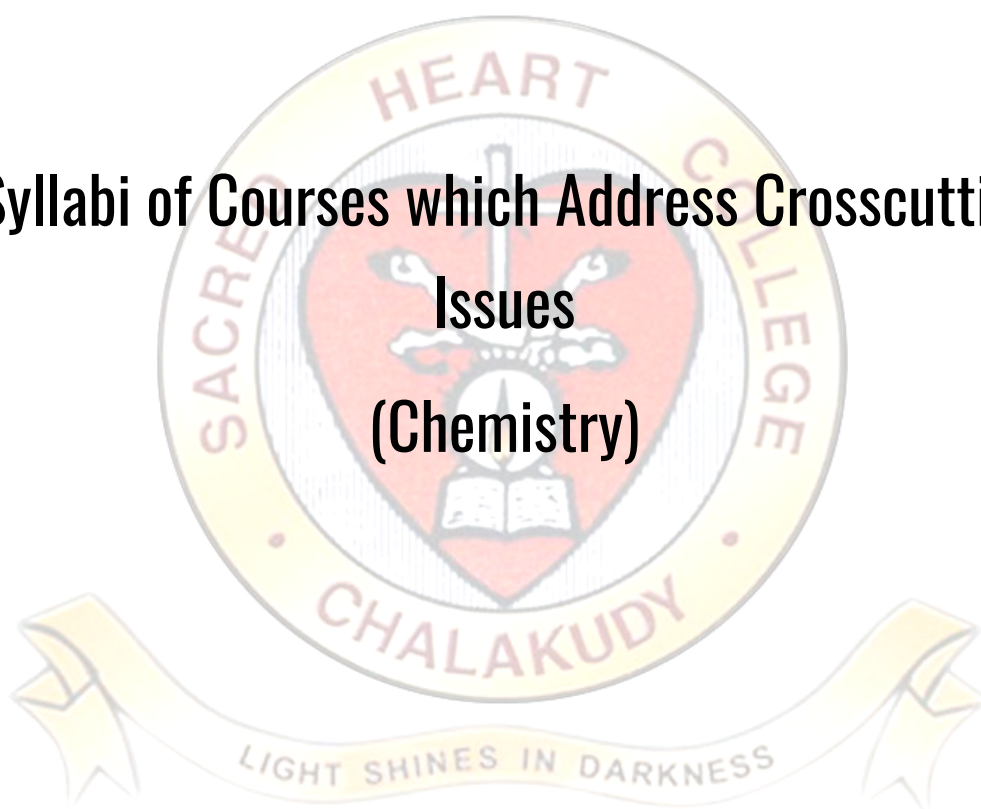


**Syllabi of Courses which Address Crosscutting
Issues
(Chemistry)**



1.3.1. Description of courses which address the Professional Ethics, Gender, Human Values, Environment and Sustainability into the Curriculum

Sl. No.	Name of the Course	Course Code	Name of the Programme	Specify the issue(s) dealing with
1.	Physical and applied chemistry	CHE4C04	BSc. Chemistry / Complementary course	Deals with pollution prevention measures and environmental sustainability.
2.	Inorganic chemistry – III	CHE5B06	BSc. Chemistry / Core course	Environment and Sustainability.
3.	Environmental chemistry	CHE5D01	BSc. Chemistry / Open course	Environment and Sustainability.
4.	Advanced and Applied Chemistry	CHE6B12	BSc. Chemistry / Core course	Environment and Sustainability.
5.	Green and nano chemistry	CHE3E03	MSc. Chemistry / Elective course	Deals with environmental sustainability through the production of nanomaterials
6.	Industrial catalysis	CHE4E05	MSc. Chemistry / Elective course	Discusses key issues in catalysis for clean energy production and environmental sustainability.
7.	Advanced topics in chemistry	CH4C13	MSc. Chemistry / Core course	Renewable Energy, Environment and Sustainability.

SEMESTER IV

UNIVERSITY OF CALICUT

Course Code: CHE4C04

Complementary Course IV: PHYSICAL AND APPLIED CHEMISTRY

Total Hours: 48; Credits: 2; Hours/Week: 3

Module I: Colloidal Chemistry (6 hrs)

True solution, colloidal solution and suspension. Classification of colloids: Lyophilic, lyophobic, macromolecular, multimolecular and associated colloids with examples. Purification of colloids by electrodialysis and ultrafiltration. Properties of colloids: Brownian movement – Tyndall effect – Electrophoresis. Origin of charge and stability of colloids – Coagulation - Hardy Schulze rule – Protective colloids - Gold number. Emulsions. Applications of colloids: Delta formation, medicines, emulsification, cleaning action of detergents and soaps.

