University of Rajasthan
Jaipur

SYLLABUS

M.Sc. (CHEMISTRY)

(Semester Scheme)

I & II Semester Examination 2022-23

III & IV Semester Examination 2023-24

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M.Sc. CHEMISTRY

Syllabus :

Credit-based Semester System with continuous assessment.

To acquire a Master degree in Chemistry, a candidate is required to earn minimum of 120 credits with grade E or higher.

Credit registration at least once in all Compulsory Credit Course (CCC) and earning all credits for accumulation of the prescribed minimum credit with grade E or higher grade in all CCC will be binding.

SCHEME OF EXAMINATION:

- Each Semester shall have continuous assessment which shall include internal assessment in theory and practical by internal examination/seminar/oral examination/viva-voce etc, besides assessment of candidate's regularity and performance in the class.
- A candidate has to pass in the continuous assessment as well as EoSE (End of Semester Examination) paper separately.
- Each EoSE of theory paper shall carry 100 marks and will be of 3 hours duration. Candidate has to attempt five (05) questions in all. All questions carrying equal marks.
- Part 'A' of the theory paper shall contain 10 Short Answer Questions of total 20 marks, based on knowledge, understanding and applications of the topics/texts covered in the whole syllabus. Each question will carry two (02) marks for correct answer.
- Part 'B' of the theory paper will have total four questions of 20 marks each, framed by taking one question from each unit with internal choice. The limit of answer will be five pages.
- Each Laboratory EoSE will be of six hours durations and involve laboratory experiments/exercises, record and viva-voce examination with weightage in ratio of 75:25.
- The Practical examination will be conducted by board of examiners consisting of one internal (to be appointed by the Head of Department) and one external examiner (to be appointed by the University).
- The medium of instruction and examination shall be English only.

COURSE STRUCTURE

The Credit Courses of the programme have been classified as below:

- CCC: Compulsory Core Course
- ECC: Elective Core Course
- SSC: Self Study Course
- PRJ: Project Work

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M.Sc. Chemistry I & II Semester III & IV Semester

FIRST SEMESTER

S. No	Subject Code	Course Title	Course Category	Credit	Contact Hours/week				EoSE (hrs)
					L	T	P	Th	P
1.	CHE 701	Advanced Inorganic Chemistry-I	CCC	4	4	0	0	3	0
2.	CHE 702	Organic Reaction Mechanism	CCC	4	4	0	0	3	0
3.	CHE 703	Quantum, Surface and Electrochemistry	CCC	4	4	0	0	3	0
4.	CHE 711	Chemistry Core Laboratory-1	CCC	6	0	0	9	0	6
5.	CHE A01	Spectroscopy – I	ECC	4	4	0	0	3	0
6.	CHE A02	Analytical Techniques	ECC	4	4	0	0	3	0
7.	CHE A03	Green and Sustainable Chemistry	ECC	4	4	0	0	3	0
8.	CHE A11	Elective Laboratory-1	ECC	6	0	0	9	0	6

SECOND SEMESTER

S. No	Subject Code	Course Title	Course Category	Credit	Contact Hours/week				EoSE (hrs)
					L	T	P	Th	P
1.	CHE 801	Advanced Inorganic Chemistry – II	CCC	4	4	0	0	3	0
2.	CHE 802	Stereochemistry and Organic Reaction Mechanism - II	CCC	4	4	0	0	3	0
3.	CHE 803	Thermodynamics and Chemical Kinetics	CCC	4	4	0	0	3	0
4.	CHE 811	Chemistry Core Laboratory-2	CCC	6	0	0	9	0	6
5.	CHE A04	Spectroscopy – II	ECC	4	4	0	0	3	0
6.	CHE A05	Environmental Chemistry	ECC	4	4	0	0	3	0
7.	CHE D01	Biomolecules – I	ECC	4	4	0	0	3	0
8.	CHE A12	Elective Laboratory – 2	ECC	6	0	0	9	0	6

