BHARATHIDASAN UNIVERSITY **TIRUCHIRAPPALLI – 620 024**

M.Sc. Chemistry **Course Structure under CBCS**

(For the candidates admitted from the academic year 2016-2017 onwards)

Semester	Course	Title	Instruction Hours/ Week	Credit	Exam Hours	Marks Internal	Marks External	Total
I	Core Course – I (CC)	Organic Chemistry –I	6	5	3	25	75	100
	Core Course – II (CC)	Inorganic Chemistry –I	6	5	3	25	75	100
	Core Course – III (CC)	Physical Chemistry –I	6	5	3	25	75	100
	Core Practical – I (CP)	Organic Chemistry Practical –I	6	3	6	40	60	100
	Core Practical – II (CP)	Inorganic Chemistry Practical –I	6	3	6	40	60	100
		TOTAL	**30**	**21**				**500**
II	Core Course – IV (CC)	Inorganic Chemistry –II	6	5	3	25	75	100
	Core Course – V (CC)	Physical Methods in Chemistry –I	6	5	3	25	75	100
	Core Practical – III (CP)	Organic Chemistry Practical – II	6	3	6	40	60	100
	Core Practical – IV (CP)	Inorganic Chemistry Practical –II	6	3	6	40	60	100
	Elective Course – IA (EC) / Elective Course – IB (EC)	(A) Solid State Chemistry / (B) Supramolecular Chemistry	6	5	3	25	75	100
		TOTAL	**30**	**21**				**500**
III	Core Course – VI (CC)	Organic Chemistry – II	6	5	3	25	75	100
	Core Course – VII (CC)	Physical Chemistry – II	6	6	3	25	75	100
	Core Practical – V (CP)	Physical Chemistry Practical – I	6	3	6	40	60	100
	Elective Course – IIA (EC) / Elective Course – IIB (EC)	(A) Pharmaceutical Chemistry / (B) Bio-organic Chemistry	6	5	3	25	75	100
	Elective Course – III (EC)	Analytical Chemistry	6	5	3	25	75	100
		TOTAL	**30**	**24**				**500**
IV	Core Course – VIII (CC)	Physical Methods in Chemistry – II	6	5	3	25	75	100
	Core Practical – VI (CP)	Physical Chemistry Practical – II	6	3	6	40	60	100
	Elective Course – IVA (EC) / Elective Course – IVB (EC)	(A) Green Chemistry / (B) Industrial Chemistry	6	5	3	25	75	100
	Elective Course – VA (EC) / Elective Course – VB (EC)	(A) Selected Topics in Chemistry/(B) Chemistry of Nanoscience and Nanotechnology	6	5	3	25	75	100
	Project	Dissertation = 80 Marks Viva = 20 Marks	6	6	-	-	-	100
		TOTAL	**30**	**24**				**500**
		GRAND TOTAL	**120**	**90**				**2000**

Project	:100 Marks	
(Dissertation	: 80 Marks	
Viva Voice	: 20 Marks)	

Note:

Core Papers	-	8
Core Practical	-	6
Elective Papers	-	5
Project	-	1

Note:

1. Theory	Internal	25 marks	External	75 marks
2. Practical	Internal	40 marks	External	60 marks

Note:

1. Theory	Internal	25 marks	External	75 marks
2. Practical	”	40 marks	”	60 marks

3. Separate passing minimum is prescribed for Internal and External
   a) The passing minimum for CIA shall be 40% out of 25 marks (i.e. 10 marks)
   b) The passing minimum for University Examinations shall be 40% out of 75 marks (i.e. 30 marks)
   c) The passing minimum not less than 50% in the aggregate.

SEMESTER-I **HOURS/WEEK: 6**
CORE COURSE-I (CC-I) **CREDITS: 5**

ORGANIC CHEMISTRY I

OBJECTIVES

1. To understand the basic concepts of aromaticity.
2. To learn the oxidation and reducing reagents for organic synthesis.
3. To learn stereochemistry of organic compounds.
4. To know the effect of light in organic reactions.
5. To study the concerted pericyclic reactions.

UNIT I: Aromaticity

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

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), Mobius aromaticity.

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.

UNIT II: Reagents in Organic Synthesis

Oxidation: Baeyer-Villiger, Jacobsen epoxidation, Shi epoxidation, Jones reagent, PCC, PDC, IBX, DMP, CAN, TPAP, NOCl, $Mn(OAc)_3$, $Cu(OAC)_2$, Bi_2O_3, Swern oxidation, Sommelet reaction, Elbs reaction, Oxidative coupling of phenols, Prevost reaction and Woodward modification.

Reduction: palladium / platinum / rhodium / nickel based heterogeneous catalysts for hydrogenation, Wilkinson's catalyst, Noyori asymmetric hydrogenation – reductions using Li/Na/Ca in liquid ammonia.

Hydride transfer reagents from group III and group IV in reductions. (i) triacetoxyborohydride, L-selectride, K-selectride, Luche reduction, Red-Al, $NaBH_4$ and $NaCNBH_3$, trialkylsilanes and trialkylstannane, (ii) stereo/enantioselectivity reductions (Chiral Boranes, Corey-Bakshi-Shibata).

UNIT III: Stereochemistry and Conformational Analysis

Stereoisomerism – symmetry – enantiomers and diastereomers – *R* and *S* nomenclature – optical activity and chirality – types of molecules exhibiting optical activity – absolute configuration – chirality in molecules with non-carbon stereocenters (N, S and P) – molecules with more than one chiral centre – atropisomerism.

Molecular chirality – allenes, spiranes, biphenyls, helicenes and cyclophanes – methods of determining configuration – *E* and *Z* nomenclature – determination of configuration of geometrical isomers – stereochemistry of addition and elimination reactions – stereospecific and stereoselective synthesis [elementary examples].

Basic concepts of conformational analysis – conformations of cyclopentane, cyclohexane, cyclohexene and fused (decalin) and bridged (norbornane type) ring systems – anomeric effect in cyclic compounds.

UNIT IV: Organic Photochemistry

Organic photochemistry – fundamental concepts – energy transfer – characteristics of photoreactions – photoreduction and photooxidation, photosensitization.

Photoreactions of ketones and enones – Norrish Type I and II reactions – Paterno-Büchi reaction – photo-Fries rearrangement – photochemistry of alkenes, dienes and aromatic compounds – di-π-methane rearrangement.

Reactions of unactivated centres – photochemistry of α,β-unsaturated carbonyl compounds – photolytic cycloadditions and photolytic rearrangements – photo additions – Barton reaction.

UNIT V: Pericyclic Reactions

Concerted reactions – orbital symmetry and concerted symmetry – Woodward and Hoffmann rules – selection rules for electrocyclic reactions – frontier molecular orbital approach – correlation diagram – examples.

Selection rules for cycloaddition reactions – frontier molecular orbital approach – correlation diagram – examples – chelotropic and ene reactions.

Sigmatropic rearrangements – 1,3, 1,5 and 1,7-hydrogen shifts – examples – Cope and Claisen rearrangements – 1,3-dipolar cycloaddition reactions: types of dipoles, selectivity, scope and applications.

REFERENCES

UNIT I and II

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. T. H. E. Lowry and K. S. Richardson, Mechanism and Theory in Organic Chemistry; Addison-Wesley, USA, 1998.

UNIT III

7. P. S. Kalsi, Stereochemistry; Wiley eastern limited; New Delhi, 1993.
8. D. Nasipuri, Stereochemistry of Organic Compounds - Principles and Applications; 2nd Ed., New Age International, New Delhi, 1994.
9. E. L. Eliel, and S. H. Wilen, Stereochemistry of Organic Compounds; John Wiley, New York, 1994.
10. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry; 1st Ed., Oxford University Press, UK, 2000.

UNIT IV and V

11. J. D. Coyle, Organic Photochemistry; Wiley, New York, 1998.
12. J. M. Coxon, and B. Halton, Organic Photochemistry; 2nd Ed., Cambridge, University Press, UK, 1987.
13. G. R. Chatwal, Organic Phtochemistry; 1st Ed., Himalaya Publications house, Bangalore, 1998.
14. S. Sankararaman, Pericyclic Reactions - A Textbook: Reactions, Applications and Theory; Wiley-VCH, New York, 2005.

