectivity and enantioselectivity.*
4. *Analyze the product distribution and the stereochemistry of various organic products.*
5. *Evaluate the relationship between structure and reactivity*

Unit I:

A) Nature and Bonding in Organic Molecule: Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyper-conjugation, Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π-molecules orbitals, annulenes, antiaromaticity, homoaromoaticity, Aromatic character and chemistry of cyclopentadienyl anion, tropylium cation, tropone and tropolone, Frost Circles (The Polygon Method) for drawing energy levels in cyclic pi systems**.**

B) Carbenes: Types of carbenes, Structure and reactivity of carbenes, Generation and reactions, insertion, addition, rearrangement reactions of carbenes, nucleophilic attack on carbenes, Simmons-Smith reaction, Reimer-Tiemann reaction, Carbylamine reaction, Shapiro reaction, Bamford-Stevens reaction and Wolff rearrangement

C) Nitrene: Generation, structure and reactions.

Unit II:

Stereochemistry: Elements of symmetry, Concept of chirality and molecular dissymmetry, molecules with more than one chiral center, meso compounds, threo and erythro isomers, method of resolution, optical purity, topicity of ligands, enantiotopic and distereotopic ligands and faces, prochirality, Cahn-Ingold-Prelog System to describe configuration at chiral centers**.** Inter conversion of Newman, Sawhorse and Fischer projection.

Conformational analysis of cycloalkanes (5-8 membered rings), substituted cyclohexanes, mono substituted, disubstituted and trisubstituted cyclohexanes, decalin system, effect of conformation on reactivity, Conformational analysis of *n*-butane and its derivatives, 1,2-diols, 1,2-dihaloethane and related compounds

Asymmetric synthesis, optical activity in absence of chiral carbon (biphenyl, spiranes and allenes), Chirality due to helical shape. Chirality of heteroatoms, stereospecific and stereoselective synthesis**.**

Unit III:

A) Reaction mechanism: Types of reaction, Types of mechanism, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, transition states and

intermediates, methods of determining mechanisms, trapping of intermediates, checking for common intermediate, competition and cross-over experiments, isotope effects, Hard and soft acids and bases**.**

B) Reaction Kinetics: Reaction co-ordinate diagrams, rate laws and methods of determining concentration.

C) Effect of Structure on reactivity: Resonance and field effects, Steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft Equation.

D) Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The *o*/*p* ratio, ipso attack, orientation in benzene ring with more than one substituent, orientation in another ring system. Friedel-Crafts reaction, Vilsmeir-Hack reaction, Gatterman-Koch reaction, Pechman reaction, Diazonium coupling, Blanc chloromethylation, Kolbe–Schmitt reaction

Unit IV:

A) Aliphatic nucleophilic substitution: The S_N1, S_N2, mixed S_N1, S_N2 and SET and S_Ni mechanisms**.** Nucleophilicty, effect of leaving group, ambient nucleophiles and ambient substrates regiospecificity, substitution at allylic and vinylic carbon atoms, Mitsunobu reaction

B) Concept of neighbouring group participation: Anchimeric assistance with mechanism, neighboring group participation by π and σ bonds, classical and non-classical carbocations, Intramolecular displacement by hydrogen, oxygen, nitrogen, sulphur and halogen**.** Alkyl, cycloalkyl, aryl participation, participation in bicyclic system, migratory aptitude.

C**) Aromatic Nucleophilic Substitution:** A general introduction to different mechanisms of aromatic nucleophilic substitution SNAr, S_N1, benzyne and SRN1 mechanisms, arynes as reaction intermediate, Reactivity - effect of substrate structure leaving group and attacking nucleophile. The Von Richter and Smiles rearrangements, Chichibabin amination reaction. Benzyne: Structure, methods of generations and reactions

Combined References of Organic Chemistry for Semester I and II:

1. Advanced Organic Chemistry –Reaction mechanism and structure, Jerry March, John Wiley
2. Advanced Organic Chemistry -F.A .Carey and R .J .Sunberg, Plenum
3. A Guidebook to Mechanism in Organic Chemistry-Peter Skyes, Longman
4. Structure and Mechanism in Organic Chemistry-C.K .Gold, Cornell University Press
5. Organic Chemistry, R.T .Morrison Boyd .Prentice Hall
6. Modern Organic Chemistry-H.O .House, Benjamin
7. Principal of Organic Chemistry-R.O.C .Norman and J. M. Coxon, Blackie Academic and Professional
8. Reaction Mechanism in Organic Chemistry-S.M .Mukharji and S.P .Singh, Macmilan
9. Stereochemistry of Organic Compounds -D .Nasipuri, New Age International
10. Stereochemistry of Organic Compounds -P .S .Kalsi, New Age International
11. Frontier Orbitals and Organic Chemical Reactions-I .Fleming

12. Orbital Symmetry –R .E .Lehr and A .P .Marchand
13. Reactive Intermediate in Organic Chemistry-N .S .Isaacs
14. Stereochemistry of Carbon Compounds -E .L .Eliel
15. Physical Organic Chemistry-J .Hine
16. Name Reaction in Organic chemistry –Surrey
17. Advanced Organic Chemistry –L .F .Fieser and M .Fieser .
18. Organic Chemistry Vol .I and II -I .L .Finar
19. Modern Organic Chemistry -J.D .Roberts and M .C .Caserio
20. The Search for Organic Reaction Pathways)Longmann(, Peter Skyes
21. Organic Chemistry 5th Edition)McGraw Hill(, S .H .Pine
22. Organic Chemistry)Willard Grant Press Botcon(, John Mcmurry
23. A Textbook of Organic Chemistry -R .K .Bansal New Age International
24. Organic Chemistry, J .Clayden, N .Greeves, S .Warren and P .Wothers, Oxford University Press
25. Organic Chemistry, 4th Edition, G Marc Loudon, Oxford University Press

Weblink to Equivalent MOOC on NPTEL/SWAYAM if relevant:

- Introductory Organic Chemistry I- https://nptel.ac.in/courses/104106119
- Mechanisms in Organic Chemistry- https://onlinecourses.nptel.ac.in/noc22_cy42
- Mechanisms in Organic Chemistry: https://onlinecourses.nptel.ac.in/noc20_cy26/preview
- Stereochemistry- https://nptel.ac.in/courses/104105086
- Stereochemistry and Applications- https://nptel.ac.in/courses/104106127
- Structure, Stereochemistry and Reactivity of Organic Compounds and Intermediates: A Problem-solving Approach- https://nptel.ac.in/courses/104105127

SEMESTER II

Paper 6

MCH2T06: Analytical Chemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course students will be able to-

1. *Select a specific analytical technique based on sample and target analyte*
2. *Develop analytical ability and critical thinking in selection of statistics and their use in making interpretation meaningful and productive.*
3. *Explain the logic behind working of indicator used in each type of titration*
4. *Elaborate interaction of radiation with matter and its application in chemical analysis.*
5. *Develop spectral methods of analysis for desired analytes.*
6. *Apply electroanalytical techniques based on conductance and emf measurements.*

Unit I:

Introduction to analytical chemistry: Types of analysis-qualitative and quantitative. Classification of analytical methods- classical and instrumental, basis of their classification with examples. Classification of analysis based on sample size (macro, semimicro, micro and ultramicro) and constituent type (major, minor, trace and ultratrace).

Volumetric Calculations: Stoichiometric and substoichiometric volumetric analysis. Concentration units: Unified atomic mass unit and the mole, Molarity, Normality, Weight and volume percent, Mole fraction, Formality, etc and their interrelation. Standard solutions. Primary standards and secondary standards. Numerical problems based on standard solution preparation, titrimetric analysis and gravimetric analysis. Calculations involved in acid-base, precipitation, redox and complexometric reactions.

Unit II: Classical methods of analysis

***Volumetric analysis*:** General principle**.** Criteria for reactions used in titrationsTheory of indicators. Types of titrations with examples- Acid-base, precipitation, redox and complexometric. Titration curves for monoprotic and polyprotic acids and bases. Indicators used in various types of titrations. Masking and demasking agents.

***Gravimetric analysis*:** General principles and conditions of precipitation. Concepts of solubility, solubility product and precipitation equilibria. Steps involved in gravimetric analysis. Purity of precipitate: Co-precipitation and post-precipitation. Fractional precipitation. Precipitation from homogeneous solution. Particle size, crystal growth, colloidal state, aging and peptization phenomena. Ignition of precipitates.

Unit III: Optical methods of analysis-I

Spectrophotometry and Colorimetry: Principle of colorimetry. Beer's law, its verification and deviations. Instrumentation in colorimetry and spectrophotometry (single and double beam). Sensitivity

and analytical significance of molar extinction coefficient and λ_{max}. Comparison method, calibration curve method and standard addition method for quantitative estimation. Role of organic ligands in spectrophotometric analysis of metal ions. Ringbom plot and Sandell's sensitivity. Photometric titrations. Determination of pK value of indicator. Simultaneous determination. Composition and stability constant of complex by Job's and mole ratio methods. Derivative spectrophotometry. Numerical problems.

Flame photometry: Principle. Instrumentation and types of burners. Factors affecting flame photometric determination. Limitations of flame photometry. Interferences in flame photometry. Applications.

Unit IV: Electrochemical methods of analysis-I

Conductometry: Concepts of electrical resistance, conductance, resistivity and conductivity. Specific, molar and equivalent conductance and effect of dilution on them. Measurement of conductance. Kohlrausch's law, Applications of conductometry in determination of dissociation constant, solubility product. Conductometric titrations. High frequency titrations. Numerical problems.

Potentiometry: Circuit diagram of simple potentiometer. Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode and glass electrode. Reference electrodes: Calomel electrode and Ag/AgCl electrode. Theory of potentiometric titrations. Nernst equation, standard electrode potential, Determination of cell potential, n, K_f and K_{sp}. pH titrations. Buffers and buffer capacity. pH of buffer mixtures based on Henderson-Hasselbalch equation and calculations.

References

1. Quantitative analysis**:** Day and Underwood **(**Prentice**-**Hall of India**)**
2. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3. Analytical Chemistry**:** Gary D**.** Christian **(**Wiley India**).**
4. Instrumental Methods of Analysis**:** Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
5. Sample Pre-treatment and Separation: R. Anderson (John Wiley and Sons)
6. Stoichiometry: B.I.Bhatt and S.M. Vora, 2nd Edition (Tata Mc-Graw Hill publication)
7. Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
8. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
9. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
10. Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
11. Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
12. Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
13. An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
14. Fundamental of Analytical Chemistry: S. A. Skoog and D. W. West
15. Instrumental Methods of Chemical Analysis: G. W. Ewing
16. Polarography: Koltoff and Ligane
17. Electroanalytical Chemistry: Sane and Joshi (Quest Publications)

Web link for related NPTEL courses

Analytical Chemistry: https://nptel.ac.in/courses/104105084

SEMESTER II

Paper 7 (Elective)

MCH2T07: (a) Solid state and organometallic chemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student would be able to

1. *Understand the structures of various types of solids.*
2. *Establish structure-property correlation in solids.*
3. *unravel and interpret the structural aspects of metal clusters.*
4. *Explain structures and applications of organotransition compounds,*
5. *predict the mechanism of complex reactions.*
6. *establish the thermodynamic and kinetic stability of reactants and products in complex reactions.*

Unit I

Solid State Chemistry: Ionic Crystals and their structures, radius ratio rule, effect of polarization on crystals. Covalent structure type: Sphalerite and Wurtzite. Geometry of simple crystal AB type: NaCl, CsCl and NiAs. AB_2 type: Fluorite, antifluorites, Rutile structures. Li_2O, Na_2O, $CdCl_2$, CdI_2 structures. Ternary Compounds ABO_3 type: Perovskite, Barium titanate, lead titanate, $CaTiO_3$, Tolerance factor, charge neutrality and deviation structures $FeTiO_3$.

Solids of AB_2O_4 type: Normal and inverse,2-3 and 4-2 spinel, packing of oxygen in tetrahedral and octahedral sites, sites occupancy number of sites surrounding each oxygen, application of charge neutrality principles, site preferences in spinel, distorted spinel. Hausmannite (Jahn-Teller distortions), Factors causing distortion in spinel.

Unit – II

(A) Metal – Ligand Bonding in Transition Metal Complexes: Recapulization of Crystal Field Theory, Application of CFT to Tetragonal, square-planer, Trigonal bipyramidal complexes, Jahn-Teller effect, Nephelauxetic effect, Limitations of crystal field theory.

(B) Magnetic Properties of Transition Metal complexes: Abnormal magnetic properties, orbital contributions and quenching of orbital angular momentum, spin-orbit coupling. Magnetic moment, electronic spectra and structure of tetrahalocobalt (II) complexes, tetrahedral and octahedral Ni(II) complexes. High spin-low spins crossover.

Unit III

Reaction mechanism of Transition Metal Complexes-II: Substitution reaction in square planar complexes: the trans effect, cis effect, steric effect, solvent effect, effect of leaving group, effect of charge, effect of nucleophile, effect of temperature. Trans effect theories, uses of trans-effect, mechanism of substitution reactions in Pt(II) complexes. Electron transfer reactions. Types of electron transfer reactions, conditions of electron transfer, and mechanism of one-electron transfer reactions, outer sphere and inner sphere mechanisms, two electron transfer reactions complimentary and non-

complimentary reactions. Tunneling effect, cross-reaction, Marcus-Hush theory, bridged activated mechanism.

Unit-IV

Organotransition Metal Chemistry: Alkyls and Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways of alkyls and aryls of transition metals. Organocopper in Organic synthesis. Compounds of Transition Metal –Carbon Multiple bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes–synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on ligands, role inorganic synthesis.

References

1. J.E.Huheey: Inorganic Chemistry
2. F.A.Cottonand G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th and 6th Editions.
3. A.F. Willims: Theoretical Approach in inorganic chemistry.
4. Mannas Chanda: Atomic Structure and chemical Bonding
5. L. E. Orgel: An Introduction To transition metal chemistry, Ligand field theory, 2nd Edition.
6. J. J. Logowski: Modern Inorganic Chemistry
7. B.Durrant and P.J.Durrant: Advanced Inorganic Chemistry
8. J C. Bailar: Chemistry of coordination compounds.
9. W. L. Jolly: Modern Inorganic ChemistryJones: Elementry Coordination chemistry.
10. B. N. Figgis: Introduction to Ligand field.
11. M.C.Day and J.Selbin: Therotical Inorganic Chemistry.
12. J. Lewin and Wilkins: Modern Co-ordination chemistry.
13. Purcell and Kotz: Inorganic Chemistry.
14. D. Banerjea: Co-ordination chemistry, Tata Mc. Graw. Pub.
15. A.F. Wells: Structural inorganic chemistry, 5th Edition, Oxford.
16. S. G. Davies: Organotransition metal chemistry applications to organic synthesis.
17. R. C. Mehrotra: Organometallic chemistry Tata McGraw Hill. Pub.
18. G. S. Manku: Thereotical priciples of inorganic chemistry
19. A. B. P. Lever: Inorganic electronic spectroscopy.
20. R.H.Crabtree:The Organometalic chemistry of Transition metals, John Wiley.
21. D.N.Styanaryan:Electronic Absorption Spectroscopy and related techniques, University Press.
22. R. S. Drago: Physical methods in inorganic chemistry
23. F.Basolo andG.Pearson: Inorganic Reaction Mechanism
24. Organometallics II and I complexes with transition metal- carbon bonds: Manfred Bochmann-
25. Oxford Press.
26. Advanced Inorganic Chemistry Vol I and II – Satyaprakash, Tuli, Bassu and Madan- S Chand.
27. A.E.Martel; Coordination Chemistry-VolIandII,VNR.

