SYLLABUS

For
M. Sc. Course in
Chemistry

To be effective from the session 2016-17

KAZI NAZRUL UNIVERSITY
ASANSOL 713 340
WEST BENGAL, INDIA
Duration of PG Course of Studies in Chemistry will be of two years with four Semesters, viz., Semester I, Semester II, Semester III and Semester IV - each of six months’ duration coupled with four examinations viz. Semester I, Semester II, Semester III and Semester IV in chemistry at the end of each Semester. Syllabus is hereby framed according to certain schemes and structures highlighted below.

Schemes:
(i) 300 marks in Semester I & III, 350 marks for Semester II and 250 marks for Semester IV with a grand total of 1200 marks and 98 credits.
(ii) 24 credits in Semester I & III, 28 credits in Semester II and 22 credits in Semester IV with a total of 98 credits; each theoretical/practical paper of 4 credits; term paper/project of 6 credits;
(iii) 20% marks allotted for internal assessment in each paper
(iv) Four theoretical general papers (common to all students) in each of Semester I and Semester II
(v) Two practical general papers (common to all students) in each of Semester I and Semester II
(vi) Three major electives viz. Inorganic, Organic and Physical in Semester III and Semester IV; number of students in each Major paper to be decided by the department; the particular major paper once chosen by any student in Semester III, the corresponding major paper to be continued in Semester IV
(vii) For theoretical papers in Semester III, three advanced general papers (common to all students) and one major paper
(viii) For practical papers in Semester III, one advanced general paper strictly on instrumental methods in chemical analysis with computer simulation (common to all students) and one Major paper (applicable to students as selected by department)
(ix) For theoretical papers in Semester IV, one advanced general paper (common to all students) and two major papers (applicable to students as per provision made in Semester III by the department)
(x) For practical paper in Semester IV, one major practical paper (applicable to students as selected by department)
(xi) In Semester II, one Extra Departmental elective paper to be learnt by the students of the other sister departments and the students of this department be learnt from other sister departments.
(xii) In Semester IV, one paper on term paper/project work (subject matter of each major paper of Semester IV)
(xii) In all semesters each theoretical paper consisting of two units, viz., Unit I and Unit II
(xiii) Total eight questions each with 8 marks to be set in each theoretical paper with each unit containing four questions; examinees to be answered a total of five questions taking at least two from each Unit
(xiv) Duration of examination: each theoretical paper of 50 marks, each practical paper, 6 hours
(xv) For each practical paper: internal assessment, 10; experiments, 30; viva-voce (by external examiner), 10
(xvi) For term paper/project work: internal assessment, 10; presentation of seminar in presence of external expert; 30, and thereafter interaction, 10
## Course Structure

<table>
<thead>
<tr>
<th>Paper Code</th>
<th>Core Subject</th>
<th>Marks*</th>
<th>Credit**</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSCCHEMC101</td>
<td>Inorganic Chemistry General - I</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC102</td>
<td>Organic Chemistry General I</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC103</td>
<td>Physical Chemistry General I</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC104</td>
<td>Analytical Chemistry General I</td>
<td>50</td>
<td>4</td>
</tr>
</tbody>
</table>

**Theoretical Papers**

<table>
<thead>
<tr>
<th>Paper Code</th>
<th>Core Subject</th>
<th>Marks*</th>
<th>Credit**</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSCCHEMC105</td>
<td>Inorganic Chemistry General: Practical</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC106</td>
<td>Organic Chemistry General: Practical</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>300</td>
<td>24</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Paper Code</th>
<th>Core Subject</th>
<th>Marks*</th>
<th>Credit**</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSCCHEMC201</td>
<td>Inorganic Chemistry General II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC202</td>
<td>Organic Chemistry General II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC203</td>
<td>Physical Chemistry General II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC204</td>
<td>Analytical Chemistry General II</td>
<td>50</td>
<td>4</td>
</tr>
</tbody>
</table>

**Practical Papers**

<table>
<thead>
<tr>
<th>Paper Code</th>
<th>Core Subject</th>
<th>Marks*</th>
<th>Credit**</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSCCHEMC205</td>
<td>Physical Chemistry General: Practical</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC206</td>
<td>Analytical Chemistry General: Practical</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>Extra Departmental Elective#</td>
<td>Supramolecular and Medicinal Chemistry</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>350</td>
<td>28</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Paper Code</th>
<th>Core Subject</th>
<th>Marks*</th>
<th>Credit**</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSCCHEMC301</td>
<td>Advanced Inorganic Chemistry General</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC302</td>
<td>Advanced Organic Chemistry General</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMC303</td>
<td>Advanced Physical Chemistry General</td>
<td>50</td>
<td>4</td>
</tr>
</tbody>
</table>

**Theoretical Papers**

<table>
<thead>
<tr>
<th>Paper Code</th>
<th>Core Subject</th>
<th>Marks*</th>
<th>Credit**</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSCCHEMMJE301</td>
<td>Inorganic Chemistry Major I</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE302</td>
<td>Organic Chemistry Major I</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE303</td>
<td>Physical Chemistry Major I</td>
<td>50</td>
<td>4</td>
</tr>
</tbody>
</table>

**Major Electives (any one)**

**Practical Papers (MSCCHEMC304 compulsory, and any one from MSCCHEMMJE304-306)**

<table>
<thead>
<tr>
<th>Paper Code</th>
<th>Core Subject</th>
<th>Marks*</th>
<th>Credit**</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSCCHEMC304</td>
<td>Advanced Chemistry General</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE304</td>
<td>Inorganic Chemistry Major: Practical I</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE305</td>
<td>Organic Chemistry Major: Practical I</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE306</td>
<td>Physical Chemistry Major: Practical I</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>300</td>
<td>24</td>
</tr>
<tr>
<td>Paper</td>
<td>Core Subject</td>
<td>Marks*</td>
<td>Credit**</td>
</tr>
<tr>
<td>---------------</td>
<td>---------------------------------------------------</td>
<td>--------</td>
<td>----------</td>
</tr>
<tr>
<td><strong>Theoretical Papers</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MSCCHEMC401</td>
<td>Advanced Analytical Chemistry General</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td><strong>Major Electives (any one from MSCCHEMMJE401-403 and any one from MSCCHEMMJE404-406)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MSCCHEMMJE401</td>
<td>Inorganic Chemistry Major II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE402</td>
<td>Organic Chemistry Major II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE403</td>
<td>Physical Chemistry Major II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE404</td>
<td>Inorganic Chemistry Major III</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE405</td>
<td>Organic Chemistry Major III</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE406</td>
<td>Physical Chemistry Major III</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td><strong>Major Elective Practical (any one)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MSCCHEMMJE407</td>
<td>Inorganic Chemistry Major: Practical II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE408</td>
<td>Organic Chemistry Major: Practical II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td>MSCCHEMMJE409</td>
<td>Physical Chemistry Major: Practical II</td>
<td>50</td>
<td>4</td>
</tr>
<tr>
<td><strong>Term Paper/Project</strong></td>
<td>(any one from MSCCHEMC402-404)**</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MSCCHEMC402</td>
<td>Inorganic Chemistry Term Paper/Project</td>
<td>50</td>
<td>6</td>
</tr>
<tr>
<td>MSCCHEMC403</td>
<td>Organic Chemistry Term Paper/Project</td>
<td>50</td>
<td>6</td>
</tr>
<tr>
<td>MSCCHEMC404</td>
<td>Physical Chemistry Term Paper/Project</td>
<td>50</td>
<td>6</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td>250</td>
<td>22</td>
</tr>
<tr>
<td><strong>Grand Total</strong></td>
<td></td>
<td>1200</td>
<td>98</td>
</tr>
</tbody>
</table>

* Marks: Sem I + Sem II + Sem III + Sem IV = 300 + 350 + 300 + 250 = 1200;  
**Credit: Sem I + Sem II + Sem III + Sem IV = 24 + 28 + 24 + 22 = 98;  
# Number of students-intake for minor electives may depend on the availability of seats;  
** For term paper/project: preparation + presentation + viva-voce = 25 + 15 + 10 = 50.
Semester I