THIRD SEMESTER

S. No	Subject Code	Course Title	Course Category	Credit	Contact Hours/week				EoSE (hrs)
					L	T	P	Th	P
1.	CHE 901	Organotransition Metal Chemistry	CCC	4	4	0	0	3	0
2.	CHE 902	Organic Synthesis – I	CCC	4	4	0	0	3	0
3.	CHE 903	Bio-Physical Chemistry	CCC	4	4	0	0	3	0
4.	CHE 911	Core Laboratory – 3	CCC	6	0	0	9	0	6
5.		Theory Elective – 1	ECC	4	4	0	0	3	0
6.		Theory Elective – 2	ECC	4	4	0	0	3	0
7.		Theory Elective – 3	ECC	4	4	0	0	3	0
8.		Elective Laboratory-3	ECC	6	0	0	9	0	6

FOURTH SEMESTER

S. No	Subject Code	Course Title	Course Category	Credit	Contact Hours/week				EoSE (hrs)
					L	T	P	Th	P
1.	CHE X01	Solid States and Nanomaterials	CCC	4	4	0	0	3	0
2.	CHE X02	Organic Synthesis – II	CCC	4	4	0	0	3	0
3.	CHE X03	Advanced Physical Chemistry	CCC	4	4	0	0	3	0
		Theory Elective – 1	ECC	4	4	0	0	3	0
		Theory Elective – 2	ECC	4	4	0	0	3	0
		Theory Elective – 3	ECC	4	4	0	0	3	0
		Project Work	PRJ	10					

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Elective Core Courses (ECC) groups

A: Integrated / Allied Chemistry

B: Inorganic Chemistry group

C: Physical Chemistry group

D: Organic Chemistry group

E: Pharmaceutical Chemistry group

S. No.	Course Code	Elective Paper Title	Prerequisite	Semester
1.	CHE A01	Spectroscopy – I		I
2.	CHE A02	Analytical Techniques		I
3.	CHE A03	Green and Sustainable Chemistry		I
4.	CHE A04	Spectroscopy – II		II
5.	CHE A05	Environmental Chemistry		II
6.	CHE B01	Bioinorganic Chemistry	-	III
7.	CHE B02	Supramolecular Chemistry	-	III
8.	CHE B03	Inorganic Polymers	-	III
9.	CHE B04	Advanced Bioinorganic Chemistry	CHE B01	IV
10.	CHE B05	Materials and Industrial Chemistry	-	IV
11.	CHE B06	Photoinorganic Chemistry	-	IV
12.	CHE C01	Advanced Electrochemistry – I	-	III
13.	CHE C02	Advanced Chemical Kinetics – I	-	III
14.	CHE C03	Chemical Analysis	-	III
15.	CHE C04	Advanced Chemical Kinetics – II	CHE C02	IV
16.	CHE C05	Advanced Electrochemistry – II	CHE C01	IV
17.	CHE C06	Advanced Nanoscience and Nanotechnology	-	IV
18.	CHE D01	Biomolecules – I	-	II
19.	CHE D02	Heterocyclic Chemistry – I	-	III
20.	CHE D03	Natural Product – I	-	III
21.	CHE D04	Medicinal Chemistry – I	-	III
22.	CHE D05	Heterocyclic Chemistry – II	CHE D02	IV
23.	CHE D06	Natural Product – II	CHE D03	IV
24.	CHE D07	Medicinal Chemistry – II	CHE D04	IV
25.	CHE E01	Pharmaceutical Chemistry –I		III
26.	CHE E02	Biomolecules II	CHE D01	III
27.	CHE E03	Pharmaceutical Chemistry –II	CHE E01	IV
28.	CHE E04	Advanced Pharmaceutical Chemistry	-	IV
29.	CHE A11	Elective laboratory – 1	-	I
30.	CHE A12	Elective laboratory – 2	-	II
31.	CHE B11	Elective laboratory – 3	-	III
32.	CHE C11	Elective laboratory – 3	-	III
33.	CHE D11	Elective laboratory – 3	-	III
34.	CHE E11	Elective laboratory – 3	-	III
35.	CHE A21	Project Work – PRJ	-	IV

- Department will inform the students about the minimum/maximum number of Elective courses offered to students at the beginning of each semester based on the courses opted by students and availability of faculty.
- In semesters III and IV, Theory elective papers 1-3 to be opted out of one of four elective groups offered (B,C,D,E). Pharma group students may opt D04 and D07 as third elective in III and IV semester, respectively. Elective Laboratory – 3 will be according to the opted Elective Theory group.

