M.Sc., Chemistry

Poompuhar College (Autonomous)

Melaiyur-609 107

Course Structure Under CBCS

(2016-2017 onwards)

POOMPUHAR COLLEGE (AUTONOMOUS), MELAIYUR – 609 107

Course Structure under CBCS

M.Sc., Chemistry

(for the candidates admitted from the academic year 2016 – 2017 onwards)

SEMESTER	COURSE	TITLE	INSTRU HOURS/WEEK	CREDIT	EXAM Hrs	MARKS INTERNAL	MARKS EXTERNAL	TOTAL
I	Core Course – I (CC)	Organic Chemistry - I	6	4	3	25	75	100
	Core Course – II (CC)	Inorganic Chemistry - I	6	4	3	25	75	100
	Elective Course – I	Analytical Chemistry	6	4	3	25	75	100
	Core Course – III (CC)	Organic Practical - I	6	5	*	40	60	100
	Core Course – IV (CC)	Inorganic Practical - I	6	5	*	40	60	100
		Total	30	22				500
II	Core Course – V (CC)	Physical Chemistry - I	6	4	3	25	75	100
	Core Course – VI (CC)	Inorganic Chemistry - II	6	5	3	25	75	100
	Core Course – VII (CC)	Physical Methods in Chemistry - I	6	5	3	25	75	100
	Core Course – VIII (CC)	Organic Practical - II	6	5	*	40	60	100
	Core Course – IX (CC)	Inorganic Practical - II	6	4	*	40	60	100
		Total	30	23				500
III	Core Course – X (CC)	Organic Chemistry - II	6	5	3	25	75	100
	Core Course – XI (CC)	Inorganic Chemistry - III	6	5	3	25	75	100
	Core Course – XII (CC)	Physical Chemistry Practical - I	6	4	**	40	60	100
	Elective Course - II	Polymer Chemistry	6	4	3	25	75	100
	Elective Course - III	Green and Environmental Chemistry	6	4	3	25	75	100
		Total	30	22				500
IV	Core Course – XIII (CC)	Physical Chemistry - II	6	5	3	25	75	100
	Core Course – XIV (CC)	Physical Chemistry Practical – II	6	4	**	40	60	100
	Elective Course - IV	Industrial Chemistry	6	4	3	25	75	100
	Elective Course - V	Chemistry of Nano Science and Nano Technology	6	4	3	25	75	100
	Project work	Project work	6	6				100
		Total	30	23				500
		Grand Total		**90**				**2000**

* Practical examination for Organic Practicals I & II and Inorganic Chemistry Practicals I & II will be conducted at the end of second semester – 6 Hrs duration.

** Practical examination for Physical Chemistry Practicals I & II will be conducted at the end of the fourth semester – 6 Hrs duration.

SEMESTER - I **CORE COURSE – I**

ORGANIC CHEMISTRY - I

UNIT I STRUCUTURE AND BONDING

1.1 Nomenclature of alicylic, bicyclic and tricyclic compounds, [Basic skletalstrucures only with or without one substituent]

1.2 Localized chemical bonding. Electronic structure of molecules based on VB,MO and HOMO –LUMO theory. Application of Electronegativity, Dipole moment, Inductive and Field Effects.Bond distances, Bond angles, Bond Energies.

1.3 Delocalized chemical Bonding: Bond energies and Bond distances in compounds containing delocalized Bonds, Cross conjugation, Resonance, Steric inhibition of resonance, Hyper conjugation, Keto-EnolTautomerism.

UNIT II AROMATICITY AND HETEROCYCLES

2.1 Aromatic character: Five-, six-, seven-, and eight-membered rings – othersystems with aromatic sextets – Huckel's theory of aromaticity, concept of homoaromaticity and antiaromaticity.

2.2 Electron occupancy in MO's and aromaticity – NMR concept of aromaticity and antiaromaticity, systems with 2,4,8 and 10 electrons, systems of more than 10 electrons (annulenes).

2.3 Bonding properties of systems with (4n+2)π-electrons and 4nπ-electrons, alternant and non-alternant hydrocarbons (azulene type) – aromaticity in heteroaromatic molecules, sydnones and fullerenes.

2.4 Nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen, and sulphur. Synthesis, reactivity and applications of the following heterocycles: Oxazoles, Pyridazines, Pyrimidine and Pyrazines.

UNIT III STEREOCHEMISTRY AND CONFORMATIONAL ANALYSIS

3.1 Stereoisomerism –Optical Isomerism- symmetry – enantiomers and diastereomers – Conversions used in stereochemistry. Newman, Sawhorse and Ficher notations and interconversions and representations.*R* and *S* nomenclature – optical activity and chirality – types of molecules exhibitingoptical activity – absolute configuration – chirality in molecules with noncarbonstereocenters (N, S and P) – molecules with more than one chiral centre – atropisomerism.

3.2 Molecular chirality – allenes, spiranes, biphenyls.Geometrical isomerim-
E and *Z* nomenclature – determination of configuration of geometrical isomers – stereochemistry of addition and elimination reactions – stereospecific and stereoselective synthesis [elementary examples].

3.3 Basic concepts of conformational analysis – conformations of cyclohexane, cyclohexene and decalin.

UNIT IV ORGANIC PHOTOCHEMISTRY

4.1 Organic Photochemistry - Fundamental concepts - Jablonski diagram - Energy transfer. Characteristics of photoreactions, Photo reduction and photo oxidation and photosensitization.

4.2 Photo reactions of ketones and enones - Norrish type I and II reactions.ParternoBuchi reaction, Photo chemistry of alkenes, dienes and aromatic compounds- Di-π-methane rearrangement.

4.3 Reactions of unactivated centers - Photolytic cycloadditionsand photolytic rearrangements. Photo additions - Barton reaction.

UNIT V REAGENTS IN ORGANIC SYNTHESIS AND DETRMINATION OF REACTION MECHANISM

5.1 Oxidation: Baeyer-Villiger, Jacobsen epoxidation, Jones reagent, PCC, PDC, IBX, DMP, Swern oxidation, Sommelet reaction, Elbs reaction, Oxidative coupling of phenols, Prevost reaction.

5.2 Reduction: palladium / nickel based heterogeneous catalysts for hydrogenation, Wilkinson's catalyst, reductions using Li/Na/Ca in liquid ammonia. Hydride transfer reagents –$NaBH_4$ and $NaCNBH_3$.

5.3 Thermodynamic and Kinetic controlled reactions, Energy profile diagram, Intermediate vs Transition state, Product analysis and its importance, Kinetic methods, Stereochemical studies, Isotopic and substituent effects.

REFERENCE

1. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure; 7th Ed., Wiley, New York, 2013.
2. I. L. Finar, Organic Chemistry; Vol.II, 7th Ed., Pearson education Ltd, New Delhi, 2009.
3. R. K. Bansal, Organic Reaction Mechanisms; 11th Ed., Tata McGraw Hill, Noida, 2006.
4. R. T. Morrison and R. N. Boyd, Organic Chemistry, 7th Ed., Pearson, New Delhi, 2011.
5. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry; Parts A and B, 5th Ed., Springer, Germany, 2007.
6. P. S. Kalsi, Stereochemistry; Wiley eastern limited; New Delhi, 1993.
7. D. Nasipuri, Stereochemistry of Organic Compounds - Principles and Applications; 2nd Ed., New Age International, New Delhi, 1994.
8. E. L. Eliel, and S. H. Wilen, Stereochemistry of Organic Compounds; John Wiley, New York, 1994.
9. J. D. Coyle, Organic Photochemistry; Wiley, New York, 1998.
10. G. R. Chatwal, Organic Phtochemistry; 1st Ed., Himalaya Publications house, Bangalore, 1998.

FACULTY UNIVERSITY NOMINEE HOD

SEMESTER - I **CORE COURSE – II**

INORGANICCHEMISTRY - I

UNIT I MAIN GROUP CHEMISTRY

1.1 Chemistry of Boron – Borane, higher boranes, Carboranes, Borazines and boron nitrides. Chemistry of silicon – silanes, higher silanes, multiple bonded systems.Disilanes, silicon nitrides, siloxanes and silicates, P-N compounds, Cyclophospazanes, Cyclophosphazenes, S-N compounds - S_4N_4 $(SN)_x$..

