Course Structure

For

M.Sc. Chemistry

Session 2017-2018

Department of Chemistry

Dr. Shakuntala Misra National Rehabilitaion University

Mohaan Road, Lucknow

Pin: 226017

Department of Chemistry

STUDY & EVALUATION SCHEME
SEMESTER-I

Sl.No.	SUBJECT CODE	SUBJECT	PERIOD			EVALUATION SCHEME				SUBJECT TOTAL	CREDIT
						SESSIONAL EVALUATION			EXAM SEE		
			L	T	P	CT	TA/ AT	TOTAL			
THEORY SUBJECTS											
1	MCY-101	Inorganic Chemistry-I	4	0	0	15	15	30	70	100	4
2	MCY-102	Organic Chemistry-I	4	0	0	15	15	30	70	100	4
3	MCY-103	Physical Chemistry-I	4	0	0	15	15	30	70	100	4
4	MCY-104	Analytical Chemistry-I	4	0	0	15	15	30	70	100	4
											16
PRACTICAL											
5	MCY-105	Lab Course-I	0	0	4	0	15	15	35	50	4
	MCY-106	Lab Course-II	0	0	4	0	15	15	35	50	4
		Total	16	0	8	60	90	150	350	500	24

STUDY & EVALUATION SCHEME
SEMESTER-II

Sl.No.	SUBJECT CODE	SUBJECT	PERIOD			EVALUATION SCHEME				SUBJECT TOTAL	CREDIT
						SESSIONAL EVALUATION			EXAM SEE		
			L	T	P	CT	TA/ AT	TOTAL			
THEORY SUBJECTS											
1	MCY-201	Inorganic Chemistry-II	4	0	0	15	15	30	70	100	4
2	MCY-202	Organic Chemistry-II	4	0	0	15	15	30	70	100	4
3	MCY-203	Physical Chemistry-II	4	0	0	15	15	30	70	100	4
4	MCY-204	Analytical Chemistry-II	4	0	0	15	15	30	70	100	4
PRACTICAL											
5	MCY-205	Lab Course-III	0	0	4	0	15	15	35	50	4
	MCY-206	Lab Course-IV	0	0	4	0	15	15	35	50	4
		Total	16	0	8	60	90	150	350	500	24

STUDY & EVALUATION SCHEME
SEMESTER-III

Sl.No.	SUBJECT CODE	SUBJECT	PERIOD			EVALUATION SCHEME				SUBJECT TOTAL	CREDIT
						SESSIONAL EVALUATION			EXAM SEE		
			L	T	P	CT	TA/ AT	TOTAL			
THEORY SUBJECTS											
1	MCY-301	Inorganic Chemistry-III	4	0	0	15	15	30	70	100	4
2	MCY-302	Organic Chemistry-III	4	0	0	15	15	30	70	100	4
3	MCY-303	Physical Chemistry-III	4	0	0	15	15	30	70	100	4
4	MCY-304	Analytical Chemistry-III	4	0	0	15	15	30	70	100	4
PRACTICAL											
5	MCY-305	Lab Course-V	0	0	4	0	15	15	35	50	4
	MCY-306	Lab Course-VI	0	0	4	0	15	15	35	50	4
		Total	16	0	8	60	90	150	350	500	24

STUDY & EVALUATION SCHEME
SEMESTER-IV

Sl.No.	SUBJECT CODE	SUBJECT	PERIOD			EVALUATION SCHEME				SUBJECT TOTAL	CREDIT
						SESSIONAL EVALUATION			EXAM SEE		
			L	T	P	CT	TA/ AT	TOTAL			
THEORY SUBJECTS											
1	MCY-401	Elective-I	4	0	0	15	15	30	70	100	4
2	MCY-402	Elective-II	4	0	0	15	15	30	70	100	4
3	MCY-403	Elective-III	4	0	0	15	15	30	70	100	4
											12
PROJECT											
1	MCY-404	Project	0	0	8	00	00	00	100	100	8
SEMINAR											
1	MCY-405	SEMINAR	0	0	4	00	00	00	100	100	4
		Total	12	0	12	45	45	90	410	500	24

SEMESTER I

MCY-101: INORGANIC CHEMISTRY-I 60h

Unit-I

(a) Symmetry and group theory: Symmetry elements & Operation, Determination of point group of a molecule, Flow chart for assign point group, Mathematical Requirement for a point group, Group, subgroup, class subclass, Character table, and construction of character tables for c_{2v} and c_{3v} groups.

(b) Stereochemistry and Bonding in Main Group Compounds

VSEPR theory & drawbacks, Bent rule, MO theory, Energy level diagram for F_2, O_2, CO, NO. Walsh diagram (triatomic and pentatomic).

Unit-II

Chemistry of Transition Elements-I

General characteristic properties of transition elements, crystal field theory: Splitting of energies of orbitals under ocatahedral, tetrahedral and square planar environment, crystal field stabilization energy, limitations of CFT.

Unit-III

Chemistry of Transition Elements-II

Spectrochemical series, Jahn-Teller effect, stability of coordination complexes and factors effecting stability, nephelauxetic effect, ligand field theory, splitting of d orbital's in low symmetry environments, molecular orbital theory as applied to metal complexes, brief introduction to Angular Overlap Model.

Unit-IV

Chemistry of Transition Elements-III

Spectroscopic ground states, terms and symbols, selections rules, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculation of 10 Dq, B and β parameters, Magnetic moments, Magnetic properties of transition metal complexes, Inter-ion magnetic coupling, anomalous magnetic moments, magnetic exchange coupling and spin crossover, comparison of first transition series with 2^{nd} and 3^{rd} transition series.

Recommended Books:

1. J H Huheey, Inorganic Chemisry - Principles, structure and reactivity, Harper and Row Publisher, Inc. New York (1972)
2. J. D. Lee, Concise Inorganic Chemistry, Elbswith Chapman and Hall, London
3. M. C. Day and J. Selbin, Theoretical Inorganic Chemistry, Reinhold, EWAP
4. F. A. Cotton, R. G. Wilkinson. Advanced Inorganic chemistry
5. Willam L. Jooly, Modern Inorganic Chemistry
6. Manas Chanda, Atomic Structure and Chemical bonding
7. N. N. Green wood and A. Earnshaw, Chemistry of elements, Pergamon
8. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsevier
9. A. F. Wells, Structural Inorganic Chemistry –5th edition (1984).
10. H. B. Gray, Electrons and Chemical Bonding. (Section 2) W.A. Benjamin. London (1965)
11. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International Pvt.Ltd. New Delhi (1999).
12. R. S. Drago, Physical Methods in inorganic Chemistry, Affiliated East-West Press (Section 1& 2) 2nd edition, Reinhold New York (1968).

MCY -102: ORGANIC CHEMISTRY-I 60h

Unit-I

Stereochemistry:

Concept of Chirality and molecular dissymmetry, R and S nomenclature, Geometrical isomerism E and Z Nomenclature, Fischer projections, Sawhorse projections and Zig-zag notation and interconversion, Chirality without chiral centres: allenes, atropisomerism, Prostereoisomerism, Prochiral relationship, homotopic, enantiotopic and disteriotopic atoms, groups and faces. Asymmetric synthesis, enantioselective reaction (Meerwein-Ponndorf-Verley reaction, Sharpless Epoxidation), Cram's rule and Prelog's rule, Recemic modifications and their resolution, enatiomeric excess (ee), Conformation alanalysis of disubstituted cyclohexanes and decalin. Reactions of chiral molecules.

Unit-II

Structure and Reactivity :

Potential energy diagram, transition state and intermediates, methods of determining mechanism, isotope effect. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, Nitrenes, Benzyne. Effect of structure on reactivity- resonsnce and field effect, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.

Unit-III

Organic Reagents (Oxidation)

Oxidations: Metal based and non-metal based oxidations of alcohols to carbonyls (aluminium, DMSO, hypervalent iodine and TEMPO based reagents), alkenes to epoxides (Sharpless asymmetric epoxidation), alkenes to diols, Prevost reaction and Woodward modification, selenium based allylic oxidation, ketones to ester/lactones (Baeyer-Villger).

Unit-IV

Reducing Reagents (Reduction)

Reductions: Catalytic hydrogenation (Heterogeneous: Palladium/Rhodium; Homogeneous: Wilkinson), Hydride transfer reagents (i) $NaBH_4$ triacetoxyborohydride, L-selectride, K-selectride, Luche reduction; $LiAlH_4$, DIBAL-H, and Red-Al; Trialkylsilanes, Meerwein-Pondorff-Verley reduction (ii) Stereo/enantioselectiviey reductions.

