COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY

(Abstract)

Faculty of Marine Sciences – Department of Chemical Oceanography – M.Sc Hydrochemistry – Syllabus Approved – Orders issued.

CONFERENCE SECTION

No. Conf.II/2941/1/AC-Marine Sc/2020 Dated, Kochi-22, 12.10.2020.

Read: Item No. I(d.1) of the Minutes of the meeting of the Academic Council held on 08.07.2020.

ORDER

The Academic Council at its meeting held on 08.07.2020 along with the recommendations of the Standing Committee resolved to approve, vide item read above, the revision of syllabus as the outcome based education framework of the M.Sc Hydrochemistry programme offered at the Department of Chemical Oceanography, under the Faculty of Marine Sciences with effect from 08.07.2020, the date of the meeting of the Academic Council as in Appendix.

Orders are issued accordingly.

Dr. MEERA V.
REGISTRAR

To

1. Dr. Rosamma Philip, Dean, Faculty of Marine Sciences and Professor, Department of Marine Biology, Microbiology and Biochemistry, CUSAT, Kochi-16
2. Dr. S.Muraleedharan Nair, Chairman, BOS in Chemical Oceanography, CUSAT, Kochi-16
3. The Head, Department of Chemical Oceanography, CUSAT, Kochi-16
4. The Controller of Examinations/Joint Registrar (Academic)/Assistant Registrar (Academic)
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COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY

M. Sc. HYDROCHEMISTRY Program.

(Scheme, Syllabus & Outcome applicable from 2020 Admission)

M. Sc. HYDROCHEMISTRY – PROGRAMME STRUCTURE

Core courses

Semester	Course code	Course Name	Credits	Page
I	20-304-0101	Co-ordination Chemistry	3	2
	20-304-0102	Marine Environment	3	4
	20-304-0103	Quantum Mechanics	3	7
	20-304-0104	Stereochemistry, Pericyclic Reactions and Photochemistry	3	9
	20-304-0105	Practical I - Analytical Techniques	2	12
	20-304-0106	Practical II - Quantitative Chemical Analysis	2	13
		Total Credits (Core) - I Semester	16	
II	20-304-0201	Chemical Oceanography	3	16
	20-304-0202	Group Theory and Spectroscopy	3	18
	20-304-0203	Natural Products and Organic Synthesis	3	20
	20-304-0204	Thermodynamics and Statistical Mechanics	3	23
	20-304-0205	Practical III - Separation and Synthetic Methods	2	26
	20-304-0206	Practical IV - Water and Sediment Analysis	2	28
		Total Credits (Core) - II Semester	16	
III	20-304-0301	Aquatic Chemical Resources	2	31
	20-304-0302	Organic Spectroscopy	3	33
	20-304-0303	Solution Chemistry	3	36
	20-304-0304	Practical V - Instrumental Techniques 1	2	39
	20-304-0305	Practical VI - Physicochemical Methods	2	41
		Total Credits (Core) - III Semester	12	
IV	20-304-0401	Dissertation (Project Work in the Department / Universities / Scientific Institutes / Industrial Organizations etc.)*	14	
	20-304-0402	Project Viva-Voce*	2	-
		Total Credits (Core) - IV Semester	16	-

CE – Continuous Evaluation; ESE – End Semester Examination

Total number of credits for all the four semesters (Core courses)	60
Minimum number of credits required for the completion of M. Sc. (Hydrochemistry) programme	72
Minimum number of credits to be taken as electives courses	12

Elective courses** offered by the Department

Course code	Course name	Credits	Page
20-304-0001	Analytical Chemistry	3	44
20-304-0002	Applications of Coordination Compounds	2	46
20-304-0003	Aquatic Pollution	3	48
20-304-0004	Atmospheric Chemistry	3	50
20-304-0005	Chemistry of Biomolecules	2	52
20-304-0006	Chemistry of Radiation, Surface and Inorganic Materials	3	54
20-304-0007	Computational Chemistry	3	56
20-304-0008	Environment Law And EIA	2	59
20-304-0009	Estuarine Chemistry	3	61
20-304-0010	General Chemical Oceanography***	3	64
20-304-0011	General Chemical Oceanography Practical***	2	66
20-304-0012	Green Chemistry	2	67
20-304-0013	Instrumental Techniques	3	69
20-304-0014	Instrumental Techniques II- Practical VII	2	71
20-304-0015	Introduction to Hydrochemistry	3	73
20-304-0016	Marine Biogeochemistry	3	75
20-304-0017	Marine Geochemistry	3	77
20-304-0018	Marine Natural Products	3	80
20-304-0019	Marine Organic Chemistry	3	83
20-304-0020	Nanomaterials and Supramolecular Chemistry	3	85
20-304-0021	Organometallic Chemistry	3	88
20-304-0022	Polar Sciences	2	90
20-304-0023	Solid State Chemistry	3	92
20-304-0024	Water Management	3	94

Audit courses**

Course code	Course name	Credits	Total Teaching Hours	Page
20-304-0025	Good Laboratory Practice and safety	0	12	97
20-304-0026	Research Methodology	0	12	99

*The project dissertations will be assessed by the department examination committee constituted by the Department Council.
** Depends on faculty / infrastructural facilities.
*** This course is meant for M.Sc. programs other than M.Sc. Hydrochemistry.

Semester I

20-304-0101–Coordination Chemistry

Unit I - Stability of Metal Complexes

Coordination numbers and symmetries, types of ligands, nomenclature and isomerism of complexes, the stability of complexes-stepwise and overall formation constants, factors affecting the stability of complexes, chelate effect, macrocyclic effect.

Unit II - Metal-Ligand Bonding in Transition Metal Complexes

Crystal field splitting diagrams in complexes of low symmetry; ligand field theory, molecular orbital theory of octahedral complexes, Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller effects and distortions; experimental evidence for metal-ligand orbital overlap; Limitation of crystal field theory, molecular orbital theory.

Unit III - Kinetics and Mechanism of Substitution Reactions

Kinetics and mechanisms in reactions of complex ions: lability and inertness, ligand displacement reactions in octahedral and square complexes, trans-effect-theories and applications, electron transfer reactions-outer sphere and inner sphere processes. Frank Condon principle, Marcus equation

Unit IV - Electronic Spectra of Transition Metal Complexes

Micro-states**,** Term-symbols, Russel-Saunders states, d-d transition and charge-transfer transition, selection rules for electronic transition, Spectroscopic ground states, Orgel and Tanabe-Sugano diagrams for transition metal complexes ($d^1 – d^9$ states) calculation of Dq, B and β parameters, Jahn-Teller theorem, spectral consequences of Jahn-Teller effect, applications of electronic spectra in the structural studies of complexes.

Unit V - Magnetic Properties of Transition Metal Complexes

Guoy's and Faradays's method for the determination of magnetic susceptibility, calculation of magnetic moments, paramagnetism, diamagnetism, ferromagnetism, anti-ferromagnetism, temperature-independent paramagnetism; Curie law, Curie-Weiss Law. Classification of paramagnetic complexions, Spin only group, Group with large multiplet separation, Group with small multiplet separation spin-orbit coupling, quenching of orbital angular momenta, spin cross over the phenomenon, applications of magnetic data in the structural studies of complexes.

Learning Outcomes

After completion of the course, the students will be able to:

1. Predict the isomers possible for the metal complexes.
2. Explain the stability of metal complexes
3. Comprehend the bonding in transition metal complexes using crystal field theory, ligand field theory, and M.O. theories.
4. Explain inert and labile complexes and mechanism of reactions
5. Predict the structure of the complexes from their magnetic moment values.

References

1. J.E. Huheey, E.A. Keiter and R. L. Keiter. Inorganic Chemistry: Principles of Structure and reactivity, 4^{th} ed., Addison Wesley Publ. Co., 1993 (Chapter 11, 12, 13 and 15).
2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6^{th}ed. Wiley Eastern, New Delhi, 1999 (4^{th} and 5^{th} eds. preferred)
3. D.F. Shriver and P.W. Atkins. Inorganic Chemistry, 5^{th} ed., Oxford University Press, 2010
4. D. Banerjea. Coordination Chemistry, 3^{rd} ed., Tata McGraw – Hill, New Delhi. 2009
5. N.N. Greenwood and A. Earnshaw. Chemistry of the Elements, 2^{nd}ed. Pergamon Press, Exeter, Great Britain, 1997.
6. J.D. Lee. Concise Inorganic Chemistry, 5^{th}ed. Chapman and Hall, 1996.
7. G. Rodgers. Introduction to coordination, solid-state and descriptive Inorganic chemistry, 3^{rd}ed. McGraw–Hill, 2012.
8. Bodie Douglas, Darl McDaniel and John Alexander. Concept and Models of Inorganic Chemistry, 3^{rd}ed. J Wiley, 2006.
9. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong. Shriver and Atkins Inorganic Chemistry, Oxford University Press, 2006.
10. Sutton, D. Electronic Spectra of Transition Metal Complexes, McGraw-Hill: New York, 1968
11. Mabbs, F.E. and Machin, D.J. Magnetism and Transition Metal Complexes Chapman and Hall: U.K, 1973.

20-304-0102 – Marine Environment

Unit I - History of Ocean Studies

Need for ocean studies – definition of water bodies - ocean as an important component of the hydrosphere – global ocean basin and their dimension**,** development and scope of oceanography - historical account on ocean Studies – oceanographic exploration – contributions of Challenger and International Indian Ocean Expeditions and GEOSECS programmes. International oceanographic organizations - major oceanographic institutions in the world and India.

Unit II – Physical Environment

Dimensions of the ocean, physical properties of seawater, distributions of salinity, temperature and density. T - S Diagrams, general circulations, important currents of the world ocean, thermohaline circulation and the oceanic conveyor belt. Major water masses of the world's oceans. Sound transmission in the sea, ocean waves, ocean optics, tides and tidal currents in shallow seas, estuaries and rivers. Coastal processes.

Unit III – Geological Environment

The structure of the earth, ocean floor, general topography of the ocean floor, deep ocean basins, ocean plateaus, continental shelves, slopes, submarine ridges and trenches, submarine canyons, sediments, fossils, marginal seas, ocean formation.

Unit IV - Chemical Environment

origin of seawater, the structure of water, ion-water interactions, the polarized water molecule, colligative properties of seawater, comparison of river and seawater, hydrological cycle and budget. Classification of elements based on their distribution - major and minor constituents – general behaviour of elements - chemical exchanges across interfaces and residence times in seawater.

Unit V - Biological Environment

Sea as a biological environment. Divisions of the marine environment. Marine ecosystems: Rocky shores, sandy shores, estuaries, salt marshes, mangroves, coral reefs and the deep sea. Marine organisms - plankton, nekton and benthos. Marine food web dynamics, primary, secondary and tertiary production and factors influencing primary production, food chains, food webs. Bioluminescence & Biological rhythm

Learning Outcomes

After completion of the course, the students will be able to:

1. Discuss the marine environment that impacts the student's areas of oceanographic interest, and also understand the major historical events through which the science of oceanography has evolved.
2. Explain the physical oceanography concepts like the physical features, circulation patterns, ocean currents, water masses, tidal features, acoustic properties etc.
3. Discuss basic concepts about the topography of ocean floor, and familiarize with various geological features like ocean plateaus, continental shelves, slopes, submarine ridges and trenches, submarine canyons etc.
4. Discuss the properties and interactions of the substances present in the marine environment and relate the structure of the water molecule to the chemical and physical properties of the ocean.
5. Explain the factors that influence the primary productivity in the oceans and illustrate how it affects the biomass of living forms in the ocean in addition to the basic knowledge of biological rhythm concerning with marine ecosystem and organisms.

References

1. J.W. Nybakken and M.D. Bertness, Marine Biology – an ecological approach, 6th ed., Benjamin Cumins, 2004.
2. A.C. Duxbury, A.B. Duxbury and K.A. Sverdrup, An Introduction to World Oceans, 6th ed., Mc Graw Hill Publishers, 2000
3. E. Brown, Waves, Tides and Shallow Water Processes, The Open University, 2006
4. G.L. Pickard, Descriptive Physical Oceanography, Pergamon Press, 1975.
5. D.A. Rose, Introduction to Oceanography, Prentice Hall Inc., 1977.
6. T. Garrison, Oceanography 2nd, Wadsworth Publishing Company, 1995
7. F.J. Millero, Chemical Oceanography 4th ed., CRC Press, 2013
8. P.R. Paul, Invitation to Oceanography 4th ed., Jones and Bartlett Publishers, 2003
9. J.P. Riley and R. Chester, Introduction to Marine Chemistry, Academic Press, 1971
10. F.P. Shepard, Submarine Geology, Harper and Row, 1964
11. F.P. Shepard, Geological oceanography: Evolution of coasts, continental margins, and the deep-sea floor, Crane, Russak & Company, 1977
12. P.V. Mldenov, Marine Biology – A very short introduction, Oxford University Press, 2013

13. C.A.M. King. Beaches and Coast, Taylor and Francies. M.J. Keen, An Introduction to Marine Geology, Elsevier, 2007
14. D.W. Townsend, Oceanography and Marine Biology: An Introduction to Marine Science, Oxford University Press, 2012.
15. J. Rothman. Ocean Anatomy: The Curious Parts & Pieces of the World under the Sea, Storey Publishing, LLC. 2020
16. T. Gerkema. An Introduction to Tides. Cambridge University Press, 2019
17. T.S. Garrison. Essentials of Oceanography. Brooks Cole, 2017.