Module II: New Vistas in Chemistry (6 hrs)

Nanochemistry: Introduction – classification of nanomaterials (0D, 1D, 2D) - size dependence of material properties (optical, electrical and catalytic) - surface to volume ratio and its significance - application of nanomaterials in electronics, optics, catalysis and medicine. Green Chemistry: Definition and need of green chemistry - principles - atom economy - green solvents - green synthesis of Ibuprofen.

Module III: Chromatography (6 hrs)

Chromatography- Introduction - Adsorption and partition chromatography - Principle and applications of column, thin layer, paper and gas chromatography - R_f value – Relative merits of different techniques.

Module IV: Spectroscopy (10 hrs)

Origin of spectra - Interaction of electromagnetic radiation with matter. Different types of energy levels in molecules: Rotational, vibrational and electronic levels. Statement of Born

Oppenheimer approximation - Fundamental laws of spectroscopy and selection rules (derivations not required).

IR Spectroscopy: Introduction - Group frequency concept - Characteristic stretching frequencies of O-H, N-H, C-H, C=C, C=N and C=O functional groups - Fingerprint region in IR spectra.

UV-Visible Spectroscopy: Introduction - Beer-Lambert's law - Electronic transitions in molecules ($\sigma \rightarrow \sigma^*$, $n \rightarrow \sigma^*$, $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$) - Chromophore and auxochrome - Red shift and blue shift.

NMR Spectroscopy: Introduction - Chemical shift and spin-spin coupling - Application in elucidating the structure of ethanol, dimethyl ether, propanal and acetone.

Module V: Polymers (4 hrs)

Classification of polymers - Addition and condensation polymers – Thermoplastics and thermosetting plastics - Structure and applications of synthetic rubbers (Buna-S, Buna-N and neoprene), synthetic fibres (Nylon 66, Nylon 6 and dacron), thermoplastics (polyethene, polystyrene, PVC and teflon) and thermosetting plastics (bakelite and melmac). Uses of kevlar, nomex and lexan – Biodegradable polymers (PGA, PLA and PHBV) and their applications.

Module VI: Environmental Pollution (6 hrs)

Definition – Types of pollution.

Air pollution: Pollution by oxides of nitrogen, carbon and sulphur. Effects of air pollution: Depletion of ozone, green house effect and acid rain.

Water pollution: Pollution due to sewage, industrial effluents, soaps, detergents, pesticides, fertilizers and heavy metals – Eutrophication - Biological magnification and bioaccumulation - Effects of water pollution. Water quality parameters – DO, BOD and COD (elementary idea only).

Soil pollution – Pollution due to plastics. Thermal pollution and radioactive pollution: Sources, effects and control measures.

Module VII: Chemistry in Daily Life (10 hrs)

Petrochemicals: Name, carbon range and uses of fractions of petroleum distillation – Octane number - Cetane number – Flash point. LPG and CNG: Composition and uses.

Pharmaceuticals: Drug - Chemical name, generic name and trade names with examples. Antipyretics, analgesics, antibiotics, antacids, antiseptics.

Dyes: Definition – Requirements of a dye - Theories of colour and chemical constitution – Structure and applications of martius yellow, indigo and alizarin.

Food: Food additives: Food preservatives, artificial sweeteners and antioxidants. Commonly used permitted and non-permitted food colours.

Cement: Manufacture, composition and setting. Glass: Types of glasses and uses.

References:

1. B. R. Puri, L. R. Sharma, M. S. Pathania, Principles of Physical Chemistry, 46th Edn., Vishal Publishing Company, New Delhi, 2013.
2. F. Daniels, R. A. Alberty, Physical Chemistry, 5th Edn., John Wiley and Sons, Canada, 1980.
3. T. Pradeep, A Textbook of Nanoscience and Nanotechnology, McGrawhill, New Delhi, 2012.
4. V. K. Ahluwalia, Green Chemistry, Narosa Publishing House, New Delhi, 2011.
5. R. A. Day Junior, A. L. Underwood, Quantitative Analysis, 5th Edn., Prentice Hall of India Pvt. Ltd., New Delhi, 1988.
6. R. P. Budhiraja, Separation chemistry, New Age International (P) Ltd., 2007.
7. C. N. Banwell, E. M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th Edn., McGraw–Hill publishing Company Limited, New Delhi, 2002.
8. V. R. Gowarikar, Polymer Chemistry, New Age International Pvt. Ltd., New Delhi, 2010.
9. Fred. W. Billmeyer, Textbook of Polymer Science, 3rd Edn., Wiley India, Delhi, 2008.
10. A. K. De, Environmental Chemistry, 6th Edn., New Age International Pvt. Ltd., New Delhi, 2006.
11. A. K. Ahluwalia, Environmental Chemistry, Ane Books India, New Delhi, 2008.
12. Jayashree Ghosh, A Textbook of Pharmaceutical Chemistry, 3rd Edn., S. Chand and Company Ltd., New Delhi, 1999.
13. B. Sivasankar, Food processing and preservation, Prentice – Hall of India Pvt. Ltd., New Delhi, 2002.