Recommended Books:

1. Organic Synthesis: The Disconnection Approach, Stuart Warren, Paul Wyatt.
2. Stereochemistry by P. S. Kalsi (New Age International)
3. Organic Chemistry Vol.I&II. By I.L. Finar
4. Problems and Solutions by I.L.Finar
5. Modern Methods of Organic Synthesis by Carruthers, W and Iain Coldham
6. Stereochemistry of Organic Compounds- D. Nasipuri.
7. Organic Chemistry- R. T. Morrison and R. N. Boyd. (PrenticeHall)
8. Modern Organic Reactions (Benjamin) H. O. House.
9. Principle of Organic Synthesis-R. O. C. Norman and J. M. Coxon. (ELBS)
10. Reaction Mechanism in Organic Chemistry- S. M. Mukherji and S. P. Singh
11. Advanced Organic Chemistry (McGraw-Hill)- J. March
12. Basic Principles of Organic Chemistry (Benjamin) J. D. Roberts and M. C. Caserio.
13. Stereochemistry of Carbon Compounds. (McGraw-Hill) E. L. Eliel
14. Organic Stereochemistry (McGraw-Hill) by Hallas.
15. Introduction to Stereochemistry (Benjumin)- K. Mislow
16. A Guide Book to Mechanism in Organic Chemistry (Orient-Longmens)-Peter Sykes
17. Organic Chemistry (McGraw-Hill) Hendrikson, Cramand Hammond.
18. Modern organic synthesis: An Introduction, George S. Zweifel, Michael H. Nantz

MCY -103: PHYSICAL CHEMISTRY-I

60h

Unit I

Quantum Mechanics: Introduction to Exact Quantum mechanical Results

The Schrödinger equation and the postulates of quantum mechanics, operator, Eigenvalues and Eigen functions ψ, ψ^2, Hermitian operator, Normalisation and orthogonality. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Unit II

Angular Momentum

Ordinary angular momentum, generalized angular momentum, Eigenfunctions for angular momentum, Eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, spin-orbit coupling antisymmetry and Pauli exclusion principle.Perturbation theory. Simple Application of variation method and Perturbation theory.

Unit-III

Chemical Kinetics:

Theories of reaction rates, Collision ,activated complex and unimolecular reaction Lindmann Theory and activation energy and its determination, Kinetics and thermodynamic control of reactions. Reactions in solutions, Effect of pressure, dielectric constant and ionic strength; kinetics of enzyme catalysed reactions, fast reactions; study of fast reaction by relaxation method, flash photolysis and NMR methods, Theories of unimolecular reactions and catalysis.Chain reaction involving Hydrogen –Bromine , Hydrogen-Chlorine reaction and pyrolysis of acetaldehyde .

Unit-IV

Macromolecules:

Polymer- definition classification of polymer, electrically conducting, five resistant, liquid crystal polymer, kinetics and mechanism of polymerization (Chain reaction and step growth), molecular mass, number and mass average molecular mass, molecular mass determination (Osmometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures. Polymer structure and physical properties-crystalline melting point T_m. Entropy and heat of fusion. The glass transition temperature, T_g Relationship between T_m and T_g , properties requirements and polymer utilization.

Recommended Books:

1. Physical Chemistry–P. W. Atkins, Oxford University press, VIIth edition, 2002.
2. Textbook of Physical Chemistry–S. Glasstone
3. Principles of Physical Chemistry–Marron and Pruton
4. Physical Chemistry– G. M. Barrow, Tata-McGraw Hill, Vth edition, 2003.
5. Physical Chemistry- G. K. Vemulapalli, Prentice- Hall of India, 1997
6. Physical Methods in Inorganic Chemistry (DWAP)- R. S. Drago
7. Macromolecules: Structure and Function , F.Wold, Prentice Hall.
8. Chemical Kinetics- K. J. L aidler, Pearson Education, 2004
9. Basic Chemical Kinetics- G. L. Agarwal, Tata- Mc Graw Hill

MCY -104: ANALYTICAL CHEMISTRY-I 60h

Unit-I

(a) **Introduction:** Scope & objectives, Analytical chemistry and chemical analysis, Classification of analytical methods, Selection of methods, Sample processing, Steps in a quantitative analysis, Quantitative range (bipartite classification), Data organisation, Analytical validations, Limit of detection and limit of quantitation, concept of good laboratory practices.

(b) **Analytical Statistics:** Propagation of measurement uncertainties (inaccuracy and imprecision). Useful statistical test: test of significance, the F test, the student 't' test, the chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values, significant figures, regression analysis (least square method for linear and non-linear plots), statistics of sampling and detection limit evaluation.

Unit-II

Microwave spectroscopy: Selection Rules, 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, Application of Microwave Spectra.

Unit-III

Infrared spectroscopy: Review of liner harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; Anharmonicity, Morse potential energy diagram, vibrational-rotation spectroscopy, P, Q, R branches, breakdown of Born-Oppenheimer approximation; vibrations of polyatomic molecules, Selection rules, normal modes of vibration, group frequencies, Finger print region, overtones, hot bands, factor affecting the band positions and intensities, forensic application.

Unit-IV

Raman Spectroscopy: Classical and quantum theories of raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Strokes raman spectroscopy (CARS).

Books Recommended

1. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, *Modern Methods of Chemical Analysis*, 2nd Edition (1976), John Wiley, New York.

2. G. D. Christian, *Analytical Chemistry*, 5th Edition (1994), John Wiley & Sons, New York.

3. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Analytical Chemistry - An Introduction*, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.

4. J. H. Kennedy, *Analytical Chemistry: Principles*, 2nd Edition (1990), Saunders Holt, London.

SEMESTER-II

MCY -201: INORGANIC CHEMISTRY-II **60h**

Unit-I

Metal ligand equilibria in solution:

Stepwise and overall formation constant, tends in stepwise constant, factor affecting the stability of metal complexes with reference to the nature of mrtal ion and ligand, chelate effect and its thermodynamic origin.

Unit-II

Reaction mechanism of transition metal complexes:

Energy profile of reaction, reactivity of metal complexes, inert and labile complexes, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anattion reactions, reactions without metal ligand bond cleavage, Substitution reaction in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reaction, mechanism of one electron transfer reactions, outer sphere type reactions, cross reaction and Marcus-Hush theory, inner sphere type reaction.

Unit-III

Organometallic Chemistry: Ligand hapticity, synthesis, structure and bonding organometallic compounds, organometllic compounds in organic synthesis, homogeneous catalytic reactions (Hydrogenation, hydroformylation, isomerisation and polymerisation), transition metal pie complexes.

Unit-IV

Metal π - complexes:

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, Important reactions of metal carbonyls; preparations, bonding, strcture elucidation, important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

Metal Clusters: Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbony I and halide clusters, compounds with metal-metal multiple bonds.

Recommended books:

1. J. H. Huheey, Inorganic Chemistry- Principles, structure and reactivity, Harperand Row Publisher, Inc. New York (1972)
2. J. D. Lee, Concise Inorganic Chemistry, Elbs with Chapman and Hall, London
3. M.C. Day and J. Selbin, Theoretical Inorganic Chemistry, Reinhold, EWAP
4. T. S. Swain and D. S. T. Black, organometallic Chemistry
5. JohnWulff,structureandpropertiesofmaterials,Volume–4, electronicproperties, Wiley Eastern
6. F. A. Cotton, R. G. Wilkinson. Advanced Inorganic chemistry
7. Willam L. Jooly, Modern Inorganic Chemistry
8. P. L. Pauson, Organometallic Chemistry
9. H. S. Sisler, Chemistry in non–aqueous solvents, Reinhold Publishing Corporation, USA, 4th edition (1965)

MCY -202: ORGANIC CHEMISTRY-II 60 h

Unit I

Organic Reactions

Arndt-Eistert, barbier Wieland degradation, Cope elimination and rearrangement, Dakin, Duff, Elbs persulphate, Nef, Pechmann, Tiechenko, Ulmann, Vilsmeier reactions, Diels-Alder reaction (inter and intramolecular), ketene cycloaddition (inter and intramolecular), Pauson-Khand reaction. Michal Addition & Robinson annelation.

Unit-II

Pericyclic Reactions

Classification of pericyclic reactions, Woodward- Hoffmann correlation diagrams. FMO and PMO approach, Frontier orbitals of ethylene 1,3 butadiene, 1,3,5 hexatriene and allyl system, Electrocyclic reactions- conrotatory and disrotatory motion, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3, dipolar cycloadditions. Sigmatropic rearrangements.