*****

SEMESTER-I **HOURS/WEEK: 6**
CORE COURSE-II (CC-II) **CREDITS: 5**

INORGANIC CHEMISTRY I

OBJECTIVES

1. To understand the basic concepts of main group elements.
2. To learn the theories and mechanism of reactions of metal complexes.
3. To study the concepts of photochemistry and its applications.

UNIT I: Main Group Chemistry

Chemistry of boron – borane, higher boranes, carboranes, borazines and boron nitrides – chemistry of silicon – silanes, higher silanes, multiple bonded systems, disilanes, silicon nitrides.

P-N compounds, cyclophosphazanes and cyclophosphazenes – S-N compounds – S_2N_2, S_4N_4, (SN)x, polythiazyl S_xN_4 compounds – S-N cations and anions, S-P compounds – molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10} – homocyclic inorganic systems – oxocarbon anion.

Ionic model – lattice energy – Born-Lande equation – Kapustinskii equation – high T_c superconductors – solid state reactions – tarnish reaction decomposition, solid-soild reaction and photographic process – factors affecting reaction rate.

UNIT II: Principles of Coordination Chemistry

Studies of coordination compounds in solution – detection of complex formation in solution – stability constants – stepwise and overall formation constants.

Simple methods (potentiometric, pH metric and photometric methods) of determining the formation constants.

Factors affecting stability – statistical and chelate effects – forced configurations.

UNIT III: Theories of Metal-Ligand Bond

Crystal field theory – splitting of d-orbitals under various geometries – factors affecting splitting – CFSE and evidences for CFSE (structural and thermodynamic effects).

Spectrochemical series – Jahn-Teller distortion – spectral and magnetic properties of complexes – site preferences.

Limitations of CFT – ligand field theory – MO theory – sigma- and pi-bonding in complexes – Nephelauxetic effect – the angular overlap model.

UNIT IV: Reaction Mechanism in Coordination Complexes

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 applications – electron transfer reactions – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes – application of electron transfer reactions in inorganic complexes – isomerisation and racemisation reactions of complexes.

Molecular rearrangements of four- and six-coordinate complexes – interconversion of stereoisomers – reactions of coordinated ligands – template effect and its applications for the synthesis of macrocyclic ligands – unique properties.

UNIT V: Inorganic Photochemistry

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

Unimolecular charge-transfer photochemistry of cobalt(III) complexes – mechanism of 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.

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

REFERENCES

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.

*****

SEMESTER-I **HOURS/WEEK: 6**
CORE COURSE-III (CC-III) **CREDITS: 5**

PHYSICAL CHEMISTRY I

OBJECTIVES

1. To understand the concepts of group theory and quantum chemistry.
2. To learn the chemical kinetics and statistical thermodynamics.
3. To study the theories of kinetics, photochemistry and radiation chemistry.

UNIT I: Concepts of Group Theory

Symmetry elements and operations – point groups – assignment of point groups to molecules – group postulates and types of groups – group multiplication tables, sub groups, similarity transformations – conjugate elements and classes.

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

The great orthogonality theorem – construction of character table – direct product – projection operators – symmetry of hybrid orbitals.

UNIT II: Quantum Chemistry - I

Inadequacy of classical mechanics – black body radiation – Planck's quantum concept – photoelectric effect – Bohr's theory of hydrogen atom – hydrogen spectra – wave-particle dualism – uncertainty principle – decline of old quantum theory.

Schrödinger equation – postulates of quantum mechanics – operator algebra: linear operator, Hermitian operators, eigenfunctions and eigenvalues, angular momentum operator – commutation relations and related theorems – orthogonality and normalization.

Applications of wave mechanics to simple systems – particle in a box, one and three dimensional, particle with finite potential barrier – the quantum mechanical tunneling.

UNIT III: Chemical Kinetics - I

Theories of reaction rate – absolute reaction rate theory (ARRT) – transmission coefficient, reaction coordinate – potential energy surfaces – kinetic isotope effect – Hinshelwood theory – Kassel, Rice and Ramsperger theory (KRRT) – Slater's treatment.

Principle of microscopic reversibility – steady-state approximation – chain reactions: thermal and photochemical reactions between hydrogen and halogens – explosions and hydrogen-oxygen reactions.

UNIT IV: Statistical Thermodynamics

Thermodynamic probability – probability theorems – relation between entropy and probability (Boltzmann-Planck equation), ensembles, phase space, Ergodic hypothesis, microstates and macrostates, Maxwell-Boltzmann distribution law – partition functions – translational, rotational, vibrational and electronic partition functions.

Relationship between partition functions and thermodynamic properties – calculation of equilibrium constants from partition functions – heat capacities of monatomic crystals – Einstein theory and Debye theory.

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

UNIT V: Fast Reaction Techniques, Photochemistry and Radiation Chemistry

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

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

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

REFERENCES

1. F. A. Cotton, Chemical Applications of Group Theory; 3rd Ed., John Wiley and 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; University Science 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.
9. J. W. Moore and R. G. Pearson, Kinetics and Mechanism; 3rd Ed., John Wiley and Sons, New York, 1981.
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., Pragathi Prakashan, 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 of Chemistry - Classical, Statistical and Irreversible; Pearson Education, New Delhi, 2013.
16. Horia Metiu, Physical Chemistry, Thermodynamics; Taylor and Francis, Singapore, 2006.
17. K. K. Rohatgi-Mukherjee, Fundamentals of Photochemistry; 3rd Ed., New Age International Pvt. Ltd., New Delhi, 2014.
18. J. W. T. Spinks and R. J. Woods, Introduction to Radiation Chemistry; 3rd Ed., John Wiley and Sons, New York, 1990.

*****

SEMESTER-I **HOURS/WEEK: 6**
CORE PRACTICAL-I (CP-I) **CREDITS: 3**

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) and purified (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. Benzophenone oxime 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)

REFERENCES

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.

*****

SEMESTER-I **HOURS/WEEK: 6**
CORE PRACTICAL–II (CP-II) **CREDITS: 3**

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

2. **Estimation** of copper, ferric, nickel, chromium and manganese ions using photoelectric colorimeter

REFERENCES

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.

*****

SEMESTER-II **HOURS/WEEK: 6**
CORE COURSE-IV (CC-IV) **CREDITS: 5**

INORGANIC CHEMISTRY II

OBJECTIVES

1. To understand the role of metal ions in biological process.
2. To learn the basic concepts of chemotherapy.
3. To learn the principle of catalysis and reaction mechanisms of organometallics.

UNIT I: General Principles of Bioinorganic Chemistry

Occurrence and availability of inorganic elements in biological systems – biomineralization – control and assembly of advanced materials in biology – nucleation and crystal growth – various biominerals – calcium phosphate – calcium carbonate – amorphous silica, iron biominerals – strontium and barium sulphate.

Function and transport of alkali and alkaline earth metal ions: characterization of K^+, Na^+, Ca^{2+} and Mg^{2+} – complexes of alkali and alkaline earth metal ions with macrocycles – ion channels – ion pumps, catalysis and regulation of bioenergetic processes by the alkaline earth metal ions – Mg^{2+} and Ca^{2+}.

Metals at the center of photosynthesis – primary processes in photosynthesis – photosystems I and II-light absorption (energy acquisition) – exciton transport (direct energy transfer) – charge separation and electron transport – manganese catalyzed oxidation of water to O_2.

UNIT II: Amines, Proteins and Enzymes

Cobalamines: reactions of the alkyl cobalamines – one electron reduction and oxidation – Co-C bond cleavage – coenzyme B_{12} – alkylation reactions of methylcobalamin.

Heme and non-heme proteins – haemoglobin and myoglobin – oxygen transport and storage – electron transfer and oxygen activation – cytochromes, ferredoxins and rubredoxin – model systems, mononuclear non-heme iron enzymes.

Copper containing proteins – classification and examples – electron transfer – oxygen transport-oxygenation – oxidases and reductases – cytochrome oxidase – superoxide dismutase (Cu, Zn) – nickel containing enzyme: urease.

UNIT III: Medicinal Bioinorganic Chemistry

Bioinorganic chemistry of quintessentially toxic metals – lead, cadmium, mercury, aluminium, chromium, copper and plutonium – detoxification by metal chelation – drugs that act by binding at the metal sites of metalloenzymes.