SEMESTER II

Paper 7 (Elective)

MCH2T07: (b) Organic Reaction Mechanism

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Predict the orientation and stereochemistry of the product of addition and elimination reaction*
2. *Apply enolate chemistry to achieve molecular complexity*
3. *Design organic reactions in order to achieve the required product(s)*
4. *Formulate green chemistry synthesis to increase atom economy*
5. *Application of free radicals in functional group transformation*

Unit-I

A) Addition to carbon-carbon multiple bond: Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, Orientation and stereochemistry of common reactions, Addition to cyclopropanes, Hydrogenation of double bond and triple bonds. Hydrogenation of aromatic rings, hydroboration-oxidation, epoxidation, Michael addition

B) Elimination reactions: The E1, E2 and E1CB mechanisms, Stereochemistry of E2 elimination, Orientation of the double bond, Saytzeff and Hoffman's rule, Effect of substrate structure, attacking base, leaving group and medium, Mechanism and orientation in pyrolytic elimination involving selenium oxide, Cope and Chugaev elimination

Unit II:

Addition to carbon-hetero atom multiple bond: Ionization of carbon hydrogen bond and prototopy, Base and acid catalysed halogenation of ketones, keto-enol equilibria, structure and rate in enolisation, concerted and carbanion mechanism for tautomerism, geometry of carbanions, kinetic and thermodynamic control in the generation of enolates, Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters, and nitriles, Wittig reaction, Mechanisms and synthetic applications of condensation reactions involving enolates- Aldol, Knoevengel, Claisen, Mannich, Benzoin, Perkin, Stobbe reaction, Robinson annulation, Hydrolysis of esters and amide, Baylis-Hillman reactions, Ugi and Passerini reaction.

Unit III:

Free radical reactions: Generation of free radicals, Type of free radical reactions, free radical substitution, mechanism at an aromatic and aliphatic substrate, reactivity at a bridgehead position. The reactivity and selectivity principle of halogenation at an alkyl carbon, allylic carbon (NBS), hydroxylation at an aromatic carbon by means of Fenton's reagent. Auto-oxidation, chlorosulphonation (Reed Reaction) Coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, Hunsdiecker reaction, Barton reaction, Hoffmann-Loefler-Freytag reaction, McMurry coupling, Samarium(II) iodide reagents for functional group transformations and C-C bond formation.

Applications of tributytin hydride: Reduction of halides, alcohols and acids, addition to carbon-carbon double bond, cyclization of free radical intermediates, tandem radical cyclization reactions, fragmentation reactions

Unit IV

Molecular rearrangements: Definition and classification. Mechanism, stereochemistry and synthetic applications of Pinacol-Pinacolone, Wagner- Meerwein, Tiffenev–Demjnov ring expansion, Arndt-Eistert synthesis, Dienone-phenol rearrangement, rearrangement due to electron deficient nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements, Baeyer-Villiger oxidation, Dakin oxidation, [1,2]-Wittig rearrangement, Base catalysed rearrangements: Benzilic acid, Favourski, Neber, Sommlett-Hauser and Smiles rearrangement, Stevens rearrangement

Fragmentation reactions: Electron push and pull requirement, Beckmann fragmentation, Eschenmoser fragmentation, Alicyclic-Grobb rearrangement

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Weblink to Equivalent MOOC on SWAYAM if relevant:

- Essentials of Oxidation, Reduction and C-C Bond Formation. Application in Organic Synthesis- https://nptel.ac.in/courses/104101127
- Principles of Organic Synthesis- https://nptel.ac.in/courses/104103110
- Introductory Organic Chemistry II- https://onlinecourses.nptel.ac.in/noc21_cy46/preview

SEMESTER II

Paper 7 (Elective)

MCH2T07: (c) Quantum, Statistical and Nuclear Chemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Understand, the concept of statistical thermodynamics and their uses.*
2. *Understand the quantum mechanical applications in actual practice and in spectroscopy*
3. *Understand the thermodynamics of real processes*
4. *Understand the distribution laws and their applications*
5. *Understand the fundamentals of Nuclear sciences*

UNIT I: QUANTUM MECHANICS - II

Approximate methods, variation principle, its application in Linear and non-linear functions, MO theory applied to H_2^+ molecule and H_2 molecule (calculation of energy), Introduction to perturbation theory (First order correction to wave function and energy), Application to He atom.

Electronic structure of atoms: Russel Sanders terms and coupling schemes, term separation energies of the p^n configuration, term separation energies for d^n configuration, magnetic effects: spin orbit coupling and Zeeman splitting.

Hybridization, hybrid orbitals in terms of wave functions of s and p orbitals, sp and sp^2 hybridizations, Simple Hückel theory applied to: ethylene, butadiene and cyclobutadiene.

UNIT II :STATISTICAL THERMODYNAMICS

Statistical thermodynamics :Lagrange's Method of Undetermined Multipliers)Conditional Maximization(, Stirling Approximation, Concept of Distribution, Thermodynamic Probability and most probable distribution, Maxwell Boltzmann, Bose Einestein, Fermi Dirac statistics, comparison between three statistics.

Partition function, Translational partition function, Rotational partition function, Vibrational partition function, Electronic partition function, Applications of partition functions, Numerical.

UNIT III :STATISTICAL MECHANICS OF ENSEMBLES AND NON-EQUILIBRIUM THERMODYNAMICS

Atomic and Molecular quantum levels, Significance of Boltzmann Distribution law, partition Functions and ensembles, ensemble averaging, postulates of ensemble averaging, canonical, grand canonical and micro canonical ensembles, corresponding distribution laws using Lagranges method of undetermined multipliers. Ortho and para hydrogen, principle of equipartition of energy, calculation of average energy.

Nonequilibrium Thermodynamics :Conservation of mass and energy in time dependent closed and open systems, Thermodynamic criteria of irreversibility, rate of entropy production and entropy exchange in irreversible processes .The generation of the concept of Chemical Affinity and the extent of

advancement of chemical reactions, Thermodynamic constraints on the signs of chemical affinity and the velocity of chemical reaction, application to any one coupled reaction.

UNIT IV :NUCLEAR CHEMISTRY

Introduction, radioactive decay and equilibrium, thermonuclear reactions, photonuclear reactions, Radiometric titration, isotopic dilution analysis, NAA.

Nuclear models: Fermi gas model, shell model, liquid drop model, application of liquid drop models semiempirical mass equation.

Counters: proportional counter, GM counter, scintillation counter, ionization chamber counter.

References

1) Ira N .Levine, Quantum Chemistry, 5th edition)2000(, Pearson educ., Inc.New Delhi
2) A. K. Chandra, Introductory Quantum Chemistry, 4th edition)1994(, Tata Mc-graw Hill, New Delhi.
3) M.W. Hanna, "Quantum Mechanics in Chemistry", Benjamin
4) L .Pualing and E .B .Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York)1935.(
5) R .K .Prasad, Quantum Chemistry, New Age International, Delhi .
6) R .K .Prasad, Quantum Chemistry through problems and solutions, New Age International, New Delhi, 2009.
7) B .C .Reed, Quantum Mechanics, Jones and Bartlett, New Delhi, 2010.
8) R .P .Rastogi and R .R .Mishra, An Introduction to Chemical Thermodynamics, Vikas Publication, Gorakhpur, 2010.
9) P .W .Atkins'and D .Paula, Physical Chemistry, 8th Edition, Oxford University Press, 2010.
10) G .K .Vemulapalli, Physical Chemistry, Prentice –Hall of India, 1997.
11) S .Glasstone, An Introduction to Electrochemistry, East-West Press Pvt .Ltd., New Delhi, 2004.
12) H .K .Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
13) S .O .Pillai, Solid State Physics, New Age International, New Delhi, 2102.
14) N .B .Hanny, Treaties in Solid State Chemistry,
15) M .C .Day and J Selbin, Theoretical Inorganic Chemistry, Reinhold Pub .Corp., New York,
16) I Prigogine and R .Defay, Chemical Thermodynamics, Longmans, London, 1954.
17) S .R .DeGroot and P .Mazoor, Non-Equilibrium Thermodynamics, North-Holland Co., Amsterdam, 1969.
18) G .Lebon, D .Jou and Casa Vazquez, Understanding Non-equilibrium Thermodynamics, Springer, 2008.
19) I.Prigoggine, "An Introduction to Thermodynamics of Irreversible Processes, "Wiley-Interscience.
20) R .P .Rastogi, Introduction to Non-equilibrium Physical Chemistry, Elsevier, Amsterdam, 2008.
21) G .A .Somorjai, Introduction to Surface Chemistry and Catalysis, Wiley, 2010.

22) M .C .Gupta, Statistical Thermodynamics, New Age International.
23) K .Huang, Statistical Mechanics, Wiley, New Delhi, 2003.
24) Andrew Maczek, Statistical Thermodynamics, Oxford University Press Inc., New York)1998.(
25) C.N. Rao .Nuclear Chemistry
26) B .G .Harvey, Introduction to Nuclear Physics and Chemistry, Prentice Hall, Inc) .1969.(
27) H.J .Arnikar, Essentials of Nuclear Chemistry, 4th Edition)1995(, Wiely-Eastern Ltd., New Delhi.
28) L .E .Smart and E .A .Moore, Solid State Chemistry-An Introduction, CRC Tylor and Fransis, 2005.
29) D .D .Sood, A .V .R .Reddy, Fundamentals of Radiochemistry, Indian Association of Nuclear Chemists and Allied Scientists, 2007.
30) C .N .R .Rao and Gopalakrishnan, "New Directions in Solid State Chemistry" Second Edition, Cambridge University Press.
31) Anthony R .West, "Solid State Chemistry and its Applications "Wiley India Edition.
32) C .Kalidas and M .V .Sangaranarayana, Non-Equilibrium Thermodynamics.

NPTEL sources weblinks:

- Quantum Chemistry: https://archive.nptel.ac.in/courses/104/105/104105128/
- https://www.youtube.com/watch?v=InNx7cYE9DI
- https://onlinecourses.nptel.ac.in/noc22_cy02/preview
- For statistical Thermodynamics: https://onlinecourses.nptel.ac.in/noc23_me69/preview
- https://nptel.ac.in/courses/104103112
- For Nuclear Chemistry: https://onlinecourses.nptel.ac.in/noc23_cy21/preview
- https://www.youtube.com/watch?v=iMhDYarsfII
- https://archive.nptel.ac.in/courses/112/103/112103243/

SEMESTER II

Paper 7 (Elective)

MCH2T07: (d) Instrumental Methods of Analysis

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course students will be able to -

1. *Understand the importance of sampling and sample treatment.*
2. *Select appropriate sampling technique based on sample and target analyte.*
3. *Explain principle and instrumentation involved in AAS.*
4. *Deduce the necessity to remove interferences in AAS and methods involved .*
5. *Select proper technique among the available techniques.*
6. *Formulate experiments based on optical and electroanalytical techniques.*

Unit-I:

Sampling and sample treatment: Criteria for representative sample. Techniques of sampling of gases (ambient air and exhaust gases), liquids (water and milk samples), solids (soil and coal samples) and particulates. Hazards in sampling. Safety aspects in handling hazardous chemicals. Sample dissolution methods for elemental analysis: Dry and wet ashing, acid digestion, fusion processes and dissolution of organic samples.

Detection and quantification: Concepts and difference between sensitivity, limit of detection and limit of quantification, role of noise in determination of detection limit of analytical techniques. Methods of quantification: Absolute method, comparison method, calibration curve method, standard addition method and internal standard method.

Unit-II: ***Atomic absorption spectroscopy***

Principle**.** Atomic energy levels**.** Grotrian diagrams**.** Population of energy levels**.** Instrumentation**.** Sources**:** Hollow cathode lamp and electrodeless discharge lamp, factors affecting spectral width**.** Atomizers**:** Flame atomizers, graphite rod and graphite furnace**.** Cold vapour and hydride generation techniques**.** Factors affecting atomization efficiency, flame profile**.** Monochromators and detectors**.** Beam modulation**.** Detection limit and sensitivity**.** Interferences and their removal**.** Comparison of AAS and flame emission spectrometry**.** Applications of AAS**.**

Unit-III: Polarography and amperometry

Polarography: Principle of DC polarography. Instrumentation in polarography. Advantages and limitations of DME. Types of currents- residual current, migration current, diffusion current, limiting current, adsorption current, kinetic current and catalytic current. Ilkovic equation-diffusion current constant and capillary characteristics. Derivation of equation of polarographic wave and half wave potential. Experimental determination of half wave potential. Reversible, quasi reversible and irreversible electrode reactions. Polarographic maxima and maximum suppressor. Oxygen interference and deaeration. Introduction to pulse, a.c. and oscillographic techniques and their advantages. Applications of polarography in determination of dissolved oxygen, metal ion quantification and

speciation, simultaneous determination of metal ions, analysis of organic compounds. Limitations of polarography.

Amperometric titrations: Principle, types and applications in analytical chemistry.

Unit-IV: Miscellaneous techniques

Fluorometry and phosphorimetry: Principles of fluorescence and phosphorescence. Jablonski diagram. Concentration dependence of fluorescence intensity. Fluorescence quenching. Instrumentation. Applications.

Nephelometry and turbidimetry: Principle, instrumentation and applications.

Photoacoustic spectroscopy: Theory. Instrumentation. Advantages over absorption spectroscopy. Chemical and surface applications of PAS.

References

1. Quantitative analysis**:** Day and Underwood **(**Prentice**-**Hall of India**)**
2. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3. Analytical Chemistry**:** Gary D**.** Christian **(**Wiley India**).**
4. Instrumental Methods of Analysis**:** Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
5. Sample Pre-treatment and Separation: R. Anderson (John Wiley and Sons)
6. Stoichiometry: B.I.Bhatt and S.M. Vora, 2nd Edition (Tata Mc-Graw Hill publication)
7. Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
8. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
9. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
10. Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
11. Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
12. Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
13. An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
14. Fundamental of Analytical Chemistry: S. A. Skoog and D. W. West
15. Instrumental Methods of Chemical Analysis: G. W. Ewing
16. Polarography: Koltoff and Ligane
17. Electroanalytical Chemistry: Sane and Joshi (Quest Publications)

Web link for related NPTEL courses

- Analytical Chemistry: https://nptel.ac.in/courses/104105084

SEMESTER II

Practical 3

MCH2P03: On Job Training/Field Project

120 h (8 h per week) *100 Marks*

On job training or a Field Project is a skill based practical program. It has to be carried out in accordance

Annexure III of General Guidelines for M.Sc. program.

1. Every student admitted to M.Sc. Second Semester is compulsorily required to undergo this course bearing 4 credits.
2. During second semester, all students will have to undergo OJT/Internship/FP of 120 Hours.
3. Each student will be required to submit a detailed report to the Department/ College/ Institute for the work undertaken during this period **within 7 days of completion of the training** following which the evaluation and assessment for OJT/Internship/FP will be done by the college/institute concerned. The Report submitted must be according to the Learning outcomes and in tune with the rubric for evaluation.
4. College/Institute is required to assign Supervisor/Mentor to students for OJT/Internship/FP who will guide the students in attaining the outcomes of this course.
5. The Internal Examiner and External Examiner shall jointly evaluate the report submitted by the student and her/his seminar and shall immediately submit the evaluation report in the prescribed format provided along with.