Theoretical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC101: Inorganic Chemistry General I

Unit I

1. Bonding, reactivity and molecular properties – a quantum chemical approach (12 lectures)

   Fundamentals, LCAO and/or Hückel treatments of σ- and π-MOs (inorganic di-/polyatomic species, organic open-chain/cyclic units such as alkanes, alkenes, vinyl/allylic system, dienes, polyenes, sandwich molecules, boron/carborane compounds, etc) with an inner look into orbital symmetry, molecular term symbols, relative energy, transition probability, selection rules, nature and intensity of transitions (allowed/forbidden), probing reaction center, and aromaticity of inorganic, organic, coordination and organometallic species; Koopmans’ theorem, Walsh diagram, isolobal analogy

2. Coordination chemistry – stereochemistry, bonding and structure (13 lectures)

   Preamble, Orgel/Tanabe-Sugano diagram, ligand symmetry orbital, molecular orbital, Angular overlap model, spectral features, Nephelauxetic effect, Racah parameter, Franck Condon principle, vibronic coupling, band broadening, spin-orbit coupling, spin-forbidden transition, intensity stealing, magnetic properties, cooperative, anomalous and subnormal magnetic moments, lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelator/congregator/macrocycle, structural equilibrium and implication

Unit II

3. Organometallic chemistry I (10 lectures)

   Overview, valence electron count, oxidation number and formal ligand charge; carbonyl ligand, linear/cyclic π-ligand system, compounds with M-C, M=C and M≡C bonds, hydride and dihydrogen complexes; phosphine, Jesiphos and related ligands; spectral analysis and structural characterization, Dewar-Chatt-Duncanson bonding model, isolobal analogy, Agostic interaction

4. Bioinorganic and inorganic medicinal chemistry (15 lectures)

   Background, myoglobin, hemoglobin, hemocyanin, hemerythrin, cytochromes, rubredoxin, ferredoxins; biological nitrogen fixation, chlorophyll and photosynthesis; PS-I, PS-II, bioenergetics and ATP cycle, glucose storage, Na+/K+ ion pump, ionophores, metalloenzyme – catalase, peroxidase, ceruloplasmin, cytochrome oxidase, carbonic anhydrase, carboxy peptidase, metallothionein, xanthine oxidase, sulphite oxidase, nitrate reductase, superoxide dismutase, chemistry of respiration; vitamin B$_{12}$ and B$_{12}$-enzyme

   Metals in medicines: diseases due to deficiencies, carcinogenesis, applications of chelators and metal chelates of different generations; antitumour, anticancer and anti-AIDS drugs, mechanistic pathway, limitation, future dimension

Suggested books

MSCCHEMC102: Organic Chemistry General I

Unit I

1. Stereochemistry (Static and Dynamic) of organic compounds: concept and application (10 lectures)

Static stereochemistry: Molecular symmetry and chirality; axial chirality, planar chirality and helicity; topicity and prostereoisomerism; conformation of acyclic and cyclic systems (3 to 5 and 7 to 8 members ring) along with fused and bridged ring compounds; conformations of rings with multiple double bonds; stereoelectronic effects; Baldwin’s rule, stereochemistry of fused ring and bridged ring compounds (with special reference to decalin and phenanthrene systems)

Dynamic stereochemistry: Curtin-Hammett principle and Wenstein-Eliel equations; conformation, reactivity & mechanism (viz: acyclic and cyclic system focusing on nucleophilic substitution reaction, formation and cleavage of epoxide ring, addition reactions to double bonds, elimination reactions, pyrolytic syn-elimination, oxidation of cyclohexanols, etc.); elementary idea about asymmetric synthesis

2. Organic reaction mechanism (15 lectures)

Substitution reactions: Aliphatic nucleophilic substitution — $S_N1$, $S_N2$, mixed $S_N1$ and $S_N2$, SET mechanisms; neighbouring group participation by $pi$- and $sigma$-bonds, anchimeric assistance; $S_Ni$ mechanism; nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon; effect of substrate structures on reactivity, nucleophiles, leaving group and reaction medium; phase transfer catalysis, regioselectivity; Aromatic nucleophilic substitution — $S_NAr$, benzyne and $Sn1$ mechanisms; effect of substrate structures on reactivity, leaving group and attacking nucleophile; Aliphatic electrophilic substitution — $S_E1$, $S_E2$, and $S_Ei$ mechanisms; electrophilic substitution accompanied by double bond shifts; effects of substrates, leaving group and solvent polarity on the reactivity; Aromatic electrophilic substitution — the arenium ion mechanism; orientation and reactivity; energy profile diagrams; the ortho/para ratio; orientation in other ring systems; ipso attack; Free radical reactions: Types of free radical reactions; free radical substitution mechanism; mechanism at an aromatic substrate; neighbouring group assistance; reactivity for aliphatic and aromatic substrates at a bridgehead; reactivity in the attacking radicals; effects of solvents on reactivity; allyllic halogenation (NBS), oxidation of aldehydes to carboxylic acids; auto-oxidation; free radical rearrangements

Elimination reactions: E1, E2 and E1cB mechanisms; product stereochemistry; effects of substrate structures, attacking base, leaving group and the medium on reactivity; mechanism and orientation in pyrolytic elimination

Addition reactions: Addition to carbon–carbon multiple bonds — mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals; region- and chemoselectivity; orientation and reactivity; Addition to carbon–hetero multiple bonds — mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles; addition of Grignard reagents, organozinc and organolithium
reagents to carbonyl and unsaturated carbonyl compounds; Mechanism of condensation reactions involving enolates — Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions

Rearrangement reactions: Formation and stability of carbonium ions, carbanion, carbenes, nitrenes, radicals and arynes. Rearrangement involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement), reaction involving acyl cation, PPA cyclization and Fries rearrangement, rearrangement of carbenes (Wolff & Arndt-Eistert synthesis), rearrangement of nitrenes (Hoffmann, Curtius, Schmidt, Lossen, Beckmann rearrangement); sigmatropic rearrangements

Metathesis and click chemistry: Definition, classes of reactions, catalysts used, mechanistic aspects and synthetic applications of methathesis reactions and click reactions in organic chemistry with suitable examples

Unit II

3. Ultraviolet and visible (UV-vis) spectroscopy: Application
   Recapitulation of the principle, preparation of samples for UV-vis spectroscopy, effects of solvents, chromophores and auxochromes, characteristic absorptions of varying chromophoric systems, applications

4. Infrared (IR) spectroscopy: Application
   Recapitulation of the principle, Fourier transform infrared spectroscopy (FTIR), preparation of samples for infrared spectroscopy, characteristic group frequencies and applications

5. Nuclear Magnetic Resonance (NMR) spectroscopy: General principles and application
   \(^1\text{H-NMR} \) spectroscopy: General introduction and definition; chemical shifts; spin-spin interaction; shielding mechanism; mechanism of measurement; chemical shifts and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohol, phenols, enols, carboxylic acids, amines, amides & mercapto); chemical exchange; effect of deuteration; complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling, stereochemistry; hindered rotation; Karplus curve-variation of coupling constant with dihedral angles; simplification of complex spectra - nuclear magnetic double resonance, shift reagents, solvent effect; Fourier transform technique; nuclear Overhauser effect (NOE); resonance of other nuclei, \(^{19}\text{F}, \^{31}\text{P}, \) etc
   \(^{13}\text{C-NMR} \) spectroscopy - general considerations; chemical shift values (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon); coupling constant; Two Dimensional NMR Spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

6. Mass spectrometry: General principles and application
   Introduction; ion production - EI, CI, FD and FAB; factors affecting fragmentation; ion analysis; ion abundance; Mass spectral fragmentation of organic compounds; common functional groups; molecular ion peak; metastable peak; McLafferty rearrangement; nitrogen rule; high resolution mass spectrometry; examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

7. Combined spectral applications
   Applications of all the spectroscopic techniques (UV, FT-IR, NMR and Mass) in a combined manner to solve structural problems of unknown organic compounds
Suggested books


MSCCHEMC103: Physical Chemistry General I

Unit I

1. Quantum mechanics I
(13 lectures)

Drawback of classical physics: A brief discussion on Black Body radiation, photo-electric effect and Double slit experiment. Wave-particle duality. Uncertainty principle, Operators in QM, Operator algebra, Commutation relation, Eigen functions and Eigen values, Postulates of QM, Ehrenfest’s theorem, Schrodinger Equations, Theorems of QM. Few Model Systems, their solutions: Particle in 1-d Box, Selection Rules. Discussion on Bohr’s correspondence principle. Checking the validity of Schrodinger wave equation based on correspondence principle and Heisenberg’s Uncertainty principle Particle in 3-d Box, Particle in a ring and in a sphere, Tunneling.