Chemotherapy – chemotherapy with compounds of certain non-essential elements – platinum complexes in cancer therapy – cisplatin and its mode of action – cytotoxic compounds of other metals.

Gold containing drugs as anti-rheumatic agents and their mode of action – lithium in psychopharmacological drugs – radiopharmaceuticals – technetium.

UNIT IV: Organometallics

The 18 electron rule – applications and limitations – isolobal concept and its usefulness – uses of typical organometallics such as metal alloys and organometallic hydrides in organic synthesis.

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

Classification based on captivity and polarity of M-C bond, organometallic compounds of lanthanides and actinides – fluxional organometallic compounds – organometallics in medicine, agriculture, horticulture and industry.

UNIT V: Reactions and Catalysis by Organometallics

Organometallic reactions – ligand association and dissociation – oxidative addition and reductive elimination – insertion reactions.

Reactions of coordinated ligands in organometallics – hydrogenation, hydroformylation, epoxidation, metathesis.

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

REFERENCES

1. J. E. Huheey, Inorganic Chemistry; 4th Ed., Harper and Row Publishers, Singapore, 2006.
2. K. F. Purcell and J. C. Kotz, Inorganic Chemistry; Thomson Learning, Boston, 1980.
3. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry; Panima Publishing Company, New Delhi, 1997.

4. W. Kaim and B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life; 2nd Ed., John Wiley and Sons, New York, USA, 2013.
5. G. L. Eichhorn, Inorganic Biochemistry; Volumes 1 and 2, 2nd Ed., Elsevier Scientific Publishing Company, New York, 1975.
6. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry; 6th Ed., John Wiley and Sons, New York, 1999.
7. R. C. Mehrotra and A. Singh, Organometallic Chemistry; 2nd Ed., New Age International Ltd. New Delhi, 2014.
8. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals; 3rd Ed., John Wiley and Sons, New York, 2001.
9. S. E. Kegley and A. R. Pinhas, Problems and Solutions in Organometallic Chemistry; 2nd Ed., University Science Books, Oxford University Press, 1986.
10. A. J. Pearson, Advances in Metal-Organic Chemistry, Vol. 1; Jai Press, Inc., Greenwich, 1989.
11. A. W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry; 1987, Oxford University Press, Chennai.
12. I. Haiduc and J. J. Zuckerman, Basic Organometallic Chemistry; Walter De Gruyter Inc, USA, 1985.
13. P. Powell, Principles of Organometallic Chemistry; 2nd Ed., Chapman and Hall, London, 1988.
14. B. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry; 3rd Ed., John Wiley and sons, New York, 1994.
15. 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.
16. 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.

*****

SEMESTER-II **HOURS/WEEK: 6**
CORE COURSE-V (CC-V) **CREDITS: 5**

PHYSICAL METHODS IN CHEMISTRY I

OBJECTIVES

1. To understand the principles of molecular spectroscopy.
2. To study UV, NMR and IR spectroscopy of organic compounds.
3. To learn the ESR, ORD and Mass spectroscopy of organic compounds.
4. To know the effect of X-ray, electron, neutron diffractions of compounds.

UNIT I: Principles of Molecular Spectroscopy

Interaction of electromagnetic radiation with molecular systems – time evolution of the systems under radiation – Einstein transition probability for induced absorption and spontaneous and stimulated emission – transition moment and oscillator strength.

Microwave spectroscopy – rotational spectra of diatomic molecules, rigid and non-rigid rotors – intensity of spectral lines – effects of isotopic substitution – microwave spectra of polyatomic molecules – linear and symmetric top molecules – 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.

Raman spectra – rotational Raman spectra of linear and symmetric top molecules – vibrational Raman spectra – rotational fine structure – electronic spectra of diatomic molecules – vibrational coarse structure – intensity of vibrational lines in electronic spectra – rotational fine structure – fortrat diagram.

UNIT II: Nuclear Magnetic Resonance Spectroscopy

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

Simplification of complex spectra – double resonance techniques, shifts reagents – chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOH, NH, NH_2) – an elementary treatment of NOE phenomenon.

^{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 – 2D techniques: ^{1}H–^{1}H COSY, ^{1}H–^{13}C HETCOSY – NOESY.

UNIT III: UV-Visible and IR Spectroscopy

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 – disubsitituted benzene derivatives – study of steric effect in aromaticity.

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

UNIT IV: ESR, ORD and Mass Techniques

ESR – basic principles – comparison between ESR and NMR spectra – hyperfine splitting – applications to organic free radicals.

Optical rotatory dispersion and circular dichroism – introduction to theory and terminology – cotton effect – ORD curves – axial haloketone rule and its applications – the octant rule – its applications – applications of ORD to determine absolute configuration of monocyclic ketones – comparison between ORD and CD – their interrelationships.

Mass Spectrometry – instrumentation – resolution – ESI, EI, CI and FAB methods – base peak, isotopic peaks, metastable peaks – importance of metastable peaks, parent peak, recognition of molecular ion peak – fragmentation – general rules – pattern of fragmentation for various classes of compounds, McLafferty rearrangement – nitrogen rule.

Application of UV, IR, NMR and mass spectroscopy – structural elucidation of organic compounds – (minimum 15 problems should be worked out).

UNIT V: X-Ray Diffraction

X-Ray diffraction by single crystal method – space groups – systematic absences in X-ray data and identification of lattice types, glide planes and screw axes – X-ray intensities – structure factor and its relation to intensity and electron density – phase problem – structure solution by heavy atom method and direct method – determination of absolute configuration of molecules – a brief account of Cambridge Structural Database (CSD) and Protein Data Bank (PDB).

Electron diffraction by gases – scattering intensity vs. scattering angle, Wierl equation – measurement techniques.

Neutron diffraction by crystals – magnetic scattering – measurement techniques – elucidation of structure of magnetically ordered unit cell.

REFERENCES

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 Organic Compounds; 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, PHI Learning, 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 International Publishers, New Delhi, 2004.
10. W. Clegg, Crystal Structure Determination; Oxford University press, UK, 1998.
11. G. H Stout and L. H. Jensen, X-ray Structure Determination: A Practical Guide; John Wiley and Sons, New York, 1992.
12. J. P. Glusker and K. N. Trueblood, Crystal Structure Analysis: A Primer; 3rd Ed., Oxford University Press, UK, 2010.
13. D. N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques; University Press, Hyderabad, 2001.
14. 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

*****

SEMESTER-II **HOURS/WEEK: 6**
CORE PRATICAL-III (CP-III) **CREDITS: 3**

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)

a. *p*-Bromoacetanilide from aniline (acetylation and bromination)
b. Acetylsalicylic acid from methyl salicylate (hydrolysis and acetylation)
c. 1,3,5-Tribromobenzene from aniline (bromination, diazotization and hydrolysis)
d. *p*-Nitroaniline from acetanilide (nitration and hydrolysis)
e. Benzilic acid from benzoin (rearrangement)
f. *p*-Aminobenzoic acid from p-nitrotoluene (oxidation and reduction)
g. Benzanilide from benzophenone (rearrangement)
h. *p*-Bromoaniline from acetanilide (bromination and hydrolysis)
i. *m*-Nitroaniline from nitrobenzene (nitration and reduction)
j. 1,2,4-Triacetoxy benzene from hydroquinone (oxidation and acylation)

REFERENCES

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.

*****

SEMESTER-II | **HOURS/WEEK: 6**
CORE PRATICAL-IV (CP-IV) | **CREDITS: 3**

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)

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. Hexamminecobalt(III) chloride

REFERENCES

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

*****

SEMESTER-II **HOURS/WEEK: 6**
ELECTIVE COURSE-IA (EC-IA) **CREDITS: 5**

(A) SOLID STATE CHEMISTRY

OBJECTIVES

1. To learn the crystal structures of few inorganic solids.
2. To study the chemistry of crystallization and vapour phase transport.
3. To learn the applications of magnetic materials.
4. To study the chemistry of organic solids.