SEMESTER II

Practical 4

MCH2P04: Organic Chemistry

6 h per week *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Handling of the hazardous chemicals by safely*
2. *Predict and analysis of the major and minor products of a variety of organic reactions*
3. *Monitoring of the chemical reactions*
4. *Calculation of yield, percentage yield of the chemical reactions*
5. *Understand the concept of Qualitative analysis*

a. **Organic preparations:** Student is expected to carry out minimum of 7-10 single stage preparation and 3-4 two stage organic preparation from the following lists (**Total 10 preparations**). During preparation of organic compounds, the techniques such as crystallization, distillation, solvent extraction, TLC and column chromatography should be demonstrated.

2. Oxidation :Adipic acid by chromic acid oxidation of cyclohexanol.
3. Benzophenone → benzhydrol
4. Aldol condensation :Dibenzal acetone from benzaldehyde .
5. Sandmeyer reaction :p -chlorotoluene from p-toluidine
6. Cannizzaro reaction
7. Friedel Crafts Reaction :β-Benzoyl propionic acid from succinic anhydride and benzene.
8. Benzoin → 2,4,5-triphenyl imidizole
9. Sucrose → Oxalic acid
10. Methyl acetoacetate → 5-methyl-isoxazol-3-ol
11. Ethyl acetoacetate → 4-aryl-6-methyl-3,4-dihydro-2)1*H*-(pyrimidinone ester
12. Ethyl acetoacetate → Diethyl 1,4-dihydro-2,6-dimethyl-4-phenylpyridine-3,5-dicarboxylate
13. Dye preparation :Sulphanilic acid → Methyl orange
14. Dye preparation :p-nitroaniline → *p*-red
15. Acetanilide → *p*-nitroacetanilide →*p*-nitroaniline
16. Aniline → 2,4,6-tribromo aniline → 2,4,6-tribromoacetanilide
17. Nitrobenzene →m-dinitrobenzene →*m*-nitroaniline
18. toluene → *p*-nitrotoluene →*p*-nitrobenzoic acid
19. Glycine → Benzoyl glycine → 4-benzilidene-2-phenyl oxazole
20. Benzaldehyde → chalcone → chalcone dibromide
21. *Any other suitable preparation of organic molecules depending on availability of chemicals*

B) Qualitative Analysis : Separation, purification and identification of the mixture of two organic compounds)binary mixture with two solid, one solid one liquid and two liquids (using chemical methods or physical techniques. **Minimum 6-10 mixtures to be analyzed**.

References

1) Practical organic chemistry by FG Mann and BC Saunders
2) Text book of practical organic chemistry –by Vogel
3) The synthesis, identification of organic compounds –Ralph L. Shriner, Christine K.F. Hermann, Terence C. Morrill and David Y. Curtin
4) Compendious Practical Organic Chemistry : Preparations, Isolation, and Chromatography by Basavarajaiah S M, Nagesh G Y, Ramakrishna Reddy K
5) Advanced Practical organic chemistry by N.K.Vishnoi

SEMESTER II

Practical 5

MCH2P05: Analytical Chemistry

6 h per week *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Carry out calibration of glassware available in the laboratory.*
2. *Analyze the data obtained through experiments using statistical analysis parameters.*
3. *Estimate quantitatively analyte present in different samples using classical and instrumental methods of analysis.*
4. *Design experiments based on classical and instrumental techniques.*
5. *Understand the principles involved in visual and instrumental volumetric techniques.*
6. *Formulate experiments based on optical and electroanalytical techniques.*

Section (A): Classical methods and separation techniques:

Calibration, validation and computers

1. Calibration of pipette and burette.
2. Statistical analysis of data.
3. Use of MS-Excel in statistical analysis of data and curve fitting.

Volumetry

1. Determination of Na_2CO_3 in washing soda.
2. Determination of NaOH and Na_2CO_3 in a mixture.
3. Estimation of nickel in given solution by direct complexometric titration with EDTA using bromopyrogallol red.
4. Estimation of nickel in given solution by complexometric back-titration with EDTA.
5. Estimation of chloride in given solution by Mohr's titration.
6. Estimation of chloride in given solution by Volhard's titration.
7. Determination of volume strength of commercial hydrogen peroxide by redox titration with $KMnO_4$.
8. Estimation of phenol/ aniline by bromination method.
9. Estimation of glucose.
10. Estimation of acetone.
11. Estimation of formaldehyde.
12. Estimation of Mn in the presence of Fe using masking phenomenon (ferromanganese alloy).

Gravimetry

1. Estimation of barium as barium sulphate.
2. Estimation of calcium as calcium oxalate/ calcium carbonate/ calcium oxide.

Separation techniques

1. Qualitative separation of metal ions by paper chromatography for 2/3 components.
2. Determination of ion-exchange capacity of resin.
3. Separation of ions by ion exchange.

Section (B): Instrumental techniques: Electroanalytical techniques

1. Analysis of commercial vinegar by conductometric titration.
2. Estimation of phenol by conductometric titration with NaOH.
3. Determination of strength of HCl and CH_3COOH in a mixture conductometrically.
4. Determination of strength of HCl and oxalic acid in a mixture conductometrically.
5. Determination of strength of oxalic acid and CH_3COOH in a mixture conductometrically.
6. Determination of degree of dissociation and dissociation constant of acetic acid conductometrically.
7. Estimation of phenol in dilute solution by conductometric titration with NaOH.
8. Determination of strength of HCl and CH_3COOH individually and in a mixture potentiometrically.
9. Determination of Fe(II) by potentiometric titration with $K_2Cr_2O_7$.
10. Determination of three dissociation constants of H_3PO_4 by pH-metric/ potentiometric titration.

Optical methods

1. Determination of pK of indicator by colorimetry.
2. To estimate the amount of NH_4Cl colorimetrically using Nesseler's Reagent.
3. To study the complex formation between Fe(III) and salicylic acid and find the formula and stability constant of the complex colorimetrically (Job's method).
4. To determine the dissociation constant of phenolphthalein colorimetrically.
5. Estimation of iron in wastewater sample using 1,10-phenanthroline.

References

1. Quantitative analysis**:** Day and Underwood **(**Prentice**-**Hall of India**)**
2. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3. Analytical Chemistry**:** Gary D**.** Christian **(**Wiley India**).**
4. Experiments and calculations in Engineering Chemistry- S. S. Dara (S. Chand and Co.)
5. Experiments in Chemistry-D. V. Jahagirdar (Himalaya)

SEMESTER III

Paper 8

MCH3T08**: Spectroscopy-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Understand the symmetry properties of molecules*
2. *Interpret the structure of simple organic molecules using mass spectrometry*
3. *Correlate the presence of functional groups with IR frequencies*
4. *Apply the IR and Raman spectroscopy to simple molecules*

Unit - I: Symmetry properties of molecules and group theory:

Symmetry elements and symmetry operations. Properties of group. Point groups and Schoenflies symbols. Symmetry operations as a group. Matrix representations of groups. Multiplication table for C_{2v}, C_{3v} and C_{2h}. Reducible and irreducible representations. Similarity transformation. Classes of symmetry operations. Great Orthogonality Theorem. Derivation of character tables for H_2O and NH_3 using Great Orthogonality Theorem. Application of character tables in selection rules of IR, Raman and Electronic spectroscopy.

Unit - II:

A] **Mass spectrometry:** Theory, ion production(EI, CI, FD, FAB), ion analysis, ion abundance, isotopic contribution, Nitrogen-rule, types of fission processes, high resolution mass spectrometry, metastable peak, molecular ion peak, McLafferty rearrangement, mass spectral fragmentation of organic compounds alkanes, alkenes, alkynes, alcohols, amines, amides, acids, aldehydes, ketones, halides, Structure determination of organic molecules by mass spectrometry, problem based on mass spectral data

B] **Mössbauer spectroscopy**: Basic principle, experimental techniques, recoil emission and absorption, source, absorber, isomer shift, quadrupole interaction, magnetic hyperfine interaction, applications in determining electronic structure, molecular structure, crystal symmetry, magnetic structure, surface studies, biological applications.

Unit - III:

A] **Microwave spectroscopy**: Classification of molecules on the basis of M.I., rigid and non-rigid rotor, effect of isotopic substitution on transition frequencies, stark effect, microwave spectrometer, application in deriving: molecular structure, dipole moment, atomic mass and nuclear quadrupole moment.

B] **ESR spectroscopy**: Introduction, principle of ESR, ESR spectrometer, hyperfine coupling, zero field splitting, factors affecting g values, Kramer's degeneracy, application of ESR spectra to study free radicals like hydrogen, methyl radical, 1,4-semibenzoquinone, naphthalene, transition metal complexes, biological systems.

Unit IV:

A] **Infrared spectroscopy**: Diatomic molecules: Molecules as harmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, zero point energy, isotope effect. The Anharmonic oscillator, the interactions of rotations and vibrations. P,Q,R branches, vibration of polyatomic molecules, selection rules, normal modes of vibration, group frequencies, overtone and combination frequencies. Structure determination of organic molecules by IR spectroscopy, problem based on IR spectral data

B] **Raman Spectroscopy**: Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Selection rules, coherent anti-Stokes Raman spectroscopy, Structure determination from Raman and Infra-red spectroscopy.

References

1. Spectroscopic identification of organic compound-RM Silverstein, GC Bassler and TC Morril, John Wiley
2. Introduction to NMR spectroscopy-R. J. Abraham, J. Fisher and P Loftus Wiley
3. Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
4. Organic Spectroscopy-William Kemp, ELBS with McMillan
5. Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
6. Practical NMR Spectroscopy-ML Martin, JJ Delpench, and DJ Martyin
7. Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
8. Fundamentals of Molecular Spectroscopy-CN Banwell
9. Spectroscopy in Inorganic Chemistry-CNR Rao and JR Ferraro
10. Photoelectron Spectroscopy-Baber and Betteridge
11. Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten
12. NMR –Basic Principle and Application-H Guntur
13. Interpretation of NMR spectra-Roy H Bible
14. Interpretation of IR spectra-NB Coulthop
15. Electron Spin Resonance Theory and Applications-W Gordy
16. Mass Spectrometry Organic Chemical Applications, JH Banyon

SEMESTER III

Paper 9

MCH3T09**: Advanced Organic Chemistry-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Identify a pericyclic reaction and categorize it as a cycloaddition, a group transfer reaction, a sigmatropic rearrangement, or an electrocyclic reaction,*
2. *Apply frontier molecular orbital (FMO) theory to rationalize selectivity and reactivity aspects of pericyclic reactions.*
3. *Understand the reaction mechanism of various common reagents employed in organic synthesis*
4. *Understand the reactivity of sulphur, silicon and phosphorous elements.*
5. *Apply pericyclic reactions for the synthesis of complex organic molecules*

Unit I: Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system, classification of pericyclic reaction. FMO approach, Woodward-Hoffman correlation diagram method and Perturbation of Molecular Orbital (PMO) approach of pericyclic reaction under thermal and photochemical conditions Electrocyclic reactions, conrotatary and disrotatary motion for 4n and (4n+2) systems, Cycloaddition reaction with more emphasis on [2+2] and [4+2], Cycloaddition of ketenes, Secondary effects in [4+2] cycloaddition. Stereochemical effects and effect of substituents on rate of cycloaddition reaction, Diels-Alder reaction, 1,3-dipolar cycloaddition and chelotropic reaction. Sigmotropic rearrangement, suprafacial, and antarafacial shift involving carbon moieties, retention and inversion of configuration, [3,3] and [5,5] sigmotropic rearrangements, Claisen, Cope, Sommelet-Hauser rearrangements, Ene reaction

Unit II: Oxidation

Oxidation of alkanes, aromatic hydrocarbons and alkenes, Dehydrogenation with S, Se, Fremy's salt, DDQ, chloranil, Oxidation with SeO_2, Epoxidation of olefins, application of epoxides, Sharpless asymmetric epoxidation, Dihydroxylation of olefins using $KMnO_4$, OsO_4, Woodward and Prevost dihydroxylation, Oxidative cleavage of olefins, Ozonolysis, Etard Reaction

Oxidation of alcohols: Chromium reagents, pyridinium chlorochromate (PCC), pyridinium dichromate (PDC), Collin and Jones reagent, Combination of DMSO with DCC, $(COCl)_2$, NCS, SO_3 and $(CH_3CO)_2O$ for oxidation of alcohols, Oxidation with MnO_2, Oppenauer oxidation, CAN, Tetrapropyl ammonium peruthenate, Fetizon's reagent, Chemistry and synthetic applications of $Pb(OAc)_4$, Dess-Martin periodane, IBX and related hypervalent iodine based oxidations

Conversion of ketones to α, β-unsaturated ketones and α-hydroxy ketones, Baeyer-Villiger oxidation, Dakin oxidation, Tamao-Fleming Oxidation, Oxidations with Dimethyl dioxirane (DMDO) and 2-sulfonyloxaziridines and chiral version

Unit III: Reduction

Catalytic heterogeneous and homogeneous hydrogenation, Hydrogenation of alkenes, alkynes and arenes, Selectivity of reduction, Mechanism and stereochemistry of reduction, Raney Ni-catalyst, Adam catalyst, Lindlar catalyst, Wilkinson catalyst

Reduction by dissolving metals, Reduction of carbonyl compounds, conjugated systems, aromatic compounds and alkynes. Birch reduction, Hydrogenolysis

Reduction by hydride transfer reagents, Meerwein-Pondorff-Verley reduction, Reduction with $LiAlH_4$ and $NaBH_4$, stereochemical aspects of hydride addition, Derivatives of $LiAlH_4$ and $NaBH_4$, Selectivity issues, Diisobutylaluminium hydride (DIBAL-H), Sodium cyanoborohydride, Reduction with boranes and derivatives Reduction of carbonyl group to methylene, Reduction with diimide and trialkylsilanes

Unit IV: Chemistry of P, S, Si, and Boron compounds

1) Phosphours and sulphur ylide: Preparation and their synthetic application along with stereochemistry

2) Umpolung concept: Dipole inversion, generation of acyl anion, use of 1,3-dithiane, ethylmethylthiomethylsulphoxide, *bis*-phenylthiomethane, metallated enol ethers, alkylidene dithiane, ketone thioacetals, 2-propenethiobismethyl thioallyl anion, thiaminehydrochloride based generation of acyl anion

3) Organoboranes- preparation and properties of organoborane reagents e.g. RBH_2, R_2BH, R_3B, 9-BBN, catechol borane. Thexylborane, cyclohexylborane, $ICPBH_2$, IPC_2BH, Hydrboration mechanism, stereo and regioselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes, Synthesis of *EE, EZ, ZZ* dienes and alkyenes. Mechanism of addition of IPC_2BH. Allylboranes-synthesis, mechanism and uses

4) Organosilicon compounds in organic synthesis, Me_3SiCl, Me_3SiH and Peterson reaction, Synthesis and reactions of alkenyl, alkynyl and aryl silanes

References

1. Organic Chemistry, J .Clayden, N .Greeves, S .Warren and P .Wothers, Oxford University Press
2. Some Modern Methods of Organic Synthesis-W .Carruthers
3. Principles of Organic Synthesis by R. O. C. Norman and James M. Coxon (Nelson Thornes Ltd)
4. Advance Organic Chemistry Part-B-F .A .Caray and R .J .Sundberg Plenum Press
5. Modern Organic Synthesis: An Introduction by G. S. Zweifel and M. H. Nantz (Wiley)
6. Organic Synthesis by Michael Smith , 4th Edition (Academic Press)
7. Pericyclic Reactions by I. Fleming, Oxford University Press, 1999
8. S. Sankararaman, Pericyclic Reactions – A textbook. Wiley-VCH, 2005.
9. Organic synthesis: The roles of boron and silicon by S. E. Thomas (Oxford Chemistry Primers)
10. The Chemistry of Organophosphorous-A .J .Kirbi and S.G .Warren
11. Organosilicon Compound-C .Eabon
12. Organic Synthesis via Bora- H. C. Brown
13. Organoborane Chemistry-T .P .Onak
14. Organic Chemistry of Boron-W Gerrard

Weblink to Equivalent MOOC on SWAYAM if relevant:

- Organic Photochemistry and Pericyclic Reactions: Dr. N.D. Pradeep Singh Department of Chemistry IIT Kharagpur, https://nptel.ac.in/courses/104105038
- Pericyclic Reactions and Organic Photochemistry: Prof. Sankararaman, IIT Madras https://nptel.ac.in/courses/104/106/104106077/
- Essentials of Oxidation, Reduction and C-C Bond Formation. Application in Organic Synthesis https://nptel.ac.in/courses/104/101/104101127/
- Reagents in organic synthesis: Prof. Subhas C. Pan, IIT Guwahati https://archive.nptel.ac.in/courses/104/103/104103111/
- Principles of Organic Synthesis: Prof. T. Punniyamurthy, IIT Guwahati, https://archive.nptel.ac.in/courses/104/103/104103110/

SEMESTER III

Paper 10

MCH3T10**: Advanced Inorganic Chemistry**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Understand the crystal structures of simple inorganic molecules.*
2. *Understand the industrial applications of catalysis.*
3. *Apply the mechanism of metallo-enzyme actions in various life processes.*
4. *Apply simple methods of synthesis and characterization to nanomaterials.*

Unit I: Solid State Chemistry

Ionic Crystals and their structures, radius ratio rule, effect of polarization on crystals. Covalent structure type: Sphalerite and Wurtzite. Geometry of simple crystal AB type: NaCl, CsCl and NiAs. AB_2 type: Fluorite, antifluorites, Rutile structures. Li_2O, Na_2O, $CdCl_2$, CdI_2 structures.