1.2 Ionic Model- Lattice energy, Bornhober Cycle - Born-Lande Equation-kapustinskii equation- Application of Latice Energy, High Tc Superconductors - Band theory of Solids - Schotty, Frenckel defects, F center.

UNIT II PRINCIPLES OF COORDINATION CHEMISTRY

2.1 Studies of coordination compounds in solution - detection of complex formation in solution - Stereo and optical isomerism in coordination complexes. Stability constants - Stepwise and overall formation constants.

2.2 Simple methods of determining the formation constants – (Jobs continuous method of variation, mole-ratio method, polarographic methods).

2.3 Factors affecting stability - Statistical and chelate effects - Forced configurations.

UNIT III THEORIES OF METAL – LIGAND BOND

3.1 Crystal field theory (CFT) - Splitting of d orbitals under various geometries - Factors affecting splitting - Crystal Field StabilisationEnergy(CFSE) and evidence for CFSE (Structural and thermodynamic effects).

3.2 Spectrochemicalseries -john Teller distortion - Spectral and magnetic properties of complexes - Site preferences.

3.3 Limitations of CFT - ligand field theory - MO theory - Sigma and Pi bonding in complexes. Nephelauxetic effect.

UNIT IV REACTION MECHANISM IN COORDINATION CHEMISTRY

4.1 Kinetics and mechanism of reactions in solution - labile and inert complexes - ligand displacement reactions in octahedral and square planar complexes - acid hydrolysis, base hydrolysis and anation reactions – trans effect - theory and application.

4.2 Electron transfer reactions - electron exchange reactions - complementary and non- complementary types - inner sphere and outer sphere process - Application of electron transfer reactions in inorganic - isomerisation and racemisation reactions of complexes.

4.3 Molecular rearrangements of Reactions of four and six coordinate complexes -interconversionof stereoisomers - Reactions of coordinated ligands - template effect and its application.

UNIT V INORGANIC PHOTOCHEMISTRY

5.1 Electronic transitions in metal complexes, metal-centered and charge-transfer transitions – various photophysical and photochemical processes of coordination compounds.

5.2 Unimolecular charge-transfer photochemistry of cobalt(III) complexes – mechanism of Charge Transfer To Metals(CTTM), photoreduction – ligand-field photochemistry of chromium(III) complexes – Adamson's rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium polypyridine complexes, emission and redox properties.

5.3 Photochemistry of organometallic and metal carbonyl compounds – compounds with metal-metal bonding – Reinecke's salt chemical actinometer.

REFERENCE

1. M. C. Day, J. Selbin and H. H. Sisler, Theoretical Inorganic Chemistry; Literary Licensing (LLC), Montana, 2012.

2. F. A. Cotton and G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry; 6th Ed., A Wiley - Interscience Publications, John Wiley and Sons, USA, 1999.

3. J. E. Huheey, Inorganic Chemistry; 4th Ed., Harper and Row publisher, Singapore, 2006.

4. A. W. Adamson, Concept of Inorganic Photochemistry; John Wiley and Sons, New York, 1975.

5. S. F. A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum; Academic Publishers, Oxford University Press, New York, 1996.

6. A. W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry; R. E. Krieger Pubs, Florida, 1984.

7. J. Ferraudi, Elements of Inorganic Photochemistry; Wiley, New York, 1988.

8. F. Basolo and R. G. Pearson, Mechanism of Inorganic Reactions; 2nd Ed., John Wiley, New York, 1967.

9. R. K. Sharma, Inorganic Reactions Mechanism; Discovery Publishing House, New Delhi, 2007.

FACULTY UNIVERSITY NOMINEE HOD

SEMESTER - I ELECTIVE COURSE – III

ANALYTICAL CHEMISTRY

UNIT I INSTRUMENTAL METHODS OF ANALYSIS

1.1 Principles and applications of extended X-ray absorption fine structure (EXAFS) -surface extended X-ray absorption (SEXAFS).

1.2 Atomic absorption spectroscopy (AAS) -flame emission spectroscopy (FES) -turbidimetryand nepheleometry - theory and applications.

UNIT II DATA AND ERROR ANALYSIS

2.1 Various types of error - accuracy, precision, significant figures - describing data , population and sample,mean, variance, standard deviation, way of quoting uncertainty, repeatability and reproducibility of measurements.

2.2 Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t - Test, paired t- Test - analysis of variance (ANOVA) -Correlation and regression.

2.3 Curve fitting, fitting of linear equations, simple linear case, weighted linear case, analysis of residuals- general polynomial equation fitting.

UNIT III CHROMATOGRAPHY

3.1 Solvent extraction - principles of ion exchange, paper, thin-layer and column chromatographic techniques.Columns, absorbents, methods, Rf values, McReynolds constants and their uses.

3.2 HPLTC, HPLC techniques - absorbents, columns, detection methods, estimations, preparative column - GC - MS techniques–methods, principles anduses.

UNIT IV THERMOANALYTICAL METHODS AND FLUORESCENCE SPECTROSCOPY

4.1 Principles and applications of Thermogravimetryanalysis (TGA), Differential thermal analysis (DTA) and Differential scanning calorimetry (DSC)–Thermometric titrations - types -advantages.

4.2 Basic aspects of synchronous fluorescence spectroscopy.

UNIT V ELECTROANALYTICAL TECHNIQUES

5.1 Electrochemical sensors, ion sensitive electrodes, glass - membrane electrodes - solid liquid membrane electrodes, ion-selective field effect transistors (ISFETs) - sensors for the analysis of gases in solution

5.2 Amperometric titrations - principle instrumental - techniques - applications.

5.3 Fluorimetry, Phosporimetry - Instrumentation and its applications.

REFERENCE

1. D. B. Hibbert and J. J. Gooding, Data Analysis for Chemistry; Oxford University Press, UK, 2006.
2. J. Topping, Errors of Observation and Their Treatment; 4th Ed., Chapman Hall, London, 1984.
3. A. Braithwaite and J. F. Smith, Chromatographic Methods; 5th Ed., Springer,

   Germany; 1995.
4. V. K. Srivastava and K. K. Srivastava, Introduction to Chromatography; 2nd Ed., Holden Day, New York, 1985.
5. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, Instrumental Methods of Analysis; 6th Ed., CBS Publishers and Distributors, Chennai, 1986.
6. D. A. Skoog, D. M. West and D. J. Holler, Fundamentals of Analytical Chemistry,7th Ed., Harcourt College Publishers, Singapore, 2004.
7. A. Sharma, S. G. Schulman, Introduction to Fluorescence Spectroscopy; Wiley- Interscience, New York, 1999.
8. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy; 4th Ed., Tata McGraw-Hill, New Delhi, 1994.
9. A. I. Vogel, Text Book of Quantitative Inorganic Analysis; 6th Ed., Longman, New Delhi, 2000.
10. D. C. Harris, Quantitative Chemical Analysis; 4th Ed., W. H. Freeman Publications, New York, 1995.
11. S. C. Gupta, Fundamentals of Statistics; 6th Ed., Himalaya Publications, Delhi, 2006.
13. Organic Electro chemistry by Henning lund& Ole Hammerich 4th edition – Marcel Dekker inc. New York.
14. B.K. Sharma. (Industrial chemistry of chemical Engineering).

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - I

CORE COURSE – III (CORE PRACTICAL - I)

ORGANIC CHEMISTRY - I (P)

OBJECTIVES

1. To perform the qualitative analysis of a given organic mixture.
2. To carry out the preparation of organic compounds.

1. Qualitative analysis of an organic mixture containing two components

Mixtures containing two components are to be separated (pilot separation) andpurified (bulk separation) – The physical constants are to be reported (analysis).