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CHE 701: ADVANCED INORGANIC CHEMISTRY – I
(Theories of Bonding, Spectroscopic methods and Nuclear Chemistry)

UNIT - I

4 Credit (4 hrs/week)

Stereochemistry and Bonding in Main Group Compounds:
Limitations of VSEPR Theory, dπ-pπ bond, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules

Metal Ligand Bonding:
Limitation of crystal field theory, molecular orbital theory, and introduction to ligand field theory: σ-bonding in octahedral and tetrahedral complexes, π-bonding and molecular orbital theory.

UNIT - II

Electronic Spectra of Transition Metal Complexes
Spectroscopic ground states, correlation diagrams, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, Racah parameters (B) and nephelauxetic ratio (β) parameters, charge transfer spectra.

UNIT - III

Optical Rotatory Dispersion (ORD), Circular Dichroism (CD) and Magnetic Properties of Transition Metal Complexes
Spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical conformation, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

UNIT – IV

Nuclear and Radiochemistry:
Laws of radioactive decay; Detection of radiations; Geiger-Nuttal rule; GM tubes and their characteristics; Ionization chamber, Proportional counters, Scintillation counters; Solid state detectors; Calibration of counting equipments; Determination of absolute disintegration rates.
Activation analysis: Principles; Various methods of activation; Methodology; Advantages, limitations and applications.

SUGGESTED BOOKS AND REFERENCES

1. Inorganic Chemistry, Principles of structure and Reactivity, 4th Edition; James E. Huheey: Elleu A. Keiter: Richard L. Keiter.
2. Advanced Inorganic Chemistry; F.A. Cotton and G. Wilkinson.
3. Theoretical Inorganic Chemistry; Day and Selbin.
4. Concepts and Models in Inorganic Chemistry; Doughlas Mc Daniel.
5. Physical Methods in Inorganic Chemistry; R. S. Drago.
6. Chemistry of the Elements; N.N. Greenwood and A. Earnshow, Pergamon, 1984.
7. Inorganic Electronic Spectroscopy; A.B.P. Lever, Elsevier, 1968.
8. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillard and J.A. Mc Cleverty, Pregamon, 1987; Vol. 2.
9. Nuclear and Radiochemistry; G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller; 3rd Edn., Wiley: NY, 1981.
10. Essentials of Nuclear Chemistry, H. J. Arnikar; 4th Eds., New Age International: N Delhi, India, 2011.
11. Nuclear and Radiochemistry: Fundamental and Applications, 2 Vols., Jens-Volker Kratz and Karl Heinrich Lieser; 3rd Edn., John Wiley & Sons: UK, 2013.

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CHE 702: ORGANIC REACTION MECHANISM

4 Credit (4 hrs/week)

UNIT- I

Reaction Mechanism: Structure and Reactivity

A review of types of mechanisms and reactions, methods of determining reaction mechanism, thermodynamic and kinetic requirements for reaction, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett Principle, Isotope effects. Effects of structure on reactivity, resonance and field effects, steric effects. Quantitative treatment of the effect of structure on reactivity. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.

Aromaticity: Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons. Huckel's rule, energy level of π-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach, energetic and magnetic concept.

UNIT - II

Aliphatic Nucleophilic Substitution

The S_N1, S_N2, mixed S_N1-S_N2 and SET mechanisms. The S_Ni mechanism. The neighbouring group mechanism - participation by π and σ bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system. Application of NMR spectroscopy in the detection of carbocations. Nucleophilic substitution at the allylic, aliphatic trigonal and a vinylic carbon. Reactivity - effect of substrate structure, attacking nucleophile, leaving group and reaction medium. Ambident nucleophile, regioselectivity.

Aromatic Nucleophilic Substitution

The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richte, Sommelet-Hauser and Smiles rearrangements.

UNIT - III

Aliphatic Electrophilic Substitution

Bimolecular mechanisms - S_E2 and S_Ei. The S_E1 mechanism - electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and solvent polarity on reactivity.

Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity of aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenations (NBS). Oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

UNIT - IV

Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction, Sharpless asymmetric epoxidation.

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Addition to Carbon-Heteroatom Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagent, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Introduction to condensation reactions involving enolates - Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

Elimination Reactions

The E2, El and ElcB mechanisms. Steric orientation of the double bond. Reactivity, effect of substrate structure, the attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic eliminations.

SUGGESTED BOOKS AND REFERENCES

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, McGraw Hill.
2. Mechanism and Structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston).
3. Advanced Organic Chemistry Part-A. F.A. Carey and R.J. Sundberg, 5th Ed. Springer (2007).
4. Physical Organic Chemistry – J. Hine.
5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes. Longman
6. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers. Oxford University Press (2001)
7. Structure and Mechanism in Organic Chemistry. C.K. Ingold. Cornell University Press.
8. Organic Chemistry. R.T. Morrison and R N. Boyd. Prentice-Hall.
9. Modern Organic Reactions. H O House, Benjamin.
10. Principles of Organic Synthesis. R O C Norman and J.M. Coxon. Blackie Academic & Professional.
11. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.

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CHE 703: QUANTUM, SURFACE AND ELECTROCHEMISTRY

4 Credit (4 hrs//week)

UNIT – I

Introduction: Historical background – Black body Radiation, de-Broglie concept, Heisenberg's Uncertainty Principle. Postulates of Quantum Mechanics, Operators - Linear, Commutator, Hamiltonian, Hermitian and Angular Momentum Operators, Eigen Value and Eigen Functions, Schrodinger's equation, wave function, physical significance of ψ^2.

Application of Schrodinger's Equation to (i) particle in one dimensional box, (ii) particle in three dimensional box, (iii) Simple Harmonic Oscillator, (iv) Rigid Rotor and (v) Hydrogen atom; Radial and angular wave functions, quantum numbers and their significance.

UNIT-II

Angular Momentum: Ordinary angular momentum, Eigen functions and Eigen values of angular momentum, Ladder Operator, Addition of Angular Momentum; Spin, antisymmetry and Pauli's exclusion principle.

Approximation Method: The Variation theorem, linear variation principle, perturbation method (First order and nondegenarate). Application of variation method and perturbation method to Helium atom.

Molecular Orbital Theory: Basic ideas, criteria of forming MOs, LCAO Concept. Huckel's Molecular Orbital (HMO) theory for conjugated organic systems. Application of HMO to ethylene, allylic, cyclopropanyl, butadiene and cyclobutadiene system.

UNIT - III

Surface Chemistry

Adsorption: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon)

Micelles : Surface active agents, classification of surface active agents, micellization, hydrophobic interaction , critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization -phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

UNIT - IV

Electrochemistry

Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces, Guoy-Chapman, Stern, Graham Devanatham-Mottwatts, Tobin, Bockris, Devanathan models, Over potentials, exchange, current density derivation of Butler Volmer equation, Tatel plot. Polarography theory, Ilkovic equation; half wave potential and its significance.

SUGGESTED BOOKS AND REFERENCES

1. Physical Chemistry by P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry. Ira N. Levine, Prentice Hall.
4. Quantum Chemistry; R.K. Prasad, New Age International
5. Micelles, Theortical and Applied aspects; V. Morai, Plenum Press.
6. Modern Electrochemistry Vol. I & II; J.O.M. Bockris and A.K.N. Reddy Plenum Press, New York.
7. Physical Chemistry by Puri, Sharma and Pathania Vishal Publications.

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CHE 711: CHEMISTRY CORE LAB – I

6 Credit (9 hrs/week)

A. **Qualitative analysis of mixture consisting of eight cationic / anionic radicals including:**
   a. Interfering anionic radical
   b. Insolubles : oxides, sulphates and halides
   c. Less common metal ions : Tl, W, Mo, Se, Te, V, Th, Ti, Zr, Ce, Li

B. Purification techniques and Qualitative analysis

a. Demonstrations of purification, drying and storage of solvents using various techniques – distillation, steam distillation, vacuum distillation, etc.

b. Separation of Organic binary mixtures [(one liquid and one solid) or (two solids)] using H_2O, HCl, NaOH, $NaHCO_3$, Ether or other reagent and identification of components using chemical tests, IR spectra for functional group identification and preparation of derivatives.