SEMESTER V

UNIVERSITY OF CALICUT

Course Code: CHE5B06

Core Course VI: INORGANIC CHEMISTRY – III

Total Hours: 48; Credits: 3; Hours/Week: 3

Module I: Analytical Principles II (6 hrs) Qualitative Analysis:

Applications of solubility product and common ion effect in the precipitation of cations – Interfering acid radicals and their elimination (oxalate, fluoride, borate, phosphate, chromate, arsenite and arsenate) – Introduction of micro scale experiments in inorganic and organic qualitative analysis & their advantages. Preparation of Na_2CO_3 extract for inorganic qualitative analysis and its advantages. Gravimetric analysis – Mechanism of precipitate formation. Factors affecting stability of precipitates. Co-precipitation and post precipitation. Effects of digestion, washing, drying and ignition of precipitates.

Module II: Metallurgy (10 hrs)

[Prerequisites: Occurrence of metals based on standard electrode potential – Concentration of ores – Calcination and roasting – Reduction to free metal.] Electrometallurgy – Hydrometallurgy. Refining of metals: Electrolytic refining, ion exchange method, zone refining, vapour phase refining and oxidative refining – Ellingham diagrams for metal oxides – Extractive metallurgy of Al, Fe, Ni, Cu, Ti and U. Alloys: Definition – Composition and uses of German silver, brass, bronze, gunmetal and alnico. Steel: Open hearth process – classification of steel – Composition and uses of alloy steels – Composition, properties and applications of industrially important stainless steel types: Austenitic, Martensitic and Ferritic stainless steels, Aerospace and automotive applications of stainless steel. Intramedullary rods (a brief study).

Module III: Interhalogen compounds (5 hrs)

[Prerequisites: Halogens, properties, electronic configuration, electronegativity, electron affinity.] Electropositive character of iodine – General preparation and properties of interhalogen compounds (study of individual members not required) – Structure, hybridization and reactivity of ClF_3 , ICl_3 , IF_5 and IF_7 - Comparison of properties of halogens and pseudohalogens (cyanogens as example) – Structure of polyhalide ions.

Module IV: Noble Gases (3 hrs)

[Prerequisites: Why the name noble gas? electronic configuration.] Discovery – Occurrence – Separation by charcoal adsorption method – Structure of oxides, fluorides and oxy fluorides of xenon – Reaction of xenon fluorides with water – Uses of noble gases.

Module V: Inorganic Polymers & Non-aqueous Solvents (8 hrs)

[Prerequisites: Catenation, Self ionization of water.] Inorganic Polymers: Heterocatenation. Structure and applications of silicones and silicates. Phosphazenes: Preparation, properties and structure of di and tri phosphonitrilic chlorides. SN compounds: Preparation, properties and structure of S_2N_2 , S_4N_4 and $(\text{SN})_x$. Non-aqueous Solvents: Classification – General properties – Self ionization and leveling effect – Reactions in liquid ammonia, liquid N_2O_4 , liquid SO_2 and liquid HF.

Module VI: Environmental Pollution (12 hrs)

[Prerequisites: What is Pollution? quality of drinking water.]

Air pollution: Major air pollutants – Oxides of carbon, nitrogen and sulphur – Particulates – London smog and photochemical smog. Effects of air pollution: Acid rain, greenhouse effect and depletion of ozone. Control of air pollution – Alternate refrigerants. Bhopal Tragedy (a brief study).

Water pollution: Water pollution due to sewage and domestic wastes – Industrial effluents – Agricultural discharge – Eutrophication. Quality of drinking water – Indian standard and WHO standard. Water quality parameters: DO, BOD and COD – Determination of BOD and COD. Toxic metals in water (Pb, Cd and Hg) – Minamata disaster (a brief study). Control of water pollution – Need for the protection of water bodies.

Thermal pollution: noise pollution and radioactive pollution (Sources, effects and consequences). Pollution due to light.

Hiroshima, Nagasaki and Chernobyl accidents (a brief study). Local environmental movements: Silent Valley, Plachimada, Narmada.

Air pollution in Indian cities: Delhi, Agra and Kanpur.

Module VII: Solid Waste Management (4 hrs)

[Prerequisites: Aerobic and anaerobic degradation.]

House hold, municipal and industrial solid waste – Non-degradable, degradable and biodegradable waste – Hazardous waste – Pollution due to plastics. Solid waste management: Recycling, digestion, dumping, incineration, land treatment and composting. Impacts of medical waste and e-waste and their disposal. Energy production from waste.