2. Atomic and molecular spectroscopy: principle and application
(12 lectures)

Review of basic spectroscopy, Hydrogen energy levels, spectroscopic transitions and selection rules, Multi-electron Atoms, Vector model, orbital and spin angular momentum of electrons, normal and anomalous Zeeman and Paschenback effects, Stern-Gerlach experiment, LS and jj coupling, spin-orbit coupling, atomic energy terms and term symbols, hyperfine structure

Rotational spectra: diatomic molecules as rigid rotors - energy levels, selection rules and spectral features, isotope effect, intensity distribution, effect of non-rigidity on spectral features; vibrational spectra of diatomics: potential energy of an oscillator, Harmonic Oscillator approximation, energy levels and selection rules, anharmonicity and its effect on energy levels and spectral features: overtones and hot bands, vibration-rotation spectra of diatomics: origin; selection rules; P, Q and R branches; Raman spectra: origin, selection rules, classical and quantum treatment of rotational and vibrational Raman spectra of diatomics, resonance Raman spectroscopy; NMR spectra: theory, relaxation process, spin interactions - its origin, equivalent protons, qualitative idea of energy levels of AX, AX2 and AX3 systems, a few representative examples

Unit II

3. Solutions thermodynamics and electrochemistry
(15 lectures)

Partial molar quantities, significance and the determination of partial molar quantities, Thermodynamics of ideal and non-ideal binary solutions, excess functions and their determination, Activity co-efficients, Experimental determination of activity coefficients of electrolytes and non-electrolytes, Ion-Ion interactions, Debye-Huckel theory, Limiting and extended Debye Huckel equations for activity coefficients, ion-solvent interaction: Born model and Born equation, enthalpy of ion-solvent interaction and its calculation, Eley-Evan model, solvation number and methods for determination of solvation number, ion association: Bjerrum equation, fraction of ions associated, ion association constant; electrode kinetics: relation between current and rate of electrode reaction, current-overpotential relationship, Tafel equation and its importance

4. Statistical thermodynamics
(10 lectures)
Motivation for study, Entropy and Probability, Stirling approximations, Maxwell-Boltzmann Distribution, Gibbs paradox, Sackur-Tetrode equation, concept of partition functions, translational, rotational, vibrational and electronic partition functions, Thermodynamic properties in terms of partition functions, Equilibrium constant, Equipartition principle, Einstein theory of specific heat capacity of solids.
**Suggested books**


**MSCCHEMC104: Analytical Chemistry General I**

**Unit I**

1. **Statistical methods in analytical methods**

   Application of counting statistics in analytical and nuclear measurements: probability and binomial distribution, radioactivity as a statistical phenomenon, standard deviation of counting data, Poisson distribution, optimization of counting experiments

2. **Separation techniques**

   Preamble, successive extraction and separation; techniques of solvent extraction: Craig extraction and counter current distribution; ionic liquid assisted and supercritical solvent extraction, problems; chromatography: mathematical
relations of capacity, selectivity factor, distribution constant and retention time; chromatogram, elution in column chromatography: band broadening and column efficiency; van Deemter equation; column resolution, numerical problems, gas chromatography, high performance chromatography and supercritical fluid chromatography: principles, methods, comparison and applications; size-exclusion chromatography, ion chromatography and capillary electrophoresis: principles, methods and applications

Unit II

3. Thermal methods

(10 lectures)

Different methods of analysis: TGA, DTA, DSC; thermogram, applications, thermal stability of covalent and non-covalent bonds, thermal degradation, single crystal phase transformation, thermochemiluminescence, different types of titrations and their applications, solid state reaction kinetics

4. Electroanalytical methods I

(15 lectures)

Fundamentals, electrochemical cell, reference and indicator electrodes, supporting electrolyte, solvent, electrolytic process, three electrode system, DME, Ilkovic equation, Ilkovic-Heyrolsky equation, test of reversibility, current-voltage diagram, DC and AC polarography, Cottrell equation, stripping voltammetry, amperometric titration, membrane electrodes, electrode-solution interface layer, gas-sensing probe

Suggested books


Practical Papers (For Each, Full Marks: 50; Credit: 4)

**MSCCHEMC105: Inorganic Chemistry General: Practical**

1. Preparation/synthesis of inorganic and coordination compounds: selected simple salts, double salts and coordination compounds with some common inorganic and organic ligands
2. Characterization using microanalysis, conductivity measurement and spectroscopic analysis

**MSCCHEMC106: Organic Chemistry General: Practical**

1. Separation (chemical/column chromatographic) of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic samples and identification of individual components
2. Synthesis of organic compounds involving important chemical reactions (halogenations, nitration, diazotisation, Beckmann transformation, photochemical reaction, Sandmayer reaction, pinacol-pinacolone rearrangement, etc.)
Semester-II

Theoretical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC201: Inorganic Chemistry General II

Unit I

1. Chemistry of elements and their compounds (25 lectures)

   Elements – structural versatility coupled with properties; compounds – design and benign synthesis, isolation, characterization, solution structure, molecular aggregate, crystalline architecture, spectral, magnetic and catalytic properties and application in chemistry, biology and materials science

   Non-transition and transition metal ion homoleptic/heteroleptic and homonuclear/heteronuclear complexes of different dimensions with varied mono- and polydentate blockers containing carbon, nitrogen, phosphorus, chalcogen, halogen donors with/without mono-/polydentate pure/mixed bridges and counter ions

   Mono- and polynuclear compounds of lanthanoid and actinoid ions stressing on choice of different multidentate chelators and congregators with special emphasis on electric, magnetic, conducting, superconducting and fluorophoric behaviours

Unit II

2. Inorganic reaction mechanism I (13 lectures)

   Preamble, factors affecting the rate of a chemical reaction, analysis of rate data, complex rate laws, kinetically indistinguishable schemes, nucleophilicity and rate scales: Edward scale, n_Pt scale, Gutmann donor number, Drago E & C scale, trans- and cis- effects, water exchange rates, proton ambiguity, mechanistic simulation; associative, dissociative, interchange, nucleophilic, electrophilic, insertion pathways; Hammett relation, application of LFER in chemical kinetics

3. Cluster compounds (12 lectures)

   Classification, elemental clusters, cluster skeletal electron (Elm) counting, higher boron hydrides-structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, chevrel compounds, infinite metal chains, multidecker molecules, cluster-surface analogy

Suggested books


MSCCHEMC202: Organic Chemistry General II

Unit I

1. Organic name reactions (10 lectures)
   - Baeyer-Villiger oxidation; Burton reaction; Beckmann rearrangement; Birch reduction; Claisen rearrangement; Favorskii reaction; Fries rearrangement; Heck reaction; Mannich reaction; McMurry reaction; Michael addition; Perkin reaction; Sharpless asymmetric epoxidation; Stile coupling; Strecker reaction; Suzuki coupling; Wittig reaction; Yamaguchi esterification

2. Reaction intermediates (09 lectures)
   - Generation, stability & structure, and reactivity of the reaction intermediates, viz. carbocations, carbanions, carbon free-radicals, carbenes, benzynes and nitrenes

3. Synthetic polymers and biopolymers (06 lectures)
   - Introduction to polymers - synthetic polymers; principles of macromolecular synthesis; step-growth vs. chain-growth polymerizations; Dendrimers: Dendritic polymers and their potential applications; chemistry of biopolymers (carbohydrates, proteins, and nucleic acids)