Unit-III

Photochemistry:

(a) An overview of photochemistry, Jablonski diagram and photophysical processes, Franck-Condon principle.

(b) Photochemistry of alkenes and related compounds: Isomerization, Di-π-methane rearrangement and cycloadditions.

Unit-IV

(a) Photochemistry of aromatic compounds: Ring isomerization and cyclization reactions.

(b) Photochemistry of carbonyl compounds: Norrish type-I and type-II cleavage, Photoenolization, Paterno-Buchi reaction, photodimerisation of a, b- unsaturated ketones, rearrangement of enones and dienones, Photo-Fries rearrangement.

Recommended text books

1. Fundamental of Photochemistry, K. K. Rohatgi-Mukherjee, New Age International (P) Ltd., New Delhi, 1986.
2. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science, Books, CA, 2010.
3. Photochemical Synthesis, I. Ninomiya, T. Naito, Academic Press, New York, 1989.
4. Reaction mechanism in organic chemistry- S. M. Mukherjee and S. P. Singh.
5. Reactive Intermediates in Organic chemistry (John Wiley) N. S. Issacs.
6. Principle of organic synthesis- R. O. C. Norman and J. M. Coxon. (ELBS)
7. Advanced organic chemistry (Mc Graw- Hill) J. March.
8. Jagdamba Singh and L D S Yadav, Advanced Organic Chemistry / Organic Synthesis, Pragati Prakashan, 2011.
9. I. Fleming, *Pericyclic Reactions*, Oxford University Press, Oxford (1999).

MCY -203: PHYSICAL CHEMISTRY-II 60h

Unit-I

Electrochemistry-I

Theory of electrolytic conductance: Debye - Huckel theory of strong electrolytes - Debye-Huckel-Onsager (DHO) equation - validity of DHO equation. Activity coefficients of electrolytes - ionic strength, Debye-Huckel limit in glaw, modifications of DHLL, qualitative test and verification of DHLL, solubility measurements. Applications of conductance measurements.

Unit-II

Electrochemistry-II

Galvanic cells: Cells with and without transference, liquid junction potential and its determination, Donnan membrane equilibrium, Applications of EMF measurements, solubility and solubility product, pH and its measurement by glass electrodes, temperature coefficient of EMF and determination of ΔG, ΔH and ΔS.

Unit-III

Classical Thermodynamics:

Free energy, chemical potential and entropy, Gibbs-Duhem Equation partial molar properties and their significance, fugacity. Non-ideal systems: excess functions for non-ideal solutions.

Unit-IV

X-ray and electron diffraction:

Bragg condition, Symmetry of Crystals , Law of crystallography miller indices, Laue method Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflection, identification of unit cell from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

Scattering intensity vs. Scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecule. Low energy electron diffraction and structure of surfaces.

Recommended Books:

1. Thermodynamics for Chemists – S. Glasstone, D. Van Nostrand, 1965.
2. Principles of Electrochemistry-S. Glasstones
3. Modern Electrochemistry by K.N. Reddy
4. Thermodynamics A Core Course- R. C. Srivastava, S. K. Saha and A. K. Jain, Prentice- Hall of India, IInd edition, 2004.
5. Physical Chemistry–P. W. Atkins, Oxford University press, VIIth edition, 2002
6. Physical Chemistry-K. L. Kapoor (Part-V)
7. Physical Chemistry- G. K. Vemulapalli, Prentice- Hall of India, 1997.
8. Physical Chemistry- K. K. Kapoor (Part-IV)
9. Solid State Chemistry and its Application , A.R.West ,Plenum.
10. Solid State Chemistry , D.K.Chakrabarty, New Age International .

MCY -204: ANALYTICAL CHEMISTRY-II 60h

Unit-I

Voltametry: Origin of polargraphy, Current-voltage relationship, Theory of DC polarography, Instrumentation, Ilkovic equation, Qualitative and quantitative applications, Introduction to differential pulse polarography and cyclic voltametry, Amperometric titrations.

Unit-II

Atomic Absorption Spectroscopy Introduction, Principal, difference between AAS and AES: Flame and ICP sources, Advantages of AASover AES, advantages and disadvantages of AAS. Instrumentation, Single anddouble beam AAS, detection limit and sensitivity, Interferences applications.

Unit-III

(a) **Separation Methods:** Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography: Gas chromatography, High-performance liquid chromatography

(b) **Thermal Analysis:** Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods

Unit-IV

(a) **Solution Equilibria-I**: Solvents and solutions, general treatment of equilibria in aqueous medium involving monoprotic weak acid and weak base, and sails of weak acids and weak bases. Activity and concentration, Effect of electrolytes on chemical equilibria, Calculation of pH, Constructing titrarion curves from charge balance and mass balance equations, Acid-base titrations and theory of pH indicators, Redox equilibria and redox titration, Theory of redox indicators.

(b) **Solution Equilibria-II:** Complexation equilibria and complexometric titrarions, Precipitation reaction and precipitation titrations and theory of adsorption indicators, Job's method of continuous variation, mole ratio and slope tario analysis, Advantages and limitations, typical examples.

Recommended books:

1. Principal of Instrumental Analysis- D. Skoog and D. West
2. Analytical Chemistry: (J.W)G. D. Christian
3. Instrumental Methods of Inorganic Analysis (ELBS): A. I. Vogel
4. Introduction to chromatography: Bobbit
5. Instrumental Methods of analysis (CBS)- H. H. Willard, L. L. Mirrit, J. A. Dean
6. Instrumental Methods of Analysis: Chatwal and Anand
7. Chemical Instrumentation: A Systematic approch- H. A. Strobel

SEMESTER-III

MCY -301: Inorganic Chemistry III: **60 h**

Unit I

Application of Spectroscopy:

(a) Electron Spin Resonance Spectroscopy:. Hyperfine Coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) incliuding biological systems and to inorganic free radicals such as PH_4, F_2 and $[BH_3]$.

(b) Applications of multinuclear NMR with emphasis on ^{11}B, ^{19}F, ^{31}P, ^{125}Te, ^{119}Sn and ^{195}Pt NMR.

Unit II

Mossbauer Spectroscopy: Basic Principles, spectral paramaters and spectrum display. Application of the technique to theb studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds- nature of M-L bond, coordination number, structure and (3) detedcation of oxidation sate and in equivalent MB atoms.

Unit III: Bioinorganic Chemistry(A) Metal Ions in Biological System

(a) Essential and trace metals. (b) Na^+/K^+ Pump

(c) Vitamin B_{12} methyl cobalamine, Biomethylation. (d) Heme protines and oxygen uptake, sturucture and function of haemoglobin, myoglobin,homocyanins and hemerythrin , model synthetic complexes of iron , cobalt and copper

(B) **Electron Tranfer in Biology**

(a) Structure and function of metalloproteins in electron transport processes-cytochromes and ion-sulphur proteins,synthetic models.

(b) **Nitrogenase:** Biological nitrogen fixation , molybdenum nitogenase, spectroscopic and other evidence, other nitrogenises model systems.

Unit IV Selected Topics

I. Chemistry of less familiar metals: Os, Ir, Ru, Rh , Pd.
II. Platinum Phosphine complexes
III. General method of prepration and importent reactions (insertion reactions , metathetical reactions with protic compounds) of metal and metalloids amides .
IV. Prepration of important radio isotopes ($_1H^3$, $_6C^{14}$,$_{11}Na^{22}$, $_{15}P^{32}$, $_{16}S^{35}$) and applications of coordination compounds of Tc^{99} as imagining agents in nuclear Medicine

Books Suggested

1. Structural Methods in Inorganic Chemistry , E.A.V. Ebsworth, D.W.H. Rankin and S.Cradock , ELBS
2. Progress in Inorganic Chemistry vol 8 f.A.Cotton , vol 15 ed.S.J.Lippard, Wiley.
3. NMR ,NQR EPR and Mossbauer spectroscopy in inorganic chemistry ,R.V.Parish,Ellis horwood .
4. Practical NMR Spectroscopy, M.L.Martin ,J.J.Delpeuch and G.J.Martin, Heyden
5. Principles of Bioinorganic Chemistry, S.J.Lippard and J.M.Berg, University science Books.
6. Bioinorganic Chemistry,I. Bertini, H.B.gray,S.J.Lippard & J.S.valentine, University science Books.
7. Inorganic Biochemistry vol. I and II G.L.Eichhorn Elsevier.
8. Progress in inorganic chemistry vol. 18 and 38 ed.J.J.Lippard, Wiley.
9. Environmental Chemistry, A.K.De,Wiley Eastern.
10. Environmental Pollution Analysis,S.M.Khopkar, Wiley Eastern.
11. Advance Inorganic Chemistry, F.A.Cotton and G.Wilkinson.
12. Inorganic Chemistry , J.E.Huheey.
13. Nuclear and Radiochemistry,G.Friedlander and J.W.Kennedy
14. Essentials of nuclear Chemistry, H.J.Arnikar
15. Quantitative Inorganic Analysis, A.I.Vogel.