2. Preparation of organic compounds (single stage)

1. Methyl-*m*-nitrobenzoate from methylbenzoate (nitration)
2. Glucose pentaacetate from glucose (acetylation)
3. Resacetophenone from resorcinol (acetylation)
4. Benzophenoneoxime from benzophenone (addition)
5. *o*-Chlorobenzoic acid from anthranilic acid (Sandmayer reaction)
6. *p*-Benzoquinone from hydroquinone (oxidation)
7. Phenylazo-2-naphthol from aniline (diazotization)

REFERENCE

1. J. Mohan, Organic Analytical Chemistry: Theory and Practice; Narosa, 2003.
2. V. K. Ahluwalia, P. Bhagat, and R. Agarwal, Laboratory Techniques in Organic
   Chemistry; I. K. International, 2005.
3. N. S. Gnanaprakasam and G. Ramamurthy, Organic Chemistry Lab Manual; S.V. Printers, 1987.
4. A. I. Vogel, A. R. Tatchell, B. S. Furniss, A. J. Hannaford and P. W. G. Smith,Vogel ' s Textbook of Practical Organic Chemistry; 5th Ed., Prentice Hall, 1989.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - I

CORE COURSE – IV (CORE PRACTICAL - II)

INORGANIC CHEMISTRY I (P)

OBJECTIVES

1. To perform the semi-micro qualitative analysis.
2. To estimate the metal ions using colorimeter.

1. Semi-micro qualitative analysis

Mixture containing two commoncations (Pb, Bi, Ca, Cd, Fe, Cr, Al, Co, Ni, Mn, Zn, Ba, Sr, Ca, Mg, NH_4) andtwo less common cations (W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U, Li).

2. Estimation

Copper, ferric, nickel, chromium and manganese ions usingphotoelectric colorimeter

REFERENCE

1. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rd Ed., National Pubs, London, 1988.
2. G. Svehla, Text Book of Macro and Semimicro Qualitative Inorganic Analysis; 5th Ed., Longman group Ltd, London, 1987.
3. A. I. Vogel, Text Book of Quantitative Inorganic Analysis; 6th Ed., Longman,New Delhi, 2000.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - II **CORE COURSE - V**

PHYSICAL CHEMISTRY - I

UNIT I CONCEPTS OF GROUP THEORY

1.1 Symmetry elements and operations – point groups – assignment of pointgroups to molecules – group postulates and types of groups – groupmultiplication tables, sub groups, similarity transformations – conjugateelements and classes.

1.2 Matrix representation of symmetry operations and point groups – reducible andirreducible representations – properties of irreducible representation.

1.3 The great orthogonality theorem – construction of character table – directproduct – projection operators – symmetry of hybrid orbitals.

UNIT II QUANTUM CHEMISTRY - I

2.1 Inadequacy of classical mechanics – black body radiation – Planck's quantumconcept – photoelectric effect – Bohr's theory of hydrogen atom – hydrogenspectra – wave-particle dualism – uncertainty principle – decline of oldquantum theory.Schrodinger equation – postulates of quantum mechanics – operator algebra:linear operator, Hermitian operators, eigenfunctions and eigenvalues, angularmomentum operator – commutation relations and related theorems –orthogonality and normalization.

2.2 Applications of wave mechanics to simple systems – particle in a box, one andthree dimensional, particle with finite potential barrier – the quantummechanical tunneling.

UNIT III CHEMICAL KINETICS - I

3.1 Theories of reaction rate – absolute reaction rate theory (ARRT) – transmissioncoefficient, reaction coordinate – potential energy surfaces –kinetic isotopeeffect – Hinshelwood theory – Kassel, Rice and Ramsperger theory (KRRT) –Slater's treatment.

3.2 Principle of microscopic reversibility – steady-state approximation – chainreactions: thermal and photochemical reactions between hydrogen andhalogens – explosions and hydrogen-oxygen reactions.

UNIT IV STATISTICAL THERMODYNAMICS

4.1 Thermodynamic probability – probability theorems – relation between entropyand probability (Boltzmann-Planck equation), ensembles, phase space, Ergodichypothesis, microstates and macrostates, Maxwell-Boltzmann distribution law– partition functions – translational, rotational, vibrational and electronicpartition functions.Relationship between partition functions and thermodynamic properties –calculation of equilibrium constants from partition functions – heat capacitiesof monatomic crystals – Einstein theory and Debye theory.

4.2 Quantum statistics – Bose-Einstein (B.E.) and Fermi-Dirac (F.D.) distributionequations – comparison of B.E. and F.D. statistics with Boltzmann statistics –applications of quantum statistics to liquid helium, electrons in metals andPlanck's radiation law – concept of negative Kelvin temperature.

UNIT V FAST REACTION TECHNIQUES, PHOTOCHEMISTRY AND RADIATION CHEMISTRY

5.1 Introduction – flow methods (continuous and stopped flow methods) – relaxation methods (T and P jump methods) – pulse techniques (pulseradiolysis, flash photolysis) – shock tube method – molecular beam method – lifetime method.

5.2 Photophysical processes of electronically excited molecules –Jablonski diagram– Stern-Volmer equation and its applications – experimental techniques inphotochemistry – chemical actinometers– lasers and their applications.

5.3 Differences between radiation chemistry and photochemistry – sources of highenergy radiation and interaction with matter – radiolysis of water, solvatedelectrons – definition of G value, Curie, linear energy transfer (LET) and Rad –scavenging techniques – use of dosimetry and dosimeters in radiationchemistry – applications of radiation chemistry.

REFERENCE

1. F. A. Cotton, Chemical Applications of Group Theory; 3rd Ed., John Wileyand Sons, Singapore, 2003.
2. R. L. Flurry, Jr, Symmetry Groups: Theory and Chemical Applications; Prentice Hall, New Jersy, 1980.
3. S. F. A. Kettle, Symmetry and Structure; 2nd Ed., John Wiley and Sons, Chichester, 1995.
4. A. K. Chandra, Introductory Quantum Chemistry; 4th Ed., Tata McGraw Hill, Noida, 1994.5. D. A. Mcquarrie, Quantum Chemistry; UniversityScience Books, Sausalito,2008.
6. I. N. Levine, Quantum Chemistry; 5th Ed., Prentice Hall, New Jersey, 2000.
7. R. K. Prasad, Quantum Chemistry; 4th Ed., New Age International

Publishers, New Delhi, 2014.
8. K. J. Laidler, Chemical Kinetics; 3rd Ed., Tata McGraw Hill, Noida, 1987.
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10. M. Mortimer and P. G. Taylor, Chemical Kinetics and Mechanism; 1st Ed.,Royal Society of Chemistry, UK, 2002.
11. J. N. Gurtu and A. Gurtu, Advanced Physical Chemistry; 5th Ed., PragathiPrakashan, Meerut, 2006.
12. J. I. Steinfeld, J. S. Francisco and W. L. Hase, Chemical Kinetics and Dynamics; 2nd Ed., Prentice Hall, New Jersey, 1999.
13. K. S. Gupta, Chemical Kinetics and Reaction Mechanism; RBSA Publishers,Jaipur, India, 1992.
14. P. W. Atkins, Physical Chemistry; 7th Ed., Oxford University Press, Oxford,2001.
15. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students ofChemistry - Classical, Statistical and Irreversible; Pearson Education, New Delhi, 2013.
16. HoriaMetiu, Physical Chemistry, Thermodynamics; Taylor and Francis, Singapore, 2006.
17. K. K. Rohatgi-Mukherjee, Fundamentals of Photochemistry; 3rd Ed., NewAge International Pvt. Ltd., New Delhi, 2014.
18. J. W. T. Spinks and R. J. Woods, Introduction to Radiation Chemistry; 3rdEd., John Wiley and Sons, New York, 1990.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - II **CORE COURSE - VI**

INORGANIC CHEMISTRY – II

UNIT I ACIDS AND BASES

1.1 Bronsted and lewis acids and bases, protonicacid,proton affinities - differentiating and leveling solvents - acidic behavior of the binary hydrides - strength of oxyacids - hydrolysis -amphoteric oxides - non protonic concepts of acid- base reactions -lux concept.

1.2 Liquid ammonia, acetic acid, brominetrifluoride, dinitrogentetroxide, liquid hydrogen fluoride as solvents.

1.3 Classifications of acids and bases- hard or soft - acid - base strength and hardness and softness. E-C parameters for the strength of acids and bases.

UNIT II NUCLEAR CHEMISTRY

2.1 Radioactivedecay - theories of decay process - laws of radioactivity . Detection and measurement of radiations- nuclear structure - composition of nuclei - properties of nuclei - nuclear radii- nuclear spin etc.Nuclear forces - its characteristic - meson field theory - nuclear stability - nuclear models - liquid drop,shell and collective models.