Unit II

4. Chemistry of natural products: Chemistry and function (15 lectures)
   - Chemistry and function of some major groups of natural products such as terpenoids (monoterprenoids: geraniol, alpha-pinene, camphor, menthol, carvone; sesquiterpenoids: farnesol, zingiberine, caryophyllene, santonin; diterpenoids: abietic acid, taxol; triterpenoids: beta-amyrene, oleanolic acid, ursolic acid), alkaloids (papaverine, emitene, morphine, quinine, nicotine, ephedrine) and carbohydrates (monosaccharides and disaccharides); concepts on biosynthetic pathways (mevalonic acid, geranyl pyrophosphate, shikimic acid) for natural products

5. Medicinal chemistry (10 lectures)
   - Concept of drug design (physiochemical principles and basis of drug design, quantitative description, physicochemical approach of drug molecules, different methods of drug design, Free Wilson method and its application to extrathermodynamic approach); pharmacodynamic and pharmacokinetic (drug absorption, distribution, metabolism and excretion) aspects; drug targets (enzymes, receptors, nucleic acids); membranes and receptors (drug transport mechanism and absorption processes, prodrugs and bioactivation, receptor theories and receptor models, drug receptor interactions); concept on lead compounds and lead modifications; pharmacophore; structure-activity relationship (SAR); clinical trials; bioavailability; computer-aided drug design (de novo design), docking procedures and molecular modeling; discussion with suitable examples of choice.

Suggested books


MSCCHEMC203: Physical Chemistry General II

Unit I

1. Symmetry and group theory
   Concept of symmetry, symmetry elements and symmetry operations, optical activity, concept of groups, point symmetry groups, class, group multiplication tables, matrix representation, equivalent and reducible representations, irreducible representations, great orthogonality theorems statement and interpretation, proof of its corollaries, character table and its construction, number of times an irreducible representation occurs in a reducible one; the reduction of reducible representations, notation of irreducible representations, link between group theory and quantum mechanics, direct product representations, vanishing integrals and projection operators

Unit II

2. Quantum mechanics II
   Harmonic Oscillator: solution of Schrodinger equation of a harmonic oscillator using the operator method as well as the technique for solution of differential equation, selection rules for harmonic oscillator, checking the validity of Schrodinger wave equation based on correspondence principle, Heisenberg’s Uncertainty principle, QM of rotational motion; angular momentum operators and their commutation relations, operator algebra and Ladder operators for rotational motion, solution of Schrodinger equation using the operator method as well as the technique for solution of differential equation, quantum mechanics of rigid rotor and its application
   Hydrogen atom: Separation of translational and internal motion of a two-body problem, determination of radial part of the wave function, relation among principal, azimuthal and magnetic quantum number, nodal properties of angular part as well as the radial part of the hydrogen atom wave function, shape of the orbitals, space quantization, selection rules for hydrogen atom.

3. Chemical Kinetics
   Transition state theory, potential energy surfaces, concept of imaginary frequency, thermodynamic treatment of reaction rates, energy of activation, volume of activation, reactions in solutions, diffusion and activation controlled
reactions, influence of solvent dielectric constant and ionic strength on reaction rates, linear free energy relationship, effect of substituents, Hammet's and Taft's constants, Hammet's acidity functions, Oscillatory reactions

Suggested books


MSCCHEMC204: Analytical Chemistry General II

Unit I

1. **Nuclear force, structures and properties** (18 lectures)

   Fundamentals, nuclear composition, different nuclear forces; concept of nuclear angular momentum, magnetic dipole moment and electronic quadruple moment (elementary idea), nuclear magnetic dipole moment and electric quadruple moment in terms of shell model, parity of nuclear energy states; liquid drop model, formulation of semi-empirical binding energy equation, mass parabola and application of binding energy equation; nuclear reactions, Q-value and cross section of nuclear reaction, compound nucleus theory, shell model, nuclear magic number and its derivation from nuclear potential well, calculation of nuclear spin, nuclear isomerism and non-optical transitions; two body problem - properties of deuteron
and derivation of depth-range relationship, its applications in explaining nature of nuclear force, nuclear models - strong and weak interaction, collective model, Fermi gas model, nuclear excitation, idea of nuclear temperature and entropy

2. **Nuclear quadruple resonance and Mossbauer spectroscopy** (07 lectures)

NQR, Mossbauer effect - conditions, nuclear recoil, Doppler effect, instrumentation, chemical shift examples, quadrupole effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, typical spectra of iron and tin compounds

Unit II

3. **Theory of radioactive decay and radioactive equilibrium** (10 lectures)

Introduction, quantum mechanical aspects of radioactive disintegration, alpha decay paradox and its explanation in terms of tunnel effect, Geiger-Muller relationship, time-dependant perturbation theory, Golden rule and its application in explaining beta and gamma transition, selection rules

Successive disintegration, Bateman equation, secular and transient equilibrium, no equilibrium; analysis of special types of successive disintegration, formation of radionuclide in a nuclear reaction, activation analysis

4. **Surfactants and utility** (07 lectures)

Preamble, surface excess; classification of surfactants BET isotherm, LB film, membrane equilibrium, micellisation, Kraft temperature, synthetic application of micellar catalysis, mixed micelles, foaming of surfactant solution, different types of interface, emulsion and emulsifier, photochemistry and redox reaction in micellar systems, nanoemulsion and stabilisation

5. **Environmental chemistry** (08 lectures)

Sustainable development, twelve principles of green chemistry and implementations, atom economy, environmental E-factor, role of catalysts, microwave and ultrasound irradiation in green synthesis, traditional and alternative commercial syntheses of ibuprofen, adipic acid and maleic acid etc, green chemistry in action developing foam, whitening agent, detergent builders, green insecticides, biosynthesis of synthetic chemical, photochemical reactions in atmosphere, photochemical smog and stratospheric ozone depletion; chemicals from renewable feedstock

**Suggested books**


Practical Papers (For Each, Full Marks: 50; Credit: 4)

**MSCCHEMC205: Physical Chemistry General: Practical**

1. Experiments in equilibrium and kinetics
3. Instrumental methods: colorimetry, polarimetry, conductometry and potentiometry
4. Data processing and elementary numerical techniques

**MSCCHEMC206: Analytical Chemistry General: Practical**

1. Experiments on quantitative estimation: analysis of selected ores and alloys
2. Separation techniques involving ion-exchange and solvent extraction
3. Titrimetric estimation of different organic compounds
4. Beer’s law: application in different chemical matrices

Extra Departmental Electives (Full Marks: 50; Credit: 4)

**MSCCHEMMIE201: Supramolecular and Medicinal Chemistry**

Concept and language, choice of building blocks – a sheer necessity, atomic and molecular valences, supramolecular orbitals, principle of three C’s, pallet of non-covalent forces such as hydrogen bond, π–π, C-H–π, halogen–π, S–π, cation–π, hydrophobic, hydrophilic etc interactions and their harnessing towards crystal engineering.
structure directed supramolecular arrays, allostery, proton and hydride sponges, lock and key principle, host-guest interaction, self organization and self complementarity, superstructures in organic, inorganic, metallo-organic and organometallic compounds, 0D, 1D, 2D, 3D architectures and hierarchies, crystal synthesis, supramolecular devices, deliberate isolation of different functional materials, molecular receptor and specific molecular recognition

Drug discovery and history of medicinal chemistry, drug and medicine, physiochemical principles and basis of drug design, pharmacodynamic and pharmacokinetic (drug administration, dosing, absorption, distribution, metabolism and excretion) aspects; drug targets (enzymes, receptors, nucleic acids); prodrugs and bioactivation, concept on lead compounds and lead modifications; pharmacophore; structure-activity relationship, clinical trials; bioavailability; computer-aided drug design; uses of different drugs and medicines: carcinogenesis, applications of chelators and metal chelates of different generations; antitumour, anticancer and anti-AIDS drugs, mechanistic pathway, limitation, future dimension

*Suggested books*


**Semester-III**

Theoretical Papers (For Each, Full Marks: 50; Credit: 4)

**MSCCHEMC301: Advanced Inorganic Chemistry General**

**Unit I**

1. **Structure and properties of solids**
   - Fundamentals, ionic, covalent, metallic hydrogen bonded and molecular solids; perovskite, ilmenite and rutile; spinel and inverse spinel, diamond cubic, silicates: single/double chain, 3D network, pyroxene, amphibole, talc, mica, clay, zeolite; crystal defects, non-stoichiometric compounds; electronic properties of solids, F-centre, conductors, insulators, semiconductors, superconductors; ferroelectricity, antiferroelectricity, pyroelectricity, piezoelectricity, liquid crystals, cooperative magnetism.