MCY -302: Organic Chemistry III:

Unit I

(a) Aliphatic nucleophilic substitution : The SN_2, SN_1 and SET mechanism. The Neighboring group mechanism, neighboring group participation by σ and π bonds, anchimeric assistance . The SN_1 mechanism Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon. Reactivity effect of substrate structure, attacking nucleophile, leaving group and reaction medium , phase transfer catalysis and ultrasound , ambident nucleophile , regioselectivity.

(b) Aliphatic electrophilic substitution : Biomolecular mechanism – S_E2 and S_E1. The S_{E1} mechenism, electrophilic substitution accompanied by doubled bond shifts . Effect of substrates, leaving group and solvant polarity.

Unit II

(a) Aromatic Electrophilic substitution : The arenium ion mechanism, The ortho/ para ratio, ipso attack, orientation in other ring system , quantitative treatment of reactivity in substrates and electrophiles . Diazonium coupling , Vilsmeir reaction , Gatterman-koch reaction.

(b) Aromaatic Nucleophilic substitution: The $S_N Ar$, S_N1, benzyne and $S_{RN}1$ mechanisms. Reactivity-effect of Substrates structure, leaving group and attacking nucleophle.The Von Richter, Sommelet-Houser and Smiles rearrangements.

UnitIII

(a) Elimination Reactions: The E_2, E_1 and E_1cb Mechanism and their spectrum . Orentationof double bond . Reactivity- effects of substrares structures,attacking base , the leaving group and the medium .

(b) 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 attacking radicals. The effect of solvent on reactivity .Alicyclic halogination (NBS), oxidation of aldehyde to carboxylic acid, auto-oxidation , coupling of alkynes and arylation of aromatic compounds by diazonium salt.Sandemeyer reaction.Free radical rearrangement. Hunsdiecker reaction .

Unit IV

(a) Rearrangements: General mechanistic considerations- nature of migration, migratory

aptitude.A detailed study of the following rearrangements –Pinacole-pinacolone, Wagner-Meerwein,Demjanov,Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis,Neber,Beckmann,Hofman,Curtius,Schimdt,Baeyer-Villigr, Shapiro reaction.Hofmann Loffler-Freytag Reaction, Sommelet-Houser, barton Reaction.

(b) Protecting Groups: Principle of protection of Alcohols, Amine ,Carbonyl and Carboxyl group

Books Suggested:

1. Designing of Organic Synthesis , S.Warren,Wiley.
2. Modern Synthetic Reactions ,H.O.House,W.A.Benzamin.
3. Some Modern Methods of Organic Synthesis,Wcarruthers ,Cambridge univ.Press
4. Advance Organic Chemistry,Reaction Mechenism & Struture.J.March,John Wiley.
5. Principle of Organic Synthesis,R.O.C.Norman and J.M.Coxan,backie Academic & Professional.
6. Advance Organic Chemistry,Part B,F.A.Carey & R.J.Sundberg, plenum Press.

MCY -303: PHYSICAL CHEMISTRY-III 60 h

Unit-I

Non equilibrium thermodynamics: Thermodynamic criteria for non-equilibrium states, entropy production, flow, irreversible processes , forces and fluxes. Onsager reciprocal relations. Electrokinetic phenomena. Irreversible thermodynamics for biological systems. Coupled reactions.

Unit-II

Statistical Thermodynamics: Distribution of molecular states, internal energy and entropy, canonical partition function, thermodynamic relations; Determination of mean energies, heat capacities, residual entropies, equilibrium constants. FD statistics, BE statistics and their applications in electrons in metals, photons. BE condensation.

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 surface area (BET equation), surface film of liquids (electro-kinetic phenomenon), catalytic activity at surface.), transition state theory of surface reactions, rates of chemisorption and desorption, unimolecular and bimolecular surface reactions, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity.

Micelles: Surface active agent, classification of surface active agent, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactant, counter ion binding to micelles, thermodynamics of micellization – phase separation and moss action models, solubilisation, micro emulation, reverse micelles.

Unit-IV

Photochemical Process

Photochemical reactions, laws of Photochemistry Quantum Yeild and its determination, Phosphorescence and its triple state , energy level diagrams , intersystem crossing (jablonski diagram) Frank Condon Principle physical properties of excited molecules , kinetics and thermodynamics of photochemical reactions. Photoreduction photoxidations,Electron transfer

reactions, photoconduction, chemiluminiscence, photosensitization and quenching, stern-volmer equation

Recommended books:

1. Physical Chemistry–P. W. Atkins, Oxford University press, VIIth edition, 2002.
2. Physical Chemistry–G. M. Barrow,Tata- Mc Graw Hill, Vth edition, 2003.
3. Principles of Physical Chemistry– Marron and Pruton.
4. Physical chemistry- G. K. Vemulapalli, Prentice- Hall of India, 1997.
5. Thermodynamics for Chemistry – S. Glasstone, D. Van Nostrand, 1965.
6. Thermodynamics A Core Course- R. C. Srivastava, S. K. Sahaand A. K. Jain, Prentice-Hall of India, IInd edition,2004
7. Text book of Physical Chemistry– S. Glasstone
8. Physical Chemistry of Surface-A. W. Adamsen and Gaust 5th Edition Wiley
9. Photochemistry, R.P.kundall and A.Gilbert,Thomsan Nelson.
10. Organic Photochemistry , J Coxon and B.HAlten ,Cambridge University press

MCY -304: ANALYTICAL CHEMISTRY-III 60h

Unit I

(a) UV-Visible Spectroscopy: Basics of Photometry, Lambert beer's law,Woodward-Fisher rule and applicatons.

(b) Infra-red spectroscopy: Applications of FTIR in structural determination.

Unit II

Mass Spectrometry: Basic principles, ionization techniques, isptope abundance, molecular ion , fragmentation processes of organic molecules, McLafferty rearrangement,deduction of structure using mass spectral fragmentation, FAB-Mass, High resolution MS, soft ionization methods, EI-MS and MALDI-MS.

Unit III

NMR spectroscopy-I

1H NMR: Instrumentation, Magnetic and non-magnetic nuclei, Larmor frequency, absorption of radiofrequency, chemical shift and its measurement, factors influencing chemical shift, deshielding, anisotropic effect, spin-spin coupling, factors influencing coupling constant, AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, NOE effects, restricted rotation (DMF, DMA), cyclohexane ring inversion, chemical shift reagents for stereochemical assignments.

Unit IV

NMR spectroscopy-II

(a) Introduction to ^{13}C NMR, Off-resonance coupled and decoupled and DEPT method. Multinuclear NMR of Si, F and P nuclei.

(b) Interpretation of spectra of compounds based on UV-visible, IR, mass and NMR spectroscopy.

Recommended Books:

1. Instrumental Methods of analysis- Willard, Merrit, Deanand Settle.
2. Spectroscopic identification of organic compounds- R. M. Silverstein and G. C. Bassler

3. Spectroscopic methods inorganic chemistry- D. H. Williams and I. Fleming
4. Absorption spectroscopy of organic molecules- V. M. Parikh
5. Applications of spectroscopic techniques in Organic chemistry- P. S. Kalsi

SEMESTER-IV

MCY -401: Elective papers (Opt anyone out of five)

MCY -402: Elective papers (Opt anyone out of five)

MCY -403: Elective papers (Opt anyone out of five)

MCY -404 :Project

MCY -405: Seminar

Elective paper II

MCY -402(A)

Heterocyclic Chemistry 60 h

I. Nomenclature of Heterocycles

Replacement and sysmetic nomenclature (Hantzsch Windman system) for monocyclic, fused and bridged hetrocycles.

II.Aromatic Heterocycles

General chemical behavior of aromatic heterocycles , classifications (structural type) ,criteria of aromaticity (bond length, ring current and chemical shifts in 1H NMR-spectra , empirical resonance energy , delocalization energy and Dewar resonance energy , diamagnetic susceptibility exaltation).Heteroaromatic reactivity and tautomerism in aromatic hetericycles .