2.2 Artificialradioactivity **-** Nuclear reactions - Transmutation - stripping and pickup, Fission products and fission yields. Fusion, spallation and fragmentation reactions-scattering reactions - nuclear cross section - Q value. Nuclear reactors - charged particle accelerators - neutron sources - gamma ray and X-ray sources. Radioactive techniques - tracer technique – neutron activation and isotopic dilution analysis.

2.3 Application of nuclear science in agricultureand biology, radiation risks and medical benefits - natural and manmade isotopes.

UNIT III BIO- INORGANIC CHEMISTRY

3.1 Biological role of metal ions, calcium biochemistry, oxygen transport and storage, carbonic anhydrase, carboxypeptidases, FeS proteins

and non-hemeiron cytochomes of the electron transport chain, cytochrome, P-450 enzymes. coenzymeB12.

3.2 Nitrogen fixation and photosynthesis -mechanism of enzyme catalysis (lock and key method).

UNIT IV ORGANOMETALLICS

4.1 Eighteen (18) electron rule – applications and limitations –isolobal concept and itsusefulness – uses of typical organometallics such as metal alloys andorganometallic hydrides in organic synthesis.

4.2 Nitrosyl complexes – bridging and terminal nitrosyls, bent and linear nitrosyls–dinitrogen complexes –metallocene and arene complexes – metal carbenes,carbenes, carboxylate anions.

UNIT V REACTIONS AND CATALYSIS BY ORGANOMETALLICS

5.1 Organometallic reactions – ligand association and dissociation – oxidative

addition and reductive elimination – insertion reactions.

5.2 Reactions of coordinated ligands in organometallics – hydrogenation,

hydroformylation, epoxidation, metathesis.

5.3 Polymerization of olefins, olefin oxidation (Wacker process) and carbonylation ofmethanol.

REFERENCE

1. J. E. Huheey, Inorganic Chemistry; 4th Ed., Harper and Row Publishers, Singapore, 2006.
2. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry; Panima Publishing Company, New Delhi, 1997.
3. G. L. Eichhorn, Inorganic Biochemistry; Volumes 1 and 2, 2nd Ed., Elsevier Scientific Publishing Company, New York, 1975.
4. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry; 6th Ed., John Wileyand Sons, New York, 1999.
5. R. C. Mehrotra and A. Singh, Organometallic Chemistry; 2nd Ed., New Age International Ltd. New Delhi, 2014.
6. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals; 3rd Ed.,John Wiley and Sons, New York, 2001.
7. A. J. Pearson, Advances in Metal-Organic Chemistry, Vol. 1; Jai Press, Inc., Greenwich, 1989.
8. A. W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry; 1987, Oxford University Press, Chennai.
9. I. Haiduc and J. J. Zuckerman, Basic Organometallic Chemistry; Walter De GruyterInc, USA, 1985.
10. P. Powell, Principles of Organometallic Chemistry; 2nd Ed., Chapman and Hall,London, 1988.

11. B. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry; 3rd Ed., John Wiley and sons, New York, 1994.

12. M. Bochmann, Organometallics 1: Complexes with transition metal-carbon bonds;Oxford Chemistry Primers Series, No. 12, and M. Bochmann, Organometallics 2:Complexes with transition metal-carbon bonds; No. 13, 1994.

13. J. P. Collman, L. S. Hegedus, J. R. Norton and R. G. Finke, Principles and Applications of Organotransition Metal Chemistry, University Science Books, California, 1987.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - II

CORE COURSE - VII

PHYSICAL METHODS IN CHEMISTRY - I

UNIT I PRINCIPLES OF MOLECULAR SPECTROSCOPY

1.1 Interaction of electromagnetic radiation with molecular systems. Microwave spectroscopy – rotational spectra of diatomic molecules, rigid andnon-rigid rotors – intensity of spectral lines – effects of isotopic substitution –microwave spectra of polyatomic molecules – linear and symmetric topmolecules –

1.2 Raman spectra – rotational Raman spectra of linear and symmetric topmolecules – vibrational Raman spectra – rotational fine structure – electronicspectra of diatomic molecules – vibrational coarse structure – intensity ofvibrational lines in electronic spectra – rotational fine structure –fortratdiagram.

UNIT II NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

2.1 ^{1}H NMR Spectroscopy – multiplicity – coupling constant – spin-spin splitting –vicinal and geminal coupling constants –Karplus equation – long rangecoupling constants, influence of stereochemical factors on chemical shift ofprotons.

2.2 Simplification of complex spectra – double resonance techniques, shiftsreagents – chemical spin decoupling of rapidly exchangeable protons (OH, SH,COOH, NH, NH2) – an elementary treatment of NOE phenomenon.

2.3 ^{13}C NMR Spectroscopy – broad band decoupling – off resonance decoupling –chemical shifts of common functional groups – FT NMR and its importance–DEPT spectra – identification of small compounds

based on NMR data – 2Dtechniques: 1H–1H COSY, 1H–13C HETCOSY – NOESY.

UNIT III UV-VISIBLE AND IR SPECTROSCOPY

3.1 UV-Visible spectroscopy – introduction – instrumentation, sampling techniques– Woodward-Fieser and Scott's rules for conjugated dienes and polymers,ketones, aldehydes, α,β-unsaturated acids, esters, nitriles, and amides –differentiation of geometrical isomers and positional isomers –disubsititutedbenzene derivatives – study of steric effect in aromaticity.

3.2 Infrared spectroscopy – Introduction – instrumentation, sampling techniques –factors influencing group frequencies – quantitative studies – hydrogen bonding (intermolecular and intramolecular).

3.3 Infrared spectra – diatomic molecules, simple harmonic and anharmonic oscillators – diatomic vibrating rotator rotation – vibration spectrum of carbon monoxide – interaction of rotation and vibration (breakdown of Born-Oppenheimer approximation) – influence of the rotation on the spectrum of polyatomic molecules, linear and symmetric top molecules, parallel and perpendicular vibrations – influence of nuclear spin.

UNIT IV ESR, ORD AND MASS TECHNIQUES

4.1 ESR – basic principles – comparison between ESR and NMR spectra – hyperfinesplitting – applications to organic free radicals.

4.2 Optical rotatory dispersion and circular dichroism– introduction to theory andterminology – cotton effect – ORD curves – axial haloketone rule and itsapplications – the octant rule – its applications – applications of ORD todetermine absolute configuration of monocyclic ketones – comparison betweenORD and CD – their interrelationships.

4.3 Mass Spectrometry – instrumentation – resolution – ESI, EI, CI and FABmethods – base peak, isotopic peaks, metastable peaks – importance ofmetastable peaks, parent peak, recognition of molecular ion peak –fragmentation – general rules – pattern of fragmentation for various classes ofcompounds, McLafferty rearrangement – nitrogen rule.Application of UV, IR, NMR and mass spectroscopy – structural elucidation oforganic compounds.

UNIT V MOSSBAUER SPECTROSCOPY

5.1 Isomer shifts – quadrupole splitting – magnetic interactions – applications to iron and tin compounds.

5.2 NQR spectroscopy – characteristics of quadrupolar nucleus – effects of field

gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.Photo electrn spectroscopy – theory – applications of UPES and XPES.

REFERENCE

1. C. N. Banwell, Fundamentals of Molecular Spectroscopy; 4th Ed., McGraw Hill Education, Noida, 1994.
2. B. P. Straughan and S. Walker, Spectroscopy; Vol.3, Halstead Press, Sydney, 1978.
3. G. M. Barrow, Introduction to Molecular Spectroscopy; McGraw Hill, New York, 1964.
4. P. K. Ghosh, Introduction to Photoelectron Spectroscopy; John Wiley, New York,1989.
5. P. M. Silverstein and amd F. X. Western, Spectroscopic Identification of OrganicCompounds; 8th Ed., John Wiley, New York, 2014.
6. W. Kemp, Organic Spectroscopy; 3rd Ed., Palgrave, New York, 1991.
7. J. R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, PHILearning, New Delhi, 2009.
8. Y. R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical applications; S. Chand, New Delhi, 1992.
9. P. S. Kalsi, Spectroscopy of Organic Compounds; 6th Ed., New Age InternationalPublishers, New Delhi, 2004.
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11. Web Pages: Cambridge Structural Database (CSD)- http://www.ccdc.cam.ac.uk /products/csd/Protein Data Bank (PDB) http://www.rcsb.org/pdb/home/home.do
12. J. R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, PHILearning, New Delhi, 2009.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - II CORE COURSE – VIII (CORE PRATICAL - III)

ORGANIC CHEMISTRY - II (P)

OBJECTIVES

1. To carry out the qualitative analysis of an organic mixture.

2. To perform the preparation of organic compounds.

1. Quantitative analysis of organic compounds

Estimation of phenol, aniline, ketone, glucose, nitrobenzene, saponification value of an oil and iodine value of oil.