References:

1. Jeffrey A. Lee, The Scientific Endeavor: A Primer on Scientific Principles and Practice, Pearson Education, 1999.
2. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Brooks/Cole, Thomson Learning, USA, 2004.
3. A. I. Vogel, A Textbook of Quantitative Inorganic Analysis, 3rd Edn., Longmans, Green, London, 1962.
4. A. Cottrell, An introduction to metallurgy, 2nd Edn., University press, 1990.
5. D. F. Shriver, P. W. Atkins, Inorganic Chemistry, 3rd Edn., Oxford University Press, 2006.
6. F. A. Cotton, G. Wilkinson, C. Murillo, M. Bochman, Advanced Inorganic Chemistry, 6th Edn., John Wiley, New York, 1999.
7. Christian Reichardt, Thomas Welton, Solvents and solvent effect in organic chemistry, Wiley-VCH Verlag GmbH & Co., 2002.
8. S. S. Dara, A Textbook of Environmental Chemistry and Pollution Control, 8th Edn., S. Chand and Sons, New Delhi, 2008.
9. A. K. De, Environmental Chemistry, 6th Edn., New Age International (P) Ltd., New Delhi, 2006.
10. G. M. Masters, Introduction to Environmental Engineering and Science, 3rd Edn., Prentice-Hall Inc., New Delhi, 2007.
11. M. N. Rao, A. K. Datta, Waste Water treatment, Oxford & IBH Publ, Co. Pvt. Ltd., 1987.
12. R. C. Brunner, Hazardous Waste Incineration, McGraw Hill Inc., 1989.

SEMESTER V

UNIVERSITY OF CALICUT

Course Code: CHE5D01

Open Course 1: ENVIRONMENTAL CHEMISTRY

Total Hours: 48; Credits: 3; Hours/Week: 3

Module I: Introduction to Environment and Environmental pollution (4 hrs)

Environmental chemistry - introduction, Environmental segments – Lithosphere: components of soils, Hydrosphere: water resources, Biosphere, Atmosphere - regions of atmosphere – Troposphere, stratosphere, mesosphere, thermosphere. Environmental pollution – Concepts and definition – Pollutant, contaminant, receptor and sink – Classification of pollutants – Global, regional, local, persistent and non-persistent pollutants.

Module II: Air Pollution (8 hrs)

Tropospheric pollution – Gaseous air pollutants – Hydrocarbons, oxides of sulphur, nitrogen and carbon – Global warming, green house effect, acid rain – Particulates – Smog: London smog and photochemical smog – effects and control of photochemical smog – stratospheric pollution - depletion of ozone layer, chlorofluorocarbons - Automobile pollution. Control of air pollution – Alternate refrigerants – Bhopal Tragedy (a brief study). Air pollution in Indian cities (Delhi, Agra and Kanpur).

Module III: Water Pollution (10 hrs)

Impurities in water – cause of pollution – natural and anthropogenic – Marine water pollution – Underground water pollution. Source of water pollution – Industrial waste, Municipal waste, Agricultural waste, Radioactive waste, Petroleum, Pharmaceutical, heavy metal, pesticides, soaps and detergents. Types of water pollutants: Biological agents, physical agents and chemical agents – Eutrophication - biomagnification and bioaccumulation. Water quality parameters: DO, BOD, COD, alkalinity, hardness, chloride, fluoride and nitrate. Toxic metals in water and their effects: Cadmium, lead and mercury – Minamata disaster (a brief study), itai-itai disease, oil pollution in water. International standards for drinking water.

Module IV: Soil, Noise, Thermal, light and Radioactive Pollutions (8 hrs)

Soil pollution: Sources by industrial and urban wastes. Pollution due to plastics, pesticides, biomedical waste and e-waste (source, effects and control measures) – Control of soil pollution - Solid waste Management – Open dumping, landfilling, incineration, re-use, reclamation, recycle, composting. Non-degradable, degradable and biodegradable wastes. Hazardous waste. Noise Pollution – physiological response to noise, Noise categories - effect of noise – biological effects. Thermal pollution – definition, sources, harmful effects and prevention. Light pollution. Radioactive pollution (source, effects and control measures) – Hiroshima, Nagasaki and Chernobyl accidents (brief study). Endosulfan disaster in Kerala.

Module V: Pollution Control Measures (12 hrs)

Air pollution control measures – Gravitational settling chamber, fabric filter, wet scrubber, catalytic converters, stacks and chimneys, cyclone collectors, Cottrell electrostatic precipitator, extraction ventilator, zoning and green belt.

Module VI: Green Chemistry (6 hrs)

Introduction- Definition of green Chemistry, need of green chemistry, basic principles of green chemistry. Applications of green chemistry in daily life.