III. Non Aromatic Heteocycles

Strain bond angle and torsional strains and their consiquences in small ring heterocycles . Conformation of six membered heterocycles with refrence to molecular geometry , barrier to ring inversion , pyramidal inversion and 1,3 diaxial interaction . Stereo-electronic effects –anomeric and related effects . Attractive interactions-hydrogen bonding and intermolecular nucleophilic-electrophilic interactions .

IV. Heterocyclic Synthesis

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions .

V.Small Ring Heterocycles

Three membered and four membered heterocycles- synthesis and reactions of aziridines, oxiranes, thiiranes , azetidines, oxetanes and thietanes.

VI .Benzo-Fused Five Membered Heterocycles

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.

VII. Meso-Ionic Heterocycles

General c;assification,chemistry of some important meso-ionic heterocycles of type-A and B their applications.

VII. Six Membered heterocycles with One Heteroatom

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & Thopyrylium salts and pyridones . Synthesis & reactions of quinolizinium and benzopyrelium salts , coumarins and ahromones.

Six Membered Heterocycles with Two or more Heteroatoms

Synthesis and reactions of diazines , triazines, tetrazines and thiazines .

Seven and Large Membered Heterocycles

Synthesis and reactions of azepines , oxepines , thiepines, diazepines, thiazepines, diazocines, dioxocines and dithiocines.

Books Suggested

1. Heterocyclic Chemistry Vol.1-3R.R.Gupta, M.Kumar, V.Gupta, Springer Verlag

2.The Chemistry of Heterocycles, T.Eicher and S.Hauptmann, Thieme.

3. Heterocyclic Chemistry, J.A.Joule, K.Mills and G.F.Smith, Chapman and Hall.

4. Heterocyclic Chemistry, T.L.Gilchrist, LongmanScientific Technical.

5.Contemporatry Heterocyclic Chemistry, G.R.Newkome and W.W.Paudler, Wiley-Inter Science.

6.An Inrtoduction to the Heterocyclic Compounds ,R.M.Acheson , John Wiley.

7.Comprehensive Heterocyclic Chemistry, A.R.Katrizky and C.W.Rees, eds. Pergamon Press.

Elective paper II

MCY -401 (B)

Natural Product Chemistry **60h**

Unit I

Terpenoids and Carotenoids

Classification, nomenclature, isolation, general methods of structural determination, isoprene rule,stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geranoil, □-Terpeneol, Menthol, Farnesol, Abietic acid and β-Carotene.

Unit II

Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine, Quinine and Morphine.

Unit III

Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholestoral, Bile acids, Androsterone, Testosterone, Estrone, Progestrone, Aldosterone.

Unit IV

Prostaglandins

Occurrence, nomenclature, classification, biogenesis and physiologicaleffects.Synthesis of PGE2 and PGF2a.

Recommended books:

1. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
2. Organic Chemistry, Vol 2, I.L. Finar, ELBS.
3. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.

4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the
6. Americas, Ed.KurtHostettmann, M.P Gupta and A.Marston, Harwood Academic
7. Publishers.
8. Introduction to Flavonoids, B.A Bohm, Harwood Academic Publishers.
9. Chemistry of Natural products- Kalsi
10. Principles of organic synthesis by R. O. C. Norman and J.M.Coxon; Chapman and Hall
11. Classics in organic synthesis – K. C. Nicolaou & E. J. Sorensen
12. Medical Natural Products - A Biosynthetic approach by Paul M. Dewick 2nd edition(Wiley)
13. Chemical aspects of Biosynthesis – J. Mann (1994

Elective paper II

MCY -402 (C)

Photochemistry **60h**

Unit I

Photochemical Reactions: Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

Unit II

Determination of Reaction Mechanism: Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions.Types of photochemical reaction-photo-dissociation, gas-phase photolysis.

Unit III

Photophysical process: Fluorescence and fluorescence quenching, Stern Volmer plot, Measurement of fluorescence and phosphorescence and lifetimes. Introduction to time-resolved techniques for absorption and emission measurements, detection and kinetics of reactive intermediates.Examples of low temperature matrix isolation of reactive intermediates.

Unit IV

Fluorescence based sensors – examples of molecular and supramolecular systems. Conversion of solar energy to chemical and other forms of energies, solar photovoltaic cell, basic principle and design of the cell.

Recommended books

1. Physical Chemistry, Thomas Engel & Phillip Reid- Peerson's Publication
2. Fundamental of Photochemistry, K. K. Rohatgi-Mukherjee, New Age International (P) Ltd., New Delhi, 1986.
3. Principles of Fluorescence Spectroscopy, 3rd Ed., J. R. Lakowicz, Springer, New York, 2006.

4. Fundamentals of Photoinduced Electron Transfer, G. J. Kavarnos, VCH publishers Inc., New York, 1993.
5. Molecular Fluorescence: Principles and Applications, B. Valeur, Wiley-VCH Verlag GmbH, Weinheim, 2002.
6. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science, Books, CA, 2010.

Photochemical Synthesis, I. Ninomiya, T. Naito, Academic Press, New York, 1989.

Elective paper II

MCY-402 (D)

MEDICINAL CHEMISTRY **60 h**

Unit I

Introduction to Medicinal Chemistry

Role of Medicinal Chemists, Medicines, Current trends in Drug discovery, Drug Discovery Pipeline, Clinical trials, Leads and analogues: desirable properties, Sources of leads and drugs. Procedures followed in drug design, Classification of drugs: on basis of pharmacological activity, chemical structure, and origin, Methods of administration of drugs.

Unit II

Drug Design and Action

Development of new drugs, concept of lead, Compound and lead modification, Lipinski rule, concepts of prodrugs, Drug receptor interactions, PK and PD properties of drugs, and Drug metabolism, Therapeutic Index, Drug-response relationship (Agonist and Antagonists), Tachyphylaxis, structure-activity relationship (SAR) factors affecting bioactivity, Isosterism and bio-isosterism, Drug Designing: Methods of variation, Theories of drug activity (Clark's occupancy theory, The Rate theory, The two-state model, Concept of drug receptors elementary treatment of drug receptor interactions, Receptors, and their properties, types of receptors.

Unit III

Pharmacokinetics and Pharmacodynamics properties of drugs

Introduction to drug absorption, distribution, elimination using pharmacokinetics important pharmacokinetics parameters in defining drug disposition and in therapeutics, drug metabolism, biotransformation significance of drugs medicinal chemistry.

Unit IV

Synthesis and action of drugs

Based on structure or pharmacological basis with examples; Mode of action and synthesis of cardiac glycosides, local antiinfective drugs, antineoplastic agents, psychoactive drugs, antibiotics.

Recommended books:

1. Fundamentals in medicinal chemistry- G. Thomas. 2nd edition
2. Introduction to medical Chemistry, G. L. Patrick
3. Medicinal Chemistry- Ashutoshkar
4. Medicinal Chemistry- Sreeram and Yogeshwari
5. Medicinal Chemistry & Drug discovery- Burger (Volume 1-6)
6. Strategies for organic synthesis 7 design (D. Lednicer)
7. Burger's medicinal chemistry vol. 1to6

Elective paper II

MCY 402 (E)

APPLIED CHEMISTRY **60h**

Unit-I

Pharmaceutical and Drug Regulations

Regulatory aspects of pharmaceutical and bulk drug manufacture: DRA, FDA, CPMP, ICH guidelines, Drug approval processes, Patent application, WHO certification, IPR, TIFAC, TDB, NABL, NRDC, Good manufacturing practices (GMP).

Unit II

Pulp and Paper Industry:

Classification and properties of fibrous materials, general principles of some mechanical and chemical (acid, neutral and alkaline) pulping process, pulping kinetics, paper properties testing, process instrumentation, lignin as a chemical raw material, introduction to modern pulping technology, advances in pulping.

Unit III

Starch Industry:

Cellulose: occurrence, manufacture, properties, preparation from wood, industrial application of cellulose (textile and jute industry, synthetic silk). Industrial poisons.

Unit IV

Industrial Chemicals

Explosives (cordite, gun-cotton, blasting gelatin). Marine chemicals: Chitosan, Agar-Agar, Industrial carbon, surface coating, refractories and abrasives, lubricants, cutting oils.

Recommended text books:

1. Chemical process industries by N.D. Shreeve.
2. Applied chemistry for Engineer by Diamont.
3. Industrial poisons and solvents by Jacobs.
4. Chemistry of engineering materials by Jain & Jain.

Elective paper I

MCY 401 (B)

Environmental Chemistry **60h**

Unit I

Environment

Scope and significance, classification of environmental pollution: air, water and soil.

Air Pollution: Classification of air pollutants, wind stability and turbulence.