2. Preparation of organic compounds (double stage)

1. *p*-Bromoacetanilide from aniline (acetylation and bromination)
2. Acetylsalicylic acid from methyl salicylate (hydrolysis and acetylation)
3. 1,3,5-Tribromobenzene from aniline (bromination, diazotization and
4. hydrolysis)
5. *p*-Nitroaniline from acetanilide (nitration and hydrolysis)
6. Benzilic acid from benzoin (rearrangement)
7. *p*-Aminobenzoic acid from p-nitrotoluene (oxidation and reduction)
8. Benzanilide from benzophenone (rearrangement)
9. *p*-Bromoaniline from acetanilide (bromination and hydrolysis)
10. *m*-Nitroaniline from nitrobenzene (nitration and reduction)
11. 1,2,4-Triacetoxy benzene from hydroquinone (oxidation and acylation)

REFERENCE

1. J. Mohan, Organic Analytical Chemistry, Theory and Practice; Narosa, 2003.
2. V. K. Ahluwalia, P. Bhagat and R. Agarwal, Laboratory Techniques in Organic Chemistry; I. K. International, 2005.
3. N. S. Gnanaprakasam and G. Ramamurthy, Organic Chemistry Lab Manual; S. V. Printers, 1987.
4. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford and P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry; 5th Ed., Prentice Hall, 1989.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - II CORE COURSE – IX (CORE PRATICAL - IV)

INORGANIC CHEMISTRY II (P)

OBJECTIVES

1. To carry out the titrimetric and gravimetric analyses.

2. To perform the preparation of compounds.

1. Titrimetry and Gravimetry

A mixture of solution(s) should be given for estimation

Cu (V) and Ni (G)

Cu (V) and Zn (G)

Fe (V) and Zn (G)

Fe (V) and Ni (G)

Zn (C) and Cu (G)

Cu (V) and SO_4^{2-}(G)

2. Preparation of complexes

1. Tris(thiourea)copper(I) chloride
2. Tetraamminecopper(II) sulphate

3. Potassium trioxalatoferrate
4. Potassium trioxalatoaluminate(III)
5. Potassium trioxalatochromate(III)
6. Tris(thiourea)copper(I) sulphate

REFERENCE

1. A. I. Vogel, Text Book of Quantitative Inorganic Analysis; 6th Ed., Longman, New Delhi, 2000.

FACULTY UNIVERSITY NOMINEE HOD

SEMESTER - III CORE COURSE – X

ORGANIC CHEMISTRY - II

UNIT I NUCLEOPHILIC SUBSTITUTION REACTIONS

1.1 Aliphatic nucleophilic substitution – mechanisms – S_N1, S_N2, S_Ni– ion-pair in S_N1 mechanisms – neighbouring group participation - substitutions at allylic and vinylic carbons.

1.2 Correlation of structure with reactivity - solvent effects.

1.3 Rearrangements involving carbocations– Wagner-Meerwein and dienone-phenolrearrangements.

1.4 Aromatic nucleophilic substitutions – S_N1, S_NAr, Benzyne mechanism –reactivity orientation –Ullmann, Sandmeyer and Chichibabin reaction –rearrangements involving nucleophilic substitution – Stevens – Sommelet-Hauser and von-Richter rearrangements.

UNIT II ELECTROPHILIC SUBSTITUTION REACTIONS

2.1 Aromatic electrophilic substitution reaction – orientation, reactivity andmechanisms based on transition state theory with suitable reactions – 2.2 substitutions in thiophene and pyridine – N-oxide – quantitative treatment ofthe structural effects on reactivity.

2.3 Substituent effects – origin of Hammett equation – principles of Hammettcorrelation – effect of structure on reaction mechanisms - Hammett parameters –σ and ρ, modified forms of Hammett equation, Taft Equation.

2.4 Aliphatic electrophilic substitution – S_E2, S_Ei and S_E1 mechanisms – diazoniumcoupling reactions – metals as electrophile in substitution reactions anddecomposition of diazonium salts.

UNIT III ADDITION AND ELIMINATION REACTIONS

3.1 Addition to carbon-carbon multiple bonds – electrophilic, nucleophilic and freeradical additions – orientation of the addition –stereochemical factorsinfluencing the addition of bromine and hydrogen bromide, hydroxylation – hydroboration leading to formation of alcohols.

3.2 Addition to carbonyl and conjugated carbonyl systems – mechanism – Grignardreagents – 1,2- and 1,4-additions (dimethylcuprate) – addition tocarbon-oxygen double bond – Benzoin, Knoevenagel, Stobbe, Darzensglycidicester condensation and Reformatsky reactions.

3.3 Elimination reactions – mechanisms; E1, E2, E1cB – stereochemistry ofelimination, Hofmann and Saytzeff rules – competition between eliminationand substitution –pyrolytic*cis*-elimination, Chugaev reaction – examples suchas dehydration, dehydrohalogenation, Cope elimination–Bredt's rule with examples.

UNIT IV PERICYCLIC REACTIONS

4.1 Concerted reactions –stereochemistry – orbital symmetry and concerted symmetry and correlation diagram. Frontiermolecular orbital approach – Woodwardand Hoffmann rules - electrocyclic reactions - cycloaddition reactions.

4.2 Sigmatropic rearrangements – selection rules and examples with simple molecules - 1,3and 1,5 -hydrogen shifts - Cope and Claisen rearrangements.

UNIT V NATURAL PRODUCTS

5.1 Terpenes: Structural elucidation, medicinal values and synthesis of α – pinene, camphor and zingiberene.

5.2 Alkaloids: Structural elucidation, medicinal values and synthesis of quinine, reserpine, morphine – Cinchonine and papaverine (Wilkinson systhesis).

5.3 Vitamins: Physiological importance – structural elucidation of vitamins B_6, E (E_1 - ∞ Tocopherol) and K (K_1 - Phyloquinone).

REFERENCE

1. S. H. Pine and J. B. Hendrickson, D. J. Cram and G. S. Hammond, Organic Chemistry; 5th Ed., McGraw Hill, Noida, 1987.

2. T. H. E. Lowry and K. S. Richardson, Mechanism and Theory in OrganicChemistry; 3rd Ed., Benjamin-Cummings Publishing, USA, 1997.

3. J. March and M. B. Smith, Advanced Organic Chemistry: Reactions, Mechanismsand Structure, 6th Ed., Wiley, New York, 2007.

4. R. K. Bansal, Reaction Mechanism in Organic Chemistry; Tata McGraw Hill, Noida,1990.

5. F. A. Carey, and R. J. Sundberg, Advanced Organic Chemistry, Parts A and B, 5thEd., Springer, Germany, 2007.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - III **CORE COURSE – XI**

INORGANIC CHEMISTRY – III

UNIT I ELECTRONIC SPECTROSCOPY

1.1 Microstates and Term symbols for transition metal ions - Possible Term symbols for p^2 and d^2.

1.2 Hund's rule - RS and j j coupling - Selection rules - orgel diagrams for d^n, oh and Td systems. Tanabe -sugano diagram calculation of β and 10 Dq - factors affecting 10 Dq - charge transfer spectra.

UNIT II IR AND RAMAN SPECTROSCOPY

2.1 Combined use of IR and Raman spectroscopy in the structural elucidation of simple molecules like H_20, ClF_3, NO_3, ClO_3. Effect of coordination of ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cynide, thiocyanate, nitrate, sulphate and dimethylsulphoxide.