References:

1. A. K. De, Environmental Chemistry, 7 th Edn., New Age International, 2012.
2. A. K. Ahluwalia, Environmental Chemistry, The Energy and Resources Institute, 2017.
3. Balram Pani, Textbook of Environmental Chemistry, I. K. International Pvt Ltd, 2010.
4. S. K. Banergy, Environmental Chemistry, 2 nd Edn., Prentice-Hall of India Pvt. Ltd., New Delhi, 2005.
5. J. M. H. Selendy, Water and Sanitation-Related Diseases and the Changing Environment, John Wiley & Sons, 2011.
6. P. K. Goel, Water Pollution: Causes, Effects and Control, New Age International, 2006.
7. K. C. Schiffner, Air Pollution Control Equipment Selection Guide, CRC Press, 2013.
8. M. Lancaster, Green Chemistry: An Introductory Text, Royal Society of Chemistry, 2010.
9. V. K. Ahluwalia, M. Kidwai, New Trends in Green Chemistry, Springer Science & Business Media, 2012.

SEMESTER VI

UNIVERSITY OF CALICUT

Course Code: CHE6B12

Core Course XII: Advanced and Applied Chemistry

Total Hours: 48; Credits: 3; Hours/Week: 3

Module I: Colloids and Nanomaterials (6 hrs)

[Prerequisites: Colloids: Definition – classification - Synthesis – nanometer, micrometer.]
Colloids: Stability – electrical double layer – zeta potential - Aggregation – flocculation – purification of colloids - Properties and applications of colloids. Nanomaterials: Classification of nanomaterials (0D, 1D, 2D and 3D) – Top down and bottom up approaches in the synthesis – Size dependence of material properties (optical, electrical and catalytic). Variation in electronic and optical properties – Surface area to volume ratio (aspect ratio) and its significance – Metal and semiconductor nanoparticles and carbon nanotubes. Characterization of nanomaterials. Applications of nanomaterials (general idea only).

Module II: New vistas in chemistry (8 hrs)

Green Chemistry: Introduction – need of green chemistry approach – Twelve principles of green chemistry with explanations - Atom economy and microwave assisted reactions – Green solvents – Green synthesis of ibuprofen. Microwave and ultrasound assisted green synthesis: Diels-Alder reaction and Cannizzaro reaction.

Supramolecular chemistry: Introduction - types of non-covalent interactions – Molecular recognition – Host-guest interactions.

Combinatorial Chemistry: Introduction – combinatorial synthesis (elementary idea only). Applications of combinatorial synthesis (brief study).

Module III: Introduction to Computational Chemistry (6 hours)

Computational chemistry as a tool and its scope. Classification of computational chemistry methods – Molecular Mechanics methods (basic idea of force field and examples) and Electronic Structure methods (basic idea of ab initio and semi empirical methods), potential energy surface – local minima, global minima, saddle point and transition states. Geometry optimization. Softwares used in computational chemistry calculations.

Module IV: Synthetic polymers (4 hrs)

Classification – Tacticity – Synthesis and applications of addition polymers (polyethene, polystyrene, PAN and PMMA) and condensation polymers (nylon 6, nylon 66, Bakelite, kevlar and terylene) – thermosets. Zeigler Natta polymerization - advantages. Plastic identification codes. Biodegradable polymers: PLA, PGA and PHBV.

Module V: Applied inorganic chemistry (8 hrs)

Cement: Manufacture, composition and setting. Glass: Manufacture, annealing, types of glasses and uses. Refractory materials: borides and carbides. Inorganic fertilizers: Essential nutrients for plants – nitrogeous, phosphatic and potash fertilizers – examples with formula. Rocket propellants: Classification with examples. Tooth paste and Talcum powder: Composition and health effects. Chemical industries in kerala: Location, raw materials, chemistry involved in the preparation and uses of the following, caustic soda and chlorine – Travancore Cochin Chemicals Ltd., TiO_2 pigment from ilmenite – Travancore Titanium Products Ltd.

Module VI: Applied organic chemistry – I (8 hrs)

Petroleum: Carbon range and uses of various fractions of petroleum distillation – Petrol – Knocking – Octane number – Anti-knocking compounds – Diesel oil – Cetane number – Flash point – Composition and uses of LPG and CNG.

Pharmaceuticals: Medicinal chemistry – Drugs (chemical, generic and trade names with examples). Terminology: Prodrug, pharmacy, pharmacology, pharmacodynamics and pharmacokinetics (elementary idea only). Antipyretics, analgesics, antacids, antihistamines, antibiotics, antiseptics, disinfectants (definition and examples, structures not expected) – Preparation of paracetamol and aspirin.

Cleansing agents: Soaps and detergents: Preparation of soap by saponification of oils and fats, classification, advantages and disadvantages of soaps and detergents – TFM of soap – Cleaning action. Shampoos: Ingredients and functions.