C. **Experiments based on**

Surface tension

i. To study surface tension concentration relationship for solution (Gibbs equation).
ii. To determine the critical micelle concentration (CMC) of SDS and CTAB by surface tension techniques.

Adsorption

i. Adsorption of Oxalic acid
ii. Acetic acid on charcoal

Viscosity, Solubility and Molecular weight determination

i. Experiments based on determination of viscosity of given liquid using Ostwald's viscometer.
ii. Study the variation of viscosity of pure liquid with temperature and determination of temperature coefficient of viscosity of the liquid.
iii. Determination of Solubility of various salts like NaCl, KCl, KNO_3 and $NaNO_3$ at different temperature and draw the solubility Curve.
iv. Determination of molecular weight of given polymer (Polyvinyl alcohol, polystyrene, methyl acrylate, etc.) using viscometer
v. Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte

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CHE A01: SPECTROSCOPY –

4 Credit (4 hrs/week)

UNIT - I

Introduction: Interaction of light with matter, mechanism of absorption and emission of radiation.

Microwave Spectroscopy: Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor; stark effect, nuclear and electron spin interaction and effect of external field applications.

Vibrational Spectroscopy: Vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. P.Q.R. branches, breakdown of Oppenheimer approximation; vibrations of polyatomic molecules; selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal ligand vibrations.

Raman Spectroscopy: Origin, rotational and vibrational Raman Spectra of diatomic molecules.

UNIT - II

Electronic Spectroscopy

Atomic Spectroscopy: Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

Molecular Spectroscopy: Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

Photoelectron Spectroscopy: Photo-electric effect, ionization process, Koopman's theorem, photoelectron spectra of simple molecules, ESCA, chemical information from ESCA; Auger electron spectroscopy-basic idea.

UNIT-III

Magnetic Resonance Spectroscopy

Nuclear Magnetic Resonance: Basic Principle, Spin quantum number, interaction between Spin and a Magnetic Field, Larmor Precession, Relaxation Times; Continuous Wave NMR Spectroscopy, Fourier Transform NMR Spectroscopy; Introduction to Chemical Shift, Spin-spin coupling, Coupling constant. Nuclei other than hydrogen: Nuclei with spin ½ (^{13}C, ^{19}F, ^{31}P, ^{117}Sn, ^{119}Sn, etc.). Nuclei with spin greater than ½ (^{14}N, ^{11}B). Quadrupole effects; factors effecting chemical shift in inorganic compounds - geometry, electronegativity, charge, oxidation state, coordination number. Coupling between two or more than two types of NMR active nucleus in a compound (e.g. $CHFCl_2$, $HPFCl$, $OP(O)FH$, $HP(O)F_2$, BH_4).

Electron Spin Resonance: Basic principles, zero field splitting and Kramer's degeneracy, Isotropic and anisotropic Hyperfine coupling, spin-orbit coupling and significance of g tensors, factors affecting the 'g' value, its applications to the study of free radicals & fast reactions andapplication to transition metal complexes; spin Hamiltonian, spin densities and McConnell relationship. Applications - spin polarization for atoms and transition metal ions.

UNIT-IV

Mossbauer Spectroscopy: Basic principles, spectral parameters and spectrum display, applications of the techniques to the studies of (i) bonding and structures of Fe^{2+} and Fe^{3+} compounds including those

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of intermediate spin; (ii) Sn^{2+} and Sn^{4+} compounds, nature of M-L bond, coordination number, structure; and (iii) detection of oxidation state and in equivalent MB atoms.

Electron Microscopy: Basic principles of Electron Microscopy SEM, TEM, AFM; and their applications in structural analysis.

SUGGESTED BOOKS AND REFERENCES

1. Fundamentals of Molecular Spectroscopy, Banewell and McCash
2. Modern Spectroscopy, J.M. Hollas, John Wiley.
3. Applied Electron Spectroscopy for Chemical Analysis D. H. Windawi and F.L. Ho, Wiley Interscience.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Electronic Absorption Spectroscopy and related Techniques, D N Sanyanarayana
8. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
9. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
10. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
11. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper & Row.
12. NMR Spectroscopy in Inorganic Chemistry, J.A. Iggo, Oxford University Press: Oxford, 1999, pp 1-21; 31-35.
13. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.