2.2 Effect of isotopic substitution on the Vibrationalspectra of molecules - Vibrational spectra of metal carbonyls with references to the nature of bonding geometry and number of C-O stretching vibrations (Group theoretical treatment).

UNIT III NMR SPECTROSCOPY

3.1 Chemical shift and coupling constants (spin – spin coupling involving different nuclei ^{1}H, ^{31}P, ^{13}C) interpretation and application to inorganic compounds. Effects of quadrupolar nuclei (^{1}H, ^{10}B, ^{11}B) on the ^{1}H NMR spectrum.

3.2 NMR paramagnetic molecules - isotopic shifts , contact and pseudo contact interactions. Lanthanide shift reagents, Stereochemistry of non-rigid molecules. Satellite spectra - Applications of ^{1}H, ^{31}P, ^{13}C NMR of inorganic molecules.

UNIT IV

4.1 Basic principles - "g" values and its types - factors affecting "g" values - Hyperfine spiliting - Applications of ESR to Free radicals and Inorganic molecules.

4.2 Magnetic properties - Dia, para, ferro and Antiferro magnetisms - first order and second order, Zeeman effect – Temperature independent paramagnetism

UNIT V X-RAY CRYSTALLOGRAPHY

5.1 Solid state: difference between point group and space group - screw axis - glid planes . Crystal symmetry elements - crystal classes - crystal systems - unit cell - bravis lattices, asymmetric unit space group - equivalent positions - relations between molecular symmetry and crystallographic symmetry - basic concepts. The concept of reciprocal lattice and its applications - X ray diffraction by single crystal - structure factor - systematic absences - determination of space group - heavy atom method.

5.2 Neutron diffraction - elementarytreatment - comparison of x ray diffraction, electron diffraction - basic principles.

REFERENCE

1. B.N Figgis "introduction to ligand fields" wiley eastern, new delhi, (Units I,II,III and IV)
2. James E. Huheey, Ellen A. Keiter and richard L. Keiter , "inorganic chemistry" 4th edition Addison, wesly (Unit I)
3. R.S Drago "Physical methods in inorganic chemistry " (Unit -II)
4. A.F.A Kettle, "Coordination compounds " ELS (Unit – I,II,III, and IV)
5. E.A.V ebsworth, David W.H Rankin, Stepehn Cradock "Structural methods in inorganic chemistry"ELBS 1988 (Unit I,II,III and IV)
6. D.F Shriver, P.W Atkins and C.H Lanford "Inorganic chemistry" 2nd edition.
7. LenoidV.Azaroff, Elements of X-ray crystallography McGraw – Hill Co, New york (Unit - III)
8. Antony R.West "Solid state chemistry and its application "John wiley, New york (Unit - III)
9. P.J Wealthy "The determination of molecular sstrucutre"
10. A.B.P Lever "Inorganic electronic spectroscopy" @ndedition . Elsevier, London 1984 (Unit - I)
11. Nakamoto "Infra red spectra of coordination compounds".

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - III **CORE COURSE – XII (CORE PRATICAL - V)**

PHYSICAL CHEMISTRY I (P)

OBJECTIVES

To perform the various techniques of physical chemistry experiments.

Any ten experiments (to be decided by the course teacher) out of the following

experiments.

1. Kinetics-acid hydrolysis of ester–comparison of strengths of acids.
2. Kinetics-acid hydrolysis of ester–determination of energy of activation (Ea).
3. Kinetics-saponification of ester–determination of ethyl acetate by conductometry.
4. Kinetics-persulfate-iodine reaction –determination of order, effective of ionic strength on rate constant.
5. Determination of molecular weight of substance by transition temperature method.
6. Determination of molecular weight of substances by Rast method.

7. Determination of Critical Solution Temperature (CST) of phenol-water system and effect of impurity on CST.
8. Study of phase diagram of two components forming a simple eutectic.
9. Study of phase diagram of two compounds forming a compound.
10. Study of phase diagram of three components system.
11. Determination of molecular weight of substances by cryoscopy.
12. Determination of integral and differential heat of solutions by colorimetry.
13. Polymerization-rate of polymerization of acrylamide.
14. Distribution law – study of Iodine-Iodine equilibrium.
15. Distribution law – study of association of benzoic acid in benzene.
16. Adsorption – oxalic acid/acetic acid on charcoal using Freundlich isotherm.

REFERENCE

1. B. P. Levitt, Findlay's Practical Physical Chemistry; 9th Ed., Longman, 1985.
2. J. N. Gurtu and R. Kapoor, Advanced Experimental Chemistry; Vol. 1-Physical, S. Chand and Co., New Delhi, 1987.

FACULTY UNIVERSITY NOMINEE HOD

SEMESTER - III ELECTIVE COURSE – II

POLYMERCHEMISTRY

UNIT I CLASSIFICATION AND MOLECULAR WEIGHT DETERMINATION

1.1 Basic concepts of polymer science-molecular forces and chemical bonding in polymers-classification of polymers-addition polymers, condensation polymers, biopolymers – polymer synthesis-polymerization techniques.

1.2 Molar mass and size ofpolymers, Number average and weight average molecular weight-methods of molecular weight determination - Osmometry, Viscosity,Light scattering,sedimentation, Ultracentrifuge -Molecular weight distribution curve.

UNIT II SYNTHESIS AND KINETICS

2.1 Kinetics of polymerization-free radical chain polymerization,cationic polymerization, anionic polymerization, copolymerization.

2.2 Degree of polymerization,Chain length,chain transfer,chain termination, stereo regular polymerization,Zeigler Natta Catalysts.

UNIT III CHARACTERIZATION

3.1 Crystalline nature-x-ray diffraction-Study of polymers,degree of crystallinity,Differential scanning calorimetry, Thermogravimetric analysis of polymers.Glass transition temperature-Factors affecting glass transitiontemperature, the properties associated with glass transition temperature andcrystallinity andmelting point-Relation to structure.

UNIT IV CHEMICAL REACTIONS

4.1 Hydrolysis,Acidolysis, Hydrogenation,Addition and Substitution reactions-Cyclization,Cross Linking-Vulcanization, Graft and Block Copolymers.

4.2 Types of Degradation-Thermal,Mechanical,Oxidative, Hydrolyticand photo degradation

UNIT V PHYSICAL PROPERTIES AND APPLICATIONS

5.1 Mechanical- Stress- strain measurements; Electrical- Conducting polymers-Polyacetylene,polyaniline. Industry important polymers-Natural and synthetic rubber,polyesters,polytetrafluoroethylene (PTFE),polystyrene,lon ExchangeResins, Nafion, Polyacylonitrile – Carbon fibres, Polyvinyl chloride and polyacrylates.

REFERENCE

1. V.R Gowariker et al , Science Wiley Eastern , 1986.
2. K.J Sounders, Organic Ploymer Chemistry, Chapman and hall, 1976.
3. Raymond, B. Seymour, PloymerChemistry - An Introduction , Marcel Dekker Inc NY 1981.
4. Fred W Billmayer Jr. Text book of polymer science, Hohh Wiley And Sons 3rd Ed 1981.
5. K.Gupta Fundamentals of polymer science and engineering, Tata McGraw Hill 1981.
6. Stepak, Ploymer characterization of processing technology, Academic Press London.
7. Stone, Inorganic polymers, Academic Press , New York.
8. B.K Sharma , polymer chemistry, Krishna PrakashanMandir, Meerut.

FACULTY UNIVERSITY NOMINEE HOD

SEMESTER - III ELECTIVE COURSE – III

GREEN AND ENVIRONMENTAL CHEMISTRY

UNIT I INTRODUCTION TO GREEN CHEMISTRY

1.1 Green chemistry - relevance and goals, Anastastwelve principles of green chemistry - tools of green chemistry - Alternative starting materials, reagents, catalyst, solvents and process with suitable examples.

1.2 Microwave mediated organic synthesis (MAOS),Explosive - Specific effects of microwave - Heatreaction - Solid support reactions.

1.3 Typical reactions - Hydrolysis, Saponification, Acetolysis - Principle, Instrumentation and advantages.

UNIT II IONIC LIQUID AND PTC

2.1 Introduction - Synthesis of ionic liquids - Physical properties - application in alkylation, Diels – alder reactions - Phase transfer catalyst - Synthesis - Applications.