Ternary Compounds ABO_3 type: Perovskite, Barium titanate, lead titanate, $CaTiO_3$, Tolerance factor, charge neutrality and deviation structures $FeTiO_3$.

Solids of AB_2O_4 type: Normal and inverse,2-3 and 4-2 spinel, packing of oxygen in tetrahedral and octahedral sites, sites occupancy number of sites surrounding each oxygen, application of charge neutrality principles, site preferences in spinel, distorted spinel. Hausmannite (Jahn-Teller distortions), Factors causing distortion in spinel.

Unit II: Organometallic Chemistry

Introduction of Organometallic Chemistry, counting of electrons, 16-18 rule, Ligand substitution reactions, Oxidative Addition: Concerted, S_N2 and radical mechanism, Reductive elimination, Migratory insertion and elimination reactions, Migration and insertion reactions Alpha-Migratory insertion and Alpha-Elimination Reactions, beta-migratory insertion, Beta-Elimination Reaction, Alpha-Abstraction and Beta-Abstraction, 4-Center Reactions [2+2] Reactions, External Attack by a Ligand and Reductive Coupling

Hydrogenation Reaction [mobohydride and dihydride catalyst] Stereoselective hydrogenation reaction, Wilkinson catalyst, Schrock-Osborn catalysts for hydrogenation, Carbonylation Reaction: Monsanto Acetic Acid Process, Hydroformylation, Hydrocarboxylation and Hydrocyanation, Ziegler-Natta polymerization

Palladium catalyzed cross-coupling reactions-Heck reaction, carbonylation, Wacker oxidation, Kumada, Stille, Sonogashira, Negishi and Suzuki coupling reactions and their importance, Applications of $Co_2(CO)_8$**,** $Ni(CO)_4$, $Fe(CO)_5$ and in organic synthesis. Transition metal carbenes, Fischer and Schrock carbenes, Olefin metathesis by I^{st} and II^{nd} generation catalyst, Schrock and Grubbs catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, application in the synthesis of homo and heterocyclic compounds, polymerization and synthesis of small organic molecules.

Unit -III

A) Metallo enzymes: The principle involved and role of various metals in i) Zn-enzyme: Carboxyl peptidase & Carbonic anhydrase. ii) Fe-enzyme: Catalase Peroxidase & Cytochrome P-450 iii) Cu-enzyme: Super Oxide dismutase iv) Molybdenum: Oxatransferase enzymes, Xanthine oxidase, Co-enzyme vitamin B_{12}, Structure of vitamin B_{12}. Co-C bond cleavage, Mutase activity of co- Enzyme B-12, Alkylation reactions of Methyl Cobalamin.

B) Electron transfer in biology: Structure and functions of metalloproteins in electron transfer proteins, cytochromes and Fe-S proteins, non-heme iron proteins; Rubredoxins, Synthetic models. Biological nitrogen fixation (*in-vitro* and *in-vivo*).

Unit-IV: Nanomaterials and Microscopic Techniques

A) Nanoparticles and nanostructure materials: Introduction, methods of synthesis: conventional and biogenic synthesis. Molecular Precursor routes to inorganic solids: Nanoporous Materials: Zeolites, metal oxides, composites & molecular sieves, composition-structure, preparation & applications.

B) Carbon-based nanomaterials: Introduction, synthesis methods: CNT, graphene-based materials, graphitic carbon nitride, quantum dot, carbon dot.

C) Techniques for nanomaterials authentication: X-Ray diffraction, Fourier Transform Infrared Spectroscopy, UV-Diffuse Reflectance Spectroscopy, X-ray Photoelectron Spectroscopy, Scanning Electron Microscopy, Transmission Electron Microscopy, Atomic Force Microscopy, Energy Dispersive X-Ray Analysis, Brunauer-Emmett-Teller analysis, Thermogravimetric Analysis.

References

1. Inorganic Chemistry, Third Edition, Shriver and Atkins, Oxford University Press.
2. Inorganic Chemistry, Fourth Edition, Catherine E. Housecroft and Alan G. Sharpe, Pearson, England.
3. Principles of Inorganic Chemistry, thirty third edition, B. R. Puri, L. R. Sharma, K. C. Kalia, Milestone Publisher & Disruptors, Delhi.
4. Organometallic Chemistry, Revised Second Edition, R. C. Mehrotra, A. Singh, New Age International Publication, New Delhi.
5. Basic Inorganic Chemistry, Third Edition, F. Albert Cotton, Geoffrey Wilkinson, John Wiley & Sons Inc.
6. Essentials of Bio-Inorganic Chemistry, Neerja Gupta, Monal Singh, Pragati Edition, Meerut.
7. Inorganic Chemistry, Gary L. Miessler and Donald A. Tarr, Pearson Education International, New York.
8. Inorganic Chemistry, Fourth Edition, James E. Huheey, Ellen A. Keitler, Richard L. Keitler, Pearson Education International, New York.

9. Emerging Nanomaterials and Their Impact on Society in the 21st century, N. B. Singh, Md. A.B. Hasan Susan, R.G. Chaudhary, Material Research Forum, Millerville, USA.
10. Concept and Models of Inorganic Chemistry, Third Edition, B. Douglas, D. McDaniel, J. Alexander, John Wiley & Sons Inc., New York.
11. Inorganic Chemistry, K. F. Purcell, J. C. Kotz, Cengage Learning, Delhi.
12. Nanoscale Materials in Chemistry, K. I. Kalbunde, John Wiley, New York.
13. Biogenic Sustainable Nanotechnology, R. P. Singh, A. R. Rai, A. Abdala, R. G. Chaudhary, Elsevier, Amsterdam, Netherland.
14. Introduction To Nanoscience and Nanotechnology, Chris Binns, John Wiley & Sons Inc., New York.
15. Carbon nanomaterials: synthesis, structure, properties and applications, R. Mathur, B. Singh, S. Pande, Taylor & Francis, Boca Raton.
16. Nanomaterials and Nanocomposites: Synthesis, Properties, Characterization Techniques, and Applications, R. K. Goyal, Taylor & Francis, Boca Raton.

SEMESTER III

Paper 11

MCH3T11**: Elective (a) Inorganic Chemistry Special-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student would be able to*

1. *Understand structure and bonding in transition metal pi complexes*
2. *Elaborate advance materials including supramolecules and advanced nanomaterials.*
3. *Classify and characterize the coordination polymers*
4. *Understand mechanism of photophysical and photochemical processes*
5. *Explain various redox processes in complexes.*

Unit-I

Transition Metal Pi Complexes-Carbon multiple bonds. Nature of bonding, structural characteristics and synthesis, properties of transition metal pi- Complexes with unsaturated organic molecules, alkenes alkynes, allyl, diene, dienyl, arene and trienyl complexes. Application of transition metal, organometallic intermediates in organic synthesis relating to nucleophilic and electrophilic attack on ligands, role in organic synthesis.

Unit-II

A) Supramolecular chemistry: Definition, intermolecular bonds, concepts and perspectives, cationic recognition, anionic recognition, neural molecular recognition: self-assembly concept and its application in molecular and supramolecular chemistry, supra molecular chemistry, supramolecular devices and machines.

B) Inorganic pharmaceuticals: Lithium drugs, gold antiarithritic drugs, Bismuth drugs in the treatment of gastric ulcers, Cyclams as anti-HIV agents, Radio-diagnostic agents, contrast agents for MRI and X-ray imaging.

C) Nano structural materials: Nanofibres, MXenes (two-dimensional inorganic compounds), Molecular Precursor routes to Nanoporous Materials: Zeolites and molecular sieves, porous lamellar solids, composition-structure, preparation and applications.

Unit-III

A) **Coordination Polymers**: Coordination polymers and their classification. Synthesis and applications of coordination polymers. Use of polymeric ligands in synthesis of coordination polymers. Organosilicon polymers. Synthesis and their uses.

B) **Characterization of coordination polymers on the basis of**:

i) Spectra (UV, Visible, IR and NMR)

ii) Magnetic and thermal (TGA, DTA and DSC) studies

Unit-IV

A] Photophysical and photochemical properties of Gold(I) complexes: Introduction, Binuclear and trinuclear complexes, Mixed metal Systems, Photochemical reactivity, Solid state studies, Mononuclear Gold(I) complexes, Mononuclear three coordinate Gold(I) complexes

B) Redox reactions by Excited Metal Complexes: Energy transfer under conditions of weak interaction and strong interaction – exciplex formation, conditions of excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2- bipyridine and 1,10-Phenanthroline complexes.), illustration of reducing and oxidizing character of ruthenium(II); role of spin-orbit coupling, lie time of these processes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants in to high energy products, chemical energy in to light.

C) Excited States of Metal Complexes: Electronically excited states of metal complexes, charge transfer spectra, charge transfer excitations, methods for obtaining charge transfer spectra.

References

1. Anderson J.C.,LeverK.D.,Alexander J.M and Rawlings,R.D.,ELBS
2. GrayG.W.Ed.Thermotropic Liquid Crystals,John Wiley
3. Kelkar and Hatz Handbook of Liquid Crystals,ChemieVerlag.
4. Kalbunde K.I.,Nanoscale Materials in Chemistry,JohnWiley,NY.
5. Shull R.D.,McMichael R.D. and SwartzendrubL.J.,Studies of Magnetic Properties of Fine particles and their relevance to Mataerials Science, Elsevier Pub. Amsterdam
6. Optoelectronic Properties of Inorganic Compounds, D. Max Roundhill and John P. Fakler, Jr. Plenum Press, New York

SEMESTER III

Paper 11

MCH3T11**: Elective (b) Organic Chemistry Special-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Learn the important aspects of steroids and terpenoids.*
2. *Understand the biosynthesis of natural products.*
3. *Analyze the enzyme reactions involved in various life processes*
4. *Illustrate the structure elucidation of unknown naturally occurring organic compound*
5. *Apply the knowledge of organic reactions for the total synthesis of useful natural products*

Unit I

A) Terpenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, and synthesis of the following representative molecules: Citral, Geraniol, α-terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β-carotene, Vitamin A.

B) Genesis of biological isoprene unit, Biosynthesis (**ONLY**) of the following tepenoids: myrecene, linalool, geraniol, α-terpeneol, limonene, camphor, α-pinene, β-pinene, farnesol, β-bisabolene and squalene.

Unit- II

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, generalmethods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring,role of alkaloids in plants Structure, stereochemistry, and total synthesis of the following: Ephedrine, (+)-coniine, Nicotine, Atropine, Quinine, Reserpine and Morphine.

Biosynthesis (**ONLY**) of the followings: hygrine, tropinone, nicotine, pelletierine, conine.

Unit-III

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and total synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone and Aldosterone. Biosynthesis of steroids (lanosterol)

Unit IV

A) Plant Pigments: Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteolin, Quercetin, Myrcetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Cyanidin-7-arabinoside, Cyanidin, Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and The Shikimate pathway: Biosynthesis of Cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavanoids.

B) Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE2 and PGF2 (E. J. Corey and Gilbert Stork synthesis only) and iodolactonization reaction.

References

1. Organic Chemistry Vol. II - I. L. Finar
2. Chemistry of Plant Natural Products: Sunil Kumar Talapatra and B. Talapatra (Springer)
3. Classical Methods in Structure Elucidation of Natural Products: *R. W. Hoffmann*, Wiley-VCH
4. A Fragrant Introduction to Terpenoid Chemistry: Charles S Sell (RSC)
5. Chemistry of Alkloids-S .W .Pelletier
6. Chemistry of Steroids-L .F .Fisher and M .Fisher
7. The Molecules of Nature-J .B .Hendricsion
8. Biogenesis of Natural Compound -Benfield
9. Natural Product Chemistry and Biological Significance -J .Mann, R .S Devison, J .B .Hobbs, D .V .Banthripde and J .B .Horborne
10. Introduction to Flavonoids-B .A .Bohm, Harwood
11. Chemistry of Naturally Occurring Quinines-R .H .Thomson
12. The Systematic Identification of Flavonoids -Marby, Markham, and Thomos

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Weblink to Equivalent MOOC on SWAYAM if relevant:

- Classics in total synthesis: Prof. Krishna P. Kaliappan, IIT Bombay (Useful for total synthesis of alkaloids, steroids and prostaglandins) https://archive.nptel.ac.in/courses/104/101/104101133/

SEMESTER III

Paper 11

MCH3T11**: Elective (c) Physical Chemistry Special-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Understand, the concept of statistical function, and applications*
2. *Understand the applications of electrochemistry in various fields*
3. *Understand the theories of advanced chemical dynamics*
4. *Understand the various photophysical processes and their applications*

UNIT I: ELECTRICAL AND THERMAL PROPERTIES OF SOLIDS

A) Classical free electron theory, electrical conductivity, thermal conductivity, Wiedemann-Franz Law, Lorenz number, Electronic distribution in solids using Fermi Dirac Statistics, The Fermi Distribution function and effect of temperature, Quantum theory of free electrons, periodic potential, The Kronig-Penney Model, Brillouin Zones, Distinction between metals, insulators and intrinsic semiconductors based on above theory.

B) Thermal Properties: Specific heat of solids, Classical theory, Einstein's theory of heat capacities, Debye theory of heat capacities or Debye T-cubed law.