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CHE A02: ANALYTICAL TECHNIQUES

4 Credit (4 hrs/week)

UNIT I

Statistics – Introduction to Chemometrics

Limitations of analytical methods, Errors and classification, Determinant, constant and indeterminate, accuracy, precision, minimization of errors, significant figures and computation rules, mean and standard deviation, distribution of random errors, variance and confidence interval, paired *t*-test, least square method, correlation and regression, linear regression.

UNIT II

Sampling in analysis

Definition, theory, basis and techniques of sampling, sampling statistics, sampling and physical state, crushing and grinding, hazards in sampling, techniques of sampling of gases, fluid, solids, and particulates, minimization of variables, transmission and storage of samples, high pressure ashing techniques (HPAT), particulate matter, its separation in gas stream, filtering and gravity separation, analysis of particulate matter like asbestos, mica, dust and aerosols etc.

Solvent extraction method in analysis

Principle, classification, theory, instrumentation and applications.

UNIT III

Conductometry:

Important laws, definitions, relations, effect of dilution on conductivity, measurement of conductivity, types of conductometric titrations, its applications and limitations.

Potentiometry:

Principle, instrumentation, types of potentiometric titrations and its applications, pH measurements, determination of pH, ion selective electrodes, instrumentation and applications.

UNIT IV

Coulometry:

Introductions, principle, experimental details of coulometry at constant current and constant potential, titrational applications.

Atomic Absorption Spectroscopy:

Introduction, principle, Grotrian diagram, instrumentation, applications, detection limit, sensitivity and disadvantages.

SUGGESTED BOOKS AND REFERENCES

1. Mendham J., Denney R.C., Barnes J. D., Thomas M.J.K., Vogels' text book of quantitative chemical analysis, 6th edition, Prentice Hall, 2000.
2. Skoog Douglas A., Holler F. James, Nieman Timothy A., Principles of instrumental analysis, Saunders College Pub., 1998.
3. Day R. A and A. L. Underwood, Quantitative analysis, Prentice Hall, 1999.
4. Drago R. S., Physical methods in Chemistry, Saunders, 1999.
5. Peters D.G, J. M. Hayes and G. M. Hefige, A brief introduction to Modern chemical analysis, Philadelphia: Saunders, 1976.
6. Ebsworth E.A.V, DWA Rankin and C. Craddock, Structural methods in inorganic chemistry, ELBS.
7. Elian JAD Butter Worth, Photoelectron spectroscopy.
8. Eliel E.L, Stereochemistry of carbon compounds, Tata-McGraw-Hill

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CHE A03: GREEN AND SUSTAINABLE CHEMISTRY

4 Credit (4 hrs/week)

UNIT – I

Introduction, principle and concepts of Green Chemistry

Need for green chemistry; Inception and evolution of green chemistry; Twelve principles of green chemistry with their explanations and examples; Designing a green synthesis using these principles; Green chemistry in day to day life.

UNIT – II

Non-traditional greener alternative approaches

Different approaches to green synthesis: (a) Uses of green reagents in organic synthesis - Dimethyl carbonate, polymer supported reagents - per acids and chromic acid (b) Green catalysts, role of catalysis in sustainable development, homogeneous and heterogeneous catalysts; Introduction, advantages and applications of - (i) Nanocatalysts, (ii) Phase transfer catalysts, (iii) Biocatalysts, (iv) Organocatalysts, in organic synthesis.

UNIT – III

Applications of non-conventional energy sources

Introduction of microwave induced synthesis: Microwave activation, equipment, time and energy benefits, limitations; Organic transformations under microwaves - Fries rearrangement, Diels-Alder reaction, decarboxylation, saponification of ester, alkylation of reactive methylene compounds; Heterocyclic synthesis - β-Lactams, pyrrole, quinoline.

Introduction of ultrasound assisted green synthesis: Instrumentation, physical aspects, applications in organic transformations.