2.2 Support catalysts and Biocatalysts for green chemistry - Introduction - the concept of atom economy - supported metal catalyst, meson porous silica - the use of bio Catalysts for green chemistry, alternative synthesis reagents and reaction conditions.

2.3 A Photochemical alternative to Friedel - Craftsreactions - Dimethyl Carbonate as a ethylating agent - the design and applications of green super critical carbon dioxide for synthetic chemistry.

UNIT III RETERO SYNTHESIS

3.1 Disconnection approach -Synthon - Synthetic Equivalent - C-X - C-C disconnections. FGI - Diels alder reactions ,Wurtz connection, Michael reaction, Protecting Groups, C-OH, C-NH_2, C-COOH.

UNIT IV WATER AND AIR POLLUTION

4.1 Water - properties of water, water cycle, water pollution - sources of water pollution - impact of Gulf War, Earth Summit - Water sharing Disputes.

4.2 Air - Climate change, Global warming, Greenhouse effect, Hazardous solid waste - Sources, Transport, Disposal, hospital wastes.

4.3 Alternative fuels - Hydrogen, Bio Diesel, Indoor air pollution, Acid Rain, Smog, Deforestation, Desertification, Bio-diversity Loss and their effects.

UNIT V INDUSTRIAL WASTE AND TREATMENT PROCESS

5.1 Introduction - the problems of substances and the chemical industry - characteristics of industrial wastes - types of industrial wastes - solid industrial wastes - principles of industrial waste.

5.2 Treatment - Protection of biosphere - Basic trends in Biosphere protection for industrial wastes - treatment of wastes (or) Effluents with organic impurities - treatment of wastes (or) Effluents with inorganic impurities. Effluents of industrial units and their purification - the treatment of some industrial effluents - Stationary chemicals analysis of industrial effluents (or) sewage - the nature and treatment of some important chemical wastes - methods of treating industrial sludge.

REFERENCE

1. Green chemistry - Environmental benign reactions - V.K Ahiuwalia, Ane Books India (Publisher) (2006)
2. Green chemistry - Designing chemistry for the environment - edited by Paul T. Anastas& Tracy c.Williamson, Second Edition (1998)
3. Green chemistry - Frontiers in bengin chemical synthesis and process - edited by Paul T.Anastas& Tracy C. Williamson, Oxford Universitry Press (1998)
4. Green Chemistry - Environment friendly alternatives, Edited by RashmiSangi& M.M Srivastava , Narora Publishing House , (2003)

5. Industrial Chemistry (including chemical engineering) - B. K Sharma 10th edition.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - IV **CORE COURSE – XIII**

PHYSICAL CHEMISTRY - II

UNIT I QUANTUM CHEMISTRY - II & GROUP THEORY

1.1 Application of Wave mechanics, the rigid rotator, harmonic oscillator-Hydrogen atom solution -shapes and nodal properties of orbitals-Space quantization-electron spin-Many electron atoms-one electron orbital-Pauli principle- derminental form of wave function ,Helium atom and effective nuclear charge-Approximation method-

Variationmethods, application to Hydrogen and Helium atoms-Perturbation method for nondegenerate systems.

1.2 Angular momentum in many electron systems-Spin orbit interaction L-Sand j-j coupling schemes.

1.3 Atomic Structure calculation –Self consistent method for atoms-Hartree and HartreeFock method for atoms.

1.4 Vibrational spectra- symmetry properties of normal molecules-Symmetry co-ordinates-Selection-rules for fundamental Vibrational transition- IR and Raman activity of fundamentals in CO_2,H_2O,N_2F_2-The rule of mutual exclusion and Fermi resonance.

UNIT II ELECTROCHEMISTRY - I

2.1 Electrolytic conductance, Debye –Huckel –Onsager theory - Debye Falkenhagen and Wien effect. Electrode – Electrolyte equilibrium, Electrode Potential - concentration cells - liquid junction potentials.

2.2 Process at electrode - The rate of charge transfer - Current density - Butler -Volmer equation - Tafel equation - Electrical double layer potential - theory of multiple layers at electrode - electrolyte interfaces - Double layer capacity - Electro kinetic phenomena , Applications : Fuel cells and power storage like rechargeable batteries (Lead acid, Ni-Cd and Li -ion)

UNIT III ELECTROCHEMISTRY – II

3.1 Principles and applications of Polarography - instrumentation, Types of cells, Advantages of dropping mercury electrode, interpretation of current voltage curves, tests for reversibility, determination of n values (usefulness of illkovic equation), Polarographic maxima, current time curves.

3.2 Modern developments, Oscillographic polarography, AC polarography, Cyclic voltammetry, Advantages over Polarographic techniques - test of reversibility of electron transfer reactions - Chronopotentiometry - apparatus used, advantages over polarography - controlled potential coulometry.

UNIT IV SURFACE CHEMISTRY AND CHEMICAL KINETICS - II

4.1 Surface phenomena – Gibbs adsorption isotherm – solid-liquid interfaces –

contact angle and wetting – solid-gas interface – physisorption and chemisorption – Langmuir, BET isotherms – surface area determination. Kinetics of surface reactions involving adsorbed species – Langmuir- Hinshelwood mechanism, Langmuir-Rideal mechanism – Rideal-Eley mechanism – some interfacial aspects on micelles, reverse micelles, microemulsions and membranes.

4.2 Application of ARRT to solution kinetics – effect of solvent and ionic strength, influence of pressure on rates in solution – enzyme catalysis – mechanism of single substrate reactions – Michaelis-Menten law – acidity functions – kinetics of processes in micellar and reverse micellar systems.

UNIT V MOLECULAR THERMODYNAMICS - II

5.1 Third law – thermodynamics – significance – Nernst heat theorem and other forms of stating the third law – thermodynamic quantities at absolute zero – apparent exceptions to the third law.

5.2 Thermodynamics of systems of variable composition – partial molar properties –chemical potential – relationship between partial molar quantities – Gibbs- Duhem equation and its applications (the experimental determination of partial molar properties not included).

5.3 Thermodynamic properties of real gases – fugacity concept – calculation of fugacity of real gas – activity and activity coefficient – concept – definition – standard states and experimental determinations of activity and activity coefficient of electrolytes.

REFERENCE

1. A. K. Chandra, Introductory Quantum Chemistry; 4th Ed., Tata McGraw Hill, Noida, 1994.
2. D. A. Mcquarrie, Quantum Chemistry; University Science Books, Herndon, 2008.
3. J. P. Lowe, and K. A. Peterson, Quantum Chemistry; 3rd Ed., Academic Press, Cambridge, 2005.
4. I. N. Levine, Quantum Chemistry; 7th Ed., Prentice Hall, New Jersey, 2013.
5. R. K. Prasad, Quantum Chemistry; 4th Ed., New Age International Publishers, New Delhi, 2014.
6. F. A. Cotton, Chemical Applications of Group Theory; 3rd Ed., Wiley Eastern, New Delhi, 1990.
7. P. Atkins and J. de Paula, Physical Chemistry; 9th Ed., W. H. Freeman Publications, New York, 2009.
8. S. Glasstone, Introduction to Electrochemistry; Maurice Press, Philadelphia, 2008.
9. L. Antropov, Theoretical Electrochemistry; University Press of the Pacific, USA, 2001.
10. S. Glasstone, An Introduction to Electrochemistry; Read Books, New Delhi, 2007.
11. J. O' M Bockris and A. K. N. Reddy, Modern Electrochemistry; Vol. 1 and 2, 2nd Ed., Plenum Press, New York, 1998.
12. R. G. Compton, Electrode Kinetics: Reactions; Elsevier Science Press, Chennai,1987.
13. G. W. Castellan, Physical Chemistry; Narosa, New Delhi, 1986.
14. K. J. Laidler, Chemical Kinetics; 3rd Ed., Prentice Hall, New Jersey, 1987.
15. J. W. Moore and R. G. Pearson, Kinetics and Mechanism; 3rd Ed., John Wiley and Sons, New York, 1981.