UNIT II: ELECTROCHEMISTRY OF SOLUTION

A) OHP and IHP, potential profile across double layer region, potential difference across electrified interface; Structure of the double layer: Helmholtz-Perrin, Gouy Chapman model, Stern region, Graham Devanathan- Mottwatts, Tobin, Bockris, Devnathan Models.

B) Over potentials, exchange current density, derivation of Butler Volmer equation under near equilibrium and non-equilibrium conditions, Tafel plot

C) Electrical double lever, theories of double layer, electro-capillary phenomena, electro-capillary curve. Electro-osmosis, electrophoreses. Streaming and Sedimentation potentials. Zeta potentials and its determination by electrophoresis, influence of ions on Zeta potential.

UNIT III: CHEMICAL DYNAMICS - I

A) Dynamics of complex reactions: reversible, parallel, consecutive, concurrent and branching reactions, free radical and chain reactions, reaction between Hydrogen – Bromine and Hydrogen – Chlorine (thermal and photochemical), decomposition of ethane, acetaldehyde, N_2O_5, Rice Herzfeld mechanism, Oscillatory autocatalytic and Belousov-Zhabotinsky reactions, Lotka-Volterra mechanism, the brusselator and the oregonator.

B) **Fast Reactions:** relaxation methods, flow methods, flash photolysis, magnetic resonance method, relaxation time and numerical.

UNIT IV: PHOTOCHEMISTRY

A) **Photophysical phenomenon:** Introduction, photo and photochemical excitation and de-excitation, fluorescence, delayed fluorescence, and phosphorescence, fluorescence quenching: concentration

quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer between photoexcited donor and acceptor systems. Stern-Volmer relation, critical energy transfer distances, energy transfer efficiency, examples and analytical significance, bimolecular collisions, quenching and Stern-Volmer equation.

B) **Photochemical reactions:** photoreduction, photooxidation, photodimerization, photochemical substitution, photoisomerization, photosensitization, chemiluminescence, photochemistry of environment: Greenhouse effect.

References

1. G. M. Panchenkov and V. P. Labadev, " Chemical Kinetics and catalysis", MIR Publishing
2. E.A. Moelwyn- Hughes, "Chemical Kinetics and Kinetics of Solutions", Academic
3. K. J. Laidler, Chemical Kinetics, Third Edition (1987), Harper and Row, New York
4. J. Raja Ram and J. C. Kuriacose, Kinetics and Mechanism of Chemical Transformations MacMilllan Indian Ltd., New Delhi (1993)
5. J.G. Calvert and J.N. Pitts, Jr., Photochemistry, John Wiley and Sons, New York (1966).
6. K. K. Rohtagi-Mukherjee, Fundamentals of Photochemistry, New Age International, New Delhi(1986).
7. R. P. Wayne, Principles and Applications of Photochemistry, Oxford University Press, Oxford(1988).
8. N. J. Turro, Modern Molecular Photochemistry, Univ. Science Books, Sansalito (1991).
9. J. F. L. Lakowicz, Principles of Fluorescence Spectroscopy, 2nd Edition (1999), PlenumPublishers, NewYork.
10. F.W.Sears, " Introdction to Thermodynamics, Kinetic Theory of Gases and statistical mechanics". AddisonWesley
11. H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
12. M. C. Day and J Selbin, Theoretical Inorganic Chemistry, Reinhold Pub. Corp., New York,
13. N. J. Turro, V. Ramamurthy and J. C. Scaiano, Principles of Photochemistry – An Introduction, Viva Books, New Delhi, 2015.
14. G. A. Somorjai, Introduction to Surface Chemistry and Catalysis, Wiley, 2010.
15. M. C. Gupta, Statistical Thermodynamics, New Age International.
16. K. Huang, Statistical Mechanics, Wiley, New Delhi, 2003.
17. Andrew Maczek, Statistical Thermodynamics, Oxford University Press Inc., New York (1998).
18. B. K. Agarwal and M. Eisner, Statistical Mechanics, Wiley Eastern, New Delhi (1988).
19. D. A. McQuarrie, Statistical mechanics, Harper and Row Publishers, New York (1976).
20. J.O.M.Bokris and A.K.N.Reddy, "Modern Elcrtrochemistry". Wiley
21. S. Glasstone, "Introduction to Electrochemistry" Affilisated East West Press, New Delhi.
22. S. O. Pillai, Solid State Physics, New Age International, New Delhi, 2102.
23. D. R. Crow, " The Principle of electrochemistry", Chapman Hall
24. G. K. Agrawal, Basic Chemical Kinetics, Tata-Mc-Graw Hill Pvt., Ltd. 1990

25. K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol-VI, 2011.
26. Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.

NPTEL sources weblinks:

- Electrochemistry of solutions: https://archive.nptel.ac.in/courses/104/106/104106129/
- Chemical Dynamics https://nptel.ac.in/courses/104101128
- https://onlinecourses.nptel.ac.in/noc20_cy22/preview
- https://nsdl.niscpr.res.in/bitstream/123456789/251/1/Photochemistry%20revised.pdf

SEMESTER III

Paper 11

MCH3T11**: Elective (d) Analytical Chemistry Special-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *Explain the principles involved in radiation chemistry.*
2. *Compare various detectors used in radiochemistry and select among them for desired analysis.*
3. *Compare various voltammetric techniques for given type of analysis.*
4. *Understand the electrodes used in different voltammetric techniques and their comparison.*
5. *Design experiments for water quality assessment based on parameter under study.*

Unit-I: Radioanalytical Chemistry

Radioactivity, Law of radioactive decay, Half life and mean life, Elementary principles of GM and proportional counters, Gamma Ray Spectrometer, Ionization chamber, HPGe detector, NaI(Tl) detector**.** Preparation of some commonly used radioisotopes (^{22}Na, ^{60}Co, ^{131}I, ^{65}Zn, ^{32}P)**,** Use of radioactive isotopes in analytical and physico-chemical problems, Neutron Activation Analysis, Isotope Dilution Analysis, Radiometric titrations (Principle, Instrumentation, applications, merits and demerits), Radiochromatography, Carbon dating, Numericals based on above.

Unit-II: Stripping voltammetry

Stripping Voltammetry**:** Principle and technique in anodic and cathodic stripping voltammetry, applications to metal ion analysis, limitations**.**

Adsorptive stripping voltammetry: Principle, technique, applications to metal ions and organic analysis**.** Advantages over anodic stripping voltammetry**.** Catalytic effects in voltammetry**.**

Working electrodes: Mercury electrodes, carbon electrodes, film electrodes**.**

Electrochemical sensors (*Chemically modified electrodes****):*** Biosensors, catalytic sensors and gas sensors**.** Comparison of voltammetry with AAS and ICP-AES**.**

Unit-III: Electroanalytical methods

Electrogravimery: Theory of electrolysis. Electrode reactions. Decomposition potential. Overvoltage. Characteristics of deposits and completion of deposition. Instrumentation. Application in separation of metals.

Cyclic voltammetry**:** Principle and technique**.** Randles-Sevcik equation**.** Interpretation of voltammogram- reversible, irreversible and quasi-reversible systems**.** Applications of cyclic voltammetry in study of reaction mechanism and adsorption processes**.**

Unit IV: Water pollution and analysis

Sources of water pollution, composition of potable water, importance of water analysis, sampling and sample preservation, physico-chemical analysis of water. Mineral analysis (temperature, pH, conductivity, turbidity, solids, alkalinity, chloride, fluoride, sulphates, hardness), Demand analysis

(DO, BOD, COD, TOC), nutrients (nitrogen-total, nitrate, nitrite, phosphate) and heavy metals (As, Cd, Cr, Hg and Pb). A brief idea of coagulation and flocculation. Water treatment plants: Sand filters and other types of filters.

References

1. Essentials of Nuclear Chemistry: H. J. Arnikar (Willey Eastern Ltd)
2. Substoichiometry in Radioanalytical Chemistry: J. Ruzicka and J Stary (Pergamon Press)
3. Introduction to Radiation Chemistry: J. W. T. Spinks and R. J. Woods
4. Radiochemistry: A. N. Nesmeyanov (Mir Publications)
5. Instrumental Methods of Analysis: Willard, Meriit and Dean(Van Nostrand)
6. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
7. Vogel's Text Book of Quantitative Inorganic Analysis: Bassett, Denney, Jeffery and Mendham (ELBS)
8. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
9. Atomic Absorption Spectroscopy: Robinson (Marcol Dekker)
10. Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
11. Analysis of Water: Rodier
12. Laboratory manual of water analysis: Moghe and Ramteke (NEERI)
13. Electroanalytical chemistry: Joseph Wang
14. Electroanalytical stripping methods: Brainina and Neyman (Wiley-Interscience)
15. Trace analysis: S. Lahiri (Narosa Publishing House)
16. Electroanalytical Chemistry: Bard (Marcel-Dekker)
17. Chemistry in Engineering and Technology- Vol I and II: J.C. Kuriacose and J. Rajaram (Tata-McGraw Hill)

SEMESTER III

Practical 6

Practical based on Elective Paper (Any one of the four special practicals)

MCH3P06: Elective (a) Inorganic Chemistry Special Practical

4 h per week *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *Prepare various complexes by wet chemical methods.*
2. *Carry out characterization of prepared complexes.*
3. *Interpret the electronic and magnetic properties of complexes.*
4. *Elucidate the spin states of various complexes using susceptibility studies.*
5. *Deduce the structures of crystalline solids.*
6. *Carry out photochemical reactions in complexes*

A) Complex preparations: Preparation and characterization of following complexes/organometallic compound including their structural elucidation by the available physical methods**. (**element analysis molecular weight determination, conductance and magnetic measurement and special studies**)**

1. Preparation of *cis* and *trans* potassium dioxalatodiaquochromate(III)
2. Preparation of hexa-aminecobalt(III) chloride
3. Preparation of *tris* (acetylacetonato) manganese(III)
4. Preparation of N-N *bis* (salicyldehyde) ethylene diaminonato nickel(II)
5. Preparation of trinitrotriaminocobalt(III)
6. Preparation of chloropentammine cobalt(III) chloride
7. To prepare copper(II) acetylacetonate complex
8. To prepare *cis* and *trans* bis (glycinato) Cu(II) monohydrate complex
9. To prepare dipyridineiodine(I) nitrate
10. Preparation of ammonium nickel(II) sulphate
11. *Any other complex depending on availability of chemicals.*

* Minimum 5 complexes should be prepared.

B. Nanomaterials and Synthesis Techniques

1. Preparation of Metal oxides and mixed oxides Nanomaterials by Conventional Methods (NiO, ZnO, TiO_2, CuO, Fe_2O_3, Fe_3O_4, Co_3O_4, $ZnFe_2O_4$, $ZnMn_2O_4$, $CuAl_2O_4$ and $NiFe_2O_4$)
2. Preparation of Metal oxides and mixed oxides Nanomaterials by Biogenic Methods (NiO, ZnO, TiO_2, CuO, Fe_3O_4, Fe_2O_3, Co_3O_4, $ZnFe_2O_4$, $ZnMn_2O_4$, $CuAl_2O_4$ and $NiFe_2O_4$)
3. Preparation of graphene oxide via *Hummer's* Method.
4. Preparation of graphitic carbon nitride using Urea, Thiourea, Melamine.

C) Separation techniques

1. Paper and thin layer chromatography

2. Ion exchange
3. Solvent extraction

D) Bioinorganic Chemistry

1. Extraction and absorption spectral study of chlorophyll from green leaves of student choice.

2. Separation of chlorophyll and their electronic spectral studies.

3. Preparation of plant extract using different parts of different biological sources.

References

1. Advanced Inorganic Analysis, S. K. Agarwal, K. Lal, Pragati Edition, Meerut.
2. Practical Inorganic Chemistry, G. Pass, H. Sutcliffe, Springer.
3. Practical Inorganic Chemistry - Marr & Rocket
4. Basic Concept of Analytical Chemistry - Khopkar S. M.
5. Vogel A: A Textbook of Quantitative Inorganic Analysis, Longman
6. Preparation And Properties of Solid-State Materials – Wilcox, Vol. IV & II, Dekker
7. The Structure and Properties of Materials – Vol IV, John Wulff, Wiley Eastern
8. Dutt P. K.: General And Inorganic Chemistry (Sarat Book House)
9. Fenton, David E.: Biocoordination Chemistry, Oxford
10. Jolly, W. L.: Inorganic Chemistry (4^{Th} Ed) Addison-Wesley
11. Bertini, et al: Bioinorganic Chemistry (Viva)
12. Katakis, D. And Gordon, G: Mechanism of Inorganic Reactions (J. Wiley)
13. Nanomaterials and Nanocomposites: Synthesis, Properties, Characterization Techniques, and Applications, R. K. Goyal, Taylor & Francis, Boca Raton.
14. Biogenic Sustainable Nanotechnology, R. P. Singh, A.R. Rai, A. Abdala, R. G. Chaudhary, Elsevier, Amsterdam, Netherland.

SEMESTER III

Practical 6

MCH3P06: Elective (b) Organic Chemistry Special Practical

4 h per week *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Understand the types of reactions involved in organic synthesis.*
2. *Realize the various functional groups which are commonly present in simple organic molecules.*
3. *Develop skills to understand the reactions of different functional groups by the hands-on experience.*
4. *Characterize the synthesized compounds using IR spectroscopy*
5. *Draw the structures using Chem-Draw*

A) Organic preparations: Student is expected to carry out 4-7 two or three stage preparation from the following list. During preparation of organic compounds, the techniques such as crystallization, distillation, solvent extraction, TLC and column chromatography should be demonstrated.

1. Aniline → acetanilide →p-bromoacetanilide →p-bromoaniline
2. Aniline → Acetanilide →p-nitroacetanilide →p-nitroaniline
3. Benzaldehyde)thiamine hydrochloride→ (benzoin → benzil → benzilic acid
4. p-Nitrotoluene →p-nitrobenzoic acid→ PABA →p-iodobenzoic acid
5. p-Cresol → p-cresylacetate → 2-hydroxy-5-methyl acetophenone → 2-hydroxy chalcone
6. Benzophenone → Benzophenone oxime → Benzanilide → Benzoic acid +aniline
7. Aniline → aniline hydrogen sulphate → sulphanilic acid → Orange II
8. Aniline → N-arylglycine → indoxyl → indigo
9. Phthalimide → Anthranilic acid → Phenyl glycine-o-carboxylic acid → Indigo
10. Phalic anhydride → Phthalimide → Anthranilic acid → o-chlorobenzoic acid
11. Phalic anhydride → Phthalimide → Anthranilic acid →Diphenic acid
12. *Any other suitable three stage preparation as per the availability of chemicals*

B) Qualitative Analysis : Separation of the components of a mixture of three organic compounds)three solids, two solids and one liquid, two liquids and one solid, all three liquids and identification of any two components using chemical methods or physical techniques .Minimum 4-6 mixtures to be analyzed.

C) IR spectroscopy: The IR spectrum of minimum four synthesized compounds from the Section A should be interpreted.

D) Use of Computers- Chem Draw, Chem Sketch for drawing simple organic molecules, aliphatic and aromatic compounds should be demonstrated (2 hour activity).