20-304-0103 – Quantum Mechanics

Unit 1 - Wave Mechanics

Planck's quantum theory, wave-particle duality. Uncertainty principle, operators and commutation relations: postulates of quantum mechanics and Schrodinger equation free particle, particle in a box, degeneracy, harmonic oscillator, rigid rotator and the hydrogen atom, Angular momentum, including spin; coupling of angular momenta including spin - orbit coupling.

Unit I1 - The Variation Method and Perturbation Theory.

Application to (1) Hydrogen atom, Hydrogen atom in an electric field, (2) Helium atom: Antisymmetric wave functions of many-electron atoms, Slater determinants, Hartree and Hartree-Fock self-consistent field model for atoms. Electronic configuration of atoms, spectroscopic term symbols, spin-orbit coupling.

Unit III - MO Theory

Chemical bonding: Born – Oppenheimer approximation, Hydrogen molecule ion. Simple Mo theory for homo and heteronuclear diatomics, LCAO–MO, non-crossing rule, correlation diagrams for homo and heteronuclear diatomics, dipole moments of homonuclear diatomic molecules.

Unit IV - VB Theory:

Heitler-London Wavefunction for hydrogen molecule, Q and J integrals, Covalent and ionic structures, singlets and triplets. Defects in the simple MO and VB theories, electron correlation problem, configuration interaction, equivalence of MO and VB theories, Coulson-Fischer function, hybridization in LiB and CO. Hybridization- construction of sp, Sp^2, Sp^3, dsp^2, and d^2sp^3 hybrids and non-equivalent sp, Sp^2, and Sp^3 hybrids. Valance MOs of CO, H 2 O, NO 3 and CH 4.

Unit V - HMO Theory

Simple Huckel theory for p-electrons, Huckel pi electron theory and its applications to ethylene, butadiene and benzene. Frontier orbitals, Extended Huckel theory. Advanced MO methods: SCF theory for molecules, Slater determinants, electron repulsion integrals. Roothan's equation. ZDO approximations, PPP, CNDO and INDO approximations. Hellman-Feynman theorem: some simple applications

Learning Outcomes

After completion of the course, the students will be able to:

1. Understand the basic principles and concepts of quantum mechanics.
2. Solve the Schrödinger equation for simple model systems of relevance within chemistry.
3. Approximate Schrödinger equation for multi electron systems.
4. Understand the basic concept of VB theory.
5. Apply Huckel theory in simple conjugated molecules.

20-304-0104 – Stereochemistry, Pericyclic Reactions and Photochemistry

Unit I- Nomenclature and Aromaticity

IUPAC system for nomenclature of acyclic and cyclic organic molecules with or without functional groups. Nomenclature for regio and stereoisomers. Criteria for aromaticity. Huckel rule and Craig's rule. Aromaticity of benzenoid and non benzenoid compounds. Aromaticity of annulenes, fused rings, catenanes, rotaxanes, metallocenes, cyclic carbocations and carbanions, mesoionic compounds, fullerene, carbon nanotube and graphene. Anti-aromaticity and homo aromaticity. Study of aromaticity via NMR technique.

Unit II - Stereochemistry and Conformational Analysis

Basic concepts in chirality, axial, planar, and helical chirality. Stereochemistry and absolute configuration of molecules with C, N, and S based chiral centers, molecules with more than one chiral centers, allenes, biphenyls, binaphthyls, ansa compounds, cyclophane compounds, spiranes, exocyclic alkylidene cycloalkenes. Topocity and prostereoisomerism. Geometrical isomerism. Principles of asymmetric synthesis. Enantio and diastereoselective synthesis. Stereoselective addition to carbonyl group: Crams and Felkin-Anh Model. Chiral reagents and chiral catalysts. Conformations of alkane, cycloalkanes and biased systems. Effect of conformation on the reactivity of cyclohexane, decalin and their substituted derivatives**.**

Unit III - Physical Organic Chemistry

Relation between thermodynamic stability and rate of reaction, Kinetic versus thermodynamic control, Hammond postulates, potential energy diagram, Hammet equation and linear free energy relationship, substitution and reaction constants, Taft equation, Salt and solvent effects, labeling and kinetic isotopic effect.

Unit IV - Pericyclic Reactions

Classification of pericyclic reactions: electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions. Woodward Hoffman's rules: Frontier Orbital and orbital symmetry correlation approaches, PMO method. Fluxional molecules. Stereochemical aspects in Diels-Alder, 1, 3 dipolar cycloaddition and ene reactions. Pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans, and Sommelet-Hauser rearrangements.

Unit V - Photochemistry

General principles, fate of excited state, jablonsky diagram, photochemistry of alkenes, dienes and polyenes, carbonyl compounds, Norrish type I and II reactions, Patterno–Buchi reaction, Fries and Di-π methane rearrangements. Photochemistry of fragmentation reactions such as Barton and Hofmann-Loffler-Freytag reactions.

Learning Outcomes

After completion of the course, the students will be able to:

1. Analyse the nomenclature and aromatic nature of various organic molecules.
2. Determine the stereochemistry and conformations of organic molecules, stereochemical and conformational effect in the reactivity, and research field application in the creation of new functional organic molecules.
3. Differentiate kinetic and thermodynamic product yield depend upon the various physical and chemical process
4. Understand the thermal and photochemical processes, the favourability of reaction and stereochemistry of reaction products when the processes are continued in 4nπ and (4n+2) π systems
5. Explain the role of light in the electronic excited state process of organic molecules and some photochemical reactions.

References

1. T. W. Graham Solomons, Craig B. Fryhle, Scott A. Snyder, Organic Chemistry, 12th ed., 2016
2. R. S. Dhillon, C. Baskar & S. Baskar, “Systematic Nomenclature of Organic Compounds”, Wiley, Dreamtech Press, 1st ed., 2019
3. P. S. Kalsi, Stereochemistry: Conformation and Mechanism, New Age Publishers, 10th ed., 2019
4. L. Poppe, M. Nógrádi, J. Nagy, G. Hornyánszky, Z. Boros, Stereochemistry and stereoselective synthesis: An Introduction, Wiley, 1st ed., 2016
5. Michael B Smith, “March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure”, 8th ed., Wiley, 2019.
6. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, New Academic Science; 4th Revised ed., 2012
7. Pierre Vogel, Kendall N. Houk, Organic Chemistry: Theory, Reactivity and Mechanisms in Modern Synthesis, Wiley, 1st ed., 2019
8. Sunil Kumar, Vinod Kumar S.P. Singh Pericyclic Reactions: A Mechanistic and Problem-Solving Approach, Elsevier, 1st ed., 2015

9. S. Sankararaman, Roald Hoffmann, Pericyclic Reactions - A Textbook: Reactions, Applications and Theory, Wiley, 1st ed., 2015
10. Ian Fleming, Pericyclic Reactions, Oxford University Press, 2015
11. Jagdamba Singh, Photochemistry and Pericyclic Reactions, New Age International Publishers, 4th ed., 2019
12. V. Balzani, P. Ceroni, A. Juris, Photochemistry and Photophysics: Concepts, Research, Applications, Wiley, 1st ed., 2014.
13. J. Clayden, N.Greeves, S. Warren, Organic Chemistry, Oxford University Press, 2nd ed., 2014
14. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Principles of Molecular Photochemistry, Viva Books, 2nd ed., 2019.

20-304-0105 – Practical I - Analytical Techniques

1. Spectrophotometric estimation of Fe, Cr, Mn, Ni, Cu.
2. Flame photometry – Determination of sodium, potassium, calcium and lithium.
3. Electrochemical methods
   a) Conductometry – Cell constant, conductivity of a weak acid, solubility of sparingly soluble salt, conductometric titrations
   b) Potentiometry – Measurement of electrode potential, activity coefficients and potentiometric titrations
   c) Polarography – Estimations of cations and organic compounds. Estimation of trace metals by stripping voltammetry
   d) Nephelometry/ Turbidimetry – estimation of sulphate, transparency of water
   e) Amperometry - Estimation of metals.

Learning Outcomes

After completion of the course, the students will be able to:

1. Estimate the concentration of metals using a spectrophotometer
2. Determine the concentration of alkali and alkaline earth metals using flame photometer
3. Apply electrochemical methods in sample analysis

References

1. J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham. Vogel's Text Book of Quantitative Inorganic Analysis, 5th edn., Longman Scientific and Technical, 1989
2. H.H. Williard, L.L. Merit, J.A. Dean and F.A. Settle. Instrumental Methods of Analysis, 7th edn., CBS Publ. And Distrib, 1989.
3. AOAC, Official Methods of Analysis of AOAC 19th edn., Washington, 2012
4. K.Grasshoff. M. Ehrhardt and K. Kremling. Methods of Seawater Analysis 3rd edn., Wiley-VCH, 1999
5. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.
6. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001
7. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005
8. APHA, Standard Methods for the Examination of Water and Wastewater, 23rd ed., 2017

20-304-0106 – Practical II - Quantitative Chemical Analysis

1. Separation and estimation of simple binary mixtures of metal ions in solutions
2. Titrimetric estimations:
    a. Complexometric titrations using EDTA for the estimation of Ca, Mg, Zn, Ni, hardness of water
    b. Redox titrations with ceric sulphate, dichromate and permanganate for the estimations of ferrous iron, zinc.
3. Estimations of
    a. Phenol, salicylic acid, aniline and sulphanilic acid (Bromate-bromide method)
    b. Glucose and sucrose (Fehling's method)
    c. Acids and esters in a mixture
    d. Carboxylic acids and carboxylic groups (iodometric method)
    e. Estimation of Nitrogen (Kjeldhal's method)
    f. Iodine value and saponification value of vegetable oils

Learning Outcomes

After completion of the course, the students will be able to:

1. Develop excellent laboratory practice skills to arrange the lab and analytical tools depending on specific purposes, data management and archiving.
2. Use EDTA titrations for the estimation of Ca, Mg, Zn, Ni
3. Estimate different organic chemicals in the sample.

References

1. J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham. Vogel's Text Book of Quantitative Inorganic Analysis, 5th edn., Longman Scientific and Technical, 1989.
2. B.S. Furniss, A.J. Hannaford, P.W.G. Smith and A.R Tatchell. Vogel's textbook of Practical Organic Chemistry, 5th ed., Longman Scientific and Technical, 1989
3. Mann and Saunders. Practical Organic Chemistry,4th ed., Orient Longman, 2004.
4. F.J. Welcher, Standard Methods of Chemical Analysis: Vol. 2, R.E. Kreiger Pub., 2006
5. G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.
6. J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry,

Macmillan, 1979

7. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., McMillian, 1968.

Semester II

20-304-0201 – Chemical Oceanography

Unit I - Introduction

Introduction to marine chemistry, the origin of seawater, structure of water, ion-water interactions, the polarized water molecule, colligative properties of seawater, oxidation-reduction potential of seawater, history of oceanography, important oceanographic expeds and oceanographic institutions of the world and India. International collaboration in marine science, Antarctica and polymetallic nodule programmes of India.

Unit II - Major and Minor Elements

Composition of seawater, constancy of relative composition, concept of chlorinity and salinity, methods of measurement. Major and minor elements of seawater - conservative and con-conservative behaviour, geochemical balance, abundance and residence time. Trace elements - concept, origin, types of distribution and fate. Chemical speciation. Water mass identification using T-S diagrams, PO and NO plots. Primary, cosmogenic and artificial nuclides. Applications of radioisotopes in oceanography.

Unit III - Dissolved Gases

Dissolved gases, reactive and non-reactive gases – sources and fluxes. argon as a reference gas, factors affecting the concentration of gases in seawater. Carbon dioxide system – origin, importance and factors governing the distribution, alkalinity, buffer capacity, lysocline and carbonate compensation depth, ocean acidification. Dissolved oxygen - origin and factors governing the distribution, AOU, oxygen minimum zone formation in the ocean, origin and consequences of ocean hypoxia. H_2S and alteration of associated elemental chemistry.

Unit IV - Nutrients Cycle

Dissolved and particulate organic matter - origin, elemental and chemical composition, distribution and fate, ectocrines, extracellular metabolites and humic substances. Blue carbon-**c**arbon sequestration in the coastal systems and contribute to the global carbon budget. Micronutrient elements - nitrogen, phosphorus and silicon, their cycles, distribution profiles and their effect on phytoplankton growth, N/P ratio.