16. M. Mortimer and P. G. Taylor, Chemical Kinetics and Mechanism; 1st Ed., Royal Society of Chemistry, UK, 2002.
17. I. Amdur and G. G. Hammes, Chemical Kinetics Principles and Selected Topics; 3rd Ed., McGraw Hill, New York, 2008.
18. M. Gratzel and K. Kalyanasundaram, Kinetics and Catalysis in Microheterogeneous Systems; Academic Press, New York, 1991.
19. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry - Classical, Statistical and Irreversible; Pearson Education, New Delhi, 2013.
20. R. K. Dave, Chemical Kinetics; Campus Books, 2000.
21. S. Glasstone, Thermodynamics for Chemists; 3rd Ed., Narahari Press, Bangalore, 2007.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - IV **CORE COURSE – XIV (CORE PRATICAL - VI)**

PHYSICAL CHEMISTRY - II (P)

OBJECTIVES

To perform the various electrical experiments.

Any ten experiments (to be decided by the course teacher) out of the following

experiments.

1. Conductometry– acid-alkali titrations.
2. Conductometry– precipitation titrations.
3. Conductometry– displacement titrations.
4. Conductometry– determination of dissociation constant of weak acids.
5. Conductometry– solubility product of sparingly soluble silver salts.
6. Verification of Onsager equation - conductivity method.
7. Determination of degree of hydrolysis and hydrolysis constant of a substance.
8. Potentiometric titrations – acid alkali titrations.
9. Potentiometric titrations – precipitation titrations.
10. Potentiometric titrations – redox titrations.
11. Potentiometry– determination of dissociation constant of weak acids.
12. Potentiometry– determination of solubility of silver salts.
13. Potentiometry– determination of activity and activity coefficient of ions.
14. pH Titration of *ortho*-phosphoric acid.
15. To determine the relative strength of two acids by conductance measurements.
16. To determine the pH of a buffer solution using a quinhydrone electrode.

REFERENCE

1. J. B. Yadav, Advanced Practical Physical Chemistry; 20th Ed., GOEL Publishing House, Krishna Prakashan Media Ltd., Chennai, 2001.

2. B. P. Levitt, Findlay' s Practical Physical Chemistry; 9th Ed., Longman, London, 1985.

3. J. N. Gurtur and R. Kapoor, Advanced Experimental Chemistry; Vol. 1-Physical, S. Chand and Co. Ltd, New Delhi, 1997.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - IV **ELECTIVE COURSE – IV**

INDUSTRIAL CHEMISTRY

UNIT I

1.1 Basic idea about unit operation -Flowcharts - Chemical conversion - Batch versus continuous processing - Chemical process selection - design - chemical process control.

1.2 Chemical process economics - Marketevaluation - plantlocation - management for productivity and creativity - Research and development and its role in chemical industries.

UNIT II FUELS

2.1 Fossil fuels - classification and unique features - Coal, Petroleum, natural gas, Biofuels: Biomass - Biodiesel, Nuclear fuels; for various types of nuclear reactors. Hydrogen as fuel in the future, hydrogen storage materials. Fuel extinguisher, fire retardant materials - Fire retarding wood - procedures for handling toxic chemicals.

UNIT III OILS, FATS, WAXES AND SOAPS

3.1 Introduction - Distinction between oils and fats - properties and its classifications - animal fats and oils - difference between animal, Vegetable and mineral oils - isolation of essential oils and their uses - Saponification value, Ester value, Acid value, iodide value - Wijs method - Reichert meissel value - Consideration in soap making - manufacture of toilet and transparent soaps - oil to be used for soap - cleaning action of soap.

UNIT IV PULP AND PAPER

4.1 Introduction - manufacture of pulp - Sulphite (or)Kraft pulp - soda pulp - sulphate pulp - Reg pulp - beating , refining , filling, sizing and colouring - Manufacture of paper – Calendaring - uses - Ecological problems of Indian pulp and paper inducting.

UNIT V PAINTS, PIGMENTS AND VARNISHES

5.1 Introduction - composition of pigments, white pigments - White lead , Zinc oxide, Lithophone, titanium dioxide. Blue pigments - Ultra marine blue , Cobalt blue, and iron blue. Red pigments - Red lead,. Green pigments - Chrome green, guignets green, reinmann's green. Block pigments - Yellow pigments - Toners - metallic powders as pigments. Paints - classification of paints - Distempers - Constituents of paints - manufacture of paints - setting of the paints -requirements of the good pains – emulsion paints - constituents of emulsion paints - advantages - chemical action of emulsion paints, Luminescent paints - Fire retardant paints - special application of paints.

5.2 Varnishes - Raw materials - manufacture of varnishes - Enamels (or) gloss finisher - Lacquers - solvents and thinners - oils.

REFERENCE

1. Chemical process industries - Norrish shreve, R. and Joseph A. Brink Jr. McGraw hill, industrial book company, London.
2. Production and properties of industrial chemicals - Brain A.C.S Reinhold - New York.
3. Petroleum products hand book, Guthrie V. McGraw hill, Tokyo.
4. Industrial chemistry (including chemical engineering) - B.K Sharma 10th edition.
5. Outines of chemical technology - For the 21stcenturay - M. GopalaRao and Matshall sitting 3rd edition.

FACULTY **UNIVERSITY NOMINEE** **HOD**

SEMESTER - IV **ELECTIVE COURSE – V**

(CHEMISTRY OF NANOSCIENCE AND NANOTECHNOLOGY)

UNIT I SYNTHETIC METHODS

1.1 Definition of nanodimensional materials – historical milestones – unique properties due to nanosize, quantum dots, classification of nanomaterials.

1.2 General methods of synthesis of nanomaterials – hydrothermal synthesis, solvothermal synthesis – microwave irradiation– sol-gel and precipitation technologies – combustion flame – chemical vapour condensation process – gas-phase condensation synthesis – reverse micelle synthesis – polymer-mediated synthesis – protein microtubule-mediated synthesis – synthesis of nanomaterials using microorganisms and other biological agents – sonochemical synthesis – hydrodynamic cavitation.

1.3 Inorganic nanomaterials – typical examples – nano TiO2/ZnO/CdO/CdS, organic nanomaterials – examples – rotaxanes and catenanes

UNIT II CHARACTERISATION OF NANOSCALE MATERIALS

2.1 Principles of Atomic Force Microscopy (AFM) – Transmission Electron Microscopy(TEM).

2.2 Resolution and Scanning Transmission Electron Microscopy (STEM) – Scanning Tunneling Microscopy (STM) – Scanning Nearfield Optical Microscopy (SNOM).

2.3 Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.

UNIT III REACTIONS IN NANOPARTICLES

3.1 Reactions in nanospace – nanoconfinement – nanocapsules

3.2 Cavitands, cucurbiturils, zeolites, M.O.Fs, porous silicon, nanocatalysis, Rotaxanes and catenanes

UNIT IV CARBON CLUSTERS AND NANOSTRUCTURES

4.1 Nature of carbon bond − new carbon structures − carbon clusters – discovery of C60−alkali doped C60−superconductivity in C60−larger and smaller fullerenes.

4.2 Carbon nanotubes – synthesis − single walled carbon nanotubes − structure and characterization − mechanism of formation − chemically modified carbon nanotubes − doping − functionalizing nanotubes − applications of carbon nanotubes.

4.3 Nanowires −synthetic strategies − gas phase and solution phase growth – growth control − properties.

UNIT V NANO TECHNOLOGY AND NANODEVICES

5.1 Application of nanotechnology - agriculture, medicine, sensors, solar energy, fuel cells, food industry, nuclear power plant and - environmental pollution.

5.2 Protein nano array, nanopipettes, molecular diodes, self assemblednano transistors, nanoparticle mediated transfection.

5.3 Protein nanoarray, nanopipettes, molecular diodes, self-assembled nanotransistors, nanoparticle mediated transfection.

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5. H. Fujita (Ed.), Micromachines as Tools in Nanotechnology; Springer-Verlag, Berlin, 2003.
6. BengtNolting, Methods in Modern Biophysics; 3rd Ed., Springer-Verlarg, Berlin, 2009.
7. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties, Elsevier, Chennai, 2000.
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9. T. Tang and P. Sheng (Eds), Nanoscience and Technology, Novel Structures and Phenomena; Taylor andFrancis, New York, 2003.
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12. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/
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