Unit II

Human environmental disturbances: Green House Effect, carbon dioxide and other Green House gases, control measures, ozone depletion problem, acid rain sources and distribution of acid rain, effect of acid rain on aquatic and terrestrial ecosystems, remedial control measures.

Unit III

Water Pollutin: Classification of water pollutants.

Wastewater: Constituents, BOD, COD measurements, municipal waste water, industrial wastewater and storm water, principle of wastewater treatment, treatment processes-physical, chemical and biological processes.

Unit IV

Solid Wastes: Characterization of solid waste, recycling, land filling.

Hazardous Wastes: Identifying hazardous, methods of identification, waste listed as hazardous waste.

Natural Environmental Hazards: Classification of hazards.

Recommended books:

1. Rogers Manual of Industrial Chemistry, Vol. 1. Ed. By C. C. Furnas (Nastrand).
2. Outline of Chemical Technology by Dryden (Ed. And revised by Gopal Rao and Sitting) (Affiliated East-West Press.

Elective paper I

MCY 401 (D)

Waste Management and Pollution Control **60h**

Unit I:

Industrial Pollution

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs. Radionuclide analysis. Disposal of wastes and their management.

Unit II

Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes.

Unit III

Wastes: Types, Waste listed as Hazardous wastes, methods of identification of hazardous wastes, recycling, landfilling, radioactive wastes. Lethal dose, tolerance limit. Solid Wastes: Wastes from thermal power Plants. Silica Fumes – Characterization and utilizations. Fly-ash–Genesis and uses.

Unit IV

Liquid waste: Effluents from coke oven – Processing of valuable materials. Effluents from phenol plant.recovery of phenols. Effluents from plants dealing with inorganic chemicals. Metal recovery: Cr, Ni, V from electroplating wastes and spent catalysts.

Recommended books:

1. Brunner R.C., 1989, Hazardous Waste Incineration, McGraw Hill Inc. 480p
2. Clark R.S., Marine Pollution, Clanderson Press Oxford (TB)
3. Cunningham, W.P. Cooper, T.H. Gorhani, E & Hepworth, M.T. 2001, Environmental Encyclopedia, Jaico Publ. House, Mumabai, 1196p
4. De A.K., Environmental Chemistry, Wiley Eastern Ltd.
5. Heywood, V.H &Waston, R.T. 1995. Global Biodiversity Assessment. Cambridge Univ. Press 1140p.
6. Jadhav, H &Bhosale, V.M. 1995. Environmental Protection and Laws. Himalaya Pub. House, Delhi 284 p.
7. Mckinney, M.L. & School, R.M. 1996. Environmental Science Systems & Solutions, Web enhanced edition. 639p.
8. Mhaskar A.K., Matter Hazardous, Techno-Science Publication (TB)
9. Miller T.G. Jr. Environmental Science, Wadsworth Publishing Co. (TB)
10. Rao M N. &Datta, A.K. 1987. Waste Water treatment. Oxford & IBH Publ. Co. Pvt. Ltd. 345p.
11. Sharma B.K., 2001. Environmental Chemistry. Geol Publ. House, Meerut
12. Trivedi R.K., Handbook of Environmental Laws, Rules Guidelines, Compliances and Standards, Vol I and II, Enviro Medi

Elective paper I

MCY 401 (C)

Materials Chemistry **60h**

Unit I & II

Inorganic materials: Design and synthesis of inorganic materials, requirements and constraints, combination properties of composites, functional materials, active materials; solid state reactions for synthesis of inorganic materials: ceramic methods, precursor method and sol-gel synthesis, physical and chemical vapour depositions; carbides, nitrides, structural and functional ceramics, intermetallics; intrinsic and extrinsic properties: electrical, optical and magnetic properties; ceramic superconductors, magnetic ceramics, Nanomaterials.

Unit III & IV

Organic materials: Molecular electronics: molecular materials for electronics and molecular scale electronics: Molecular properties, molecular arrangement and molecular interactions, piezoelectric and pyroelectric organic materials; molecular magnets based on transition metal complexes and organic ferromagnets, organic non-linear optical materials: photochromic organic materials and their classes; conducting polymers: polyacetylene, polypyrrole, polyaniline and polythiophene; conductive change transfer materials: TTFTCNQ, metal–dithiolate systems, fullerenes. Langmuir-Blodgett films, molecular electronic logic and architectures.

Elective paper I

MCY 401 (A)

Organotransition Metal Chemistry

I. Compounds of Transition Metal-Carbon Multiple bonds: 60h

Alkylidenes alkylidynes, low valent carbenes – synthesis, nature of bondas, structural characterisitics,nucleophilic and electrophilic reactions on ligands .

II. Transition Metal –Complexes

Transition metal –Complexes with unsaturated organic molecules : alkenes, alkynes allyl,dienes Dienyl and arene complexes –preprations , properties nature of bonding and structural features .Important reactions related to nucleophilic and electrophilic attack on ligands .

III. Transition Metal Compounds With Bond To Hydrogen: Covalent hydrides : synthesis and important reactions

IV. . Transition Metal Compounds With Bond To Carbon in Catalysis:

A. General idea of important catalytic steps: ligand coordination and dissociation, insertion and elimination, nucleophilic attack on coordinated ligands,oxidative addition and reductive elimination reductions.

B. Hydrogenation of alkenes using Wilkinson's catalyst, Hydroformylation of alkenes using Co and Rh catalysts, Carbonylationof methanol to acetic acid (Monsanto process), Oxidation of alkenes (Wacker process)

V. Fluxional Organometalic compounds:

Fluxionality and dynamic equilibria in compounds such as C2-olefine , C3- allyl and dienyl complexes.

VI Organometallic Compounds of Lanthanides and Actinides : 5Hrs

Methods of prepration , properties and structural features.

Books Suggested

1.Principle and Applications of Organotransition Metal chemistry : J.P.Collman

2.L.S.Hegsdus,J.R.Nortan and R.G.Finke, University Science Books

3.Principles of Organometallic Compounds Edn-II:P.P.Power

4.Organometallic Chemistry : R.C.Mehrotra snd A.Singh, New Age Inernational.

Elective paper I

MCY 401 (E)

Supramolecular, Bioinorganic and Bioorganic Chemistry

Unit-I

Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures. Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands.

Unit-II

Bioinorganic Chemistry: Role of metal ions in biological processes, structure and properties of metalloproteins in electron transport processes, cytochromes, ferrodoxins and iorn sulphur proteins, Biological nitrogen fixation, PS-I, PS-II, Oxygen uptake proteins.

Unit-III

Molecules of life: Amino acids and proteins, Carbohydrates-polysaccharides, lipids, cell membranes and nucleic acids

Structure and function: Protein structure, Ramachandran plot, protein folding: DNA/RNA structures, various forms (a, b, c, z) of DNA, t-RNA structure, transcription and translation, gene expression and DNA binding protein-zinc-finger protein.

Metabolism and Energetics: Glycolysis , citric acid cycle , oxidative phosphorylation and transport through membranes

Unit-IV

Enzyme kinetics, inhibition, drug action (selected examples)

Metalloenzymes: Hydrolytic and redox enzymes: Carbonic anhydrase and superoxide dismutase

Oxygen uptake proteins: Hemerythrin and hemocyanin

Molecular recognition: Molecular organization, Chiral recognition and role of sugar in biological recognition

Recommended books

1. Lehn, J. M. Supramolecular Chemistry: Concepts & Perspectives Wiley-VCH (1995).
2. Atwood, J. L. & Steed, J. W. Supramolecular Chemistry: A Concise Introduction John Wiley & Sons (2000).
3. D.L. Nelson and M.M. Cox, Lehninger Principles of Biochemistry 3rd Edition ((2002) McMillan North Publication
4. Balzani, V. Photochemistry of Coordination Compounds Academic Press (1970).
5. Desiraju, G. R., Ed. Perspectives in Supramolecular Chemistry, Vol. 2: Crystal Engineering and Molecular Recognition Wiley: Chichester (1995).
6. P.S.Kalsi, Bioorganic, Bioinorganic and Supramolecular Chemistry
7. L. Stryer, Biochemistry, 5th Edition, (2002) Freeman &Co. New York
8. D. Voet, J. G. Voet, Biochemistry 3rd Edition (2004), Wiley International Publication.
9. I. Bertini, H. B. Gray, S. J. Lippard, J.S. Valentine, 1st South Asian Edn., (1998) Viva Books Pvt. Limited, New Delhi M. B. Smith, Organic Synthesis, (1998) Mc Graw Hill Inc, New York

Elective Paper III

MCY 403 (A)

Advanced Quantum Chemistry **60h**

Unit I

Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (first order and non-degenerate).Applications of variation method and perturbation theory to the Helium atom. (Ground and excited state)

Hartree-Fock theory

Introduction to extended Huckel theory, Slater-Condon rules, Hartree-Fock equation, Koopmans and Brilouintheories, Roothan equation, Gaussian basis sets.