UNIT I: Crystal Structure and Crystal Engineering of Organic Solids

Types of close packing – hcp and ccp – packing efficiency – SC, BCC, and FCC, radius ratio rule – applications – polyhedral description of solids – structure types: Na_2O, Cs_2O, rutile, perovskite (ABO_3), ReO_3, K_2NiF_4, spinels and antispinels.

Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis – polymorphism and pseudopolymorphism – supramolecular isomorphism, polymorphism and crystal engineering of pharmaceutical phases.

UNIT II: Metallo Organic Frameworks

M.O.Fs (Metallo Organic Frameworks) – organometallic systems – combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. Design of nanoporous solids.

Interligand hydrogen bonds in metal complexes – implications for drug design – crystal engineering of NLO and OLED materials.

UNIT III: Preparative Methods in Solid State Chemistry

Experimental procedure, coprecipitation as a precursor to solid state reaction, other precursor methods, kinetics of solid state reactions – crystallizations of solutions, melts, glasses and gels, solutions and gels: zeolite synthesis – precipitation from solution or melt: flux method, epitaxial growth of thin layers, verneuil flame fusion method.

Graphite intercalation compounds, transition metal dichalcogenide and other intercalation compounds, ion exchange reaction, synthesis of new metastable phases by 'Chimie Douce'.

Electrochemical reduction methods – preparation of thin films, chemical and electrochemical methods, physical methods – growth of single crystals, Czochralski method, Bridgman-Stockbarger methods – zone melting.

Vapour phase transport, hydrothermal methods, comparison of different methods – high pressure and hydrothermal methods and dry high pressure methods.

UNIT IV: Magnetic Materials and Optical Properties

Selected examples of magnetic materials and their properties – metals and alloys, transition metal oxides, spinels, garnets, ilmenite and perovskites.

Magnetoplumbites – applications – structure/property relations – transformer, information storage, magnetic bubble memory devices, permanent magnets.

Luminescence, Lasers and phosphors – definitions and general comments, configurational coordinate model, some phosphor materials, anti-Stokes phosphors – lasers – the ruby laser, Neodymium lasers

UNIT V: Organic Solid State Chemistry

Topochemical control of solid state organic reactions – intramolecular reactions – conformational effects – intermolecular reactions – molecular packing effects – photodimerization of 2-ethoxycinnamic acid (α form, β form, γ form) – photopolymerization of 2,5-distyrylpyrazine – photopolymerizations of diacetylenes.

Asymmetric syntheses – dimerization of anthracene – control of molecular packing arrangements.

Organic reactions within inorganic host structures – electrically conductive organic solids – organic metals, conjugated systems, doped polyacetylene, polyparaphenylene, polypyrrole – organic charge transfer complexes – new superconductors

REFERENCES

1. A. R. West, Solid State Chemistry and Its Applications; 2nd Ed., John Wiley and sons, New York, 2014 (Unit III – V).
2. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, 1995.
3. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, Amsterdam, 1989.
4. G. R. Desiraju, and T. Steiner, The Weak Hydrogen Bond in Structural Chemistry and Biology; Oxford University Press: Oxford, 2002.
5. G. A. Jeffrey, Introduction to Hydrogen Bonding; Oxford University Press, New York, 1997.
6. J. M. Lehn, Transition Metals in Supramolecular Chemistry; Vol 5, John Wiley and Sons, New York, 1999.
7. C. N. R. Rao, Current Science, 2001, 81, 1030.
8. Journals:
   (i) Crystal Growth and Design.http://www.pubs.acs.org/journals/cgdefu/index.html
   (ii) Crystal Engineering Communication, http://www.rsc.org /Publishing/ Journals /ce/ index.asp

*****

SEMESTER-II **HOURS/WEEK: 6**
ELECTIVE COURSE-IB (EC-IB) **CREDITS: 5**

(B) SUPRAMOLECULAR CHEMISTRY

OBJECTIVES

1. To know the fundamentals of supramolecules.
2. To learn co-receptor molecules and multiple recognition
3. To study the supramolecular reactivity and catalysis.

UNIT I: Concepts of Supramolecular Chemistry

Concepts and languages of supramolecular chemistry – various types of non-covalent interactions – hydrogen bonds, C-H···X interactions, halogen bonds – π-π interactions, non–bonded interactions – various types of molecular recognition.

Crystal engineering of organic solids – hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis – polymorphism and pseudopolymorphism – supramolecular isomorphism / polymorphism – crystal engineering of pharmaceutical phases.

UNIT II: Metallo Organic Frameworks

M.O.F (Metallo Organic Frameworks) – organometallic systems – combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. – design of nanoporous solids – interligand hydrogen bonds in metal complexes – implications for drug design – crystal engineering of NLO materials, OLED.

UNIT III: Co-receptor Molecules and Multiple Recognition

Dinuclear and polynulclear metal ion cryptates – linear recognition of molecular length by ditopic co-receptors – heterotopic co-receptors – cyclophane receptors, amphiphilic receptors and large molecular cages – multiple recognition in metalloreceptors – supramolecular dynamics.

UNIT IV: Supramolecular Reactivity and Catalysis

Catalysis by reactive macrocyclic cation receptor molecules – catalysis by reactive anion receptor molecules – catalysis with cyclophane type receptors – supramolecular metallocatalysis – cocatalysis – catalysis of synthetic reactions – biomolecular and abiotic catalysis.

Supramolecular chemistry in solution – cyclodextrin, micelles, dendrimers, gelators – classification and typical reactions – applications.

UNIT V: Supramolecular Devices

Supramolecular devices and sensors – various types of supramolecular devices – an overview – supramolecular photochemistry – molecular and supramolecular photonic devices – light conversion and energy transfer devices – molecular and supramolecular electronic devices – electronic conducting devices – molecular wires, modified and switchable molecular wires – molecular and supramolecular ionic devices – tubular mesophases, molecular protonics – switching devices – electro-photo switch – ion and molecule sensors – role of supramolecular chemistry in the development of nanoscience and technology.

REFERENCES

1. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, Germany, 1995.
2. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, United States, 1989.
3. G. R. Desiraju, and T. Steiner, The Weak Hydrogen Bond in Structural Chemistry and Biology; Oxford University Press, Oxford, 1999.
4. G. A Jeffrey, Introduction to Hydrogen Bonding; Oxford University Press: UK, 1997.
5. J. M. Lehn, Transition Metals in Supramolecular Chemistry; John Wiley and Sons: New York, 1999.
6. G. R. Desiraju, Current Science; 2001, 81, 1038.
7. Web source:
   (i) Crystal Growth and Design,
   http://www.pubs.acs.org/journals/cgdefu/index.html
   (ii) Crystal Engineering
   Communicationhttp://www.rsc.org/Publishing/Journals/ce/index.asp

*****

SEMESTER-III **HOURS/WEEK: 6**
CORE COURSE-VI (CC-VI) **CREDITS: 5**

ORGANIC CHEMISTRY II

OBJECTIVES

1. To understand the nucleophilic and electrophilic substitution reactions.
2. To learn the addition and elimination reactions.
3. To study a variety of heterocycles.
4. To know the chemistry of terpenoids, steroids and alkaloids.

UNIT I: Nucleophilic Substitution Reactions

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

Reactivity – effect of structure, nucleophile, leaving group and stereochemical factors – correlation of structure with reactivity – solvent effects – rearrangements involving carbocations – Wagner-Meerwein and dienone-phenol rearrangements.

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

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

Substituent effects – origins of Hammett equation – principles of Hammett correlation – effect of structure on reaction mechanisms Hammett parameters – σ and ρ, modified forms of Hammett equation, Taft Equation.

Aliphatic electrophilic substitution – S_E2, S_Ei and S_E1 mechanisms – diazonium coupling reactions – metals as electrophile in substitution reactions and decomposition of diazonium salts.

UNIT III: Addition and Elimination Reactions

Addition to carbon-carbon multiple bonds – electrophilic, nucleophilic and free radical additions – orientation of the addition – stereochemical factors influencing the addition of bromine and hydrogen bromide, hydroxylation, 1,2-

dihydroxylation – hydroboration leading to formation of alcohols – oxidation and ozonolysis.

Addition to carbonyl and conjugated carbonyl systems – mechanism – Grignard reagents – 1,2- and 1,4-additions (lithium dimethylcuprate) – addition to carbon-oxygen double bond – Benzoin, Knoevenagel, Stobbe, Darzens glycidic ester condensation and Reformatsky reactions.