Unit V - Marine Analysis

Protocols and general methods of collection, preservation, pre-treatment and post-treatment of water and sediment samples. Water samplers – Nansen, Niskin, microlayer samplers. Sediment samplers – grabs, corers. General methods of estimation of salinity, major elements, dissolved oxygen, nutrients, trace metals and organic constituents.

Learning Outcomes

After completion of the course, the students will be able to:

1. Gain a comprehensive understanding of the properties and interactions of the substances present in the marine environment
2. Explain the differences between conservative and non-conservative elements and discuss their behaviour, distribution and cycling in the oceans with specific examples of nutrients, major and minor elements.
3. Explain the importance of dissolved gases in seawater and their role in the key processes operating in the marine environment
4. Familiarize with chemical oceanographic practicals like sampling protocols for different types of samples, preservation of samples and analytical methods for various parameters.
5. Identify marine chemical programmes that impact the student's areas of oceanographic interest, and know-how to access and understand information on these processes

References

1. F.J. Millero. Chemical Oceanography 4th ed., CRC Press, Boca Raton, 2013
2. K.S. Stowe. Ocean Science 2nd ed., John Wiley & Sons 1983
3. J.P. Riley and R. Chester. Introduction to Marine Chemistry, Academic Press1971
4. The Open University. Seawater: its Composition, Properties and Behaviour, 2nded., Oceanography Series, Pergamon, 1995.
5. D.F. Martin, Marine Chemistry, vol I and II, Marcel Dekker, New York, 1970
6. R.A. Horne. Marine Chemistry, Wiley-Interscience, London.
7. J.P. Riley and G. Skirrow. Chemical Oceanography, Vols. I to III, Academic Press, 1975
8. R. Sen Gupta and E. Desa. The Indian Ocean – A perspective, Oxford & IBH (Pub), 2001
9. S. B. Libes, An Introduction to Marine Biogeochemistry 2nd ed., Wiley, 2009
10. M.E.Q. Pilson. An Introduction to the Chemistry of the Sea 2nd ed., Cambridge University Press, 2013
11. A.H. Arias and S.E. Botte. Coastal and Deep Ocean Pollution. CRC Press, 2020.
12. N. Rasul and I. Stewart. Oceanographic and Biological Aspects of the Red Sea, Springer, 2019

20-304-0202 – Group Theory and Spectroscopy

Unit I - Group Theory

Basic principles, symmetry elements, point groups, molecular symmetry, matrix representation, group multiplication tables, group representations and character table. Great Orthogonality Theorem (GOT). Construction of irreducible representations, character table and direct product representations, total character calculation, transition moment integral, vanishing of integrals, identification of IR and Raman active vibrations (e.g., H_2O, NH_3, CH_4 , SF_6), electronic spectra, projection operator, setting up of molecular orbitals: hybridization treatment, and construction of hybrid orbitals (e.g., BF_3 & CH_4). Symmetry adapted linear combinations (SALC) and its construction using projection operator, MO's of cyclopropenyl cation, and benzene.

Unit II - Microwave Spectroscopy

Principles of moments of inertia, Rotation spectra of diatomic molecule: Rigid rotor approach-selection rules, intensity of spectral lines and Non-Rigid rotor approach - selection rules. Rotation spectra of polyatomic molecule, effect of low-frequency vibrations, effect of isotopic substitution, effect of nuclear spin, inversion phenomena, torsional vibration, asymmetric, symmetric and spherical top molecules, Stark effect, and determination of bond length.

Unit III – IR and Raman Spectroscopy

Vibrational spectra of diatomic molecules: harmonic and an-harmonic vibrations, selection rules for vibrational transition. Morse function, fundamental, overtones, and hot bands. Vibrational spectra of polyatomic molecules, normal modes of vibrations, rotational character of vibration spectra, different modes of vibrations, vibration-rotation spectra of di-atomic and polyatomic molecule, Fermi resonance and FTIR. Raman spectroscopy: classical and quantum theory. Pure rotational, pure vibrational and vibrational-rotational Raman spectra: selection rules, mutual exclusion principle, rotational constant, vibrational frequency and bond length calculation.

Unit IV - Electronic spectroscopy

Jablonski diagram, Franck - Condon principle, electronic transitions: intensity and type, Kasha's rule, and electronic states of diatomic molecules. Electronic-vibration transitions: Rotational fine structure, electronic spectra of poly atomic and conjugated molecules, photoelectron spectroscopy.

Unit V – NMR, ESR and Mossbauer Spectroscopy

NMR: Basic principle, spin active nuclei, chemical shift and factors affecting chemical shift value, shielding effects, chemical and magnetic equivalence, spin-spin interaction, coupling constant and factors influencing coupling constant, Karplus relation, measurement techniques, principles and applications: FT-NMR, COSY, NOE and INEPT. Electron Spin Resonance spectroscopy: theory, basic principle, g factor, hyperfine interactions, equivalent and non-equivalent protons, Kramer's theorem. Mossbauer spectroscopy: basic principle, recoil effect, isomer shift and factors affecting isomer shift, nuclear quadruple splitting, Idntification of Mossbauer of inorganic complexes.

Learning Outcomes

After completion of the course, the students will be able to:

1. Understand the basic principles of group theory.
2. Construct the character tables of simple molecules.
3. Describe the basic principles of spectroscopy used in chemical analysis.
4. Discuss the quantum mechanical treatment for spectroscopy
5. Solve problems in spectroscopy

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3. P. W. Atkins and J de Paula. Physical Chemistry, Oxford University Press, 9th edition, 2010
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8. M. C. Day and J.Selbin. Theoretical Inorganic Chemistry, Van Nostrand – Reinhold, 3rd edition,1976
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20-304-0203 – Natural Products and Organic Synthesis

Unit I - Reaction Intermediates and Mechanism

Generation, structure, stability, and reactivity of intermediates such as carbocations, carbanions, carbon-free radicals, carbenes, nitrenes, and arynes. Non-classical carbocations, and neighbouring group participation. The effect of substrate, reagent, leaving group, solvent and neighbouring groups on organic reactions. Organic reaction mechanisms with special reference in substitution, elimination and addition reactions.

Unit II – Organic Named Reactions

Carbocation chemistry: Wagner-Meerwein, Pinacol-pinacolone, Noyori annulation, Prins reaction etc. Carbanion chemistry: Knoevenagel, Michael addition, Favorski Rearrangement, Wittig reaction, Baeyer-Villiger oxidation, Julia elimination etc. Carbene Chemistry: Wolff rearrangement, Simmon smith reaction etc. Nitrene chemistry: Hoffmann, Curtius, Lossen, Beckmann rearrangement etc. Free radical chemistry: Sandmayer reaction, Gomberg reaction, Barton deoxygenation and decarboxylation, McMurry coupling.

Mannich reaction, Robinson annulation, Stork enamine, Heck coupling, sharpless asymmetric epoxidation, Woodward and Prevost hydroxylation, Oppenauer oxidation, Clemmensen and Wolf-Kishner and Birch reduction, Meerwein-Pondorff-Verley reduction.

Unit III – Reagents in Organic Synthesis

Complex metal hydrides: organolithium, organomagnesium, and organozinc reagents, Gilman,s reagents, lithium diisopropyl amide, dicyclohexyl carbodimide, 1, 3-dithiane (reactivity umpolung), trimethylsily iodide, tri-n-butyltin hydride, osmium tetroxide, DDQ, DCC, selenium oxide, phase transfer catalysts, crown ethers, and Merrifield resin, Wilkinson’s catalyst, Bakers’s yeast.

Unit IV – Chemistry of Heterocyclic Compounds

Nomenclature and classification of heterocycles. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S); three and four-membered heterocylic ring (azirine, oxirane, azitidine, oxetene, oxitane and thetane), five and six-membered heterocyclic rings and fused ring compounds: indole, quinoline, isoquinoline, coumarin, flavone, purine and pyrimidine bases.

Unit V – Chemistry of Natural Products

Broad classification and basic structural aspects of terpenoids, alkaloids, plant pigments, steroids and lipids, Determination of carbon skeleton of alkaloid using Hofmann, Emde, and

Von Braun degradation methods, Synthesis and structural elucidation of camphor and nicotine, Structure and synthesis of cyanin, papaverine, quercetin, testosterone, progesterone and prostaglandins. General bio-synthetic pathway of alkaloid, terpenoids, and steroids.

Learning Outcomes

After completion of the course, the students will be able to:

1. Identify the most probable intermediate, type of mechanism and the effect of "substrate to solvents" in organic reactions.
2. Acquire a general idea of important organic named reactions, its mechanism and applications in the synthetic field.
3. Identify the reagents, its nature, function and suitability in various organic reactions.
4. Recognize the organic reaction mechanism, which is following heterocyclic chemistry.
5. Classify and elucidate the expected structure of natural products in the view of general organic reactions.

References

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6. T. W. Graham Solomons, Craig B. Fryhle, Scott A. Snyder, Organic Chemistry, 12th ed., 2016
7. Richard O. C. Norman, J. M. Coxon, Principles of Organic Synthesis, CRC Press, 3rd ed., 2017
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20-304-0204 – Thermodynamics and Statistical Mechanics

Unit I - Laws of Thermodynamics

Concept of entropy. Reversible and irreversible process. Clausius inequality, free energies and maxwell's relations. Gibbs-Helmholtz equations. Third law of thermodynamics and calculation of entropy. Criteria of spontaneity. Free energy and entropy of mixing. Fundamental equations in open systems. Gibbs Duhem equation. Partial molar quantities. Chemical potential: fugacity, activity and activity coefficients

Unit II – Thermodynamics of Solutions

Duhem Marghules equation. Clausius-Clapeyron equation and its applications. Equilibrium constants: Temperature dependence of equilibrium constants. Van-Hoff equation. van't Hoff's reaction isochore and isotherm. Relation between K_P , K_C and K_X. Fundamentals and advances in the study of Phase Equilibria. Phase diagram of two and three-component systems.

Unit III – Statistical Mechanics

Thermodynamic probability, Stirling's approximation, Ensemble, Boltzmann distribution and molecular partition function, Translational, rotational and vibrational partition functions, Relationship between partition functions and thermodynamic properties, Sackur-Tetrode equation. Statistical formulation of the third law of thermodynamics, Residual entropy, Quantum Statistics: Fermi-Dirac and Bose-Einstein and Maxwell Boltzmann statistics, Heat capacity of solids-the vibrational properties of solids, Einstein's theory, Debye theory, Limitations of these theories.

Unit IV - Thermodynamics of Irreversible Processes

Postulates of irreversible processes**. N**on-equilibrium stationary states. Entropy production: rate of entropy production. Entropy production via heat transfer and chemical reactions. Phenomenological relations. Onsager reciprocal relations. Onsager relations in thermodynamics and chemical kinetics point of view. Thermal osmosis. Thermoelectric phenomena: Seebeck, Peltier, Thomson effect and their comparison.

Unit V - Bioenergetics

Coupled reactions. ATP and its role in bioenergetics. High energy bond. Free energy and entropy change in ATP hydrolysis. Thermodynamics aspects of metabolism, and respiration and glycolysis. Biological redox reactions.

Learning Outcomes

After completion of the course, the students will be able to:

1. Explain fundamental thermodynamic properties, energy and entropy concept of the systems, and solve the problems behind it.
2. Understand the role of Clausius-Clapeyron equations, and Van-Hoff equations, and the Gibbs phase rule in the equilibrium media and solutions.
3. Describe fundamental idea on the way of the distribution of particles, the relation between thermodynamic properties and partition function and statistical interpretation of various thermodynamic properties.
4. Become familiar with postulates, entropy production, thermal osmosis, thermoelectric phenomena and Onsager relations of irreversible thermodynamic processes.
5. Investigate the role of thermodynamic process in various metabolic pathways of living cells and find the queries and answers behind it.

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6. K. Stowe, An Introduction to Thermodynamics and Statistical Mechanics, Cambridge, 2016
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14. Y. Demirel, V. Gerbaud, Non-equilibrium Thermodynamics: Transport and Rate Processes in Physical, Chemical and Biological Systems, Elsevier, 4th ed., 2018

20-304-0205 – Practical III - Separation and Synthetic Methods

1. Separation and identification of organic binary mixtures
    a) Separation of components by physical and chemical methods
    b) Purification of components by suitable methods
    c) Characterization of functional groups, if any, by systematic analysis
    d) Preparation and purification of solid derivatives
    e) Determination of physical constants
2. Preparation of organic compounds

Preparation of organic compounds involving nitration, sulphonation, halogenation, diazotization, Friedal-craft reaction, Claisen condensation, Grignard reaction, benzoin condensation, benzilic acid rearrangement and catalytic hydrogenation.

3. Chromatographic techniques

Chromatographic techniques: Column Chromatography, Paper Chromatography, Thin layer Chromatography

4. Synthesis and characterization

Synthesis and Characterization (Metal content and interpretation of IR and electronic spectra)

a) Inorganic complex compounds (common transition metals and common oxygen, nitrogen or Sulphur donor ligands)
b) Organometallic compounds

Learning Outcomes

After completion of the course, the students will be able to:

1. Separate, characterize and identify organic liquid mixtures
2. Separate, characterize and purify organic liquid mixtures using multiple chromatographic methods
3. Synthesis and characterize the fundamental organic molecules.