Configuration interaction and MC-SCF

Introduction to CI; full and truncated CI theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods.

Unit II

Semi-Empirical theories

A review of the Huckel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties.

Unit III

Computer experiments using quantum chemistry- software packages such as GAUSSIAN.GAMESS/ MOPAC/ AM1 and modelling software e.g. MM2/ AMBER/ CHARM.

Unit IV

Density functional theory

Derivation of Hohnberg-Kohn theorem, kohn-Sham formulation, N- and V- representabilities, review of the performance of the existing local (e.g. Slater Xa and other methods) and non-local functional, treatment of chemical concepts with the density functional theory.

Recommended books:

1. Modern quantum chemistry, N.S. Ostlund and A. Szabo, McGraw Hill
2. Methods of molecular quantum mechanics, R. McWeeny and B. T. Sutclife, Academic Press
3. Density functional theory of atoms and molecules, R.G. Parr and W. Yang, Oxford
4. Exploring chemistry with electron structure methods, J. B. Foresman and E. Frish, Gaussian Inc.
5. Semi-empirical MO theory, J. Pople and D. L. Beveridge

Elective Paper III

MCY 403 (B)

Solid State Chemistry **60h**

Unit I

Solid State Reactions

General principles, classification of chemical reactions of solids, Experimental procedures, Accumulating pressure measurement of evolved gases, mass loss measurement, Non-isothermal methods, Absorption and evolution of heat, Diffraction methods, Co-precipitation as a precursor to solid state reactions, Kinetics of solid state reactions.

Unit II

Crystal Defects and Non-Stoichiometry

Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, Vacancies- Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colourcentres, non-stoichiometry and defects.

Unit III

Electronic Properties and Band Theory

Metals, insulators and semiconductors, electronic structure of solids-band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junction, super conductors.

Optical properties: Optical reflectance, photoconduction-photoelectric effects. Magnetic Properties- Classification of materials: Quantum theory of paramagnetic-cooperative phenomenon- magnetic domains, Hysteresius.

Unit IV

Applications

Phase Transitions: Classification; Landau's Theory; Nucleationgrowth, Martensitic transformations; Examples; Metal-insulator transitions.

Solid state synthesis: Conventional and novel methods; Specific examples; rational synthesis of solids. Characterization by diffraction.

Recommended books:

1. C.N.R. Rao and J. Gopalakrishnan, New directions in solid state chemistry, Cambridge University Press, London, 1986.
2. Comprehensive chemical kinetics, C.H. Bamford& C.F.H. Tipper, Elsevier.
3. A.R. West, Solid State Chemistry and its applications, John Wiley, New York 1984.
4. L.V. Azaroff, Introduction to Solids, Tata McGraw Hill Publishing Company Ltd., New Delhi, 1990.
5. D.M. Adams, Inorganic Solids, John Wiley and Sons, New York, 1974.
6. N.N. Greenwood, Ionic Crystals, Lattice Defects, nonstoichiometry, Butterworths, London, 1968.
7. C. Kittel, Introduction to solid state physics, JohnWiley and Sons, New York, d1986.
8. M. Ali Omar, Elementary solid state physics: Principles and Applications, Addison-Wesley Publishing Company, California, 1975.
9. P.A. Cox, The electronic structure and chemistry of solids, Oxford University Press, Oxford, 1987.
10. C.N.R. Rao and K.J. Rao, Phase transitions in solids, McGraw Hill Book Co., New York, 1978.
11. T.V. Ramakrishna and C.N.R. Rao, Superconductivity today, Wiley- Easter, 1992.
12. G. Burns, Solid State Physics, Academic Press, New York, 1985.
13. J.M. Hong and C.N.R. Rao, Preparation and characterization of materials, Academic Press, New York, 1981.

Elective Paper III

MCY 403 (C)

Chemical Dynamics: **60 h**

I.Theories of reaction rates: The theory of absolute reaction rates , Transmission coefficient. The review of theories of rates of unimolecular reactions . Hinshelwood Kassel Rice Rampsberger, RRKM and with special refrence to slater's theory. Thermodynamics of reaction rates /

II. Fast reaction Kinetics: Relaxation phenomenon, techniques for rate measurement .T jump ,P jump and Shock Wave. The stopped flow technique.The radical detectionary mass spectrometry and laser induced magnetic resonance.

III Molecular reaction dynamics: The scope of reaction dynamics in terms of reactive encounter,energy requirement; steric requirement, diffusion controlled reations.Metarial balance equation and it's solution collision of structureless particles, kinetic isotope effect. The experimental observation of activated complex.Activation parameters.Reaction between ions. Dynamic of molecular collisions, Potential energy surfaces, dynamic calculation & transition state theory . Adiabatic theory of reactions.

IV. Experimental reactions dynamics:

The bulb method. The molecular beam method from the sand point of reagent specification and product distribution . The laser induced fluorescence.

Book Sugested

1.Chemical kinetics ,Keith J.Laidler, Tara Macgraw Hill Kepmit (1995).

2.Kinetics and Mechenism, Frost and Peorson John Wiley (1963).

3.Physical Chemistry, IRAN Levine , Tata Macgraw Hill (1995).

4. Physical Chemistry, ALKMs Oxford University Press(1998).

5.Chemical Kinetics, Michel J.Pilling , Paul.W.Seakins, Science Publications(1995)

Elective Paper III

MCY 403 (D)

Statistical thermodynamics: **60 h**

I.Elements of Statistical Thermodynamics: Microsates, Macrostates,Permutations and Combinatons.Combinatory rule. Derivation of Lagrange's method of undetermined multipliers. Stirling's approximation.Partition func6tion and it's physical interpretation.Boltzmann Distribution law and its applications. Signi9ficane of b and its mathematical evaluation .Partition function and its relationship with internal energy .Helmholtz and Gibbs Free energy, Entropy,Enthalpy ,heat capacity and pressure.

II.Statistical Thermodynamics of Independent Systems: Distribution Laws and their limit of applicability .Partition function for independent and distinguishable(Localised) ,independent and distinguishable and indistinguishable systems . Partition function for mixture of gases.Cannonical and Grand Cannonical partition functions. Relation of Grand Cannonical partition function with thermodynamic stste functions .Detailed statistical study of two phase assembly of one component system.

III. Applications of Statistical Thermodynamics to Chemical Systems : Statistical interpretation of chemical equilibrium. Molecular interpretation of basic laws of thermodynamics.Statistical thermodynamics of an ideal crystal . Statistical derivation of equation of state for non-ideal fluids. Statistical thermodynamics of gaseous mixture .Statistical view of isomolecular and isotopic exchange reaction rate .Statistical evaluation of residual entropy.

IV. Nucler Spin- Statics and Functions : Symmetry and nuclear spin , ortho and para nuclear states, ortho and para hydrogen, Nuclear spin extended to special cases. Mean Distribution and Mean Square Deviation .Fluctuations in energy in a Cannonical ensemble, Fluctuations in density , radioactive disintegration and Brownian movement.

Book Suggested

1.Classical and Statistical thermodynamics, Ashley H.Carter, Prentice Hall(2001).

2. Thermodynamics and Statistical Mechenics, Kerson Huang, Second edition , Wiley (1982)

3.Fundamental of Classical and Statistical thermodynamics, BImalendu Narayan Roy, John Wiley & Sons (1982).

4.Macroscopic and Statistical thermodynamics, Yi-Chen Cheng, World Scientific (2006).

5.Matter in Equilibrium: Statistical Mechenics and Thermodynamics , Stephen R.Berry,Stuart A.Rice and John Ross, Oxford University Press(2001) 2nd edition.

6.Statistical Mechenics: Fundamentals and Modern Applications, Richard E.Wilde and Surjit Singh , Wiley-Interscience (1998).

7. Statistical thermodynamics Gupta M.C. , New Age International (P) Ltd. Publication second edition (1990).

Elective Paper III

MCY 403 (E)

Mathematics in Chemistry **60 h**

Unit I

Vectors

Vectors, dot, cross and triple products. The gradient, divergence and curl. Vector calculus, Gauss theorem (Derivation not required), application to molecular geometry

Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probably errors, examples from the kinetic theory of gases., curve fitting (including least square fit) with a general polynomial fit.