Elimination reactions – mechanisms; E1, E2, E1cB – stereochemistry of elimination, Hofmann's and Zaitsev's rules – competition between elimination and substitution – pyrolytic *cis*-elimination, Chugaev reaction – examples such as dehydration, dehydrohalogenation, Hofmann degradation, Cope elimination – Bredt's rule with examples.

UNIT IV: Heterocycles

Nomenclature: Trivial, systematic and replacement nomenclature – non-aromatic heterocycles – synthesis of tetrahydrofurans – pyrrolidines – tetrahydropyrans – piperidines.

Synthesis and reactivity of heterocycles: aziridines – oxiranes – thiiranes – azetidines – oxetanes – oxazoles – imidazoles – thiazoles – isooxazoles.

Synthesis and reactivity of aromatic heterocycles: pyrazoles – isothiazoles – triazoles – pyrimidines – purines – triazines – pyridazines – pyrazines.

UNIT V: Natural Products

Terpenoids: introduction – biosynthesis of menthol, camphor – total synthesis: Takasago synthesis of menthol, Corey's synthesis of longifolene, Curran's synthesis of hirsutene.

Steroids: introduction – partial synthesis of androsterone and testosterone (from Cholesterol) – total synthesis: Johnson's synthesis of progesterone and Vollhardt's synthesis of estrone.

Alkaloids: introduction – biosynthesis of nicotine, camptothecin – total synthesis: Corey's synthesis of epibatidine, Comin's asymmetric synthesis of Camptothecin and Woodward's synthesis of reserpine.

REFERENCES

UNIT I, II and III

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 Organic Chemistry; 3rd Ed., Benjamin-Cummings Publishing, USA, 1997.

3. J. March and M. B. Smith, Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th Ed., Wiley, New York, 2007.
4. R. K. Bansal, Reaction Mechanism in Organic Chemistry; Tata McGraw Hill, Noida, 1990.
5. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, 2nd Ed., Oxford University Press, UK, 2012.
6. F. A. Carey, and R. J. Sundberg, Advanced Organic Chemistry, Parts A and B, 5th Ed., Springer, Germany, 2007.
7. I. L. Finar, Organic Chemistry; Vol.II, 7th Ed., Pearson Education Ltd., New Jersey, 2009.
8. E. J. Corey, and X-M. Cheng, The Logic of Chemical Synthesis; 1st Ed., Wiley-Interscience, New York, 1995.

UNIT IV and V

9. T. L. Gilchrist, Heterocyclic Chemistry; 3rd Ed., Prentice Hall, New Jersey, 1997.
10. R. K. Bansal, Heterocyclic Chemistry; 3rd Ed., Wiley Eastern Ltd, New Delhi, 1999.
11. K. C. Nicolaou and E. J. Sorensen, Classics in Total Synthesis, Targets, Strategies, Methods; Wiley VCH, Germany, 1996.
12. Longifolene: F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry; Vol.2. 5th Ed., Springer, Berlin, 2008.
13. Androsterone and Testosterone: J. Chem. Soc. Perkin Trans. I; 1986, 117.
14. Epibatidine: J. Org. Chem; 1993, 58, 5600.
15. Estrone, Estradiol and 2-Methoxyestradiol: J. Org. Chem; 2009, 74, 6362.

*****

SEMESTER-III **HOURS/WEEK: 6**
CORE COURSE-VII (CC-VII) **CREDITS: 6**

PHYSICAL CHEMISTRY II

Objectives

1. To study the applications of quantum chemistry and group theory.
2. To understand electrochemistry, adsorption and classical thermodynamics.

UNIT I: Quantum Chemistry - II and Group Theory

Applications of wave mechanics – the harmonic oscillator, rigid rotator – hydrogen and hydrogen like atoms – shapes and nodal properties of orbitals – space quantization – approximation methods – methods of variation, application to hydrogen and helium atoms – perturbation method – non-degenerate systems – helium atom – effective nuclear charge.

Electron spin – many electron atoms – Pauli's principle – Slater determinants – atomic structure calculation – self-consistent field method – Hartree-Fock method for atoms – angular momentum in many electron systems – spin-orbit interaction, L-S and j-j coupling schemes.

Symmetry adapted linear combinations (SALC) – vibrational spectra – symmetry properties of normal molecules – symmetry coordinates – 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

Ion transport in solution – migration, convection and diffusion – Fick's laws of diffusion conduction – Debye-Huckel theory – ionic atmosphere – Debye-Huckel-Onsager equation – verification and extension – Debye-Falkenhagen effect and Wien effect, Debye-Huckel limiting law – activity coefficients and ionic strength – Bjerrum model.

The electrode – electrolyte interface – electrical double layer and multi layers – theories – electrocapillary curves – Lipmann equation and Lipmann potential.

Electrokinetic phenomena – classification – Tiselius method of separation of proteins – membrane potential – electrocatalysis.

UNIT III: Electrochemistry – II

Dynamics of electron transfer – Marcus theory – tunneling – the rate of charge transfer – current density – Butler-Volmer equation – Taft equation –

polarization and overvoltage – mechanism of hydrogen evolution and oxygen evolution reactions.

Principles of electrodeposition of metals – corrosion and passivity – Pourbaix and Evans diagrams – methods of protection of metals from corrosion.

Power storage systems – fuel cells – construction and functioning – applications – photovoltaic cells.

UNIT IV: Surface Chemistry and Chemical Kinetics-II

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.

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: Classical Thermodynamics

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.

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).

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.

Thermodynamics of irreversible processes: coupled flow – Onsager's reciprocal relations – entropy production.

REFERENCES

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.

*****

SEMESTER-III **HOURS/WEEK: 6**
CORE PRACTICAL-V (CP-V) **CREDITS: 3**

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.

a. Kinetics-acid hydrolysis of ester–comparison of strengths of acids.
b. Kinetics-acid hydrolysis of ester–determination of energy of activation (Ea).
c. Kinetics-saponification of ester–determination of ethyl acetate by conductometry.
d. Kinetics-persulfate-iodine reaction –determination of order, effective of ionic strength on rate constant.
e. Determination of molecular weight of substance by transition temperature method.
f. Determination of molecular weight of substances by Rast method.
g. Determination of Critical Solution Temperature (CST) of phenol-water system and effect of impurity on CST.
h. Study of phase diagram of two components forming a simple eutectic.
i. Study of phase diagram of two compounds forming a compound.
j. Study of phase diagram of three components system.
k. Determination of molecular weight of substances by cryoscopy.
l. Determination of integral and differential heat of solutions by colorimetry.
m. Polymerization-rate of polymerization of acrylamide.
n. Distribution law – study of Iodine-Iodine equilibrium.
o. Distribution law – study of association of benzoic acid in benzene.
p. Adsorption – oxalic acid/acetic acid on charcoal using Freundlich isotherm.

REFERENCES

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.

*****

SEMESTER-III **HOURS/WEEK: 6**
ELECTIVE COURSE-IIA (EC-IIA) **CREDITS: 5**

(A) PHARMACEUTICAL CHEMISTRY

OBJECTIVES

1. To understand the basics of pharmaceutical chemistry.
2. To study the antibiotics and their activity.
3. To learn the analgesic and antipyretic activities.
4. To know the activities of anaesthetics and local anaesthetics.
5. To understand concept of clinical chemistry.

UNIT I: Basics of Pharmaceutical Chemistry

Definitions – the terms – drugs, pharmacology, pharmacy, chemotherapy, therapeutics – pharmacologically active principles in plants – first aid – important rules of first aids, cuts, fractures, bleeding for blood, maintaining breathing burns and first aid box – tuberculosis (T.B.), jaundice, piles, typhoid, malaria, cholera – causes – symptoms, diagnosis – prevention and treatment – medicinally important compounds of iron – ferrous gluconate, ferrous sulphate and ferric ammonium citrate.

UNIT II: Antibiotics

Definition – introduction – classification and biological actions – penicillin, chloramphenicol, streptomycin and tetracycline – structure, properties and therapeutic uses – chemical structure and pharmacological activity – effect of unsaturation, chain length, isomerism, halogens, amino groups, hydroxyl groups and acid groups.