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1. P. B. Cranwell, L. M. Harwood, C.J. Moody, Experimental Organic Chemistry, Wiley-Blackwell, 3rd ed., 2017
2. A.I. Vogel, A. R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogel's Textbook of Practical Organic Chemistry, Prentice Hall, 5th ed., 1989

3. A.I. Vogel, Elementary Practical Organic Chemistry: Quantitative Organic Analysis, Pearson Education, 2^{nd} ed., 2010
4. F. G. Mann, B. C. Saunders, Practical Organic Chemistry,4^{th} ed., 2009
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6. R. Keese, M. P. Brändle, T.P. Toube, Practical Organic Synthesis: A Student′s Guide, Wiley, 1^{st} ed., 2006
7. A. Hassner, I. Namboothiri, Organic Syntheses Based on Name Reactions: A Practical Guide to 750 Transformations, Elsevier, 3^{rd} ed., 2011
8. N. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 6^{th} ed., Wiley-Inter science, 2009.

20-304-0206 – Practical IV - Water and Sediment Analysis

1. Sampling of water (microlayer, surface, sub-surface) and sediment (surficial and sub-surface)
2. Filtration and separation of different phases (dissolved, colloidal and particulate). Storage and preservation of water and sediment samples for environmental analysis.
3. Determination of dissolved oxygen, oxygen saturation, biochemical oxygen demand, chemical oxygen demand, dissolved organic carbon and particulate organic matter.
4. Determination of trace gases (methane, nitrous oxide and carbon dioxide) and hydrogen sulphide
5. Determination of pH (sensor and spectrophotometer), Eh and alkalinity.
6. Determination of nutrients – nitrate, nitrite, ammonia, urea and total nitrogen – reactive and total phosphate – silicate.
7. Determination of pigments (Chlorophyll a, b, c and phaeopigments) and primary productivity.
8. Determination of sediment texture, organic carbon, total nitrogen and total Sulphur

Learning Outcomes

After completion of the course, the students will be able to:

1. Use sampling and storage techniques in marine sampling
2. Analyse samples for basic hydrographical parameters
3. Interpret carbonate chemistry in the aquatic system

References

1. K.Grasshoff. M. Ehrhardt and K. Kremling. Methods of Seawater Analysis 3rd edn., Wiley-VCH, 1999
2. APHA, Standard Methods for the Examination of Water and Wastewater, 23rd ed., 2017
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1984

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7. T.R. Crompton. Analysis of Seawater: A Guide for the Analytical and Environmental Chemist. Springer, 2006

Semester III

20-304-0301– Aquatic Chemical Resources

Unit I - Aquatic Resources

Introduction. Classification - Renewable and non-renewable energy resources, Types of Marine Resources. - Marine Mineral Resources. - Marine Energy Resources. - Marine Food Resources. Water Resources , Occurrence, Effects, and Removal,. Marine Macroalgae and Microalgae and Bioproduction: fish, aquaculture products, fish oils, crustacean and mollusc shells; Benefits and Challenges. Bioproduction of Chitin and Its Derivatives, Isolation and Extraction of Chitin and Chitosan, Structure, Source and Properties of Chitin/Chitosan, Derivatives of Chitin/Chitosan, Utilization of Chitin/Chitosan for Chemicals and Materials Microalgae Groups, Bioproduction, Feedstock Products and Coproducts, Animal Feed, Human Food, Nutraceuticals, Biopolymersfor Chemicals and Fuels: Feedstock Products and Coproducts: Bioethanol, Biodiesel, Biobutanol, Bio-oil.

Unit II - Renewable Energy Resources

Solar, wind, water (hydro), biomass and geothermal; Solar energy, wind power, hydropower, tidal and wave power, geothermal heat;

Unit III - Non-renewable Energy Resources

classification . Construction material, including sand, gravel, and other high bulk materials. Industrial materials, including silica sand, aragonite, phosphates, and sulfur. Metallic minerals, like gold, platinum, tin, titanium, and rare earth metals. Metalliferous oxides, which contain manganese, copper, nickel, and cobalt. Metalliferous sulfides, including copper, lead, zinc, chromium, and gold. Manganese nodules, VMS ore deposits. Fossil fuels (coal, petroleum and natural gas); Aquifers; Nuclear fuels -- As energy sources and their demands; Oil reserves-Petroleum products, Octane, gasoline, lubricants; Gas hydrates, Inorganic Chemicals from the sea; Extraction and recovery of chemicals - Halide, Magnesium, Potassium and Gold.

Unit IV - Overview on Marine Energy Sources

Kinetic Energy (winds and currents); Potential Energy (tides); Mechanical Energy (waves); OTEC. Osmotic Pressure, Tidal Energy, Current Energy, Wave Energy, Biomass Conversion,Ocean thermal Energy; Geothermal Energy-Hydroelectric Power; Hydrokinetic Energy; Nuclear Energy; Benefits and challenges.

Unit V – Desalination: Distillation, Solar evaporation, Freezing, Electrodialysis, Reverse Osmosis, Ion-exchange and Hydrate formation; Flash Desalinization , freezing And Salt Absorbtion. Principles and applications; Advantages and limitations.

Learning Outcomes

After completion of the course, the students will be able to:

1. Classify Renewable and non-renewable energy resources and discuss its importance.
2. Describe the different energy sources for sustainable development.
3. Apply scientific methodologies to extract commercially important chemicals from the sea
4. Explain simple methodologies for harvesting energy from the sea.
5. Apply different methodologies for desalination of seawater.

References

1. E.D Howe. Fundamentals of Water Desalination, Marcel Dekkar, 1974.
2. H.G. Heitmann. Saline Water Processing, Wiley-VCH, 1989.
3. B. F. Chhapgar. Understanding the Sea, BNHS, Oxford University Press, New York, 2013.
4. P. R. Pinet. Invitation to Oceanography, Jones & Bartlelt Publishers, Marsachuselts, 3rd ed., 2010.
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8. M. K. Francesca and Y. Ning. Fuels , Chemicals and Materials from the oceans and aquatic sources; John Wiley and Sons Ltd, 2017.

20-304-0302 – Organic Spectroscopy

Unit I - Chirooptical Spectroscopy

ORD, CD, Octant rule, axial halo ketone rule and Cotton effect. Applications of chiroptical spectroscopy.

Unit II - UV-Vis and Emission Spectroscopy

Basic principles and laws of UV-Vis spectroscopy. Electronic transitions in organic molecules. Woodward-Fieser and Fieser-Kuhn rules. Estimation of λ_{max} of substituted aromatic ketones, aldehydes and acids. Influence of substituent, solvent, ring size and strain on spectral characteristics. Fundamentals of emission spectroscopy. Kasha's rule. Molecular characterization via absorption and emission spectra.

Unit III - IR Spectroscopy

Principles of characteristic group absorption of organic molecules, spectral feature of major functional groups. Effect of substituents, ring size, vibrational coupling and hydrogen bonding on vibrational frequency.

Unit IV - NMR Spectroscopy

NMR phenomena. Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shifts and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic equivalence of spins, local paramagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales. Spin-Spin coupling. Structural correlation to coupling constants, First-order and non-first order spectra, Pascal's triangle, AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, Karplus curve: variation of coupling constant with dihedral angle. Simplification methods of complex spectra by high field NMR, shift reagents, chemical exchange and double resonance. Distinction of enantiotopic and diastereotopic faces via NMR. Applications of NOE, COSY, DEPT, INEPT, APT and INADEQUATE techniques.

Unit V - Mass Spectroscopy

Basic principles. Ionization techniques (EI, ESI, CI, FAB, FD). Isotopic abundance. Molecular ion, Basic fragmentation types and rule, Factors influencing fragmentation, Fragmentation patterns. Nitrogen and ring rules. Mc-Lafferty rearrangement. Applications: HRMS, MALDI-MS, LC-MS, GC-MS.

Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, NMR, and Mass spectroscopy.

Learning Outcomes

After completion of the course, the students will be able to:

- Explain the fundamental idea of octant rule, axial halo ketone rule, cotton effect and their applications to determine the chirality of chiral organic molecules.
- Characterize conjugated organic molecules via absorption and emission spectral features, l_{max} value, and influence of substituent, solvent, ring size and strain.
- Identify different functional groups and bonds present in the organic molecules through well-known IR stretching and bending vibrational values of corresponding groups
- Determine the basic structure of organic molecules using NMR data and identify whole structure with exact stereochemistry effectively using various kinds of NMR techniques.
- Count the molecular weight of a variety of organic compounds via selective fragmentation techniques and identify the compounds which have isotopes.

References

1. P. L. Polavarapu, Chiroptical Spectroscopy: Fundamentals and Applications, CRC Press,1st ed., 2016
2. D. L. Pavia, G. M. Lampman, G.S. Kriz, J. A. Vyvyan, Introduction to Spectroscopy, Cengage, 5th ed., 2015.
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14. L. D. Field, H. L. Li, A. M. Magill, Organic Structures from Spectra, Wiley, 6th ed., 2020

20-304-0303 – Solution Chemistry

Unit I - Theories of Reaction Rates

Potential energy surfaces for bimolecular reactions, Collision theory, Transition state theory, Activation/thermodynamic parameters and Eyring equation. Various theories of Unimolecular reactions: Lindemann-Christiansen hypothesis, Hinshelwood, RRK, RRKM theories and non RRKM behaviour, Elementary reactions in solutions: influence of solvent properties on rate, Different types of molecular interactions in solutions, Diffusion and activation controlled reactions.

Unit II - Kinetics in The Excited States and Fast Reaction

Relaxation methods, Stopped flow methods, Laser Flash Photolysis, Flow tube methods, and Laser-based experiment techniques. Jablonski diagram: Franck-Condon principle, Kasha's rule and characteristics of absorption and emission. Kinetics of Unimolecular and bimolecular photophysical and photochemical processes, Quenching of fluorescence, fluorescence resonance energy transfer (FRET), Theory of energy transfer for donor-acceptor pair, Theory of collisional quenching, static quenching and combined dynamic and static quenching.

Unit III - Electrolyte and Non-Electrolyte Solution Theories

Van Laar theory, Vander Waal theory, Scatchard-Hildebrand theory. Lattice theory, Prigogine cell theory, Flory equation of state theory, Prigogine-flory-Patterson theory, Extended real association solution (ERAS) model and Kirkwood-buff theory. Drude and Nernst's electrostriction model and Born's model, Debye-Huckel Theory and applications, Debye-Falkenhagen and Wien effect, conductance with high potential gradients, Debye-Huckel limiting law and its extensions, activity and activity coefficients, ionic strength.

Unit IV - Electrode Kinetics

Current-potential relationship: Butler-Volmer, Tafel equation and their significance. Metal/Solution interfaces, Influence of double electrode layer on reaction constants. Different types of overpotentials and its effect on electrochemical reaction rates. Marcus kinetics and quadratic dependence of Gibbs free energies. Mechanism of hydrogen evolution and oxygen reduction in acid and alkaline media.

Unit V - Corrosion

Corrosion: Different types and its Environmental Impact. Thermodynamics of electrode potentials and corrosion. Fundamentals of Pitting-Bedworth ratio, Evans diagram, and Pourbaix diagrams. Pourbaix diagrams of water, iron and aluminium. Kinetics of corrosion:

polarization and corrosion rate, and corrosion rate measurements. Polarization: measurements and problems, Polarization diagram of corroding metals. Calculation of IR drops in an electrolyte. Stern Geary equation; mixed potential theory and prevention of corrosion.

Learning Outcomes

After completion of the course, the students will be able to:

1. Explain rate theories to solve problems behind of rate constant, rate and efficiency of uni and bimolecular reactions.
2. Discuss the kinetics of fast reactions and excited states which can then apply to figure out the mechanism of the complex physical and photophysical process.
3. Apply Debye theories and extended theories of Vander Waals for electrolyte and non-electrolyte solutions.
4. Explain the electrode double layer and various over potential involved during the operation of the cell, and their effect on electrochemical reaction rates.
5. Apply theories to analyze activity, activity coefficients, ionic strength, current, and overpotential under given conditions, and rate and amount of corrosion.