2. **Metal ion promoted reactions**
   - Fundamentals, simple cycle, catalytic cycle, pliancy of substrates, Tolman catalytic loop, homogeneous/heterogeneous catalysis: Wacker-Smidt synthesis, Monsanto acetic acid process, hydrogenation by Wilkinson’s catalyst, water gas shift reaction (WGSR), Fischer-Tropsch synthesis, hydrosilation, hydrophosphilynation, hydroamination, hydrocyanation and hydroboration reactions, reactions on inorganic functional groups

**Unit II**

3. **Molecular magnetism I**
   - Classification of magnetic materials, van Vleck equation and its application, Curie-Weiss law and its implication, Lande interval rule, microstates, multiplet, multiplet width, hole formalism, zero-field splitting, spin-orbit coupling, quenching of orbital contribution, Fermi contact and pseudo-contact shifts, chemical shift reagent

4. **Supramolecular Chemistry I**
   - (12 lectures)
Concept and language, scientific/technological landscape, building block, atomic and molecular valences, supramolecular orbitals, pallet of non-covalent forces and their harnessing towards crystal engineering, structure directed supramolecular arrays, crystal synthesis, deliberate isolation of different functional materials

**Suggested books**


**MSCCHEMC302: Advanced Organic Chemistry General**

**Unit I**

1. **Green chemistry: Concept, practice and aspects in current synthetic chemistry**
   
   The concept and ‘Twelve Principles’ of green chemistry; current-day need in chemical and industrial sectors; atom-economy; choice of catalysts, solvents, energy consideration and reaction media, and eco-friendliness and sustainability of a chemical process; tools of green chemistry; real-world cases of practicing green chemistry

2. **Organic synthesis focusing on carbon-heteroatom bonds**
   
   *Organoboron chemistry*: Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates; *Organosilicon chemistry*: Chemistry of organosilicon compounds, synthetic uses of silyl ethers, silylenol ethers, TMSCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon Baeyer-Villiger rearrangement; *Organophosphorous chemistry*: Chemistry of organophosphorus compounds, phosphorus ylides – Wittig reaction and its modifications, phosphine oxides and its applications; *Organosulphur chemistry*: Chemistry of organosulphur compounds, sulphur- stabilized anions and cations, sulphonium salts, sulphonium and sulfoxonium ylides

**Unit II**

3. **Protection-deprotection and retrosynthetic strategy applied in organic reactions**
   
   *Protection-deprotection*: Principle of protection-deprotection and its role in organic synthesis, different methods for protection-deprotection of common functional groups (alcoholic and phenolic hydroxyl(s), amino, carbonyl and carboxylic groups)

   *Retrosynthetic strategy*: The disconnection approach – basic principles, one-group and two-group disconnections; strategies of retrosynthesis; retrosynthetic analysis for ibogamine, valeranone, squalene, estrone, progesterone and ginkgolide B

4. **Pericyclic reaction I**
   
   Definition and classification of pericyclic reactions; methods of analyzing pericyclic reactions (Molecular Orbital Symmetry Correlation Method, Frontier Orbital Method (FMO), and Transition State Aromaticity Method); *Electrocyclic reactions*: Definition, classification, Woodward-Hoffmann Rules for electrocyclic reactions, examples of different types of electrocyclic reactions (three-, four-, five- six-, seven- and eight-membered ring systems); *Cycloaddition reactions*: Definition, classification, Woodward-Hoffmann Rules for cycloaddition reactions, examples of different types of cycloaddition reactions – [2π + 2 π]-cycloadditions, [4π + 2 π]-cycloadditions, dienes and dienophiles, Diels-Alder reaction,
′cis′ rule, Alder’s ′endo′ rule, regioselectivity, 1,3-dipolar cycloadditions, higher order cycloadditions ([4π + 4 π]-, [6π + 4 π]-, [8π + 2 π]- and [14π + 2 π]-cycloadditions).

5. Organic photochemistry I

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, Cis-trans isomeriation, Paterno-Buchi reaction, Norrish type I and II reactions, di-pi-methane rearrangement, photochemical reactions of carbonyl compounds

Suggested books


P. T. Anastas (Series editor), Handbook of Green Chemistry, Wiley-VCH Book Series

James H Clark (Series Editor-in-Chief), RSC Green Chemistry, Royal Society of Chemistry Book Series


D. W Allen, D. Loakes and J. C Tebby (Series Editors), Organophosphorous Chemistry, RSC Book Series.


MSCCHEMC303: Advanced Physical Chemistry General

Unit I

1. Applications of group theory in chemistry (13 lectures)
   Molecular vibrations, Normal mode analysis, symmetry of normal modes, Selection rules for infrared and Raman spectra, Hybridization, Construction of Symmetry adapted linear combination of atomic orbitals (SALC), Molecular orbital description of different organic, inorganic and organometallic molecules. Application of group theory to ligand and crystal field theory, construction of energy level diagrams, correlation diagrams. Symmetry and chemical reactions; Woodward-Hoffmann rules.

2. Crystallography and surface chemistry (12 lectures)
   Crystal symmetry, translation, glide plane and screw axis, Bravis lattice, space groups and its determination, stereographic projection, Fourier series, electron density and structure factor, methods for solving the phase problems, Bzones and Fermi level in lattice, concept of particle-hole in conduction process, band theory, theory of conductors, semiconductors and insulators.

   Solid surfaces: External and internal surfaces; Bulk and surface structure of FCC, BCC and HCP metals; Notation of surface structures; Relaxation and reconstruction of surfaces; homogeneous and heterogeneous surfaces. Solid-gas interfaces: Types of adsorption; Adsorption isotherms – Langmuir, Tempkin and BET. Determination of surface area of adsorbents; temperature dependence of adsorption isotherms.

Unit II

3. Chemistry of Polymers (08 lectures)

4. Biophysical chemistry (08 lectures)
5. Spectroscopy (09 lectures)

Maxwell’s field equations, transition between states, selection rules and forbidden transitions; NMR: Relaxation and exchange phenomena, theories of chemical shift and nuclear spin-spin coupling in 2-spin systems with applications, pulsed NMR (spin echo); Electronic: n-π*, π- π* and CT transitions; vibrational: simple polyatomic molecules, normal modes, influence of nuclear spin on vibration-rotation spectra of polyatomics, time-resolved IR, 2-d IR, principles of 1D and 2D NMR. Principles of ESR and Mossbauer spectroscopy.