Pesticides: Insecticides, rodenticides and fungicides (definition and examples) – Organo chlorine pesticides – Structure of Endosulfan, DDT and BHC. Organo phosphorus pesticides – malathion, parathion. Harmful effects of pesticides. Herbicides – glyphosate – side effects.

Module VII: Applied organic chemistry – II (8 hrs)

Dyes: Definition – Requirements of a dye – Theories of colour and chemical constitution – Classification based on structure and mode of application to the fabric – Preparation and uses of Rosaniline and Indigo. Composition of hair dyes. Food adulterants: Common food adulterants in various food materials and their identification: Milk, vegetable oils, tea, coffee powder and chilli powder. Food additives: Food preservatives, artificial sweeteners and antioxidants (definition and examples, structures not required) – Structure of BHT, BHA and Ajinomoto – Common permitted and non-permitted food colours (structures not required) – Natural pigments in fruits and vegetables (carotenoids, chlorophylls and flavonoids). Artificial ripening of fruits. Composition of chocolate, milk powder and soft drinks.

References:

1. M. A. Shah, Tokeer Ahmad, Principles of Nanoscience and Nanotechnology, Narosa Publishing House, New Delhi, 2010.
2. T. Pradeep, A Textbook of Nanoscience and Nanotechnology, McGrawhill, New Delhi, 2012.
3. P. N. Prasad, Nanophotonics, John Wiley & Sons, 2004.
4. P. W. Atkins, J. de Paula, Atkin's Physical Chemistry, 8 th Edn., Oxford University Press, 2006.
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8. I. N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.
9. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons Ltd., 1999.
10. V. R. Gowarikar, Polymer Chemistry, New Age International (P) Ltd., New Delhi, 2010.
11. Fred. W. Billmeyer, Textbook of Polymer Science, 3rd Edn., Wiley India, Delhi, 2008.
12. M. S. Bhatnagar, Polymer Chemistry, S Chand and Company Pvt. Ltd., New Delhi, 2014.

SEMESTER III

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN)

CHE3E03- GREEN AND NANO CHEMISTRY (ELECTIVE) (4credits, 54 h)

Unit I: Introduction to green chemistry (9h)

Green chemistry-relevance and goals, Anastas' twelve principles of green chemistry - Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

UNIT-2: Microwave mediated organic synthesis (MAOS) (9h)

Microwave activation, advantage of microwave exposure, specific effects of microwave – Neat reactions, solid supports reactions, Functional group transformations, condensations reactions, oxidations – reductions reactions, multi-component reactions.

Unit 3: Alternative synthesis, reagents and reaction conditions (9h)

Introduction, synthesis of ionic liquids, physical properties, applications in alkylation – hydroformylations, epoxidations, synthesis of ethers, Friedel-Craft reactions, Diels-Alder reactions, Knoevenagel condensations, Wittig reactions, Phase transfer catalyst - Synthesis – applications. A photochemical alternative to Friedel-Crafts reactions - Dimethyl carbonate as a methylating agent – the design and applications of green oxidants – super critical carbon dioxide for synthetic chemistry.

Unit 4: Nanomaterials – An Introduction & Synthetic Methods (9h)

Definition of nano dimensional 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 Vapor 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 5: Techniques for Characterisation of nanoscale materials (9h)

Principles of Atomic force microscopy (AFM), Transmission electron microscopy (TEM)- Resolution and scanning transition electron microscopy (STEM), Scanning Tunneling Microscopy (STM), Scanning near field optical microscopy (SNOM), Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.

Unit 6: Carbon Clusters and Nanostructures (9h)

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. Application of carbon nanotubes. Nanowires: Synthetic strategies, Gas phase and solution phase growth, Growth control - Properties.

References:

1. V. K. Ahluwalia, Green Chemistry – Environmentally benign reactions, AneBooks India (Publisher), (2006).
2. V. K. Ahluwalia, Green Chemistry: A Textbook, Narosa Publishing House, 2013.
3. Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas & Tracy C. Williamson. Second Edition, (1998).
4. Green Chemistry–Frontier in benign chemical synthesis and processes-edited by Paul T. Anastas & Tracy C. Williamson. Oxford University Press, (1998).
5. Green Chemistry – Environment friendly alternatives- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, (2003).
6. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley –VCH, Weinheim, 2004.
7. H. Fujita (Ed.), Micromachines as tools in nanotechnology, Springer- Verlag, Berlin, 2003.

SEMESTER IV

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN)

CHE4E05 - INDUSTRIAL CATALYSIS (ELECTIVE) (4 Credits, 72h)

Unit 1: Introduction to Adsorption process (9h)

Intermolecular interactions, physisorption. The forces of adsorption. Dispersion and repulsive forces. Classical electrostatic interactions. Adsorbate-adsorbate interactions, chemisorption, potential energy curves, thermodynamics of adsorption. Isothermal and adiabatic heats of adsorption. Variation of heats of adsorption with coverage. Adsorption isotherms, Langmuir, BET and Freundlich. Kinetics of chemisorptions. Activated and nonactivated chemisorptions. Absolute rate theory. Electronic theories. Hysteresis and shapes of capillaries.