References

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15. K. J. Vetter, Electrochemical Kinetics: Theoretical Aspects, Academic Press, 2013

20-304-0304 – Practical V - Instrumental Techniques I

1. Water/sediment/biological sample preparation for trace metals analysis
2. Analysis of metals using,
   a. Atomic Absorption Spectrophotometry
      i. Flame methods – Copper, cadmium, zinc, lead, manganese, iron
      ii. Hydride generation – Mercury, arsenic, selenium, tin
      iii. Graphite furnace method
   b. Inductively coupled plasma (ICP-OES)- Copper, cadmium, zinc, lead, manganese, iron
3. Voltammetry- Speciation analysis of iron in the samples
4. Ion chromatography- Determination of cations and anions in the water samples

Learning Outcomes

After completion of the course, the students will be able to:

1. Prepare aquatic samples for trace metal analysis.
2. Analyse samples for trace metals using sophisticated instruments
3. Determine cations and anions in the water samples using ion chromatography

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1. D.T.E. Hunt and A.L. Wilson. The Chemical Analysis of Water, 2nd ed., Royal Society of Chemistry, 1986
2. Instrumental Manuals of AAS, Fluorescence Spectrophotometer, GC and CHN Analyzer.
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Sediments, UNESCO, 1982. R.M Silverstein, Spectrometric identification of organic compounds

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13. T.R Chrompton, Analysis of Oceanic Waters and Sediments, CRC press, 2016

20-304-0305 – Practical VI - Physicochemical Methods

1. Phase Diagram
    a) Simple eutectic
    b) Miscible liquids
    c) Partially miscible liquids
    d) Critical solution temperature and effect of electrolytes and non-electrolytes
    e) Three-component system
2. Distribution Coefficients
    a) Partition coefficient
    b) $I\text{-}I_3$ equilibrium
3. Kinetics

    Acid-base catalysed hydrolysis of esters, the dependence of temperature and ionic strength on the rate of reactions.
4. Refractometry
    a) Identification of simple organic liquids and oils
    b) Molar refraction of solids
    c) Study of complex formation

Learning Outcomes

After completion of the course, the students will be able to:

1. Construct phase diagram of 1, 2 and 3 component systems and determine unknown concentration
2. Determine the partition coefficient of substance between two liquid media and its unknown concentration.
3. Identify organic liquids, oils and solids using refractometry
4. Conduct acid and base catalyzed hydrolysis of esters, and investigate factors responsible for altering the rate of reaction.

References

1. F. W. Gray, A Manual of Practical Physical Chemistry Paperback, Wentworth Press, 2016
2. A. Findlay, Practical Physical Chemistry, Franklin Classics Trade Press, 2018

3. J. B. Yadav, Advanced Practical Physical Chemistry, Viva Books, Krishna Prakashan Media (P) Ltd, 2015.
4. B. Vishwanathan, P.S. Raghavan, Practical Physical Chemistry, Viva Books, 1st ed., 2012
5. C. W Garland, J. W Nibler, D. P Shoemaker, Experiments in Physical Chemistry, McGraw Hill, 8th ed., 2009

Elective courses

20-304-0001 – Analytical Chemistry

Unit I – UV-Vis Spectrometry

UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments-sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.

Unit II - Fluorescence Spectrometry

Fluorometers: photoluminescence and concentration-electron transition in photoluminescence, instrumentation details. Introduction to photoacoustic spectroscopy.

Unit II - IR Spectrometry

Instrumentation, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR and MDIR absorption spectrometry. Application in qualitative and quantitative analysis.

Unit IV - Electroanalytical Methods

Potentiometry: techniques based on potential measurements, different types of indicator electrodes, glass electrode, ion-selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, Potentiometric titrations-types and applications.

Unit V - Polarography and Voltammetric Techniques

Potential and current variations at the microelectrode systems, conventional techniques for concentration determination, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography. Anodic stripping voltammetry, Organic polarography. Biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications.

Learning Outcomes

After completion of the course, the students will be able to:

1. Apply UV-Vis spectrophotometer in analytical chemistry.
2. Explain the IR spectra of simple molecules.
3. Discribe the instrumentation of molecular spectrophotometers.
4. Use electrochemical tools in quantitative and qualitative analysis.
5. Explain the use of polarography and voltammetric techniques in analytical techniques.

References

1. J. Bassett, R.C. Denney, G.H.Jeffery and J.Mendham. Vogel's Text Book of Quantitative Inorganic Analysis 4th edn., ELBS, 1982
2. R. Caulcutt and R.Boddy. Statistics for Analytical Chemists, Chapman and Hall, 1983
3. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch. Fundamentals of Analytical Chemistry, 9th edn., Cengage Learning, 2013.
4. F.W. Fifield and D.Kealey. Principles and Practice of Analytical Chemistry 5th edn., Wiley-Blackwell, 2000.
5. D.A. Skoog and J.J. Leary. Principles of Instrumental Analysis 4th edn., Saunders College Publ., 1992.
6. Jürg P. Seiler, Good Laboratory Practice – the Why and the How, Springer-Verlag Berlin Heidelberg New York.

20-304-0002 – Applications of Coordination Compounds

Unit I – Complexes in Inorganic Qualitative Analysis

Separation, masking, reductive complexation, identification of metals.

Unit II– Complexes in Gravimetric Analysis

Role of organic precipitants in gravimetric analysis, important inorganic precipitants, criteria for the choice of organic precipitants

Unit III– Complexometric Titrations

Chelates in complexometric titration, stability of metal –EDTA complexes, metallochromic indicators, titration methods employing EDTA, determination of water hardness

Unit IV– Complexes in Solvent Extraction

Principles of solvent extraction, classification of extractions, extraction by chelation, separation of metals, solvent extraction with crown ethers and cryptands

Unit V– Metal Complexes as Catalysts

Homogeneous catalysis using organometallic compounds: Reactions of organometallic complexes, ligand cone angle oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack of coordinated ligands, olefin hydrogenation, hydroformylation, Wacker process, olefin metathesis, Monsanto acetic acid synthesis,. Application of complexation in leaching, solvent extraction, flotation and purification of metals

Learning Outcomes

After completion of the course, the students will be able to:

1. Understand the role of coordination compounds in the qualitative analysis of metal ions.
2. Explain the role of organic ligands in gravimetric analysis of metal ions
3. Discuss the application of complexes with multidentate ligands in volumetric analysis of metal ions.
4. Explain the role of metal complexes in solvent extraction of metal ions.
5. Discuss the application of metal complexes as catalysts and their uses in metallurgy.

Reference:

1. J.E. Huheey, E.A. Keiter and R. L. Keiter. Inorganic Chemistry: Principles of Structure and reactivity, 4^{th} ed., Addison Wesley Publ. Co., 1993 (Chapter 11, 12, 13 and 15).
2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6^{th}ed. Wiley Eastern,

New Delhi, 1999 (4^{th} and 5^{th} eds. preferred)

3. D.F. Shriver and P.W. Atkins. Inorganic Chemistry, 5^{th}ed., Oxford University Press, 2010
4. D. Banerjea. Coordination Chemistry, 3^{rd} ed., Tata McGraw – Hill, New Delhi. 2009
5. N.N. Greenwood and A. Earnshaw. Chemistry of the Elements, 2^{nd}ed. Pergamon Press, Exeter, Great Britain, 1997.
6. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch. Fundamentals of Analytical Chemistry, 9^{th} edn., Cengage Learning, 2013.
7. J. Bassett, R.C. Denney, G.H.Jeffery and J.Mendham. Vogel's Text Book of Quantitative Inorganic Analysis 4^{th}edn., ELBS, 1982
8. R. Gopalan and V. Ramalingam Concise coordination chemistry, Vikas Publishing House Pt Ltd..2009

20-304-0003 – Aquatic Pollution

Unit I - Introduction

Major aquatic pollutants and their classification; nature, sources and transport pathways. Marine pollution – Definition (GESAMP), Conservative and non-conservative pollutants; Effect of mining and dredging operation in Aquatic system.

Unit II- Major Marine Pollutants

Types, sources and ecological effects on marine environment – Sewage, Inorganic Chemicals, heavy metal, pesticide, oil, nuclear, thermal, plastic and micro-plastic pollution.

Unit III- Impacts of Toxic Chemicals

Heavy Metals and their sources, toxic effects and impacts, Bio-accumulation and Bio-magnification; Organic Pesticides, types and their toxicity; Polycyclic Aromatic Hydrocarbons, Polychlorinated biphenyls, Radioactive substances

Unit IV - Ecological Impacts

Ocean Acidification, Ocean as a carbon sink, Carbon dioxide in the Ocean and its impact on marine life; Eutrophication, causes and Impacts, Consequences and their remediation; Marine debris and impact on Aquatic life; Prevention and Reduction; Biofouling and corrosion, prevention methods.

Unit V– Monitoring and Control Measures

Pollution monitoring –Physical, chemical and biological methods. Biological indicators, Sentinel organism concept, bioavailability and bioconcentration; Microbial indicators and their potentials; sewage treatment and their designs; Aerobic and anaerobic treatment, softening, disinfection, coagulation, sedimentation, Flocculation.

Learning Outcomes

After completion of the course, the students will be able to:

1. Describe marine pollution and their classification
2. Acquire the knowledge of various marine pollutants and their ecological impacts
3. Discuss the methods for marine pollution monitoring
4. Use ocean management and marine pollution reduction programs.
5. Distinguish bioaccumulation, biomagnification and biotransformation

References

1. Metcalf and Eddy, Wastewater engineering, treatment and resources recovery, 5th ed., McGraw-Hill Science, 2013.
2. V.M. Ehlers and E.W. Steel, Municipal and Rural Sanitation, 5th ed., McGraw-Hill Book Company, Inc., 1987.
3. J.Albaiges, Marine Pollution, Hemisphere Publ. Corp., 1989.
4. E.D.Goldberg, The Health of the Ocean, The UNESCO Press, 1976.
5. L.Landner, Chemicals in the Aquatic Environment, Springer Verlag, 1989.
6. P. Dent, Marine Pollution Year Book, Pergamon Press, 1990.
7. J.W.Moore and S.Ramamoorthy, Organic Chemicals in Natural Waters, Springer Verlag, 1984.
8. J.W.Moore, Inorganic Contaminants of Surface Water, Springer Verlag, 1991.
9. D.J.H.Philips, Quantitative Aquatic Biological Indicators, Applied Science, 1980.
10. D.W.Connell and G.J.Miller, Chemistry and Ecotoxicology of Pollution, John Wiley and Sons 1984.
11. Carl J. Sindermann, Coastal pollution: Effects on living resources and humans (Marine Science Series) 2005.
12. Churchill, R. R and A.V. Lowe, The Law of the Sea, 3rd ed. (Manchester: Manchester University Press) 1983.
13. R. B. Clark,. Marine pollution, Fifth ed. Oxford University Press, New York Inc., 2001
14. J.P. Riley and G. Skirrow, Chemical Oceanography (3rd vol) Academic Press, New York, 1975
15. E. D. Goldberg, The health of the oceans, UNESCO Press. 1976
16. R.B. Clark, Marine Pollution, Oxford Science Publications, 1986.
17. J.D.H. Phillips, Quantitative aquatic biological indicators, Applied Science Publishers, 1980
18. B.K Sharma, and Kaur, H. Krishna Prakasham Mandir, Thermal and radioactive pollution, 1994.
19. K.A. Chandler, Butter Worths Marine and offshore corrosion, 1985

20-304-0004 – Atmospheric Chemistry

Unit I - Composition and Process

Chemical composition of earth's atmosphere, dust, aerosols and clouds. Classification of aerosols, size fractions of dust. Sources and impacts of dust in atmosphere. Cyclic processes – Carbon, Oxygen, Nitrogen and Sulphur cycles. The temperature profile of the Atmosphere – temperature regulation in the thermosphere, stratosphere and troposphere. Greenhouse effect.

Unit II – Reactions

Photochemical processes – photodissociation and ionisation, Reactions of electronically excited species, adiabatic processes and correlation rules. Chemical kinetics – Unimolecular, bimolecular, and termolecular reactions. Condensed-phase, surface and heterogeneous reactions.

Unit III – Ozone

Oxygen only chemistry, reaction scheme, Chapman layers. Influence of trace constituents – catalytic cycles, Null cycles, holding cycles and reservoirs, natural sources and sinks of catalytic species. Heterogeneous and homogenous chemistry. Consequences of ozone perturbation, ozone variations and trends.

Unit IV - Earths Troposphere

Sources, sinks and transport, Oxidation and transformation – Photochemical chain initiation, oxidation steps, Tropospheric ozone production, Biogenic volatile organic compounds, heterogeneous processes and cloud chemistry.

Unit V - Air Pollution

primary and secondary pollutants, sulphur dioxide chemistry, smoke and sulphur pollution, acid rain, photochemical ozone and smog. Ion chemistry in the atmosphere, ionization mechanisms, ions in the stratosphere and troposphere

Learning Outcomes

After completion of the course, the students will be able to:

1. Describe the chemical composition of atmospheric air

2. Explain the chemical processes/reactions in atmospheric layers
3. Describe the formation, reactions, importance and depletion of ozone in the atmosphere.
4. Explain ion chemistry in the stratosphere and troposphere
5. Explain air pollution and its consequences

References

1. R.P. Wayne. Chemistry of Atmospheres, 3rd edn., Oxford University Press, 2000
2. P.V. Hobbs, Introduction to Atmospheric Chemistry, Cambridge University Press, 2000
3. Nigel Bunce. Environmental Chemistry, Wuerz Publishing Ltd., Canada, 1990.
4. D.J. Jacob. Introduction to Atmospheric Chemistry, Princeton University Press, 2000.
5. B. J. Finlayson-Pitts and J. N. Pitts, Jr.Chemistry of the Upper and Lower Atmosphere, Academic Press, 1999.
6. Claudio Tomasi, Sandro Fuzzi, and Alexander Kokhanovsky, Atmospheric Aerosols: Life Cycles and Effects on Air Quality and Climate, 1st ed., Wiley-VCH Verlag GmbH & Co. KGaA, 2017.
7. National Research Council, Classification of Dusts Relative to Electrical Equipment in Class II Hazardous Locations, The National Academies Press, 1982.