Electrochemical synthesis: Introduction, synthesis of sebacic acid and adiponitrile.

UNIT – IV

Environmentally Benign Solutions to Organic Solvents

Ionic liquids as green solvents: Introduction, properties and types of ionic liquids. Synthetic applications - Diels-Alder reaction, epoxidation and Heck reaction.

Aqueous phase reactions: Enhancement of selectivity, efficiency. Synthetic applications - 1,3-Dipolar Cycloadditions. Carbon-Carbon bond-forming processes and bromination reactions.

Fluorous solvents in green chemistry: Scope, definition and their synthetic applicability.

Role of supercritical carbon dioxide in green chemistry.

Ethyl lactate as a renewable green solvent: Properties and applications.

SUGGESTED BOOKS AND REFERENCES:

1. P.A.G. Blackie, Organic synthesis in water, Springer.
2. P.T. Anastas, J.C. Warner, Green Chemistry, theory and practice, Oxford University Press.
3. M. Lancaster, Green Chemistry: An introductory text, Royal Society of Chemistry.
4. V. Polshettiwar, T. Asefa, G. Hutchings, Nanocatalysis: Synthesis and applications, Wiley.
5. M.A. Ryan, M. Tinnesand, Introduction to Green Chemistry, American Chemical Society.
6. P.T. Anastas, Handbook of Green Chemistry, John Wiley and Sons.
7. V.K. Ahluwalia, M. Kidwai, New Trends in Green Chemistry, Springer.

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CHE A11: CHEMISTRY ELECTIVE I AB-1

A. Laboratory Estimations — 6 Credits (9 hrs/week)

i. Estimation of an acid using another standard acid
ii. Estimation of a base using another standard base
iii. Estimation of boric acid
iv. Determination of percentage purity of commercial soda
v. Determination of percentage of $CaCO_3$ in precipitated chalk sample
vi. Determination of percentage purity of caustic soda
vii. Determination of alkali content-antacid tablet using HCl

B. Organic Preparations (single step)

i. Preparation of *p*-bromoacetanilide from acetanilide.
ii. Preparation of *p*-bromoaniline from *p*-bromoacetanilide.
iii. Preparation of *m*-dinitrobenzene from nitrobenzene.
iv. Preparation of *m*-nitroaniline from *m*-dinitrobenzene.
v. Synthesis of adipic acid from cyclohexanol.
vi. Preparation of 1,1-bis-2-naphthol (BINOL) from β-naphthol.
vii. Green synthesis of 7-hydroxy-4-methylcoumarin (Pechmann condensation).
viii. More one step preparations may be carried out according to requirement of curriculum

C. Experiments based on -

Phase Equilibrium:

i. Determination of congruent composition and temperature of a binary system (e.g., diphenylamine-benzophenone system).
ii. To construct the phase diagram for three component system (e.g., chloroform-acetic acid water).
iii. Study of distribution of benzoic acid in benzene and water to show that benzoic acid dimerise in benzene.
iv. Determine the equilibrium constant for the reaction $KI + I_2 \rightarrow KI_3$ by distribution method.

Conductometry

v. Varification of Onsager's equation for strong electrolytes (NaCl, HCl, KNO_3, KCl) and determination of constant A and B.
vi. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometerically.
vii. Determination of the strength of strong and weak acids in a given mixture conductometrically.

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CHE 801: ADVANCED INORGANIC CHEMISTRY– II

(Group Theory, Molecular rearrangement processes & Inorganic reaction mechanisms)

4 Credit (4 hrs/week)

UNIT-I

Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definition of group, subgroup, conjugacy relation and classes. Point symmetry group. Schonfilies symbols, representations of groups by matrices (representation for the C_{nh}, C_{nv}, etc, group to be worked out explicity). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Derivation of character table for C_{2v} and C_{3v} point group. Symmetry aspects of molecular vibrations of H_2O molecule.

UNIT-II

Molecular Rearrangement Processes

Electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reductant, chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

UNIT-III

Inorganic Reaction Mechanism- I

Basic principles; lability, inertness, stability and instability of coordination compounds; general principles and mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes; potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation mechanism, Swain -Scott equation.