Suggested books

X. Clegg, Crystal Structure Determination, Oxford University Press, Oxford,
A. R. West, Basic Solid State Chemistry, Wiley
G. A. Somorjai, Y Li., Introduction to Surface Chemistry and Catalysis, Wiley.
P. J. Flory, Principles of Polymer Chemistry, Cornell University Press.
J. P. Allen, Biophysical Chemistry, Wiley
I. N. Levine, Quantum Chemistry: Molecular Spectroscopy,


Major Electives (any one)

**MSCCHEMMJE301: Inorganic Chemistry Major I**

**Unit I**

1. **Synthetic methodology in inorganic, coordination and organometallic chemistry**  
   (15 lectures)
   
   Ligand design/synthesis, ligand topology, molecular mechanics/engineering, tailoring/appending of pendant arm; coordination compound design/synthesis using classical/benign method, self-assembly, atom economy, thermolysis, photolysis, sonolysis, electrolysis, sol-gel method, hydrothermal method, cryochemistry, top-down and bottom-up methods for nano-structured solids

2. **Organometallic chemistry II**  
   (10 lectures)
   
   Reactions occurring in metal-bound state: ligand substitution, oxidative addition, reductive elimination; reactions triggered by modification on ligand framework: insertion and deinsertion, ligand-based nucleophilic addition, nucleophilic abstraction, electrophilic reactions; applications to organic synthesis: enantioselective functional group interconversion, chiral synthesis, protection and deprotection; transmetallation and cyclisation reactions, bioorganometallics, organo-dendrimer, surface organometallic chemistry

**Unit II**

3. **Spectral (IR, NMR, EPR, UV-Vis Mossbauer, etc.) studies of inorganic, coordination and organometallic species**  
   (25 lectures)
   
   Fundamentals, elucidation of geometric structure, electronic structure, stereochemistry, bonding, molecular aggregate, superstructure and reaction pathway in halide, pseudohalide, carbonyl, nitrosyl, DMSO, poly(pyridine, azoheterocycle, oxime, quinone, macrocycle containing compounds and organometallic complexes; enumeration and characterization: geometrical (cis/trans, fac/mer) and stereo (optical) isomers in different polyhedra; ligational motif and chelate loop, structural distortion, effective pi-acceptance centre, oxidation state, spin state, redox site of non-innocent ligands, mu-bonding and hapticity, electrophilicity/nucleophilicity, quasi- and superaromaticity, fluxionality, matalloligand, probing chemical reactivity and reaction pathways (intramolecular/intermolecular, stereoretentivity/stereodynamicity), covalency of ML bonding and comment on bonding theories

*Suggested books*


Unit I

1. VBT and MOT: Concept, molecular structure and reactivity (05 lectures)
   Orbital, atomic orbitals, hybridization of atomic orbitals, HOMO, LUMO, molecular structure and reactivity –
   Basic concepts and understanding with the help of Valence Bond Theory (VBT) and Molecular Orbital Theory (MOT)

2. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) (05 lectures)
   Chiroptical properties of organic molecules; ORD and CD principles and applications; ORD and CD curves:
   Cotton effect; empirical and semiempirical rules

3. Asymmetric synthesis (15 lectures)
   Principles and newer methods of asymmetric synthesis (including enzymatic and catalytic nexus); enantio- and
   diastereoselective synthesis; reactions of enolates (α–substitution); addition to C=C double bonds (electrophile-induced
   cyclisation, iodolactonisation, hydroboration, conjugate additions); asymmetric hydrogenation with special reference to Ru-
   BINAP catalysts; asymmetric reduction of prochiral ketones with Baker’s Yeast and CBS-catalyst; asymmetric epoxidation
   with special reference to Sharpless and Jacobsen epoxidation; asymmetric aldol reactions, asymmetric Michael reaction;
   Few important industrial applications of asymmetric synthesis

Unit II

4. Chemistry of heterocyclic compounds: Synthesis, properties and reactions (15 lectures)
   Nomenclature of bicyclic and tricyclic fused systems; heterocyclic synthesis – principles of heterocyclic synthesis
   involving cyclization reactions and cycloaddition reactions; synthesis and reactivity of 3-, 4-, 5-, 6- & 7-membered
   heterocycles with one, two or more heteroatoms (aziridines, oxiranes, thiranes, azetidines, oxetanes, thietanes, diazines,
   triazines, thiazines, azaepines, oxepines); benzo-fused five and six-membered heterocycles - synthesis and reactions
   including medicinal applications of benzopyrroles, benzofurans, benzothiophenes, quinolizinum and benzopyrylium salts,
   coumarins and chromones; phosphorus and selenium containing heterocycles; role of heterocyclic compounds in biological
   systems; heterocycles in pharmaceutical industry.

5. Organometallic chemistry (10 lectures)
   Application of transition metals in organic synthesis – preparative, structural and mechanistic aspects; Davies rule,
   catalytic nucleophilic addition and substitution reactions; coupling reaction – Heck, Stille, Suzuki coupling Ziegler Naata
   reaction; olefin metathesis; Tebbe’s reagent, Pauson-Khand reactions; Volhsrdt co-trimerisation, functional organometallic
   compounds; use of non-transition metals- Indium, tin, zinc in organic synthesis

Suggested books


MSCCHEMMJE303: Physical Chemistry Major I

Unit I

1. Classical mechanics

Newton’s prescription for classical mechanics, Laws of motion: law of inertia, law of causality, Superposition principle of force, introduction to the idea of law of force for motion, Conservative and non-conservative force, definition of potential energy, conservation of total mechanical energy for conservative system and its implication, principle of least action, generalized coordinate systems, Legendre transformation, Poission bracket Lagrangian equation of motion and definition of generalized momentum, Hamiltonian equation of motion.

2. Approximate methods in quantum chemistry

Variation theorem, application to ground states of various systems. Linear variation method, Secular determinant, Introduction to matrix mechanics-eigen values and eigen vectors, Variation method for excited states. Time-independent
perturbation theory for nondegenerate states, Perturbation of a two-level system, Many level systems, Degenerate perturbation theory and Stark effect, Hellman-Feynman and Virial Theorems. Time-dependent perturbation theory, Rabi Oscillation, Many level system; the variation of constants, the effect of slowly switched constant perturbation, The effect of oscillating perturbation, Transition rates to continuum. A semi-classical treatment to radiation-matter interaction. Fermi Golden rule, Einstein transition probabilities, lifetime and energy uncertainty.

Unit II

3. Statistical Mechanics  


Suggested books


Practical Papers (For Each, Full Marks: 50; Credit: 4)

**MSCCHEMC304: Advanced Chemistry General** (compulsory for all)

1. Instrumental methods in chemical analysis: use of different instruments like UV-Vis, FTIR, Fluorimeter, Thermal Analyser, CHN(S) Analyser, Electrochemical Analyser, etc in various chemical analyses and computer simulation

**MSCCHEMMJE304: Inorganic Chemistry Major: Practical I**

1. Synthesis of di-, tri- and polydentate Schiff bases and related chelators/congregators
2. Isolation of the complexes with synthesized ligands in (1) and ones commercially available
3. Spectroscopic (IR, UV-Vis, Fluorescence, etc) characterization of the ligands and complexes
4. Determination of composition and formation constants of selected systems by pH-metric and spectrophotometric methods

**MSCCHEMMJE305: Organic Chemistry Major: Practical I**

1. Quantitative estimation of organic compounds
   a) Sugars (glucose, cane sugar), (b) phenol, (c) aniline, (d) acetone, (e) nitrogen by Kjeldahl method, (e) saponification and iodine value of oil
2. Organic preparation (single and/or two-step process)
   Preparation of organic compounds by conventional and green chemical methods (involving single and/or two-step process) followed by purification and characterization by spectroscopic technique

**MSCCHEMMJE306: Physical Chemistry Major: Practical I**

1. Determination of dissociation constants by measuring conductivity of weak acids
2. Determination of weak acids’ dissociation constant via potentiometric titration
Semester-IV

Theoretical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC401: Advanced Analytical Chemistry General

Unit I

1. Complexes in aqueous solution (09 lectures)
   pH-potentiometric, spectrophotometric methods (slope-ratio, mole-ratio and Job’s method of continuous variation of measuring stability constants of complexes, Bjerrum half n method, stability of mixed ligand complexes and calculations; determination of composition, evaluation of thermodynamic parameters, factors influencing the stability of complexes

2. Advanced spectroscopic methods including hyphenated ones (16 lectures)
   Instrumentation, presentation of spectra, Applications of heteronuclear NMR spectroscopy; $^{11}$B, $^{13}$C, $^{14}$N, $^{17}$O, $^{19}$F and $^{31}$P-NMR, $^{195}$Pt. CD/ORD: methods, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application. EPR: anisotropy, intensity, hyperfine splitting, Kramer’s theorem, photoelectron spectroscopy, ESCA, UPS, Auger, AES, XRF and EXFAS; Synergistic benefit: spectroscopic and other tools in structure elucidation