20-304-0005 – Chemistry of Biomolecules

Unit I – Introduction to Biomolecules

Metal ions in biological system, Essential and trace elements, Role of different metal ions in biological systems. Metals in medicine: therapeutic applications. Toxic effects of metals (Cd, Hg, Cr and Pb). Broad classification of Metallo biomolecules includes transport and storage proteins, enzymes and non-proteins in terms of their biological functions. Classification, structural and function aspects of organic biomolecules such as amino acids, proteins, nucleic acids, and carbohydrates.

Unit II – Chemistry of Transport and Storage Proteins

Structural features and functions of electron carriers: cytochromes, blue copper proteins and iron-sulphur proteins; metal storage and carriers: ceruloplasmin, ferritin, transferrin; and oxygen binding proteins: myoglobin, haemoglobin, hemerythrin, and hemocyanin. Di-oxygen binding and trigger mechanism in biological systems: cooperative and non-cooperative di-oxygen binding. Features and functions of cytochrome c oxidase, and cytochrome P-450.Heme to hematin.Sickle cell anaemia and effect of carbon monoxide in biological systems.

Unit III – Chemistry of Metalloenzymes

Structural features and functions of hydrolases: carbonic anhydrase, carboxypeptidases and aminopeptidases; oxidoreductases: superoxide dismutase, nitrogenases, hydrogenases and oxidases; and isomerases: coenzymes. Vitamin B_{12}: Structural features and biological importance. Salient features and importance of biological nitrogen fixation. Structure and active site of nitrogenase enzyme.

Unit IV – Chemistry of Non-Proteins

Chlorophyll: structural features and significance in photosynthesis. Photosystem-I and photosystem-II in photosynthesis. Siderophores: active site, structure and biological functions. Molecular mechanism of ion transport across the membrane. Sodium pump, ionophores, and crown ether complexes of $Na^+$and K^+.

Unit V – Chemistry of Proteins and Nucleic Acids

Synthesis of amino acids and polypeptides, Functions and structure of protein: peptide bond and its characters, limitations on folding, Ramachandran plot, influence of side chains. Functions of nucleic acids- structure of RNA and DNA, base pairing, double helices, DNA replication, transcription, and translation. Significance of molecular recognition in DNA and protein structure.

Learning Outcomes

After completion of the course, the students will be able to:

1. Discuss the role of metal ions, amino acids, proteins, nucleic acids and carbohydrates in biological systems.
2. Explain the structural features and biological functions of transport and storage proteins.
3. Describe different kinds of metalloenzymes and its responsibilities in biological systems as an active site.
4. Explain the pathway and mechanism of (i) ion transport and (ii) oxidation of water and reduction of CO_2 to release oxygen and carbon dioxidein photosynthesis.
5. Recognize the influence of structural peculiarities of proteins and nucleic acid in biological functions.

References

1. F. A Cotton, G. Wilkinson, Advanced Inorganic Chemistry, Wiley, 6th ed., 2007
2. J.D. Lee, Concise Inorganic Chemistry, Oxford University Press, 5th ed., 2008
3. D. L. Nelson, M. Cox, Lehninger Principles of Biochemistry, WH Freeman, 7thed, 2017
4. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India, 4thed, 2006.
5. P. S. Kalsi, J. S. Kalsi, Bioorganic, Bioinorganic and Supramolecular Chemistry, New Age International Pvt. Ltd. 2017
6. J. E. McMurry, T. Begley, The Organic Chemistry of Biological Pathways, W.H.Freeman& Co Ltd, 2005
7. D. V. Vranken, G. A. Weiss, Introduction to Bioorganic Chemistry and Chemical Biology, Garland Science, 1sted, 2012
8. R. M. Roat–Malone, Bioinorganic Chemistry: A Short Course, Wiley-Blackwell, 3rd ed., 2020
9. G. R. Chatwal, Bio Organic Chemistry, Himalaya Publishing House, 2010
10. R. R. Crichton, Biological Inorganic Chemistry: An Introduction, Elsevier Science, 1sted, 2007
11. W. Kaim, B. Schwederski, A. Klein, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, Wiley India Pvt Ltd, 2nded, 2012.

20-304-0006 – Chemistry of Radiation, Surface and Inorganic Materials

Unit I – Nuclear Chemistry

Structure and stability. Binding energy and magic numbers. Nuclear reactions: energetics and types of nuclear reactions. Equations of radioactive decay and growth. Neutron captures cross-section and critical size.

Unit II – Radiation Chemistry

Radioactive elements and their decay kinetics. Radioactive equilibrium: transient and secular equilibrium, alpha and beta decay, gamma emission. Radiation and radioactivity measurements: ionization chamber, proportional counter, the Geiger counter, scintillation counter and semiconductor detectors.

Applications of nuclear and radiation chemistry: neutron activation analysis, radioactive tracers, radiometric titrations and radiation dosimetry.

Unit III - Surface Chemistry

Surface tension. Adsorption on solids: Langmuir, Freundlich and BET isotherm-derivation. Colloids: Preparation, properties and stability of colloids. Zeta potential, electrokinetic phenomena and donnan membrane equilibrium. Micro and nanoemulsions. Macromolecules: Introduction, classification and nomenclature. Molecular weight determination methods.

Unit IV - Inorganic Advanced Materials

Solid Electrolytes: Mixed oxides, cationic, anionic solid electrolytes. Solid oxide fuel cells. Rechargeable battery materials. Solid-state chemistry of metal nitrides and fluorides. Intercalation chemistry and metal-rich phases. Inorganic pigments and inorganic phosphors, Basics of molecular materials chemistry - one-dimensional metals. Molecular magnets and inorganic liquid crystals.

Unit V - Spectroscopic Identification of Inorganic Compounds

Structural elucidation of coordination compounds have ligands such as NH_3, H_2O, CO, NO, OH^-, SO_2^-, CN^-, SCN^-, NO^-, CH_3COO^- and halogen. ^{11}B, ^{31}P and ^{19}F NMR analysis of metal nuclides. ESR spectra: Application to Cu (II) complexes and inorganic free radicals. Mossbauer Spectroscopy: application to the studies of Fe and Sn complexes.

Learning Outcomes

After completion of the course, the students will be able to:

1. Discuss the fundamentals of different nuclear reactions and radioactive decay process.

2. Explain the radioactivity of elements, properties and its application in the industrial, medicinal and other fields.
3. Explain various theories based on adsorption of solids, its limitations and importance, and the fundamentals of colloids and macromolecules.
4. Acquire a basic idea on preparation, functions, properties, and applications of advanced solid-state materials
5. Analyze the structure and properties of various inorganic materials using spectroscopic techniques such as NMR, IR, ESR, EPR and Mossbauer spectroscopy.

References

1. G. Friedlander, J. W. Kennedy, E. S. Macias, J. M. Miller, Nuclear and Radiochemistry, Wiley India Pvt. Ltd, 3rd ed., 2013
2. H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International Private Limited, 4th ed., 2011
3. K. W. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, Wiley, 4th ed., 2019
4. G. Raj, Surface Chemistry, Krishan Prakashan, 4th ed., 2014
5. K. L. Kapoor, A Textbook of Physical Chemistry - Dynamics of Chemical Reactions, McGraw Hill Education, 3rd ed., 2017
6. R. S. Drago, Physical Methods in Inorganic Chemistry, affiliated east west press pvt. Ltd., 2012
7. D. W. H. Rankin, Norbert Mitzel, Carole Morrison, Structural Methods in Molecular Inorganic Chemistry, Wiley-Blackwell, 2013
8. H. R. Allcock, Introduction to Materials Chemistry, 2nd ed., 2019

20-304-0007 – Computational Chemistry

Unit I - Introduction

Computation and modeling: Introduction, definition, and scope. Classification of computational methods - Classical methods: molecular mechanics and molecular dynamics, and Quantum mechanics methods: ab initio method, semi empirical methods, basis set approximation, and density functional methods, comparison of methods, principles and applications. Computable Quantities: Potential energy surface, chemical properties and conformational search. Born - Oppenheimer approximation, geometry optimization, saddle point and stationary points.

Unit II – Molecular Mechanics and Computer Simulation Methods

Molecular mechanics: Force field - calculation of interaction and energy, important features of classical empirical force fields like AMBER, CVFF and CHARMM, molecular modeling by molecular mechanics. Molecular dynamic simulation methods: MD simulation using simple models, molecular dynamics with continuous potentials and finite difference methods. Monte Carlo method: Calculation of properties by integration, Monte Carlo simulation of rigid molecules. Calculation of thermodynamic properties, practical aspects of computer simulation, simulation result analysis and error estimation.

Unit III - AB Initio and Density Functional Methods

Hartee-Fock approximation, Self-consistent field treatment of polyatomic molecules, Hartee-Fock method in closed and open shell systems: restricted HF calculation in closed systems, restricted open shell Hartree-Fock (ROHF) and unrestricted Hartree-Fock (UHF) calculations in open shell systems. Density Functional theory, basic principles and calculations, Kohn-Sham approach: the first and the second Hohenberg-Kohn theorems.

Unit IV – Semiempirical and Basis Set Approximation

Approximations in semi-empirical methods, Simple Huckel method: Theory, energy calculation expression of a molecular species, LCAO approximation based expression in molecular wave function, secular equations, slater determinants, and the single matrix equation. Extended Huckel method: minimal valence basis set, calculation of Fock matrix elements and overlap integral, strength, weakness and applications of semi empirical methods. Complete neglect of differential overlap method, basic principle. Hydrogen-like, slater-type and Gaussian type basis functions, classification of basis sets and their nomenclature.

Unit V – Gaussian Program and Calculations

Input files and graphics program for structural determination, main features of Gaussian output files. Graphics programs: Gaussview, Chemcraft, Molda and Molden for analyzing Gaussian output data. Normal modes of vibration: identification and visualization, molecular orbitals: calculation, and interpretation, single point energy calculations, geometry optimization, and frequency calculations. Transition state: transition states optimization and characterization, the normal mode and International Rescue Committee (IRC) analyses.

Learning Outcomes

After completion of the course, the students will be able to:

1. Explain the basic concept, classification and principles of computational chemistry
2. Define molecular mechanics and computer simulation methods, and identify the advantages and disadvantages of these methods for modelling/simulating various scientific problems.
3. Explain the theory behind quantum mechanical methods and therefore design and conduct calculations in several types of systems.
4. Describe the proper methods for determining thermodynamic and electronic properties of molecular systems and be able to analyse the calculated properties critically.
5. Describe Gaussian programs for calculating the preferable geometry, energies, chemical properties, and electronic properties of molecules.

References/Readings

1. C. J. Cramer, Essentials of computational Chemistry: Theories and models, Wiley-Blackwell; 2nd ed., 2004.
2. D. Sullivan, Fundamentals of Computational Chemistry, NY Research Press, 2018.
3. F. Jensen, Introduction to Computational Chemistry, Wiley-Blackwell, 3rd ed., 2017.
4. E. G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer, 3rd ed., 2016.
5. S. Wilson, Methods in Computational Chemistry, Springer, 1992
6. D. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, Wiley-Blackwell, 1st ed., 2001.
7. D. Sholl, J. A Steckel, Density Functional Theory: A Practical Introduction, Wiley-Blackwell, 1st ed., 2009.
8. Thomas Engel & W. Hehre, Quantum Chemistry and Spectroscopy, Pearson education, 3rd ed., 2013.

9. R. Kumari, Computers and their Applications to Chemistry, Alpha Science International Ltd, 2nd revised ed., 2005.
10. K. L. Kapoor, A Textbook of Physical Chemistry, Computational Aspects in Physical Chemistry, McGraw Hill Education, 4th ed., 2019.
11. L. Parrill, Kenny B. Lipkowitz, Reviews in Computational Chemistry, Wiley-Interscience, 1st ed., 2017.

20-304-0008 – Environmental Law and EIA

Unit I – Environment and Sustainable Development:

National and International Perspectives - Population and Development. Environmental Policy and Law: Environmental Policy: Pre & Post Independence Period and Role of Government - Five-year Plans - Forest Policy - Conservation strategy - Water Policy; Conservation of Natural Resources and its Management; Constitution and Environment: Right to Environment - Constitutional provisions on Environment and its Protection - Role of Judiciary on Environmental issues - Evolving of new Principles - Polluter pays principle - Precautionary principle - Public trust doctrine.