References

1. Practical organic chemistry by FG Mann and BC Saunders
2. Text book of practical organic chemistry –by Vogel
3. The synthesis, identification of organic compounds –Ralph L. Shriner, Christine K.F. Hermann, Terence C. Morrill and David Y. Curtin

4. Compendious Practical Organic Chemistry: Preparations, Isolation, and Chromatography by Basavarajaiah S M, Nagesh G Y, Ramakrishna Reddy K
5. Advanced Practical organic chemistry by N.K. Vishnoi

SEMESTER III

Practical 6

MCH3P06: Elective (c) Physical Chemistry Special Practical

4 h per week *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Inculcate the potential of establishing any new laboratory at UG or PG level.*
2. *Execute the theoretical principles in practical*
3. *Analyze and interpret the results of their performances*
4. *Inculcate the skills of preparing, maintaining and developing the chemicals and reagents*
5. *Understand the role of laboratory safety and preparedness*

Thermodynamics:

1. Determination of partial molar volume of solute and solvent **(**ethanol-water, methanol-water, KCl-water mixture**)**

Solutions:

2. Study the variation of solubility of potassium hydrogen tartarate with ionic strength using a salt having a common ion and hence determine the mean ionic activity coefficients**.**
3. Determination of temp**.** dependence of the solubility of a compound in two solvents having similar intermolecular interactions**(**benzoic acid in water and DMSO – water mixture**)** and calculation of the partial molar heat of solution**.**

Phase equilibrium:

1. To study the effect of addition of an electrolyte such as NaCl, KCl,Na_2SO_4,K_2SO_4 etc**.** on the solubility of an organic acid**(**benzoic acid or salicylic acid**).**
2. To determine the heat of crystallization of $CuSO_4$,$5H_2O$
3. To determine the heat of reaction involving precipitation of a salt $BaSO_4$
4. To determine transition temperature of $CaCl_2$ by thermometric method and to determine transition temperature of $CaCl_2$, sodium bromide by solubility method

Kinetics:

1. To determine the activation energy of hydrolysis of an ester by acid**.**
2. Kinetics of reaction between sodium thiosulphate and KI**.** Determination of rate constant; study of influence of ionic strength
3. Kinetics of decomposition of H_2O_2 catalysed by iodide ion**.** Also determination of activation energy of reaction**.**
4. Clock reaction**-** activation energy of bromide**-**bromate reaction**.**
5. Temp dependence of persulfate**-**iodide reaction by iodine clock method and calculation of thermodynamic and Arrhenius activation parameters**.** Study of ionic strength effect on persulfate**-**iodide reaction**.**
6. Kinetics of B**-**Z reaction; Kinetics of modified B**-**Z reaction
7. Investigate the Autocatalytic reaction between potassium permanganate and oxalic acid**.**
8. Determination of pKa value of a weak acid by chemical kinetic method **(**formate**-**iodine reaction**)**

Conductometry:

1. Estimate the concentration of H_2SO_4, CH_3COOH, $CuSO_4.5H_2O$ in a given solution by carrying out conductometric titration against NaOH solution.
2. Determine the eq. conductance of strong electrolyte (KCl, NaCl, HCl, KNO_3) at several concentration and hence verify Onsager's equation.
3. Carry out the following precipitation titration conductometrically. a. 50 ml.0.02N $AgNO_3$ with 1N HCl; b.50 ml.0.02N $AgNO_3$ with 1N KCl; c. 50 ml 0.004 N $MgSO_4$ with 0.1 N $Ba(OH)_2$; d. 50 ml 0.002 N $BaCl_2$ with 1 N Li_2SO_4; e. 50 ml.0.02 N $BaCl_2$ with 1N K_2SO_4
4. To determine degree of hydrolysis of aniline hydrochloride and hence to determine the hydrolysis constant of salt by conductometric method.
5. To determine pK of weak acids, succinic acid, acetic acid, Malonic acids, (dibasic acids).
6. Complexation between $Hg^{2+}$and I^- conductometrically.
7. To determine solubility product of lead chromate.
8. Kinetic study of saponification ethyl acetate by conductometry.

Potentiometry:

1. To prepare calomel electrode and to determine the potential of calomel electrode by potentiometry.
2. To determine stability constant of Fe^{3+} with potassium dichromate in presence of dilute sulphuric acid by redox titration.
3. To determine solubility product of Silver chloride by potentiometric method.
4. Determination of redox potential of the couples(Fe^{2+}/Fe^{3+},Co^{3+}/Co^{2+},Cr^{3+}/Cr^{2+},MnO_4^- /Mn2+(any two) and equilibrium constant.
5. Study of complex formation by potentiometry e.g.Ag^+-S_2O_3-^{2}, Fe^{3+}-SCN^-,Ag^+-NH_3(any two) and calculation of stability constant.
6. Transport number by potentiometry.
7. To determine degree of hydrolysis of aniline hydrochloride and hence to determine the hydrolysis constant of salt by potentiometry method.
8. To determine pK of weak acids, succinic acid, acetic acid, Malonic acids, (dibasic acids).
9. Complexation between $Hg^{2+}$and I^- conductometrically.

Spectrophotometry:

1. To verify Beers law for solution of potassium permanganate and to find molar extinction coefficient.
2. To determine the indicator constant (pK_{In}) of methyl orange/red spectrophotometrically.
3. To determine the stability constant of reaction between Ferric ion solution and SCN^- ion solution by Job's method.
4. To determine the stability constant between Fe^{3+} and SCN^- ion solution by Ostwald and Frank method.

Polarography:

1. Determination of the half-wave potential of the cadmium ion in 1M potassium chloride solution.
2. Investigation of the influence of dissolved oxygen.
3. Determination of cadmium in solution.
4. Determination of lead and copper in steel.

Adsorption:

1. To verify Freundlich adsorption isotherm.
2. To verify Langmuir adsorption isotherm.
3. To verify Gibbs adsorption isotherm and to find surface excess concentration of solute.
4. Study of variation of surface tension of solution of n-propyl alcohol with concentration and hence determine the limiting cross section area of alcohol molecule

Transport Number:

1. To determine transport number by Hittorff's method
2. To determine the transport number by moving boundary method

References

1. Vogel A: A Textbook Of Quantitative Inorganic Analysis, Longman
2. Das and Behra, Practical Physical Chemistry
3. Carl W. Garland, Joseph W. Nibler and David P. Shoemaker, Experiments in Physical Chemistry, Mc-Graw Hill, 8th Edition, 2009.
4. Farrington Daniels, Joseph Howard Mathews, John Warren Williams, Paul Bender, Robert A. Alberty, Experimental Physical Chemistry, Mc-Graw Hill, Fifth Edition, 1956.
5. John W. Shriver and Michael George, Experimental Physical Chemistry, Lab Manual and Data Analysis, The University of Alabama in Huntsville, Fall 2006
6. Day And Underwood: Quantitative Analysis
7. Merits And Thomas: Advanced Analytical Chemistry
8. Ewing, G. W.: Instrumental Methods of Chemical Analysis, Mcgraw-Hill
9. Drago, R.S: Physical Methods in Inorganic Chemistry
10. Christian G.D: Analytical Chemistry
11. Khopkar S.M.: Basic Concept of Analytical Chemistry
12. Koltath And Ligane: Polorography
13. Braun: Instrumental Methods of Chemical Analysis
14. Willard, Merritt and Dean: Instrumental Methods of Chemical Analysis ,Van Nostrand
15. Strouts,Crifi; Llan And Wisin: Analytical Chemistry
16. Skoog S.A. And West D. W.: Fundamental of Analytical Chemistry
17. Dilts R.V.: Analytical Chemistry
18. Jahgirdar D.V : Experiments in Chemistry
19. Chondhekar T.K: Systematic Experiments in Physical Chemistry, Rajbhoj S.W., Anjali Pubn.
20. Wlehov G. J: Standard Methods of Chemical analysis 6th Ed

SEMESTER III

Practical 6

MCH3P06: Elective (d) Analytical Chemistry Special Practical

4 h per week *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *Understand the fundamental principles forming basis for the instrumental methods of analysis.*
2. *Select most suitable technique for the desired analysis.*
3. *Identify experimental conditions necessary to carry out the analysis of different samples.*
4. *Compare results obtained through different techniques.*
5. *Formulate experiments based on optical and electroanalytical techniques.*
6. *Demonstrate working of each instrument used in analysis.*

pH-metry

1. Determination of percent Na_2CO_3 in soda ash by pH-metric titration.
2. Determination of isoelectric point of amino acid.
3. Determination of three dissociation constants of phosphoric acid.

Conductometry

1. Estimation of acids in mixtures.
2. Displacement titration of CH_3COONa with HCl.
3. Precipitation titration of $MgSO_4$ and $BaCl_2$.
4. Titration of mixture of CH_3COOH, H_2SO_4 and $CuSO_4$ with NaOH.
5. Determination of dissociation constants of weak acids.

Potentiometry

1. Estimation of Cl^-, Br^- and I^- in a mixture.
2. Determination of percent purity of phenol by potentiometric titration with NaOH.
3. Estimation of acids in mixtures.
4. Potentiometric titration of phosphoric acid with NaOH.

Electrogravimetry

1. Estimation of nickel and copper individually as well as in mixture.

Spectrophotometry

1. Simultaneous determination of chromium and manganese in given mixture.
2. Simultaneous determination of two dyes in a mixture.
3. Estimation of Mn in steel.
4. Estimation of Cu/Ni in alloys.
5. Estimation of iron in water sample using 1,10-phenanthroline.
6. Estimation of Fe(III) in given solution by photometric titration with EDTA (salicylic acid method).

Flame photometry

1. Estimation of Li, Na, K, Ca in vegetable/ soil / water samples.

Polarography

1. Determination of $E_{1/2}$ of Cd^{2+} and Zn^{2+} at DME.
2. Estimation of Cd^{2+} and Zn^{2+} in respective solutions by calibration curve and standard addition methods.

Cyclic voltammetry

1. Study of cyclic voltammograms of $K_3[Fe(CN)_6]$.

Turbidimetry and nephelometry

1. Estimation of sulphate in water sample by turbidimetry.
2. Estimation of phosphate by nephelometry.
3. Determination of molecular weight of polymer.

Polarimetry

1. Determination of specific and molar rotation of optically active compound.
2. Kinetics of inversion of cane sugar in the presence of HCl.
3. Determination of percentage of two optically active substances (d-glucose and d-tartaric acid) in mixture.

References

1. Quantitative analysis**:** Day and Underwood **(**Prentice-Hall of India**)**
2. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3. Analytical Chemistry**:** Gary D**.** Christian **(**Wiley India**).**
4. Experiments and calculations in Engineering Chemistry- S. S. Dara (S. Chand and Co.)
5. Experiments in Chemistry-D. V. Jahagirdar (Himalaya)
6. Advanced Practical Chemistry-J. B. Yadav (Goel Publishing House)
7. Advanced Practical Chemistry-Jagdamba Singh (Pragati Prakashan)

SEMESTER III

Practical 7

MCH3P07: Research Project (RP)

8 h per week *100 Marks*

The objective of research project is to train the student in identifying the problem of research, develop the hypothesis, design the experiments/surveys to test the hypothesis, collect and analyse the data and draw conclusions from it. In addition, the aim is also to prepare the student to present the data in various forms such as project report, presentation in conferences and seminars and research paper. Research project is also aimed to prepare the student for doctoral research after the completion of the programme.

The student will have to carry out a research-based project work in the third and fourth semester. The project work may be carried out in the parent department or any other institute in collaboration with the parent institute. For this, the student will be attached to any of the national/regional/private research institute/organization for the duration of the third semester. If the student is working in the organisation other than the parent department, then it will be the responsibility of the student to attend the classes and other departmental activities in order to be eligible to appear for the examination. The student will be allotted the supervisor in the third semester; after which the student will finalize the topic of the project work in consultation with the supervisor.

The research project of the student will be evaluated on the basis of the project report submitted by him/her and the power point presentation made by him/her in the presence of internal and external examiner during the examination.

SEMESTER IV

Paper 12

MCH 4T12: Spectroscopy-II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Interpret the structures of simple molecules using physical methods of analysis*
2. *Understand and interpret the NMR data*
3. *Analyze X ray diffraction data*
4. *Develop the skills of analytical ability*
5. *Execute out the combined application of spectral method*

Unit I:

A) Ultraviolet and visible spectroscopy: Natural line width, line broadening, transition probability, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels. General nature of band spectra. Beer- Lambert Law, limitations, Frank-Condon principle, various electronic transitions, effect of solvent and conjugation on electronic transitions, Fieser Wooodward rules for dienes, aldehydes and ketones. Structure differentiation of organic molecules by UV Spectroscopy

B) Photoelectron spectroscopy: Basic principles, photoelectric effect, ionization process, Koopman theorem, PES and XPES, PES of simple molecules, ESCA, chemical information from ESCA, Auger electron spectroscopy.

Unit II:

Nuclear Magnetic Resonance Spectroscopy: Magnetic properties of nuclei, resonance condition, NMR instrumentation, chemical shift, spin spin interaction, shielding mechanism, factors affecting chemical shift, PMR spectra for different types of organic molecules, effect of deuteration, complex spin spin interaction (1^{st} order spectra), stereochemistry, variations of coupling constant with dihedral angle, electronegativity, Karplus equation etc., classification of molecules as AX, AX_2, AMX, A_2B_2, Shift reagents. NMR studies of ^{13}C, chemical shift in aliphatic, olefinic, alkyne, aromatic, heteroatomic and carbonyl compounds, ^{19}F, ^{31}P. Structure determination of organic molecules by NMR spectroscopy

Unit III:

A) Application of NMR spectroscopy: FT-NMR, advantages of FT-NMR, two-dimensional NMR spectroscopy-COSY, HETCOR, NOSEY, DEPT, INEPT, APT, INADEQUATE techniques, Nuclear Overhauser effect, use of NMR in medical diagnosis

B) Problems based on structure determination of organic molecules by using NMR (^1H and ^{13}C nuclei) data, Structure elucidation using combined techniques including UV, IR, NMR and mass spectrometry (based on data and copies of the spectra)

Unit IV:

Diffraction techniques: X ray diffraction: Braggs condition, Miller indices, Laue method, Bragg method, Debye Scherrer method, identification of unit cells from systematic absences in diffraction pattern, structure of simple lattices and x-ray intensity, structure factor and its relation to intensity and electron density, absolute configuration of molecules.

Electron diffraction: scattering intensity vs scattering angle, Wierl equation, measurement techniques, elucidation of structure of simple gas phase molecules, low energy electron diffraction and structure of surfaces.

Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques, elucidation of structure of magnetically ordered unit cell.