Unit 2: Kinetics and Catalysis (9h)

Adsorption and catalysis. Adsorption and reaction rate. Strength of adsorption bond and catalysis. Adsorption equilibrium and catalysis. Kinetics of heterogeneous catalysis: diffusion steps neglected. Unimolecular reactions. Bimolecular reactions. Langmuir-Hinshelwood and Eley-Rideal mechanism. Kinetics of heterogeneous catalysis: diffusion controlling. Mechanism of diffusion. Diffusion and reaction in pores. Selectivity and diffusion. Electronic factors in catalysis by metals, electronic factors in catalysis by semiconductors, geometric factors and catalysis.

Unit 3: Catalyst - Preparative Methods (9h)

Surface area and porosity measurement. Measurement of acidity of surfaces. Support materials. Preparation and structure of supports. Surface properties. Preparation of catalysts. Introduction of precursor compound. Pre-activation treatment. Activation process. General methods of synthesis of zeolites. Mechanism of nuclear formation and crystal growth. Structures of some selected zeolites. Zeolites A, X and Y. Pentasils. ZSM-5. ZSM-11. Shape selective catalysis by zeolites.

Unit 4: Deactivation of Catalysts (9h)

Deactivation of catalysts. Classification of catalyst deactivation processes. Poisoning of catalysts. Coke formation on catalysts. Metal deposition on catalysts. Sintering of catalysts. Regeneration of deactivated catalysts. Feasibility of regeneration. Description of coke deposit and kinetics of regeneration.

UNIT 5: Phase Transfer Catalysis (9h)

Basic concepts in phase transfer catalysis. Phase transfer catalyzed reactions. Basic steps of phase transfer catalysis. Effect of reaction variables on transfer and intrinsic rates. Outline of compounds used as phase transfer catalysts. Use of quaternary salts. Macrocyclic and macrobicyclic ligands. PEG's and related compounds. Use of dual phase transfer catalyst or co-catalyst in phase transfer systems. Separation and recovery of phase transfer catalysts. Insoluble phase transfer catalysts.

UNIT 6: Biocatalysis (9h)

Enzymes. An introduction to enzymes. Enzymes as proteins. Classification and nomenclature of enzymes. Structure of enzymes. How enzymes work. Effect on reaction rate. Thermodynamic definitions. Catalytic power and specificity of enzymes. Optimization of weak interactions between enzyme and substrate in the transition state. Binding energy, reaction specificity and catalysis. Specific catalytic groups contributing to catalysis. Immobilized biocatalysts. Definition and classification of immobilized biocatalysts. Immobilization of coenzymes.

UNIT 7: Industrial Catalysis-1 (9h)

Oil based chemistry. Catalytic reforming. Catalytic cracking. Paraffin cracking. Naphthenic cracking. Aromatic hydrocarbon cracking. Isomerization. Hydrotreatment. Hydrodesulphurization. Hydrocracking. Steam cracking. Hydrocarbons from synthesis gas. Fisher-Tropsch process. Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

UNIT 8: Industrial Catalysis-II (9h)

Hydroformylation of olefins. Carbonylation of organic substrates. Conversion of methanol to acetic acid. Synthesis of vinyl acetate and acetic anhydride. Palladium catalyzed oxidation of ethylene. Acrylonitrile synthesis. Zeigler-Natta catalysts for olefin polymerization. Propene polymerization with silica supported metallocene/MAO catalysts.

References:

1. A. Clark, "Theory of adsorption and catalysis", Academic Press, 1970.
2. J.M. Thomas & W.J. Thomas, "Introduction to principles of heterogeneous catalysis", Academic Press, New York, 1967.
3. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.
4. D.K Chakraborty, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.
5. J.R. Anderson and M. Boudart (Eds), "Catalysis, Science and Technology", Vol 6, Springer- Verlag, Berlin Heildberg, 1984.
6. R.B. Anderson, "Experimental methods in catalysis research", Vol I, II, Academic press, NY, 1981.
7. R. Szostak, "Molecular sieves: principles of synthesis and identification", Van Nostrand, NY, 1989.
8. R. Hughes, "Deactivation of catalysts", Academic press, London, 1984.
9. C.M. Starks, C.L. Liotta and M. Halpern, "Phase Transfer Catalysis – Fundamentals, Applications and Industrial Perspectives", Chapman & Hall, New York, 1994.
10. A.L. Lehninger, "Principles of Biochemistry", Worth Publishers, USA, 1987.
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SEMESTER IV