Unit II – International Conventions

International conventions in the development of Environmental Laws and its Policy - From Stockholm to recent conventions (Special Emphasis on Major conventions & Protocols)

Unit III – Environmental Laws

The Water Act, 1974 - Pollution of Air, Modalities of control, The Air Act, 1981 - Noise Pollution and its control, Noise Pollution control order - Disposal of Waste, laws on waste, disposal and its control - Transboundary Pollution hazards & RegulationWildlife Protection Act, 1972 - Forest Conservation Act, 1980, Environment protection act, 1986: Environment Protection Rules. International scenario, maritime law, coastal zone regulation, ECO-Mark,

Unit IV – Environmental Impact Assessment (EIA)

Introductory Background: Nexus between development and environment; comparison between economic and ecological criteria: the concept of externality: shared resources: global commons: carrying capacity: origin and evolution of EIA: relationship of EIA to sustainable development: EIA in project planning and implementation: EIA process: evaluation of proposed actions: scoping EIA methodologies: role of GIS in EIA baseline study: risk assessment and risk management: mitigation measures: comparison of alternatives: review and decision making: compensatory actions: green belts: a review of procedures, practices and guidelines in India. Case studies: river valley projects: thermal power plants: mining projects: oil refineries and petrochemicals: tourism coastal zone development.

Unit V – Environmental Audit

Environmental auditing and its importance, types of audits, general audit methodology and basic auditing structure, 1SO14000 requirements of Rule 14 for Environmental Audit under

Environmental Protection Act of 1986, definitions, Consumption audits, pollution audits, hazardous issues and its voluntary audits.

Learning Outcomes

After completion of the course, the students will be able to:

1. Describe the Environmental Policy and Law sustainable natural resource management
2. Explain the importance of international conventions for environmental protection and formulating laws
3. Discuss the international law of sea and coastal zone regulation.
4. Describe the importance of environmental impact assessment for the mitigation of pollutants in the country.
5. Explain the process of environmental auditing and its importance.

References

1. Canter Larry. Environment Impact Assessment, 2nd edn., McGraw Hill Science, 1995.
2. G.J. Rau, and C.D. Wooten. Environmental Impact Analysis Handbook, McGraw Hill. Reference Book, 1980.
3. Glasson, John, Rikki Therievel and Andrew Chadwic. Introduction to Environmental Impact Assessment, 4th edn., Routledge, 2012
4. Kulkarni, Vijay and T.V. Ramchandra. Environmental Management, The Energy and Resources Institute (TERI), 2009
5. Eccleston, Charles H. Environmental Impact Assessment: A Guide to Best Professional Practices, CRC Press, 2011
6. Morris, Peter and RikiTherivel. Methods of Environmental Impact Assessment (Natural and Built Environment Series). Routledge, 2009
7. P. Leelakrishnan. Environmental Law in India, 3rd ed., Butterworths Wadhwa, 2008.
8. Lal's commentaries on Water and Air Pollution laws along with Environment (Protection) Act and Rules, 1986.

20-304-0009 – Estuarine Chemistry

Unit I – Introduction

Classification and nomenclature of estuaries; Physical characteristics of estuaries – Classification on the basis of fluid dynamics principles – Tides and tidal currents in estuaries – Tide producing forces – salinity intrusion– gravity-driven freshwater flow – Estuarine circulation patterns, stratification, mixing and, residence times, depth-averaged and breadth – averaged models.

Unit II – Chemical Environment

Salinity distribution in estuaries – a chemical perspective, flushing time, mixing and flushing times; Conservative and non – conservative properties of dissolved constituents during estuarine mixing, heavy metals in estuaries and the processes affecting its distribution; ion speciation of dissolved elements in the estuary, Behavior of dissolved gases, redox chemistry, Redfield ratio, introduction to nutrient cycling,

Unit III - Estuarine Sediments

Physico-chemical characteristic of estuarine sediments, anoxic sediments and pore water; erosion, transportation, and deposition; coagulation and the turbidity maximum; organic geochemistry and early diagenesis

Unit IV - Biogeochemical Processes

Primary productivity in estuarine waters, mechanism and pathways of organic matter production and transformations; humic material and its importance in estuaries; biogeochemical process related to elements like carbon, nitrogen, phosphorous and silicon in the estuarine environments and their cycles. Aerobic and anaerobic environments, losses, decomposition, labile and refractory phase, fermentation, nitrate and sulfate reduction, methanogenesis.

Unit V - Estuaries in India

Important estuaries in India and Kerala: Ecological, social and economic values; Estuarine conservation and restoration strategies in India, legislature and regulations.

Learning Outcomes

After completion of the course, the students will be able to:

1. Describe the physical and chemical characteristics of the estuaries and their transition features
2. Identify the chemical processes taking place in estuarine waters and how, and to what extent these chemical processes could be affected by other geological, physical and biological processes.
3. Explain the relevance of estuarine sediments to understanding the depositional and transportation features of elements, and also their diagenetic characteristics.
4. Develop a broad appreciation of biogeochemistry of estuaries and state the factors that influence the primary productivity in estuaries and illustrate how it affects the biomass in the estuarine realm
5. Discuss the relevance of important estuaries in India and their rich natural resources to offer tremendous potential for socio-economic development.

References

1. J. D. Burton and P.S. Liss, Estuarine Chemistry, Academic Press, 1976
2. E. Wolanski and D. Mc Clusky, Biogeochemistry, Elsevier Inc, 2012
3. K.R Dyer, Coastal and Estuarine Sediment Dynamics, Wiley, 1986,
4. D. McLusky, Treatise on Esturine and Coastal Science, Academic Press, 2012
5. T. S. Bianchi, Biogeochemistry of Estuaries, Oxford University Press, 2007
6. E. Olausson and I. Cato, Chemistry and Biogeochemistry of Estuaries, Wiley 1980
7. P.C. Head, Practical Estuarine Chemistry, Cambridge University Press,1985
8. J.P. Riley and R. Chester, Chemical Oceanography (Vol.7), Academic Press, 1978
9. Waves, Tides and Shallow-Water Processes, 1991, The Open University, 2005
10. K.R Dyer, Estuarine Hydrography and Sedimentation, Cambridge University Press, 1980
11. D.A. Hansell and C. A. Carlson, Biogeochemistry of Marine Dissolved Organic Matter, Academic Press, 2002
12. T. S. Balanchi, Biogeochemistry of Estuaries, Oxford University Press, London, 2007
13. S.Z. Qasim, Indian Estuaries. Allied Publishers Pvt. Ltd. Mumbai.
14. Zhen-Gang Ji, Hydrodynamics and Water Quality: Modeling Rivers, Lakes, and Estuaries, Wiely, 2017.

15. Central Board for the Prevention and Control of Water Pollution. Scheme for Zoning and Classification of Indian Rivers, Estuaries, and Coastal Waters: Sweet water, 1979.
16. E. Wolanski, J. Day M. Elliott and R. Ramesh. Coasts and Estuaries, Elsevier, 2019.
17. L. B. de Miranda, F.P. Andutta, B. Kjerfve and B.M. e Castro Filho. Fundamentals of Estuarine Physical Oceanography, Springer, 2017
18. T.S. Garrison. Essentials of Oceanography. Brooks Cole, 2017.

20-304-0010 – General Chemical Oceanography

Unit I - Introduction

Marine chemistry as an analytical problem, the ocean as a chemical system, origin of seawater, structure of water, ion-water interactions, the polarized water molecule, Colligative properties of seawater, derivations of expressions for boiling point elevation and freezing point depression, comparison of river and seawater, hydrological cycle and budget.

Unit II - Sampling and Storage

Protocols and techniques for the sampling of water and sediment, Water samplers – Nansen, Niskin, microlayer samplers. Sediment samplers – grabs, corers. Sample pre-treatment techniques, separation and storage techniques for major ions, minor ions, nutrients, trace metals, organic compounds and their estimations.

Unit III - Major and Minor Elements

History of oceanography, important oceanographic expeds and oceanographic institutions of the world, the composition of seawater, salinity and chlorinity concepts, the major and minor constituents, constancy of relative composition, minor elements, residence time, the geochemical balance of oceans. Primary, cosmogenic and artificial nuclides. Applications of radioisotopes in oceanography.

Unit IV - Dissolved Gases

Dissolved gases, reactive and non – reactive gases – sources and fluxes. Factors affecting the concentration of gases in seawater, pH, alkalinity, specific alkalinity, buffer capacity, carbon dioxide equilibria, precipitation and dissolution of carbonates. Lysocline and carbonate compensation depth, ocean acidification. Dissolved oxygen - origin and factors governing the distribution, AOU.

Unit V – Nutrients

Dissolved and particulate organic matter - origin, elemental and chemical composition, distribution and fate. Ectocrines. Extracellular metabolites and humic substances. Blue carbon**-c**arbon sequestration in the coastal systems and contribution to the global carbon budget. Micronutrient elements - nitrogen, phosphorus and silicon, their cycles, distribution profiles and their effect on phytoplankton growth, N/P ratio.

Learning Outcomes

After completion of the course, the students will be able to:

1. Explain the chemical composition of seawater and their properties in the marine environment.
2. Distinguish conservative and non-conservative behaviour of major and minor elements and discuss their behaviour and distribution in the oceans
3. Explain the importance of dissolved gases in seawater and their distribution in the oceans, seasonal variations, physical and biological processes affecting their concentrations
4. Discuss the theoretical background of chemical oceanographic practical to sample collection and analysis
5. Describe the importance, major forms, distribution, and cycling of inorganic nutrients and organic matter in the sea

References

1. F.J. Millero, Chemical Oceanography 4th ed, CRC Press, 2013
2. K.S. Stowe. Ocean Science 2nd, John Wiley & Sons, 1983
3. J.P. Riley and R. Chester. Introduction to Marine Chemistry, Academic Press, 1971
4. The Open University. Seawater: its Composition, Properties and Behaviour 2nd ed., Oceanography Series, Pergamon, 1995
5. D.F. Martin, Marine Chemistry, Marcel Dekker, New York, 1970
6. R.A. Horne. Marine Chemistry, Wiley-Interscience, London.
7. J.P. Riley and G. Skirrow. Chemical Oceanography, Vols. I to III, Academic Press, 1975
8. R. Sen Gupta and E. Desa. The Indian Ocean – A perspective, Oxford & IBH (Pub), 2001.
9. S. B. Libes, An Introduction to Marine Biogeochemistry 2nd, Wiley, 2009
10. M.E.Q. Pilson. An Introduction to the Chemistry of the Sea 2nd ed., Cambridge University Press, 2013

20-304-0011 – General Chemical Oceanography - (practical)

1. Sampling of seawater (surface/sub-surface) samples
2. Filtration and storage of samples
3. Determination of salinity (chemical method)
4. Determination of dissolved oxygen
5. Determination of BOD and COD
6. Determination of pH, Eh and alkalinity
7. Determination of nutrients – nitrate, nitrite, phosphate and silicate
8. Determination of pigments (Chlorophyll a, b, c and phaeopigments)
9. General methods of determination of cations in seawater using a flame photometer.
10. Estimation of trace metals using AAS practical demonstration

Learning Outcomes

After completion of the course, the students will be able to:

4. Use sampling and storage techniques in marine sampling
5. Analyse samples for basic hydrographical parameters
6. Interpret carbonate chemistry in the aquatic system

References

1. K.Grasshoff. M. Ehrhardt and K. Kremling. Methods of Seawater Analysis 3rd edn., Wiley-VCH, 1999
2. APHA, Standard Methods for the Examination of Water and Wastewater, 23rd ed., 2017
3. IOC Manuals and Guides-12. Chemical Methods for use in Marine Environmental Monitoring, UNESCO. 1983
4. IOC Manuals and Guides-15. Procedure for Sampling Sea Surface Micro-layer, UNESCO, 1985
5. J.D. Strickland and T.R. Parsons. A Practical Handbook of Seawater Analysis, Unipub, 1984
6. T.R. Parsons, Y. Maita and C.M.Lalli. A Manual of Chemical and Biological Methods for Seawater Analysis, Pergamon Press, 1984
7. T.R. Crompton. Analysis of Seawater: A Guide for the Analytical and Environmental Chemist. Springer, 2006

20-304-0012 – Green Chemistry

Unit I – Introduction

Definition, basic concept, the need for green chemistry, sustainable development, principles of green chemistry with illustrated examples. Evaluating chemical reactions according to their yield and atom efficiency.

Unit II – Green Raw Materials and Products

Use of renewable starting materials - caprolactam via ammoximation, commodity chemicals from glucose and biomass conversion. Biodegradable commercial products of comparatively low persistence - polylactides, polyaspartates

Unit III – Greener Solvents and Catalysts

The use of Ionic, supercritical and fluorous media and solventless and aqueous systems as alternative. Use of heterogeneous catalysis, zeolites, biocatalysts, phase transfer catalysts and oxidations using molecular oxygen or peroxides.