Unit II

3. Electroanalytical methods II (09 lecturers)
   Instrumentation: cyclic voltammetry, differential pulse voltammetry, coulometry, electrogravimetry, LSV; methods, low-temperature accessory, interfacing, conjunctive study, switching potential, electrode potential, pathways of electron transfer: EEE, EC, EC', ECE; electro-induced reactions; conventional secondary batteries: Ni-Cd, Ni-Fe, Ag-Zn, ZEBRA system; surface-modified study, materials preparation

4. Application of radiotracers and radiopharmaceuticals (09 lectures)
   Radiotracers: isotope dilution; DIDA, IIDA and substoichiometric methods of analysis, application, nuclear activation analysis: principles, classifications and methods of nuclear activation analysis; special types of derivative activation analysis, depth profile activation analysis, cyclic activation analysis, charged-particle activation analysis (CPAA): PGNAA, PIXE, PIGE, IPAA, RBS; general considerations and factors; biosynthesis, factors in labeling: efficiency, isotope effect, specific methods of labeling

Radiopharmaceuticals: design of a new radiopharmaceutical: nuclear pharmacy: concept, pharmaceuticals and radiopharmaceuticals; radionuclide generators; ideal radiopharmaceuticals, methods of radiolabelling, specific radiopharmaceuticals for diagnostic and therapeutic purposes

5. Chemical and biological effects of radiation (07 lectures)
   Ionizing radiation and its physical and chemical effect in target, water, radiolysis; definition of different units in radiation chemistry, calculation of radiation dose, biological effects, source of human data, lethal dose, permissible level of radiation dose; primary radiological products of water and their characterization, dosimetric concepts and quantities, thermoluminescence and lyoluminescence
Suggested books


Major Electives (any one from 0402-0407 and any one from 0405-0407)

**MSCCHEMMJE401: Inorganic Chemistry Major II**

**Unit I**

1. **Electrochemical studies of redox non-innocent ligands and metal complexes**

   Fundamentals, experimental findings of CV, DPV and coulometry, delving reversible, quasi-reversible and irreversible electrochemical and chemical processes in model compounds; electro-induced reactions: protic/electroprotic equilibrium, electrocatalysis, electropolymerisation, electrocrystallisation, electrochemiluminescence; electrosynthesis, evaluating comproportionation constant, photoelectrochemistry, spectroelectrochemistry, excimer and its structure, excited state potential and chemical simulation, redox orbital, redox series, redox isomer, electron hopping, spatially isolated orbital; synergistic experiments and exposing electron transfer site, model case correlating biological processes

2. **Mechanism of electron transfer reactions**

   Fundamentals, complementary and non-complementary redox reactions, outer-sphere reaction, inner-sphere reaction, effect of bridging ligand in inner-sphere reaction, kinetics and mechanism, electron tunneling hypothesis, heteronuclear redox reaction and simplified Marcus theory; Marcus cross relationship and its application, remote attack, doubly-bridged process, ligand exchange, intervalence electron transfer, induced reaction, electron transport in biological systems and their simulations

**Unit II**

3. **Inorganic photochemistry**

   Preamble, photoexcitation, fluorescence, phosphorescence, photosensitization, quenching, charge and energy transfer, prompt and delayed reactions, excimer structure, substitution, fragmentation, isomerisation, exchange and redox
reactions; chemiluminescence, photochromism; chemical actinometry and determination of quantum yield, inorganic photochemistry in biological processes and their model studies; applications of photochemical reactions of coordination compounds - synthesis and catalysis, solar energy conversion and storage

4. Inorganic and organometallic reaction mechanism

Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to dⁿ ion complexes: operational tests, aquation and anation, reactions without metal-ligand bond breaking, kinetics of chelate formation, reaction mechanisms of organometallic systems, studies on fast reactions, kinetic and activation parameters - tools to propose a plausible mechanism; stereochemical changes: types of ligand rearrangements, isomerism in 4-, 5- and 6-coordinated complexes; reactions of coordinated ligands: model choice of metal and ligand, acid-base reaction, hydrolysis of esters, amides and peptides, aldol condensation, trans-amination, template reactions, organic synthesis with special reference to macrocyclic ligand; variable-temperature reactions in fluxional organometallic compounds

Suggested books


**MSCCHEMMJE402: Organic Chemistry Major II**

**Unit I**

1. **Advanced techniques in organic synthesis**
   (17 lectures)
   Recent advances in organic synthesis focusing on the successful application of microwave (MW) irradiation, ultrasound (US) irradiation, visible light, ball-milling, and syntheses under solid-phase, room-temperature synthesis (ambient conditions)

2. **Organic photochemistry II**
   (8 lectures)
   Photochemistry of arenes; photoreaction in solid state; method of generation and detection (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications; cyclization of radicals; photo-induced oxidations and reductions

**Unit II**

3. **Structure-function relationship in carbohydrates, proteins, lipids, nucleic acids and enzymes**
   (18 lectures)
   *Carbohydrates*: Basic structure and type of sugars, reactions, protection and deprotection, deoxy-sugars, amino sugars, glycal sugars and their synthetic aspects, mutarotations, carbohydrates as chiral pools in organic synthesis; *Proteins*: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of proteins, Ramachandran Diagram, forces responsible for holding of secondary structures, α-helix, β-sheets, tertiary structure of protein-folding, quaternary structure, biosynthesis of peptide chain; *Lipids*: Fatty acids, structure and function of triacylglycerols, glycerophospholipids, properties of lipid bi-layers, biological membranes, fluid mosaic model of membrane structure; *Nucleic acids*: Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding, structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it; *Enzymes*: Chemical and biological catalysis, properties of enzymes like catalytic power, specificity and regulation, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis; mechanism of enzyme action: transition state theory, examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease
4. Co-enzyme chemistry

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, Structure and biological functions for pyridoxal phosphate, NAD+, NADP+, FMN, FAD; mechanisms of reactions catalyzed by the above cofactors

Suggested books


MSCCHEMMJE403: Physical Chemistry Major II

Unit I

1. Quantum mechanics of many electron systems (18 lectures)


2. Molecular interactions (07 lectures)

Hamiltonian in absence and presence of external fields, forces in molecules, Hellmann-Feynmann theorem, perturbative treatment of electric polarisability, intermolecular interaction - calculation of dispersion energy, the London formula

Unit II

3. Irreversible thermodynamics and introductory course on non-equilibrium statistical mechanics (18 lectures)


4. Electric and magnetic properties of molecules (07 lectures)

Dielectric polarization; Debye equation and its limitation; Onsager’s reaction field model; electric polarizability of molecules; magnetic susceptibility - diamagnetic and paramagnetic, Currie law

Suggested books

A. Szabo, N. S. Ostlund, Modern Quantum Chemistry, Dover Publications, Inc, NY
D. W. Davies, The Electric and Magnetic Properties of Molecules,
R. Zwanzig, Nonequilibrium Statistical Mechanics, Oxford University Press.