Unit II

Matrix algebra

Addition and multiplication, inverse, adjoint and transpose of matrices, special matrices (symmetric, skew-symmetric, hermitian, skew-hermitian, unit, diagonal, unitary) and their properties, Matrix equations: Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence.

Introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants (example from Huckel theory)

Introduction to tensors: polarizability and magnetic susceptibility as examples.

Unit III

Differential calculus

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution) exact and inexact differentials with their applications to thermodynamics & kinetic properties.

Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution reduction formulae, application of integral calculus.

Functions of several variables, partial differentiation, coordinate transformation (Cartesian to spherical polar), curve sketching.

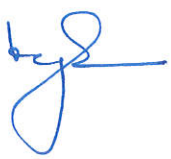
Unit IV

Elementary Differentials Equations

Variables-separable and exact first order differential equations, homogeneous, exact and linear equations, Applications to chemical kinetics, secular equilibria, quantum chemistry etc. Solutions of differentials equations by the power series method, polynomial (derivation not required), Polynomial in harmonic oscillator, rigid rotator and hydrogen atoms. Fourier series, solutions of harmonic oscillator and Legendre equation, spherical harmonics, second order differential equations and their solutions, elementary understanding of logarithms.

Recommended books

1. The Chemistry Mathematics Book, E. Steiner, Oxford University Press
2. Mathematics for Chemistry, Doggett and Sublitt, Longmann
3. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill
4. Chemical Mathematics, D. M. Hirst, Longmann
5. Applied Mathematics for Physical Chemistry, J. R. Barrante, Prentice Hall
6. Basic Management for Chemist, Tebutt, Wiley.



MCY-105: Lab Course-I

a. Inorganic Chemistry

1. Quantitative separation and determination of pairs of metal ions using gravimetric and volumetric methods.
2. Complexometric titrations.
3. Preparation, to purification and structural elucidation of following complexes by available phyco-chemical and spectral methods.
    a. Chloropentaaminecobalt (III) chloride .
    b. Bis (cyclopentadienyl) iron (II), Ferrocene.

b. Organic Chemistry

One step synthesis and physicochemical and spectra studies of the following:

1. S–Benzyl isothiouronium chloride from benzylchloride
2. ortho- Benzoyl benzoic acid from phthalic anhydride
3. Resacetophenone from resorcinol
4. para- Nitrobenzoic acid from paranitrotoluene
5. Anthraquinone from anthracene
6. Benzhydrol from Benzophenone

MCY-106: Lab Course- II

c. Physical Chemistry

1. Simultaneous determination of surface tension and viscosity with survismeter.
2. Determination of molecular weight of the polymer by viscosity method.
3. Preparation of buffer solutions and determination of their pH values.
4. Potentiometric titration of phosphoric acid using NaOH and standard Potassium hydrogen phthalate.
5. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion)
6. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.
7. Determination of pKa of an indicator.

8. Adsorption: study of surface tension – concentration – relationship for solutions (Gibbs equation)

d. Analytical Chemistry

Chromatographic Separation

1. Thin Layer Chromatography: separation of mixture of ortho and para – Nitroanilines or of given sample
2. Paper chromatography – identification of alpha amino acids or of given sample
3. Determination of Fe spectrophotometrically using o-phenanthroline.
4. Determination of Li+/K+/Na+ by flame photometry.

References:

1. Inorganic experiments, J. Derek Woolins, VCH
2. Findley's practical physical chemistry, revised B.P. Levitt, longmann
3. Vogels, text book of practical organic chemistry, pearson education.
4. Microscale Inorganic Chemistry, Z. Szafran, R. M. Pike and M. M. Singh, Wiley
5. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand
6. The systematic identification of organic compounds, R.L. Shriner and D.Y Curtin
7. Semimicro qualitative organic analysis, N.D. Cheronis, J.B. Entrikin and E.M. Hodnett
8. Experimental organic chemistry, M.P. Doyie and W.S. Mungall
9. Small scale organic preparation, P.J. Hill
10. Organometallic synthesis, J. J. Fisch and R. B. King, Academic
11. Experimental physical chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, McGraw Hill Interscience
12. Experiments in physical chemistry, J.C. Ghosh, Bharti Bhawan

MCY-205: Lab Course-III

a. Inorganic/Analytical Chemistry

1. Preparation of selected coordination complexes and their characterization by physical, magnetic and spectral techniques.
2. Volumetric analysis: redox, complexometric and precipitation titrations.
3. Job's method of continuous variation.
4. Column Chromatography: separation of mixture of ortho and para-Nitroanilines or of given sample.
5. Determination of Pb/Cd by AAS.

b. Organic/Analytical Chemistry

Two stages preparation and physicochemical and spectral analysis of the following:

1. Sym-tribromobenzene from aniline.
2. m-Nitrobenzoic acid from methyl benzoate
3. para -Nitroaniline from acetanilide.
4. Benzanilide from benzophenone.
5. para –Amino benzene sulphanamide from acetanilide
6. Anthraquinone from phthalic anhydride.
7. Preparation of Benzilic acid from Benzoin

MCY-206: Lab Course IV

Physical Chemistry

1. To determine the adsorption isotherm of acetic acid from aqueous solution by charcoal.
    a. Freundlich adsorption isotherm
    b. Langmuir adsorption isotherm
    c. BET adsorption isotherm
2. Determination of the specific rotation of sucrose & tartaric acid.
3. Determination of molar conductivity of a weak electrolyte for different concentrations & calculation of the dissociation constant of an acid.
4. Determination of the rate constant for the oxidation of iodide ions by hygrogen peroxide studying the kinetics as an iodine clock reaction.
5. Electrochemistry: Determination of solubility and solubility product of sparingly soluble salts ($PbSO_4$, $BaSO_4$) conductometrically, Potentiometry, pHmetry:

References:

1. Inorganic experiments, J. Derek Woolins, VCH
2. Microscale Inorganic Chemistry, Z. Szafran, R. M. Pike and M. M. Singh, Wiley
3. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand
4. Systematic identification of organic compounds, R.L. Shriner and D.Y Curtin
5. Semimicro qualitative organic analysis, N.D. Cheronis, J.B. Entrikin and E.M. Hodnett
6. Experimental organic chemistry, M.P. Doyie and W.S. Mungall
7. Small scale organic preparation, P.J. Hill
8. Organometallic synthesis, J. J. Fisch and R. B. King, Academic
9. Experimental physical chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, McGraw Hill Interscience
10. Findley's practical physical chemistry, revised B.P. Levitt, longmann
11. Vogls, text book of practical organic chemistry, pearson education.
12. Experiments in physical chemistry, J.C. Ghosh, Bharti Bhawan

MCY 305: Lab Course-V

1. Extraction of Natural Products:

1. Caffeine from tea leaves.
2. Citric acid from lemon.
3. Lactose and casein from milk

2. Representative Synthesis, purification and structural analysis of drug molecules:

1. Synthesis of paracetamol, aspirin etc.
2. Synthesis of drugs intermediates.
3. Preparation of 1, 1`-Bi-2-naphthol

3. Determination of partition coefficient of a drug between water & n-octanol.

4 Determination of Nitro compounds TiCl3 method

5. Non-Aquous titration; Determination of Sodium benzoate/Sodium monoglutamate (Azinomotto/Mebendazole/diazapam) in glacial acetic using perchloric acid as titrate.

MCY 306: Lab Course VI

4.Instrumental Analysis of Drug molecules:

i) Gas Chromatography, ii) Infra-Red Spectroscopy, iii) Nuclear Magnetic Resonance Spectroscopy, iv) Mass Spectrometry and v) High performance Liquid Chromatography

5. Polymer Chemistry

a. Polymer Chemistry Molecular weight determination by viscocity method
b. Osmometry -determination of molecular weight of polymers by osmotic pressure method,
c. Viscometry -same with dilute solution viscometry of polymers, same with GPC.

References:

1. Experimental physical chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, McGraw Hill Interscience
2. Findley's practical physical chemistry, revised B.P. Levitt, longmann
3. Vogls, text book of practical organic chemistry, pearson education.
4. Experiments in physical chemistry, J.C. Ghosh, Bharti Bhawan
5. D. G. Hundiwale, V. D. Athawale, U. R. Kapadi, V. V. Gite, Experiments in Polymer Science, New Age International Pvt. Ltd., New Delhi, 2009.
6. F. J. Davis, Polymer Chemistry-Practical Approach in Chemistry, Oxford University Press, Oxford, 2004.
7. Quantitative organic analysis, Vogel's.