UNIT III: Analgesic and Antipyretics

Narcotic analgesic – analgesic action of morphine – derivatives of morphine – heroin and apomorphine – synthetic analgesics – pethidine, methadone – non-narcotic analgesic – aspirin, paracetamol and phenacetin – analgin – preparation, properties and uses – ibuprofen and ketoprofen – structure and uses.

UNIT IV: Anaesthetics and Local Anaesthetics

Characteristics of anaesthetics – classification of anaesthetics – general anaesthetics – volatile anaesthetics – ether, chloroform and halothane – advantages and disadvantages – non-volatile anaesthetics (intravenous anaesthetics) – methohexitone and propanidid – structure and uses – cocaine and amethocaine – structure and uses – benzocaine and procaine – structure, synthesis and uses.

UNIT V: Clinical Chemistry

Determination of sugar (glucose) in serum – *o*-toluidine method – diagnostic test for sugar in urine – Benedict's test – detection of diabetes – detection of cholesterol in urine – detection of anaemia – estimation of haemoglobin (Hb concentration) – red cell count.

REFERENCES

1. Jayashree Ghosh, A Text Book of Pharmaceutical Chemistry; 5th Ed., S. Chand and Company Ltd., New Delhi, 2014.
2. S. Lakshmi; Pharmaceutical Chemistry; 1st Ed., S. Chand and Company Ltd., New Delhi, 1995.
3. Bhagavathi Sundari; Applied Chemistry; 1st Ed., MJP Publishers, Chennai, 2006.

*****

SEMESTER-III **HOURS/WEEK: 6**
ELECTIVE COURSE-IIB (EC-IIB) **CREDITS: 5**

(B) BIO-ORGANIC CHEMISTRY

OBJECTIVES

1. To learn the preparation, properties of amino acids and proteins.
2. To study the activity of enzymes and cofactors.
3. To know basics of lipids and nucleic acids.
4. To learn the concept of bioenergetics.
5. To learn the principles of lead and analogue synthesis.

UNIT I: Amino Acids and Proteins

Structure, classification, synthesis and properties of amino acids – biosynthesis of amino acids – peptides – N-terminal and C-terminal residue analysis – solid phase peptide synthesis.

Proteins – classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins – biological roles of proteins.

UNIT II: Enzymes and Cofactors

Chemical nature of enzymes – characteristics of enzymes – colloidal nature, catalytic nature.

Mechanism of enzymes – Michaelis-Menten hypothesis – Fischer's lock and key model – regulation of enzyme activity.

Structure and biological functions of coenzyme A, NAD+, FAD and vitamin B12.

UNIT III: Lipids and Nucleic Acids

Lipids – definition – simple lipids – fats and oils – compound lipids – phospholipids, glycolipids – physical properties – solubility, melting point, surface tension, emulsification and geometric isomerism – chemical properties – reaction involving -COOH group, -OH group and double bonds.

Nucleic Acid – definition – nucleosides and nucleotides – deoxyribonucleic acid (DNA) – internucleotides linkages – base composition – double helical structure.

UNIT IV: Bioenergetics

Concept of energy – thermodynamic principles – first law, second law, combining the two laws – relationship between standard free energy change and equilibrium constant.

Standard free energy values of chemical reactions – Adenosine triphosphate (ATP) as universal currency of free energy in biological systems – ATP hydrolysis and equilibria of coupled reactions – inter conversion of adenine nucleotides.

UNIT V: Lead and Analogue Synthesis

Designing organic synthesis – disconnection approach – synthons and synthetic equivalents – one group disconnections: alcohol, acid and ketone – functional group interconversions.

Asymmetric synthesis – basic principles – stereoselective and stereospecific reactions – reagents, catalysts and their applications (wherever applicable) in alkylation and hydrogenation – Jacobsen's catalyst – Evan's catalyst.

REFERENCES

1. J. L. Jain, Fundamentals of Biochemistry; S. Chand and Co., New Delhi, 2007 [Unit- I, II, III, IV].
2. N. C. Price and L. Stevens, Fundamental of Enzymology; Oxford University Press, UK, 1999 [Unit-II].
3. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry: Part-A and Part-B; 5th Ed., Springer, Germany, 2008 [Unit-I, II, III].
4. S. Warren, Designing Organic Synthesis: The Disconnection Approach; 2nd Ed., Wiley, New York, 2008 [Unit-V].
5. H. B. Kagan, Asymmetric Synthesis; Thieme Medical Publishers, Germany, 2009 [Unit – V].

*****

SEMESTER-III **HOURS/WEEK: 6**
ELECTIVE COURSE-III (EC-III) **CREDITS: 5**

ANALYTICAL CHEMISTRY

OBJECTIVES

1. To learn the instrumental methods
2. To learn the nature of errors and their types.
3. To understand the various techniques in chromatography.
4. To understand the principles and instrumentation of thermoanalytical and fluorescence techniques.
5. To studying detail the electroanalytical techniques.

UNIT I: Instrumental Methods of Analysis

Principles and applications of extended X-ray absorption fine structure (EXAFS) – surface extended X-ray absorption (SEXAFS) – atomic absorption spectroscopy (AAS) – flame emission spectroscopy (FES) – turbidimetry – theory and applications.

UNIT II: Data and Error Analysis

Various types of error – accuracy, precision, significant figures – frequency distributions, the binomial distribution, the Poisson distribution and normal distribution – describing data, population and sample, mean, variance, standard deviation, way of quoting uncertainty, robust estimators, repeatability and reproducibility of measurements.

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.

Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – general polynomial equation fitting, linearizing transformations, exponential function fit – r and its abuse – multiple linear regression analysis, elementary aspects.

UNIT III: Chromatography

Solvent extraction – principles of ion exchange, paper, thin-layer and column chromatography techniques – columns, adsorbents, methods, R_f values, McReynold's constants and their uses – HPTLC, HPLC techniques – adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques – methods, principles and uses.

UNIT IV: Thermoanalytical Methods and Fluorescence Spectroscopy

Principles – instrumentations and applications of thermogravimetry analysis (TGA), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) –thermometric titrations – types – advantages.

Basic aspects of synchronous fluorescence spectroscopy – spectral hole burning – flow cytometry – fluorometers (quantization) – instrumentation – applications.

UNIT V: Electroanalytical Techniques

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.

Polarography – principles and instrumentation – dropping mercury electrode – advantages – Ilkovic equation – applications of polarography – polarographic maxima – oscillographic polarography, AC polarography – cyclic voltammetry – advantages over polarographic techniques – chronopotentiometry – advantages – controlled potential coulometry – amperometric titrations: principles – techniques – applications – estimation of lead.

REFERENCES

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.

*****

SEMESTER-IV **HOURS/WEEK: 6**
CORE COURSE-VIII (CC-VIII) **CREDITS: 5**

PHYSICAL METHODS IN CHEMISTRY II

OBJECTIVES

1. To understand electronic spectroscopy of metal complexes.
2. To study in detail IR, Raman and NMR of inorganic compounds.
3. To learn the EPR, Mossbauer and magnetic properties of metal complexes.

UNIT I: Electronic Spectroscopy

Microstates, terms and energy levels for d1 – d9 ions in cubic and square fields – intensity of bands – group theoretical approach to selection rules – effect of distortion and spin-orbit coupling on spectra – evaluation of 10Dq and β for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of $[Ru(bipy)_3]^{2+}$.

Optical rotatory dispersion and circular dichroism and magnetic circular dichroism – applications to metal complexes.

UNIT II: Infrared and Raman Spectroscopy

Vibrations in simple molecules (H_2O, CO_2) and their symmetry notation for molecular vibrations – group vibrations and the limitations – combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO_4^- effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate and dimethyl sulfoxide.

Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding – geometry and number of C-O stretching vibrations (group theoretical treatment) – applications of Raman spectroscopy – resonance Raman spectroscopy.

UNIT III: NMR Spectroscopy

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^{1}H, ^{19}F, ^{31}P, ^{13}C) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei (^{2}H, ^{10}B, ^{11}B) on the ^{1}H NMR spectra.

Systems with chemical exchange – evaluation of thermodynamic parameters in simple systems – study of fluxional behaviour of molecules – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – lanthanide shift reagents.