References

2. Spectroscopic identification of organic compound-RM Silverstein,GC Bassler and TC Morril, John Wally
3. Introduction to NMR spectroscopy-R. J. Abraham, J. Fisher and P Loftus Wiely
4. Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
5. Organic Spectroscopy-William Kemp, ELBS with McMillan
6. Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
7. Practical NMR Spectroscopy-ML Martin, JJ Delpench, and DJ Martyin
8. Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
9. Fundamentals of Molecular Spectroscopy-CN Banwell
10. Spectroscopy in Organic Chemistry-CNR Rao and JR Ferraro
11. Photoelectron Spectroscopy-Baber and Betteridge
12. Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten
13. NMR –Basic Principle and Application-H Guntur
14. Interpretation of NMR spectra-Roy H Bible
15. Interpretation of IR spectra-NB Coulthop
16. Electron Spin Resonance Theory and Applications-W gordy
17. Mass Spectrometry Organic Chemical Applications, JH Banyon

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Weblink to Equivalent MOOC on SWAYAM if relevant:

- Application of Spectroscopic Methods in Molecular Structure Determination https://nptel.ac.in/courses/101/104/104106075/

SEMESTER IV

Paper 13

MCH 4T13: Advanced Organic Chemistry II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Recognize the chemical reactions of carbonyl compounds and alkenes under photochemical conditions*
2. *Understand the stereochemistry of complex organic molecules*
3. *Apply the knowledge of enaolate chemistry in modern organic synthesis*
4. *Demonstrate the applications of stereochemistry of common organic reactions*
5. *Analyze the philosophy of synthesis of small molecules*

Unit I: Organic Photochemistry

Interaction of radiation with matter, types of excitation, rate of excited molecules, quenching, Quantum efficiency, quantum yield, transfer of excitation energy, singlet and triplet states, experimental methods in photochemistry of carbonyl compounds, and transition, Norrish type I and Norrish type II reactions Paterno–Buchi reaction, Photoreduction, Photochemistry of enones, Hydrogen abstraction rearrangement of unsaturated ketones and cyclohexadienones

Photochemistry of *p*-benzoquinones, photochemistry of aromatic compounds with reference to isomerization, addition and substitution Photochemical isomerization of *cis* and *trans* alkenes, Photochemical cyclization of reaction, Photo-Fries rearrangement, di-pi methane rearrangement, Photo theory reaction of anilides, photochemistry of vision, DeMayo reaction

Unit II:

Advanced Stereochemistry

A) Recapitulation of Stereochemical concepts- enantiomers, diastereomers, homo topic and heterotopic ligands, racemization and resolution methods, Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer, Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram's rule, Felkin Anh rule, Houk model, Cram's chelate model. Asymmetric synthesis, use of chiral auxiliaries, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation

B) Stereochemistry of fused and bridged ring systems: Nomenclature, synthesis; stereochemical aspects of Perhydrophenanthrene, Perhydroanthracene, hydrindane, Steroids; Bridged system (bi, tri and polycyclo system) including heteroatoms, Bredt's Rule. Conformations of following compounds with justification of each: *cis* and *trans*-1,3- and l,4-di-t-butyl-cyclohexanes; Cis-4-di-t-butylcis-2,5-dihydroxycyclohexane; Twistane; bicyclo-[2.2.2]octane; Trans-anti-trans-Perhydro-anthracene and the lactone; cyclohexane-l,4-dione; 1,2,2,6,6-penta-methyl-4- hydroxy-4-phenylpiperidine; ψ-tropine; 2-hydroxy-2-phenyl quinolizidine; 4-*t*-butyl-4-methyl-l,3-dioxane; *cis*-and *trans*-2,5-di-t-butyl-l,3-dithianes; *cis*-2,5-di-t-butyl-l,3,2- dioxaphosphorinan-2-one

Unit III:

Alkylation of enolates and other carbon nucleophiles: Generation and properties of enolates and other stabilized carbaions, regioselectivity and stereoselectivity in enolate formation from ketones and esters, alkylation of enolates of ketones, aldehydes, esters, carboxylic acids, amides, and nitriles, Generation and alkylation of dianions, intramolecular alkylation of enolates, control of enantioselectivity in alkylation reactions, The nitrogen analogs of enols and enolates: Enamine and imine anions

Reactions of carbon nucleophiles with carbonyl compounds: Aldol addition and condensation reaction, mechanism, Control of regioselectivity and stereoselectivity of aldol reacions of aldehydes and ketones, Aldol addition reactions of enolates of esters and other carbonyl derivatives, Reaction of (*E*) or (*Z*)-enolates with chiral aldehydes, The Mukaiyama aldol reaction, Control of facial selectivity in aldol and Mukaiyama aldol reaction, Intramolecular aldol reaction and the Robinson annulation, Evans aldol reaction, Mannich reaction, Conjugate addition of enolates, organomettalic reagents and cyanide ion, Conjugate addition with tandem alkylations, Control of facial selectivity in conjugate addition reaction

Unit IV: Designing the synthesis based on retrosynthetic analysis

A) Disconnection Approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis

B) One Group C-C Disconnections: Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis

C) Two Group C-C Disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalisedcompounds, Michael addition and Robinson annelation, Methods of ring synthesis, Linear and convergent synthesis

References

1. N. J. Turro, "Modern Molecular Photochemistry" (MMP), University Press, Menlo Park, CA, 1978
2. A. Gilbert and J. Baggott, "Essentials of Molecular Photochemistry," CRC Press, London, UK, 1991
3. J. Mattay and A. Griesbeck, eds., "Photochemical Key Steps in Organic Synthesis", VCH, New York, 1994
4. J. D. Coyle, ed., "Photochemistry in Organic Synthesis", Royal society of Chemistry, London, 1986
5. Stereochemistry of Organic Compounds Principles and Applications by D. Nasipuri, 3rd Edition, New Age International (P) Ltd Publishers
6. Basic Stereochemistry of Organic Molecules, 2nd Edition, Book Syndicate Pvt. Ltd

7. Basic Organic Stereochemistry by Ernest L. Eliel, Samuel H. Wilen and Michael P. Doyle, 2001 edition, Wiley Interscience.
8. Advance Organic Chemistry Part-B-F .A .Caray and R .J .Sundberg Plenum Press (Useful for Unit III)
9. Organic Chemistry, J .Clayden, N .Greeves, S .Warren and P .Wothers, Oxford University Press
10. Some Modern Methods of Organic Synthesis-W .Carruthers
11. Principles of Organic Synthesis by R. O. C. Norman and James M. Coxon (Nelson Thornes Ltd)
12. Modern Organic Synthesis: An Introduction by G. S. Zweifel and M. H. Nantz (Wiley)
13. Organic Synthesis by Michael Smith , 4th Edition (Academic Press)
14. Organic Synthesis: The Disconnection Approach-S. Warren
15. Designing Organic Synthesis-S. Warren

Weblink to Equivalent MOOC on SWAYAM if relevant:

- Organic Photochemistry and Pericyclic Reactions: Dr. N.D. Pradeep Singh Department of Chemistry IIT Kharagpur, https://nptel.ac.in/courses/104105038
- Pericyclic Reactions and Organic Photochemistry: Prof. Sankararaman, IIT Madras https://nptel.ac.in/courses/104/106/104106077/
- A Study Guide in Organic RetrosynthesisL Problem Solving Approach: Prof. Samik Nanda, IIT Kharagpur https://nptel.ac.in/courses/104105087
- Stereochemistry: Prof. Amit Basak, IIT Kharagpur https://nptel.ac.in/courses/104105086
- Stereochemistry and Applications: Prof. A. R. Choudhury, IISER Mohali https://nptel.ac.in/courses/104106127
- Structure, Stereochemistry and Reactivity of Organic Compounds and Intermediates: A Problem-solving Approach: Prof. Amit Basak, IIT Kharagpur https://nptel.ac.in/courses/104105127

SEMESTER IV

Paper 14

MCH 4T14**: Advanced Physical Chemistry**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Understand the types and behavior of solids based on their structure.*
2. *Estimate various dependent parameters of under different influences.*
3. *Understand solid state reactions and synthesis process.*
4. *Understanding nano chemistry.*
5. *Identification of crystals and their analysis.*

UNIT I: SOLID STATE AND THEIR MAGNETIC PROPERTIES

A**)** Solid State Chemistry**:** Metals, Insulators and Semiconductors, Electronic structure of solids-band theory**.** Band structure of metals, Insulators and Semiconductors, Intrinsic and Extrinsic Semiconductors, p-n junction, energy band formation, forward bias and reversed bias p-n junction, their applications, Superconductors— types, Meissner effect, BCS theory, Low Temperature Superconductor **(**LTSC**)** and High Temperature Superconductor **(**HTSC**)**, Conventional and organic Superconductors, their applications**.**

B**)** Magnetic Properties**:** Behaviour of substances in magnetic field, effect of temperature, Curie and Curie-weiss law, calculation of magnetic moments, magnetic materials, their structure and properties, Applications, structure/ property relations, numerical**.**

UNIT II: ELECTRICAL PROPERTIES OF MOLECULES

Dipole moments of molecules, basic ideas of electrostatic interactions, polarizability, orientation polarization, Debye equations, limitation of the Debye theory, Clausius-Mossotti equation**.** electrostatic of dielectric medium, molecular basis of dielectric behavior, structural information from dipole moment measurements, use of individual bond dipole moments, application to disubstituted benzene derivatives, dipole moment and ionic character of a molecule, determination of dipole moment from dielectric measurements in pure liquids and in solutions**.** The energies due to dipole-dipole, dipole induced dipole and induced dipole-induced dipole interaction**.** Dispersion, dielectric loss and refractive index**.** Lennard-Jones potential**.**

UNIT III: THIN FILMS AND LIQUID CRYSTALS

(A) Preparation techniques, evaporation/sputtering, chemical processes, MOCVD, sol-gel, etc. Langmuir Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

(B) Liquid crystals: Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases, smectic-nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular rearrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

UNIT-IV: CRYSTAL STRUCTURES

A) Introduction to crystals, Unit Cell and lattice parameters, Symmetry elements in crystals, Absence of fivefold axis, Space groups, The Bravais Lattices, Miller Indices, Bragg's Equation, seven crystal system, packing in crystals, Hexagonal Closest Packing (HCP) Cubic Closest Packing (CCP), Voids, packing fraction, Numerical.

B) **Lattice Defects:** Perfect and Imperfect crystals, point defects**,** Interstitial, Schottky defect, Frenkel defect, line defect and other entities, thermodynamics of Schottky and Frankel defects. Dissociation, theory of dislocation, plane defects- Lineage boundary, grain boundary, stacking fault, 3D defects, Defects and their concentrations, ionic conductivity in solids, Non stoichiometric compounds. Electronicproperties of Non-stoichiometric oxides.

References

1. S**.** O**.** Pillai, Solid State Physics, New Age International, New Delhi, 2102**.**
2. C**.**Kittel, **"** Introduction to solid state Physics**"**,Wiley
3. L**.**V**.**Azaroff, **"** Introduction to solids**"**, McGraw Hill

SEMESTER IV

Paper 15

MCH4T15: Elective (a) Inorganic Chemistry Special II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student would be able to

1. *Understand the types and behavior cerasmic and composite materials.*
2. *Elaborate various types of ceramics and cementataceous composites.*
3. *Discuss corrosion types, reasons and solutions to corrosion problem.*
4. *Comprehend industrial materials and water treatment techniques.*
5. *Prepare a subject platform for energy sources and renewable fuel sources.*

Unit-I

a. Ceramic Materials: Classification of ceramics, dielectric properties and polarization properties of ceramics, piezo-, pyro- and ferro-electric effect of ceramics, sol-gel processing of ceramics. Examples and application of ceramics: oxides, carbides, borides, nitrides.

b. Composite Materials: Definition, glass transition temperature,fibersfor reinforced plastic composite materials (i.e. glass fibers, carbon fibres, and aramid fibers); concrets and asphalt materials. Application ofcomposite material.

Unit-II

A) Cementitious Materials: Difference between Blended and Non-Portland cements; Non-portland cements; high alumina cements, calcium sulfoaluminate cements, phosphate cements.Chemicals in cement hydration; hydration process, set retardersandaccelerators, plasticizers, slip-casting processing. Application of cementitousmaterials.

B) Bio-materials: Definition of biomaterials and biocompatibility;, Type of bio-materials: Metallic materials, Biopolymeric materials, Bioceramic materials (dense hydroxyapatite ceramics, bioactive glasses,and bioactive composites); Basic requirement of bone implants; Coating of hydroxyapatite on porous ceramics; Biomaterials in tissue attachments; Application of Biomaterials

Unit-III

A) Inorganic Chemicals as metallic Corrosion Inhibitors: Introduction, Principles of corrosion inhibitors, corrosion as an electrochemical process, Practical aspects of corrosion inhibition, Anion inhibitor properties in neutral electrolytes, some application of corrosion inhibitors (cooling water circulation-once through and open systems, engine radiation & cooling systems, central heating system, refrigeration plants and high chloride systems, water for steam raising, corrosion inhibitors for paintcoating).

B) Industrial gases: Introduction, Separation of gases from air,Hydrogen, Carbon dioxide, Carbon monoxide, Oxygen, Acetylene, Sulphur dioxide, Nitrous oxides.

C) Chemical explosives and propellants: Introduction, Potential energy of explosives , Properties of explosives, Manufacture of explosives , Explosives made by nitration, Dynamite , Commercial

high explosives containing no nitroglycerine , Initiating devices, Sporting and military explosives, Disruptive explosives for military use, Handling and storage of explosives.

Unit-IV

A) Applications of Biotechnology for the treatment of waste water: Introduction, Role of microorganism for the treatment of waste water, Application of biotechnology for a. high strength waste. b. Primary and secondary sludge c. Phenol & cyanide removal d. Solid phase extraction

B) Energy sources for future:

a. Solar Energy-Solar heating for homes and other buildings, electricity from solar thermal power collectors, electricity from photovoltaic cells.

b. Energy from biomass- Production of biomass, biofuels, biodiesel.

c. Geothermal energy,

d. water power

e. Tidal power.

f. Fuel Cells-Polymer electrolyte membrane fuel cells, Phosphoric acid fuel cell, Direct methanol fuel cell, Alkaline fuel cell, Regenerative(reversible) fuel cell, Clean cars for the future, Energy sources for the twenty first century.

References

1. Handbook of Industrial Chemistry,Vol.1, by K.H.Davis,F.S.Berner,Edited by S.C. Bhatia (CBS Publishers, Bangalore,2004)
2. Industrial inorganic chemistry, Karl Heinz Buchel, Hans-Heinrich Moretto, Peterwoditsch
3. Modern Electroplating, By M. Schlesinger and M. Paunovic (John Wiley and sons, Hoboken , New Jersey, 5th Edition2010)
4. Insight into Specialty Inorganic Chemicals-David Thompson (The Royal Society of Chemistry,1995)- Chapter 15.
5. New Trends in Green Chemistry (2nd Edition)-V.K.Ahluwalia and M.Kidwai (AnamayaPublishers, 2007)
6. Environmental Chemistry by A. K. Bagio.
7. Principles of Environmental Chemistry by James Girard Bartlett Publishers.
8. Waste Water Engineering by Calf& Eddy.
9. Waste Water treatment for pollution control by Arceivala.
10. Principles of water quality Control by T. H. Y Tebbut.
11. Manual on Sewage &Sewage treatment, Ministry of Works, New Delhi.

SEMESTER IV

Paper 15

MCH4T15: Elective (b) Organic Chemistry Special-II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Understand the reactivity of organometallic compounds*
2. *Demonstrate the applications of organometallic reagents in C-C bond formation*
3. *Understands the reactivity of heterocyclic compounds in various reaction conditions*
4. *Understand the electrophilic, nucleophilic reactions and synthesis of various heterocycles*
5. *Justify the need of protecting groups in organic synthesis*

Unit I:

Organometallic compounds of Group I and II Metals: Synthesis and applications of organolithium and organomagnesium reagents, nucleophilic addition to aldehyde, ketones, ester, epoxide, CO_2, CS_2, isocyanates, ketenes, imines, amides, lactones, Stereochemistry of Grignard addition to carbonyl compounds, *o*-metallation of arenes using organolithium compounds, Organocopper reagents: Preparation and applications in C-C bond forming reaction, mixed oragnocuprates, Gilman's reagent. Organo Hg and Cd reagents in organic synthesis, Reformatsky reaction, Barbier reaction

Unit II: Heterocycles-I

a) Ring Synthesis: Introduction, Cyclization reactions: Reaction types, displacement at saturated carbon, intramolecular nucleophilic addition to carbonyl groups, intramolecular addition of nucleophiles to other double bonds, cyclizations on to triple bonds, radical cyclizations, cabene and nitrene cyclization, electrocyclic reactions, reactions and structural effects of heterocyclic rings, ,3 - dipolar cycloadditions producing five - membered heterocycles, Hetero Diels-Alder reaction, [2+2] cycloaddition, ene reactions, Palladium catalysis in the synthesis of Benzo - Fused heterocycles

b) Three and four membered heterocylces: Aziridines, Oxiranes, Thirienes, Azetidines, Oxetanes and Thietanes

C) Azoles: Structural and chemical properties; Synthesis of pyrazole, isothiazole and isoxazole; Synthesis of imidazoles, thiazoles and oxazoles; Nucleophilic and electrophilic substitutions; Ring cleavages, Carbonyldiimidazole as coupling agent

Unit III: Heterocycles-II

A) Benzofused heterocycles: Synthesis of indole, benzofuran and benzo-thiophene, quinoline and isoquinoline Nucleophilic, electrophilic and radical substitutions; Addition reactions; Indole rings in biology, Synthesis and reactions of coumarin

B) Diazines: Structural and chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines; Nucleophilic and electrophilic substitutions.