UNIT-IV

Inorganic Reaction Mechanism- II

Substitution reactions of octahedral complexes; nature of substitution reactions; Theoretical approach to substitution mechanisms; mechanism of substitution reaction of complexes of cobalt; acid hydrolysis and base hydrolysis of Co (III) complexes.

Substitution reactions of square planar complexes; reaction of Pt (II) complexes; trans effect and its applications to synthesis of complexes; theories of trans effect; mechanism of substitution - kinetics of substitution of Pt(II) complexes; factors affecting the reactivity of square planar complexes.

SUGGESTED BOOKS AND REFERENCES

1. Inorganic Chemistry, Principles of Structure and Reactivity, 4thEdition, James E. Huheey: Ellen A. Keiter: Richard L. Keiter.
2. Advanced Inorganic Chemistry. F.A. Cotton and G. Wilkinson.
3. Theoretical Inorganic Chemistry, Day and Selbin.
4. Concepts and Models in Inorganic Chemistry, Doughlas Mc Daniel.
5. Introductory Quantum Chemistry, A.K. Chandra (Tata McGraw Hill)
6. Chemical Applications of Group Theory, F.A. Cotton.

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CHE 802: STEREOCHEMISTRY AND ORGANIC REACTION MECHANISM II

4 Credit (4 hrs/week)

UNIT I

Stereochemistry

Optical activity and chirality, elements of symmetry, specification of configuration - molecules with more than one chiral center. D/L, R/S and Threo/Erythro nomenclature.

Prochirality, Homotopic and Heterotopic ligands and faces, Enantiotopic groups and faces, Re/Si Nomenclature. Stereospecific and stereoselective reactions.

Optical activity in the absence of chiral carbon (biphenyls, allenes, spiranes, ansa compounds). Chirality due to helicity. Chirality in the compounds containing N, S and P.

Geometrical isomerism in cyclic and condensed systems, Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity.

Cram's, Prelog's and Horeau's rules. Circular birefringence, CD, ORD, Octant rule, Cotton effect. The axial haloketone rule. Determination of configuration (absolute and relative) and conformation.

UNIT II

Organic Photochemistry

Photochemical excitation – interaction of electromagnetic radiation with organic molecules, types of excitations, fate of excited molecules - Jablonskii diagram, intersystem crossing, energy transfer, photosensitization, quenching, quantum yield, Frank-condon principle.

Photochemical reactions of ketones – Norrish type I cleavage, Norrish type II cleavage; photo reductions; Paterno-Buchi reactions; photochemistry of α,β-unsaturated ketones, β,γ-unsaturated ketones.

Photochemistry of alkenes: intramolecular reactions of the olefinic bond – cis-trans isomerisation (stilbene), cyclization reactions.

Photochemistry of aromatic compounds: photochemical rearrangement, photostationary state, isomerizations.

UNIT III

Pericyclic Reactions

Characteristics and Classification of pericyclic reactions, thermal and photochemical reactions. Molecular orbital symmetry. Woodward-Hoffmann selection rules, Fukui's FMO approach, Woodward-Hoffmann's Conservation of orbital symmetry and correlation diagrams and PMO method.

Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 π electron and allyl systems. Valence Tautomerism.

Cycloadditions: antarafacial and suprafacial additions, 4n and 4n+2 π electron systems. Diels-Alder reaction – stereoselectivity (endo, exo), and regioselectivity; normal and inverse electron demand Diels-Alder reactions; asymmetric Diels-Alder reactions; retro-Diels-Alder reactions; 2+2 addition of ketenes, 1,3-dipolar cycloadditions. Cheletropic reactions.

Sigmatropic rearrangements: suprafacial and antarafacial shifts of C-H and C-C bonds. Retention & inversion of configuration. 3,3- and 5,5-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

UNIT IV

Molecular Rearrangements

Mechanistic aspects, nature of the migration, migratory aptitudes, memory effects. A detailed study of the following rearrangements: Benzil-benzilic acid rearrangement, Favorskii rearrangement, Neber rearrangement, Beckmann rearrangement, Hoffmann rearrangement, Curtius rearrangement, Lossen

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