UNIT IV: EPR Spectroscopy and Magnetic properties

Theory of EPR spectroscopy – spin densities and McConnell relationship – factors affecting the magnitude of g and A tensors in metal species – zero-field splitting and Kramers degeneracy – spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

Magnetic properties – types of magnetism – dia-, para-, ferro- and antiferro-magnetism – magnetic properties of free ions – first-order Zeeman effect – second-order Zeeman effect – states KT – states<<<KT – determination of magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism – magnetic properties of lanthanides and actinides – spin crossover in coordination compounds.

UNIT V: Mossbauer Spectroscopy

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

NQR spectroscopy – characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

REFERENCES

1. R. S. Drago, Physical Methods in Inorganic Chemistry; Affiliated East-West Press Pvt. Ltd., New Delhi, 2012.
2. R. S. Drago, Physical Methods in Chemistry; Saunders College Publications, Philadelphia, 1992.
3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6^{th} Ed., Wiley-Eastern Company, New Delhi, 1999.
4. P. J. Wheatley, The Determination of Molecular Structure; 2^{nd} Ed., Dover Publications, Mineola, 1981.
5. G. J. Leigh, N. Winterton, Modern Coordination Chemistry; Royal Society of Chemistry, UK, 2002.
6. E. A. V. Ebsworth, Structural Methods in Inorganic Chemistry; 3^{rd} Ed., ELBS, Great Britain, 1987.
7. W. Kemp, Organic Spectroscopy; 3^{rd} Ed., Palgrave, New York, 2011.
8. J. R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, PHI Learning, New Delhi, 2009.
9. Y. R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical Applications; S. Chand and Co., New Delhi, 1992.
10. P. S. Kalsi, Spectroscopy of Organic Compounds; 6^{th} Ed., New Age International Publishers, New Delhi, 2004.

*****

SEMESTER-IV **HOURS/WEEK: 6**
CORE PRATICAL-VI (CP-VI) **CREDITS: 3**

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.

a. Conductometry – acid-alkali titrations.
b. Conductometry – precipitation titrations.
c. Conductometry – displacement titrations.
d. Conductometry – determination of dissociation constant of weak acids.
e. Conductometry – solubility product of sparingly soluble silver salts.
f. Verification of Onsager equation - conductivity method.
g. Determination of degree of hydrolysis and hydrolysis constant of a substance.
h. Potentiometric titrations – acid alkali titrations.
i. Potentiometric titrations – precipitation titrations.
j. Potentiometric titrations – redox titrations.
k. Potentiometry – determination of dissociation constant of weak acids.
l. Potentiometry – determination of solubility of silver salts.
m. Potentiometry – determination of activity and activity coefficient of ions.
n. pH Titration of *ortho*-phosphoric acid.
o. To determine the relative strength of two acids by conductance measurements.
p. To determine the pH of a buffer solution using a quinhydrone electrode.

REFERENCES

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.

*****

SEMESTER-IV **HOURS/WEEK: 6**
ELECTIVE COURSE-IVA (EC-IVA) **CREDITS: 5**

(A) GREEN CHEMISTRY

OBJECTIVES

1. To learn the green chemistry and their principles.
2. To learn the importance of greener reactions.
3. To understand the phase-transfer catalyst in green chemistry.

UNIT I: Introduction to Green Chemistry

Introduction to green chemistry – twelve principles of green chemistry – planning a green synthesis in a chemical laboratory – evaluating the type of reaction involved – rearrangement, addition, substitution, elimination and pericyclic reactions.

Selection of appropriate solvent – aqueous phase reaction – reactions in ionic liquids – organic synthesis in solid state – solid supported organic synthesis – selection of starting materials – use of protecting group – use of catalyst – use of microwaves and sonication.

UNIT II: Addition and Condensation Reactions

Addition reactions – Michael addition in [aqueous medium and solid state] – Diels-Alder reactions in aqueous phase.

Condensation reactions – Aldol condensation of aldehydes with nitroalkanes and nitriles – Aldol condensation in solid phase – benzoin condensation under catalytic conditions – applications.

UNIT III: Oxidation and Reduction Reactions

Oxidation reactions – Baeyer-Villiger oxidation in aqueous phase and solid state – enzymatic Baeyer-Villiger oxidation.

Reduction reactions – Clemmensen reduction – mechanism – limitations – applications

UNIT IV: Phase-Transfer Catalyst Reactions

Phase-transfer catalyst reactions – Heck reaction – Michael addition reaction – oxidation of toluene to benzoic acid – Reimer-Tiemann reaction – Baker-Venkataraman synthesis – Williamson ether synthesis – Dozen reaction.

UNIT - V: Sonication Reactions

Sonication reactions – Barbier reaction – Reformatsky reaction – Simmons-Smith reaction – Strecker synthesis – Ullmann coupling reaction – Wurtz reaction – Bouveault reaction.

REFERENCES

1. V. K. Ahluwalia, Green Chemistry; 2nd Ed., Ane Books Pvt Ltd., New Delhi, 2016. [UNIT- I, II, III, IV, V]
2. P. T. Anastas and J. C. Warner, Green chemistry Theory and Practice; Oxford University Press, New York, 2005. [Unit-I]
3. V. K. Ahluwalia and K. Agarwal, Organic Synthesis, Special Techniques; 2nd Ed., Narosa Publishing House, New Delhi, 2007. [Unit-I]

*****

SEMESTER-IV **HOURS/WEEK: 6**
ELECTIVE COURSE-IVB (EC-IVB) **CREDITS: 5**

(B) INDUSTRIAL CHEMISTRY

OBJECTIVES

1. To know the basic ideas of an industry and industrial wastes.
2. To understand the petroleum and petrochemicals.
3. To understand the functions of portland cement.
4. To study the principles of pulp and paper.
5. To know the preparation of soaps, detergents and perfumes.

UNIT I: Basic Ideas and Industrial Wastes

Basics idea about unit operation – flow chart – chemical conversion – batch versus continuous processing – chemical process selection – design – chemical process control.

Types of industrial wastes – treatment of wastes or effluent with organic impurities – treatment of wastes or effluent with inorganic impurities – treatment of some important chemical wastes.

UNIT II: Petroleum and Petrochemicals

Introduction – saturated hydrocarbons from natural gas – uses of saturated hydrocarbons – unsaturated hydrocarbons – acetylene, ethylene, propylene, butylene – aromatic hydrocarbons – toluene and xylene.

Preparation of rectified spirit from beat – methylated spirit – preparation of absolute alcohol from rectified spirit – petrochemicals in India.

UNIT III: Manufacture of Cement

Introduction – types of cement – high alumina cement, water proof cement, slag cement, acid resisting cement, white cement, coloured cement, Pozzolana cement.

Setting of cement – properties of cement – testing of cement – uses of cement – concrete – cement industries in India.

UNIT IV: Pulp and Paper and Manufacture of Paper

Introduction – manufacture of pulp – types of pulp – sulphate or craft pulp, soda pulp, Rag pulp – beating, refining, filling, sizing and colouring.

Calendaring – uses – paper industries in India.

UNIT V: Soaps, Detergents and Perfumes

Introduction – types of soaps – hard and soft soaps – manufacture of soap (hot and continuous process only) – cleansing action of soap – detergents – surface active agents – biodegradability of surfactants, amphoteric detergents.

Introduction – production of natural perfumes – flower perfumes – jasmine, rose and lily – production of synthetic perfumes – muscone and nitro-musks.

REFERENCES

1. B. K. Sharma, Industrial Chemistry; 8th Ed., Goel Publishing House, New Delhi, 1997. (Unit–I, II, III, IV and V)
2. R. N. Shreve, and J. A. Brink Jr. Chemical Process Industries; 4th Ed., McGraw Hill, Toronto, 1977. (Unit–I, II, III, IV and V)
3. A. C. S. Brain, Production and Properties of Industrial Chemicals; Reinhold, New York, 1989. (Unit–I)

*****

SEMESTER-IV **HOURS/WEEK: 6**
ELECTIVE COURSE-VA (EC-VA) **CREDITS: 5**

(A) SELECTED TOPICS IN CHEMISTRY

OBJECTIVES

1. To understand the quantum chemical approach to chemical bonding.
2. To know the named reactions and their applications.
3. To understand the retro-synthetic methods.
4. To study the polymers and their types.
5. To learn the principles of nuclear chemistry.