C) Synthesis of following bioactive compounds: Vitamin B6, Ondansetron, Serotonin, Indometacin, Cyanamid, fentiazac, trimethoprim, papaverine

Unit IV:

A) Protection and de-protection of functional group in organic synthesis: Hydroxyl group- alkyl ether, benzyl ether,acyl, PMB, Trityl, TMS, TBDMS, THP, MOM, MEM, MIP ether; Diol- Acetone, Cyclohexanone; Amines- Benzyl, Acyl, CBZ, BOC, FMOC, Carboxyl group-Ester, DCCI, DIPCDI; Ketone and aldehydes- Glycol, Thioglycol, Ketal, Acetal; Othroesters as protecting groups, Protection deprotection approach - In Solid phase synthesis of polypeptide

B) Total synthesis selected molecules: FR-900848, cubane, biotin, longifolene and taxol, Endiandric Acid A, B, C and D

References

1. Organometallics: A concise Introduction, Ch. Elshebroicn and A. Salzer, VCH, chapters, 12-16
2. Organotransition Metal Chemistry: Applications to Organic Synthesis, S.G. Davies, Permagaon 1982.
3. Organometallics in Organic Synthesis – Swan & Black
4. Organometallic Chemistry - E.J. Elias and Gupta
5. Aromatic Heterocyclic Chemistry (Oxford Chemistry Primers) by David T. Davies
6. Heterocyclic Chemistry (3rd Edition) by Thomas. L. Gilchrist (Useful for Unit II)
7. Heterocyclic Chemistry by John A. Joule and K. Mills
8. The Chemistry of Heterocycles: Structure, Reactions, Syntheses, and Applications by Theophil Eicher and Siegfried HauptmannPrincipal of Modern Heterocyclic Chemistry-L .A .Paquelte
9. Heterocyclic Chemistry-Morton
10. An Introduction to Chemistry of Heterocyclic Compound-J .B .Acheson
11. Heterocyclic Chemistry by Dr Thomas. L. Gilchrist 3rd edition (Prentice Hall) for Unit II
12. Protective Groups in Organic Synthesis-T. W. Greene
13. Organic Chemistry, J .Clayden, N .Greeves, S .Warren and P .Wothers, Oxford University Press
14. Modern Organic Synthesis: An Introduction by G. S. Zweifel and M. H. Nantz (Wiley)

Weblink to Equivalent MOOC on SWAYAM if relevant:

- Organometallic Chemistry: Prof. D. Maiti, IIT Bombay
  https://nptel.ac.in/courses/104/101/104101079/
- Metal Mediated Synthesis: Prof. D. Maiti, IIT Bombay
  https://nptel.ac.in/courses/101/104/104101092/
- Transition Metal Organometallics in Catalysis and Biology: Prof. P. Ghosh, IIT Bombay
  https://archive.nptel.ac.in/courses/104/101/104101123/
- Classics in total synthesis: Prof. Krishna P. Kaliappan, IIT Bombay
  https://archive.nptel.ac.in/courses/104/101/104101133/
- Heterocyclic Chemistry: Prof. D. R. Mal, IIT Kharagpur
  https://archive.nptel.ac.in/courses/104/105/104105034/

SEMESTER IV

Paper 15

MCH4T15: Elective (c) Physical Chemistry Special-II

60 h (4 h per week): 15 h per unit *100 Marks*

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

1. *Execute the chemical dynamical calculations and research applications*
2. *Understand the applications of electrochemistry in industrial as well as research applications*
3. *Analyze the applications of radiation chemistry*
4. *Gain the knowledge of battery technology and their operations so as to work in the concerned research field*
5. *Understand, analyze and execute the concepts of quantum mechanics in various fields*

UNIT-I CHEMICAL DYNAMICS - II

A) Overview of Arrhenius rate law, Non-conventional equilibrium between reactants and activated complexes. Potential energy surfaces and reaction coordinate. Derivation of transition state theory-based equation for rate constant of bimolecular reaction. Prediction of rate constant using partition function and comparison with that given by collision theory. Arrhenius equation and activated complex theory. Transmission coefficient, quantum mechanical tunneling,

B) Reactions in solution: Cage effect, diffusion-controlled reactions, volume of activation its determination and correspondence with entropy of activation, Ionic reactions: Primary (Ionic strength) and Secondary salt effect and their nature.

UNIT II CORROSION AND CORROSION ANALYSIS

A) Scope and economics of corrosion, causes (Change in Gibbs free energy), Electrochemical Series and Galvanic series, dry (atmospheric) and wet (electrochemical) corrosion, other types of corrosion-Pit, Soil, chemical and electrochemical, inter-granular, waterline, microbial corrosion, measurement of corrosion by different methods, factors affecting corrosion, passivity, galvanic series, protection against corrosion, design and material selection.

B) Thermodynamics of corrosion, corrosion measurements (Weight loss, OCP measurements, polarization methods), passivity and its breakdown, corrosion prevention (electrochemical inhibitor and coating methods).

UNIT – III: RADIATION CHEMISTRY AND BATTERY TECHNOLOGY

A) Interaction of radiation with matter, radiation track spurs and γ-rays. Linear energy transfer, Bathe's equation for linear energy transfer, Bresstrahlung effect, Passage of neutron through matter, Interaction of γ -radiation with matter, photoelectric effect and Compton effect, pair production phenomena, units of measuring radiation absorption, Chemical Dosimeters, Fricke Dosimeter and Ceric Sulphate Dosimeter, Conversion of measured dose values, Radiolysis of water, Radiolysis of some aqueous solutions. Effect of radiation on biological substances, genetic effects, Radiation effects on organic compounds and Polymers.

B) Battery Technology: basic concept, classification of batteries, primary, secondary and reserve batteries, Construction, working and application of Acid Storage batteries, Lithium -MnO_2

batteries, Nickel- Metal hydride batteries, Fuel Cells, Construction and working of $H_2O_2$and methanol-O_2 Cell.

UNIT IV: THE LIQUID STATE AND SOLUTIONS

A] Introduction, The van der Waals Approximation, Cell theory, Hole Theory, Radial Distribution Function Methods, Radial Distribution Functions and the Thermodynamic Functions, Other Theories, Applications of these theories.

B] Introduction to solutions, Lattice Models, Ideal solutions, non-ideal or regular Solutions (Bragg-Williams Approximation), Incomplete Miscibility, Dilute Solutions, Polymer Solutions.

References

1. G.M.Panchenkov and V.P.Labadev, " Chemical Kinetics and catalysis", MIR Publishing
2. E.A. Moelwyn- Hughes, " Chemical Kinetics and Kinetics of Solutions", Academic
3. K.J.Laidler, Chemical Kinetics, Third Edition (1987), Harper and Row, New York
4. J.Raja Ram and J.C.Kuriacose, Kinetics and Mechanism of Chemical Transformations McMilllan IndianLtd., New Delhi (1993)
5. C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, **Vol 1**., Elsevier Publications, New York, 1969.
6. Gholam-Abbas Nazri, Gianfranco Pistoia, Lithum Batteries-Science and Technology, Springer, 2003.
7. C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, **Vol 2**., Elsevier Publications, New York, 1969.
8. S. Glasstone, K. J. Laidler and H. Eyring, The Theory of Rate Processes, Mc-Graw Hill, New York, 1941.
9. Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
10. D. Mcquarie and J. Simon, Physical Chemistry – A Molecular Approach, University Press, 2000
11. G. M. Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.
12. H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
13. S. O. Pillai, Solid State Physics, New Age International, New Delhi, 2102.
14. C.Kittel, **"** Introduction to solid state Physics**"**,Wiley
15. L.V.Azaroff, **"** Introduction to solids**"**, McGraw Hill
16. Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
17. N. B. Hanny, Treaties in Solid State Chemistry, 4th Edn,
18. N. B. Hanny, "Solid State Chemistry"
19. M. C. Day and J Selbin, Theoretical Inorganic Chemistry, Reinhold Pub. Corp., New York,
20. C.N.Rao. Nuclear Chemistry
21. B. G. Harvey, Introduction to Nuclear Physics and Chemistry, Prentice Hall, Inc. (1969).
22. H.J. Arnikar, Essentials of Nuclear Chemistry, 4th Edition (1995), Wiely-Eastern Ltd., New Delhi.

23. W. Loveland, D. Morrissey and G. Seaborg, Modern Nuclear Chemistry, Wiley-Interscience, 2006.
24. P. P. Milella, Fatigue and Corrosion in Metals, Springer, 2013.
25. Corrosion- Understanding the Basics, asminternational.org, 2000.
26. H. H. Uhlig, Corrosion and Corrsion Control – 3rd edn, John Wiley and sons, New York.
27. J. W. T. Spinks and R. J. Woods, An Introduction to Radiation Chemistry, John Wiley and sons., New Yoek, 1975.
28. K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol-VI, 2011.

SEMESTER IV

Paper 15

MCH4T15: Elective (d) Analytical Chemistry Special-II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *Understand the fundamental principles forming basis for the instrumental methods of analysis.*
2. *Select most suitable technique for the desired analysis.*
3. *Identify experimental conditions necessary to carry out the analysis of different samples.*
4. *Formulate experiments based on optical and electroanalytical techniques.*
5. *Demonstrate working of each instrument used in analysis.*

Unit-I: Optical methods of analysis-IV

Inductively coupled plasma-atomic emission spectroscopy: Principle, atomization and excitation**.** Plasma source and sample introduction**.** Instrumentation**.** Comparison of ICP-AES with AAS**.** Applications**.**

X-ray fluorescence spectroscopy: Principle**.** Instrumentation**:** wavelength and energy dispersive devices**.** Sources and detectors**.** Comparison between wavelength and energy dispersive techniques**.** Sample preparation for XRF**.** Matrix effects in XRF**.** Applications in qualitative and quantitative analysis**.**

Electron microscopy: Principle, instrumentation and applications of scanning electron microscopy **(**SEM**)** and transmission electron microscopy **(**TEM**)**

Unit-II: Electrochemical methods of analysis-IV

Ion selective electrodes: Theory of membrane potential**.** Types of ion-selective electrodes**.** Construction of solid state electrodes, liquid membrane electrodes, glass membrane electrodes and enzyme electrodes, Selectivity coefficients, Glass electrodes with special reference to H^+, Na^+ and K^+ ions**.** Applications of ISE in analysis of environmentally important anions like F^-, Cl^-, Br^-, I^-, NO_3^- and CN^-**.** Advantages of ISE**.**

Coulometry**:** Principle**.** Coulometry at constant potential and constant current**.** Instrumentation**.** Applications and advantages of coulometric titrations**.**

Electrochemical microscopy**:** Introduction to scanning probe microscopy **(**SPM**)**, scanning tunneling microscopy **(**STM**)**, atomic force microscopy **(**AFM**)** and scanning electrochemical microscopy **(**SECM**).**

Unit-III: Thermal methods of analysis

Introduction to different thermal methods, Thermogravimetry (TG and DTG), Static thermogravimetry, quasistatic thermogravimetry and dynamic thermogravimetry, Instrumentation-Balances, X-Y recorder, Stanton-Redcroft TG-750, Thermogram, Factors affecting thermogram, Applications of thermogravimetry, Differential Thermal Analysis (DTA)- Theories, DTA curves, Factors affecting DTA curve, Applications of DTA, simultaneous determination in thermal analysis, Differential Scanning Calorimetry (DSC)- Introduction, Instrumentation, DSC curves, factors affecting DSC curves, applications, Thermogravimetric titration-Theory, Instrumentation and applications.

Unit-IV: Air pollution and analysis

Air pollution and analysis-classification of air pollutants, sources of air pollution and methods of control, sampling of aerosols and gaseous pollutants and their effects, SO_2, NO_2, CO, CO_2, particulates-SPM, RSPM, High Volume Sampler, Fabric Filters, Cyclones (direct and Reverse), ESP, ozone layer, Green house effect, Heat Islands, Acid Rain.

References

1. Essentials of Nuclear Chemistry: H. J. Arnikar (Willey Eastern Ltd)
2. Substoichiometry in Radioanalytical Chemistry: J. Ruzicka and J Stary (Pergamon Press)
3. Instrumental Methods of Analysis: Willard, Meriit and Dean(Van Nostrand)
4. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
5. Vogel's Text Book of Quantitative inorganic Analysis: Bassett, Denney, Jeffery,Mendham (ELBS)
6. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
7. Atomic Absorption Spectroscopy: Robinson (Marcel Dekker)
8. Instrumental Methods of chemical Analysis: Braun (Tata McGraw-Hill)
9. Radiochemistry: A. N. Nesmeyanov (Mir Publications)
10. Analysis of Water: Rodier
11. Ion selective electrodes: Koryta (Cambridge University Press)
12. Industrial Chemistry: Arora and Singh (Anmol Publications)
13. Diffraction Methods: John Wormald (Clarendon Press)
14. Electroanalytical Chemistry: Bard (Dekker)
15. Analytical Chemistry by Open Learning (Wiley)
16. An Introduction to Electron Diffraction: Beeston (North Holand Publishing Co.)
17. Material Science and Engineering: V. Raghavan (Printice-Hall of India)
18. Practical Physical Chemistry: J. B. Yadav (Goel Publishing House)
19. Indian Pharmacoepia, Vol-I, II and III.

Web link for related NPTEL courses

Analytical Chemistry: https://nptel.ac.in/courses/104105084

SEMESTER IV

Practical 8

MCH4P08: Major Research Project

12 h per week *200 Marks*

The objective of research project is to train the student in identifying the problem of research, develop the hypothesis, design the experiments/surveys to test the hypothesis, collect and analyse the data and draw conclusions from it. In addition, the aim is also to prepare the student to present the data in various forms such as project report, presentation in conferences and seminars and research paper. Research project is also aimed to prepare the student for doctoral research after the completion of the programme.

The student will have to carry out a research-based project work in the third and fourth semester. The project work may be carried out in the parent department or any other institute in collaboration with the parent institute. For this, the student will be attached to any of the national/regional/private research institute/organization for the duration of the fourth semester. If the student is working in the organisation other than the parent department, then it will be the responsibility of the student to attend the classes and other departmental activities in order to be eligible to appear for the examination. The student will be allotted the supervisor in the third semester; after which the student will finalize the topic of the project work in consultation with the supervisor.

The research project of the student will be evaluated on the basis of the project report submitted by him/her and the power point presentation made by him/her in the presence of internal and external examiner during the examination.