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN)

CH4C13- ADVANCED TOPICS IN CHEMISTRY (4Credits, 72hrs)

Unit 1: Chemistry of Nanomaterials (9hrs)

History of nanomaterials- Classification. Size- dependence of properties. Electronic structure theory of metals and semiconductors. Quantum size effects. Synthesis of nanostructures: bottom-up-approach, top- down approach, self-assembly, lithography, molecular synthesis, template assisted synthesis. Methods of characterization: Electron microscopies-SEM, TEM. Scanning prob microscopies STM, AFM. X-ray photoelectron spectroscopy(XPS), Dynamic light scattering(DLS), X-ray diffraction(XRD). Applications: Nanoelectronics, nanosensors, nanocatalysts, nanofiltration, diagnostic and therapeutic applications and targeted drug delivery. Introduction to graphenes and fullerenes.

Unit 2: Green Chemistry (9hrs)

Introduction, the need of green chemistry, principles of green chemistry, planning of green synthesis, tools of green chemistry. Green reactions- Aldol condensation, Cannizzaro reaction and Grignard reaction. Comparison of the above green reactions with classical reactions. Green preparations. Applications of phase transfer catalysis. Introduction to microwave organic synthesis, Applications: environmental, solvents, time and energy benefits.

Unit 3: Introduction to Computational Quantum Chemistry (9hrs)

Electronic structure of molecules-Review of Hartree-Fock SCF method. Basis sets STOs and GTOs . Nomenclature of Basis sets. Semi empirical and ab initio methods. Calculations using Gaussian programme . Specification of molecular geometry using a) Cartesian coordinates and b) Internal coordinates. The Z-matrix . Z- matrices of some simple molecules like H₂, H₂O, formaldehyde ammonia and methanol.

Unit 4: Supramolecular Chemistry (9hrs)

Concepts and language. Molecular recognition: Molecular receptors for different types of molecules, design and synthesis of coreceptors and multiple recognition. Strong, weak and very weak Hydrogen bonds. Utilisation of H-bonds to create supramolecular structures. Use of H bonds in crystal engineering and molecular recognition. Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices. Some examples of self-assembly in supramolecular chemistry.

Unit 5: Medicinal Chemistry (9hrs)

Drug Design and Relationship of Functional Groups to Pharmacologic Activity: Introduction, different classes of drugs, drug action, pro drugs, physico chemical properties of drugs and their pharmacologic activity, SAR and QSAR, factors governing ability of drugs. Drug design, factors governing drug design, rational approach to drug design, general methods of drug synthesis. Immunoassays: General principles, antigen-antibody interactions, Hapten inhibition test, immunodiffusion, immunoelectrophoresis, ELISA, ELOSA, Fluorescence immunoassay and Radio immunoassay. Biosensors and chemosensors (basic idea only).

Unit 6: Combinatorial Chemistry (9hrs)

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, requirements-resins, Linkers. Reactants for solid phase synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis. Structure determination of active compounds- Deconvolution. Methods in deconvolution-recursive deconvolution, tagging use of decoded sheets. Planning and designing of combinatorial synthesis. Spider like scaffolds, drug molecules. Limitations of combinatorial chemistry.

Unit 7: Introduction to Industrial Catalysis (9hrs)

Structure and chemical nature of surfaces. Physisorption and chemisorptions. Energy exchange at surface. Determination of surface area and pore structure of catalysts - physical adsorption methods, X-ray methods, mercury intrusion method, chemisorptions methods. Determination of surface acidity-TPD method. Catalyst selectivity, effect of pore size on selectivity. Homogeneous and heterogeneous catalysts. Preparative methods for heterogeneous catalysts- precipitation and coprecipitation methods, sol gel method, flame hydrolysis. Preparation of Zeolites and silica supports. Mesoporous materials. Introduction to Phase transfer catalysis, biocatalysis, nanocatalysis and polymer supported catalysis. Application of heterogeneous catalysts in water gas shift reaction, ammonia synthesis, catalytic cracking, Fisher-Tropsch process, threeway catalysis.

Unit 8: Renewable Energy Sources (9hrs)

World's reserve of commercial energy sources and their availability, various forms of energy, Renewable and conventional energy systems, comparison - coal, oil and natural gas, availability, applications, merits and demerits. Renewable energy sources - solar energy, nature of solar radiation, components- solar heaters, solar cookers, water desalination. Photovoltaic generation – basics, merits and demerits of solar energy. i) Solid state junction solar cells:- principle of solar cells, Fabrication of CdS/Cu₂S and CdS/CuInSe₂ solar cells, performance testing, stability and efficiency consideration. Dye sensitized solar cells (DSSC)-Working principle, Fabrication of DSSCs based on TiO₂ and ZnO, stability and performance of dyes.

References:

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