UNIT I: Quantum Chemical Approach to Chemical Bonding and Molecular Structure

Diatomic molecules: Born-Oppenheimer approximation – MO theory (H_2 and H_2^+), VB theory (H_2 and H_2^+) – comparison.

HMO calculations – evaluation of coefficients and eigenvalues for simple molecules – electron density – bond order and free valence index.

Extended HMO theory – applications to simple systems – hybridization schemes.

UNIT II: Named Reactions and Applications in Organic Synthesis

Bamford-Stevens reaction – Barton-McCombie reaction (Barton Deoxygenation) – Baylis-Hillman reaction – Biginelli reaction – Corey-Chaykovsky reaction – Enamines and selective mono- and dialkylation via enamine reactions

Henry reaction – Hosomi-Sakurai reaction – Hunsdiecker reaction – Julia olefination and its modifications – Mitsunobu reaction – Mukaiyama-Aldol addition – Nazarov cyclization – Peterson olefination – Prevost reaction – Prins reaction – Staudinger reaction

Ugi reaction – Weinreb ketone synthesis – Wittig reaction and its modifications – Yamaguchi macrolactonization – Palladium based reactions: Fukuyama coupling – Heck reaction – Hiyama coupling – Sonogashira coupling – Stille coupling – Suzuki coupling – Tsuji-Trost Reaction.

UNIT III: Synthetic Methodology

Introduction to disconnections – synthons and synthetic equivalents – synthon approach – electron donors (nucleophiles) – electron acceptors (electrophiles)

Introduction of functional groups – umpolung reactions – one group disconnections: alcohols, olefins, ketones, acids – two group disconnections: 1,2-, 1,3-, 1,4- and 1,5-difunctional compounds – convergent syntheses.

Functional group interconversion – functional group addition – carbon-heteroatom bonds – methods for 3- and 4-membered rings - synthesis of mono- and difunctional open chain molecules – mono and bicyclic molecules with substituents.

UNIT IV: Polymer Chemistry

Introduction – structure – classification of polymers – polymerisation methods – importance of polymers.

Molecular weight of polymers – number average and weight average – determination of molecular weight by osmometry – light scattering, viscosity and sedimentation methods.

Kinetics of polymerisation reactions, polycondensation reactions, ionic and free radical polymerisation, copolymerisation – coordination polymers, conducting polymers, Ziegler-Natta catalyst.

UNIT V: Fundamental of Nuclear Chemistry

The nucleus – subatomic particles and their properties – nuclear binding energy – nuclear structure – Liquid-drop model and nuclear-shell model – n/p ratio – nuclear forces – modes of radioactive decay – alpha, beta and gamma particles – orbital electron capture – nuclear isomerism – internal conversion.

Q-Values of nuclear reaction, coloumbic barrier, nuclear cross section, threshold energy and excitation function – different types of nuclear reactions with accelerated particles.

Projectile capture and particles emission, spallation, fragmentation, nuclear fission, nuclear fusion – proportional counter, Geiger-Muller counter, scintillation counter and Cherenkov counter – linear accelerator, cyclotron and synchrotron.

REFERENCES

1. R. K. Prasad, Quantum Chemistry; 4th Ed., New Age International Publishers, New Delhi, 2009.
2. A. K. Chandra, Introductory Quantum Chemistry; 4th Ed., Tata McGraw Hill, New Delhi, 1994.
3. D. A. Mcquarrie, Quantum Chemistry; University Science Books, 2nd Ed., 2007.
4. I. N. Levine, Quantum Chemistry; 7th Ed., Prentice Hall, New Jersey, 2013.
5. L. Kurti and B. Czako, Strategic Applications of Named Reactions in Organic Synthesis; Elsevier, 2005.
6. A. Hassner and C. Stumer, Organic Synthesis Based on Named and Unnamed Reactions; Elsevier Science Ltd., UK, 1994.
7. G. Brahmachari, Organic Name Reactions: A Unified Approach; Alpha Science Intl. Ltd, UK, 2006.
8. S. Warren, Designing Organic Synthesis: The Disconnection Approach; 2nd Ed., Wiley, New York, 2008.
9. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Parts A and B, 5th Ed., Springer, Germany, 2007.
10. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, Cambridge, 2004.
11. C. E. Carraher, Polymer chemistry, 6th Ed, Marcel Dekker, New York, 2003.
12. F. W. Billmeyer, Jr., A Text Book of Polymer Science, 3rd Ed., John Wiley, 1994.
13. V. R. Gowariker, N. V. Viswanathan, and J. Sreedhar, Polymer Science; 1st.Ed., New Age Publishers, New Delhi, 1986.
14. G. Friedlander, E. S. Macias, J. W. Kennedy and J. M. Miller, Nuclear and Radiochemistry; 3rd Ed., John Wiley and Sons, London, 1981.
15. S. Glasstone, Source Book on Atomic Energy, Krieger Publishing Company, New Delhi, 2014.
16. H. J. Arnikar, Essentials of Nuclear Chemistry; 4th Ed., New Age International Publishers, New Delhi, 2005.

******

SEMESTER-IV **HOURS/WEEK: 6**
ELECTIVE COURSE-VB (EC-VB) **CREDITS: 5**

(B) CHEMISTRY OF NANOSCIENCE AND NANOTECHNOLOGY

OBJECTIVES

1. To know the synthetic methods of nanomaterials.
2. To understand the characterization of nanomaterials.
3. To understand carbon clusters and nanostructures.
4. To learn nanotechnology and nanodevices.

UNIT I: Synthetic Methods

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

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.

Inorganic nanomaterials – typical examples – nano TiO_2/ZnO/CdO/CdS, organic nanomaterials – examples – rotaxanes and catenanes

UNIT II: Characterisation of Nanoscale Materials

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

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

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

UNIT III: Reactions in Nanoparticles

Reactions in nanospace – nanoconfinement – nanocapsules

Cavitands, cucurbiturils, zeolites, M.O.Fs, porous silicon, nanocatalysis.

UNIT IV: Carbon Clusters and Nanostructures

Nature of carbon bond – new carbon structures – carbon clusters – discovery of C_{60}–alkali doped C_{60}–superconductivity in C_{60}–larger and smaller fullerenes.

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

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

UNIT V: Nanotechnology and Nanodevices

DNA as a nanomaterial – DNA – knots and junctions, DNA – nanomechanical device designed by Seeman.

Force measurements in simple protein molecules and polymerase – DNA complexes– molecular recognition and DNA based sensor.

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

REFERENCES

1. C. N. R. Rao, A. Muller and A. K. Cheetham (Eds), The Chemistry of Nanomaterials: Vol. 1 and 2; Wiley-VCH;Germany, Weinheim, 2004.
2. C. P. Poole, Jr: and F. J. Owens, Introduction to Nanotechnology; Wiley Interscience, New Jersey, 2003.
3. K. J. Klabunde (Ed), Nanoscale Materials in Chemistry; 2nd Ed., Wiley-Interscience, New York, 2009.
4. T. Pradeep, Nano: The Essentials in Understanding Nanoscience and Nanotechnology; 1st Ed., Tata McGraw Hill, New York, 2007.
5. H. Fujita (Ed.), Micromachines as Tools in Nanotechnology; Springer-Verlag, Berlin, 2003.
6. Bengt Nölting, Methods in Modern Biophysics; 3rd Ed., Springer-Verlarg, Berlin, 2009.
7. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties, Elsevier, Chennai, 2000.
8. W. Kain and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life; 2nd Ed., John-Wiley R Sons, New York, 2013.
9. T. Tang and P. Sheng (Eds), Nanoscience and Technology, Novel Structures and Phenomena; Taylor andFrancis, New York, 2003.
10. A. Nabok, Organic and Inorganic Nanostructures; Artech House, Boston, 2005.
11. E. A. Rietman, Molecular Engineering of Nanosystems; Springer-Verlag, New York, 2001.
12. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/
13. Nanoletters - http://pubs.acs.org/journals/nalefd/index.html
14. Nanotation - http://www.acsnanotation.org/

*****