MSCCHEMMJE404: Inorganic Chemistry Major III

Unit I

1. Supramolecular chemistry II (12 lectures)
   
   Judicious choice of geometry setter/blocker/spacer/counter ion – an essential prerequisite, hydrogen bonding, π…π, C-H…π, halogen…π, S…π, etc interactions, allosterism, proton and hydride sponges, principle of three C’s, lock and key principle, host-guest interaction, self organization and self complementarity, receptors, superstructures in inorganic, metallo-organic and organometallic compounds, 0D, 1D, 2D, 3D architectures and hierarchies, supramolecular devices

2. Inorganic materials (13 lectures)
   
   Molecules and crystals to materials, art of synthesis, predictable crystalline architecture, intermolecular and interion interactions, secondary building unit (SBU), surface functionalisation, hysteresis, robust and directional interactions, click chemistry, functional materials: conducting, superconducting, magnetic, non-linear, porous, luminous, liquid crystals, quantum dots, catalysts, molecular and electronic devices, biosensors, biomineralization, proteomics, dendrimers, molecular recognition

Unit II

3. Molecular magnetism II (13 lectures)
   
   Isolation of different molecular magnets, magnetic interactions in di- and polynuclear systems and clusters, cryogenic experiment, mechanism of exchange interaction, Bleaney-Bowers equation, antiferromagnetism (AF), ferromagnetism (F), single molecule magnet, deliberate synthetic approach of ferromagnetically coupled system, accidental orthogonality, spin canting, canted-AF, canted-F, spin frustration, admixed-spin, spinflop, metamagnetism, superparamagnetism, long-range ordering, calculation of ground state and spin manifold, magnetization versus field studies, inorganic, organic, metal-organic and organometallic magnetic materials

4. Structure-function relationship (12 lectures)
   
   A sheer necessity and an ultimatum, thermodynamic and kinetic parameters; diagnostic probes: spectroscopic, thermal, electrochemical, magnetic, crystallographic; parameters: stretching frequency, chemical shift, spin-spin coupling constant, isomer shift, potential value, bond distance, bond angle, torsion angle, crystal packing and Madelung constant, magnetic moment value, rate constant, half life, correlation diagram, room temperature and variable-temperature results, breakthrough and legacy
**Suggested books**


1. **Pericyclic reactions II** (08 lectures)

   Sigmatropic reactions: Definition, classification, stereochemistry, Woodward-Hoffmann rules, illustrations for [1,2]-, [1,3]-, [1,4]-, [1,5]-, [2,3]- and [3,3]-sigmatropic rearrangements, Claisen rearrangement, Cope rearrangement; Chelotropic reactions: Definition, Woodward-Hoffmann rules, examples of chelotropic reactions (chelotropic reactions involving SO₂, chelotropic extraction of nitrogen, chelotropic decarbonylation of ketones, chelotropic trapping of nitric oxide), synthetic applications; Ene reactions: Definition, classification, catalyzed and uncatalyzed ene reactions, stereochemistry of ene reactions – diastereoselection, oxy-ene and anionic oxy-ene-reactions, imino-ene reactions, carbonyl ene-reactions, singlet oxygen ene-reactions, retro-ene reactions.

2. **Supramolecular chemistry** (07 lectures)

   Basic concepts of supramolecular chemistry, different non-covalent forces (hydrogenbonding, cation-π, CH-π, π-stacking, hydrophobic, hydrophilic interactions etc.) leading to strong bonding of guest molecules to the host, design principle of host or receptor molecules, different experimental techniques to characterize the host–guest complexation, example of molecular receptors: crown ethers, ionophores, cyclophanes, cyclodextrins and their application in specific recognition processes.

3. **Antibiotics, antidiabetic and cardiovascular drugs: Chemical aspects** (10 lectures)

   Antibiotics: Cell wall biosynthesis, inhibitors, β-lactam rings, synthesis of penicillin; synthesis and mode of action of sulphonamides, nalidixic acid, norfloxacin, aminosalicyclic acid, ethinamide, fluconazole, chloroquin and premaquin; Antidiabetic drugs: insulinsensitizers (biguanides, thiazolidinediones), secretagogues (sulfonylureas, nonsulfonylurea secretagogues, alpha-glucosidase inhibitors, peptide analogues (injectable incretin mimetics, injectable amylin analogues); Cardiovascular drugs: Introduction to cardiovascular diseases, synthesis and mode of action of statins, amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil and methyl dopa

4. **Chemistry of polyphenolics** (12 lectures)

   Natural occurrence, chemical aspects, biological activities and therapeutic potential of some notable natural polyphenolics from the respective group: ellagitannins, flavonoinds and xanthonoides

5. **Chemistry of steroidal hormones** (07 lectures)

   Chemistry and function of some steroidal hormones – estrogens, estrone, estradiol, estriol, progesterone, testosterone, oral contraceptives, anabolic steroids

6. **Biosynthesis of some selected biologically relevant natural products** (06 lectures)

   Atropine, quinine, nicotine, abietic acid, β-carotene, cholesterol

**Suggested books**


MSCCHEMMJE406: Physical Chemistry Major III

Unit I

1. Molecular reaction dynamics (MRD) (12 lectures)
   Motivation for studying MRD, Spectator model, Molecular collisions, Vocabularies in MRD, Dynamics of elastic molecular collisions, Collision cross section, The impact parameter, Centrifugal energy and barrier, The reaction cross section, Reaction probability, opacity function, translation energy requirements of chemical reactions, Scattering as probe of the collision dynamics, The angular function, The deflection function, Scattering as a probe for the potential, Product angular distribution in reactive collisions, Potential energy surfaces (PES) for a reaction, attractive and repulsive PES, Polyan’s rules
2. Solid state chemistry (13 lectures)

Crystal structure: lattice, basis, concept of Bravais lattice, primitive and non-primitive cell for SC, BCC, FCC, HCP; construction of Wigner-Seitz cell; different lattice structures: diamond, zincblende, etc.; crystallographic point group and space group Reciprocal lattice, relation with Miller indices; Fourier transformation and Fourier space, conversion of primitive axes, Brillouin zone for 1D, 2D and 3D lattices, Determination of crystal structure: Bragg’s condition, von Laue condition, their interrelation, geometrical structure factor. Electronic structure: Classical Drude model and its limitation, DC electrical conductivity, equation of motion; Hall effect, concept of charge carrier, thermal conductivity; Sommerfeld theory, ground state properties of electron gas, Fermi energy, Fermi surface; thermal properties of metal, Electron level in periodic potential: Bloch’s theorem and its consequences; weak periodic potential, density of states, band structure; interaction of bands, tight-binding formulations; semiconductor solids and their properties.

Unit II

3. Photochemistry and Laser principles (15 lectures)


4. Alternative Energy Studies (10 lectures)

Solar energy conversion, artificial photosynthesis; Si-p-n junction solar cell, basic principles and application, Dye-sensitized solar cells; structure, components and their functions. operating principles, Efficiencies of solar cells. Quantum dot sensitized solar cell, Nano hybrid materials for solar cell application.

Suggested books

R. D. Levine, Molecular Reaction Dynamics, 2006, Oxford University Press.
A. R. West, Basic Solid State Chemistry, Wiley
L. Azzarof, Introduction to Solids, 1966
N. J. Turro, Modern Molecular Photochemistry, University Science Books
U. Mehmood et al. Review article on Recent advances in dye sensitized solar cells, Advances in Materials Science and Engineering Volume 2014, Article ID 974782.
Major Elective Practical (any one) (For Each, Full Marks: 50; Credit: 4)

MSCCHEMMJE407: Inorganic Chemistry Major: Practical II

1. Preparation of inorganic and coordination compounds using self-assembly
2. Growing of single crystals
3. Spectral, thermal, electrochemical and magnetic studies
4. Reactivities
5. Kinetic and mechanistic studies of some selected reactions (substitution and redox)

MSCCHEMMJE408: Organic Chemistry Major: Practical II

1. Preparation of organic compounds involving multiple step reactions
2. Characterization of organic compounds using spectroscopic methods

MSCCHEMMJE409: Physical Chemistry: Major II

1. Instrumental methods of studying hydrolysis, solubility and kinetics; elementary computer-based numerical methods
2. Study on charge transfer/EDA complexes
3. Determination of the binding constant of a ‘Host-Guest’ complex by spectrophotometric method
4. Determination of the thermodynamic parameters of the formation of a ‘Host-Guest’ complex
5. Fluorescence lifetime measurement
6. Study of a chemical oscillating system

Term Paper/Project work* (any one from 0411-0413)
(For Each, Full Marks: 50; Credit: 6)

MSCCHEMC402: Inorganic Chemistry Term Paper/Project
MSCCHEMC403: Organic Chemistry Term Paper/Project
MSCCHEMC404: Physical Chemistry Term Paper/Project

*In each discipline concerned MSCCHEMC402-404, topic-selection in consultation with the teacher; literature search from different reference books and using internet search; typed write-up with proper tables, structures, figures and literature to be submitted (approximately 25-30 pages with 12 font size); seminar lecture on this topic to be delivered in presence of all the teachers and an external subject expert