Unit IV – Greener Reaction Techniques

Alternative energy sources, basic concepts and advantages, fundamentals of microwave and sonochemical synthesis. Application of microwave and sonochemical methods in the synthesis of organic compounds. Examples of green photochemical reactions.

Unit V – Green Analytical Techniques

Green Analytical Chemistry versus Analytical Chemistry, Miniaturized extraction techniques, examples for green analysis.

Learning Outcomes

After completion of the course, the students will be able to:

1. Discuss the basic concepts and principles of green chemistry.
2. Identify green raw materials for the chemical industries.
3. Describe procedures and protocols for the synthesis of products in a green pathway.
4. Use energy-efficient technologies to enhance the yield of the product of chemical reactions.
5. Describe green technologies and methodologies used in analytical chemistry.

References

1. P.T. Anastas, L.G. Heine, T.C. Williamson (Editors). Green Chemical Syntheses and Processes, ACS Symposium Series 767, American Chemical Society, 2000.

2. P.T. Anastas, J.C. Warner. Green Chemistry, Theory and Practice, Oxford University Press, 2000.
3. P. Tundo, A. Perosa, F. Zachini. Methods and Reagents for Green Chemistry: An Introduction, Wiley-VCH, 2007.
4. D. J. Adams, P. J. Dyson, S. J. Taverner. Chemistry in Alternative Reaction Media 1st ed., Wiley, 2003.
5. Roger A. Sheldon, Isabel Arends, Green Chemistry and Catalysis 1st edn., Wiley-VCH. 2007.
6. V.K. Ahluwalia, Green Chemistry. Environmentally Benign Reactions, CRC Press, 2009.
7. Miguel De La Guardia, Salvador Garrigues. Handbook of Green Analytical Chemistry, Wiley & Sons, Ltd, 2012.

20-304-0013 – Instrumental Techniques

Unit I - Thermal Analysis

Theory, methodology and applications of thermogravimetric analysis (TGA), differential thermal analysis (DTA), and differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods.

Unit II - Atomic Spectral Measurements

Atomic emission and atomic absorption phenomena: Instrumentation details of AAS. Atomization methods - flame, electrothermal and plasma techniques, glow discharge and laser ablation, radiation sources: HCl, EDL-TGL, use in qualitative and quantitative analysis, interferences and background correction techniques. Flame photometry, plasma emissions (ICP-OES), detection systems, applications.

Unit III - Purification and Chromatographic Techniques

General methods of separation and purification of organic compounds - solvent extraction, soxhlet extraction and Pressurized liquid extraction, fractional crystallization, membrane dialysis.

Chromatography - classification of chromatographic techniques. Ion exchange, Column, Planar and Size Exclusion. Chromatography. Ion Chromatography- Principle, Instrumentation- Eluent generation techniques, anionic and cationic suppressors, Detectors-CD, ECD, UV-Vis. Applications. HPLC-Principle, Instrumentation and detectors – RI and UV-Vis detectors, preparative HPLC - methods and applications. Gas chromatography – principle, instrumentation and detectors – FID, ECD, NPD, MS detectors. Methods and applications.

Unit IV - Mass Spectrometry

Mass Spectrometers. Sector, Quadrupole and TOF Analyzers. MS, MS-MS detectors, MALDI, Atomic and molecular mass spectrometry. Isotope ratio mass spectrometry. Accelerator Mass Spectrometry. Multicollection ICP-MS. Instrumentation and Applications.

Unit V – NMR

NMR Techniques

Basic NMR instrumentation, DATA acquisition, Data processing, Pulse Techniques, Water suppression techniques, Coherence Transfer and Mixing, Coherence selection Phase cycling and Field gradients, Resolution and sensitivity

Learning Outcomes

After completion of the course, the students will be able to:

1. Calculate thermal stability of compounds
2. Understand the basic instrumentation of various spectrometers
3. Apply spectroscopic methodology for sample analysis
4. Interpret chromatograms/spectra of simple compounds
5. Apply stable isotope isotopes in paleoclimate studies

References

1. J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham. Vogel's Text Book of Quantitative Inorganic Analysis 4th edn., ELBS, 1982
2. R. Caulcutt and R. Boddy. Statistics for Analytical Chemists, Chapman and Hall, 1983
3. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch. Fundamentals of Analytical Chemistry, 9th edn., Cengage Learning, 2013.
4. F.W. Fifield and D.Kealey. Principles and Practice of Analytical Chemistry 5th edn., Wiley-Blackwell, 2000.
5. D.A. Skoog and J.J. Leary. Principles of Instrumental Analysis,4th edn., Saunders College Publ., 1992.
6. Gary D. Christian, Purnendu K. Dasgupta, Kevin A. Schug, Analytical Chemistry, 7th edn, Wiley publication, 2013.
7. Leo M.L. Nollet, Dimitra A. Lambropoulou, Chromatographic Analysis of the Environment: Mass Spectrometry-Based Approaches, Fourth Ed. 2017
8. Isotopic Analysis: Fundamentals and Applications Using ICP-MS, John Wiley & Sons, 2012
9. J. Cavanagh, W.J. Fairbrother, A.G. Palmer III, N.J. Skelton, Protein NMR spectroscopy: principles and practice. Elsevier, 1995
10. T.D. Claridge, High-resolution NMR techniques in organic chemistry. 27th ed., Elsevier, 2016.

20-304-0014 – Practical VII - Instrumental Techniques II

1. Extraction of organic compounds in the samples- Soxhlet extraction and PLE
2. Gas chromatography (GC) mass spectrometer, GC-Flame ionization detector, GC-Electron Capture detector– Quantitative and qualitative analysis of volatile marine organic compounds.
3. Liquid Chromatography-Mass Spectrometer, HPLC-UV -analysis of high molecular weight and non-volatile organic compounds. Separation and purification of organic compounds using preparative HPLC.
4. Interpretation Exercises using spectra:
   a) Interpretation of FTIR spectrum with reference to stretching vibrations of functional groups.
   b) Absorption spectra (UV-VIS) reading and interpretation of chromophores
   c) Interpretation of NMR spectrum with reference to the calculation of chemical shifts and general comments
   d) Identification of molecular ions in Mass spectra

Learning Outcomes

After completion of the course, the students will be able to:

1. Extract organic compounds in the samples using Soxhlet and PLE
2. Analyse organic compounds in the samples using GC, HPLC and LCMS
3. Interpret spectra of simple organic compounds

References

1. D.T.E. Hunt and A.L. Wilson. The Chemical Analysis of Water, 2nd ed., Royal Society of Chemistry, 1986
2. Instrumental Manuals of AAS, Fluorescence Spectrophotometer, GC and CHN Analyzer.
3. R.M. Silverstein and F.X. Webster, Spectrometric Identification of Organic Compounds, 6th ed., Wiley, 2006.
4. R. Dyer John. Applications of Absorption Spectroscopy of Organic Compounds, Prentice-Hall, 1978.
5. E. Pretsch, P. Bhlmann and M. Badertscher. Structure Determination of Organic

Compounds, Springer-Verlag, 4th ed., 2009.

6. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch. Fundamentals of Analytical Chemistry, 9th ed., Cengage Learning, 2013.
7. IOC Manuals and Guides-11. The determination of Petroleum Hydrocarbons in Sediments, UNESCO, 1982. R.M Silverstein, Spectrometric identification of organic compounds
8. IOC Manuals and Guides-13.Manual for Monitoring Oil and Dissolved/Dispersed Petroleum Hydrocarbons in Marine Waters and on Beaches UNESCO, 1984
9. Aquatic Environment Analytical Methods. Methods of Analysis of Hydrocarbons in Marine and Protection: Other Samples, MAFF, 1988
10. Aquatic Environment Analytical Methods. Methods of Analysis of Trace Metals in Marine and Protection: Other Samples, MAFF, 1989
11. J. Bassett, R.C. Denney, G.H.Jeffery and J.Mendham. Vogel's Text Book of Quantitative Inorganic Analysis 4th ed., ELBS, 1982.
12. Oliver Wurl. Practical Guidelines for the Analysis of Seawater. CRC Press, 2009.
13. T.R Chrompton, Analysis of Oceanic Waters and Sediments, CRC press, 2016

20-304-0015 – Introduction to Hydrochemistry

Unit I - Introduction to Water Molecule

Structure of liquid water, pure water and solubility, ortho-water and para water, the molecular orbital of water (H_2O), Hydrogen bonding in water, Hydrogen bonding and information transfer, water dimer and a small cluster, the molecular orbital of water dimer $(H_2O)_2$, the molecular orbital of water pentamer $(H_2O)_5$

Unit II - Molecular Properties of Water

Molecular vibration and adsorption of water, water dissociation, hydrogen ions, hydroxide ions, Grotthuss mechanism, molecular orbital of the H_3O^+ and OH^- ions, molecular orbital of hydrated hydroxide ion $H_3O_2^-$, the molecular orbital of dihydronium ion $H_5O_2^+$, hydration of biomolecules

Unit III - Physical Properties of Water

The phase diagram of water: density change, steam, gaseous water and water vapor, supercritical water, supercooled water, Ice phases, Ice crystal data, Hexagonal ice, Cubic ice (I_c/XI_c), stacking disordered ice, I_{sd}, Ice-two to Ice-eighteen and very high-pressure ices, Amorphous ice and glassy water, Clathrate ices I, II and H.

Unit IV - Water at Interfaces

Structure and chemical composition of aqueous interface solutions, Ultrathin water layers at the metal surface, Bulk water-metal interface, Water-oxide interface: Hematite and Silica, Water at hydrophobic surfaces, Liquid-vapor interfaces, Interfacial water properties in the presence of surfactants, Ice-vapor interface, Water- colloidal-clay interface, Specific and non – specific adsorption. Confined water, capillaries, Interfacial water and water gases interfaces, nano-bubbles (ultrafine bubbles)

Unit V - Anomalous Properties of Water

Phase anomalies P1-P13, Density anomalies D1-D22, Material anomalies M1-M18, Thermodynamic anomalies T1-T11, physical anomalies F1-F10, Properties of water and its isotopologues. Magnetic and electric effect on water, Water and microwaves, Self-generation of osmotic pressure.

Learning Outcomes

After completion of the course, the students will be able to:

- Discuss the basic properties of water.
- Describe the various physical and chemical properties of water at a wide range of temperature and pressure.
- Explain the behaviour of water molecule at the molecular level at various interfaces.
- Discuss the anomalous behaviour of water.
- This basic knowledge about water will be useful in various environmental and industrial applications.

Reference

1. D.A. Palmer R, Fernandez-Prini and A.H Harvey Aqueous systems at elevated temperatures and pressures: Physical chemistry in water, steam and hydrothermal solutions, 1st ed., Elsevier, Academic press, 2004
2. G. Ghosh, Handbook for refractive index and dispersion of water for scientist and engineers. Sujata Ghosh, 2005
3. F. Franks, Water and aqueous solutions at subzero temperatures. 7th ed., Springer Science & Business Media, 2013
4. G. H. Pollack, The fourth phase of water: beyond solid, liquid, and vapour. Ebner & Sons Publishers, 2013.
5. J. Fraxedas, Water at interfaces: A molecular approach. CRC Press. 2014.
6. M.M. Benjamin, Water chemistry. Waveland Press, 2014.
7. X.F. Pang, Water: molecular structure and properties. World Scientific, 2014.
8. Q. Chang, Colloid and interface chemistry for water quality control. Academic Press, 2016.
9. S. Ahuja, Chemistry and water: The science behind sustaining the world's most crucial resource. Elsevier, 2016.

20-304-0016 – Marine Biogeochemistry

Unit I - Organic Compounds in Sea

Dissolved and particulate organic compounds, their origin and distribution, ecological effects and fate in the seawater. Organic carbon cycle, molecular constituents of organic matter in the ocean, lipids, amino acids and proteins in seawater, carbohydrate, lignin and other low oxidation products; dissolved organic matter and their photooxidation.

Unit II - Geochemistry of Marine Sediments

Sources, components and classification of marine sediments. Dissolved constituents in pore water, sediment interstitial water interaction and diagenesis. Redox reactions, Eh-pH diagram and their applications. Organic matter accumulation in sediments, pathways of organic matter degradation and role of oxygen and nitrate, sulfate reduction, pathways of iron input into marine sediments and early diagenesis.

Unit III - Biogeochemical Processes in Sea

Biogeochemical processes in aerobic and anaerobic marine environments. Primary and bacterial production in the ocean, phytoplankton and their role in primary, new and export production. Benthic processes and burial of carbon. Harmful algal blooms and their effects on the marine ecosystem.

Unit IV - Particle Fluxes and Biogeochemical Cycles

Oceanic particle fluxes its variation and techniques of estimation. Benthic fluxes and their distribution, formation and distribution of marine carbonates. Biogeochemical cycles of carbon, nitrogen, phosphorous and silicon in the marine environment.

Unit V - Biogeochemical Processes in Estuaries/Coastal Systems

Mechanism and pathways of organic matter transformations. Humic material and its importance in estuaries. Biogeochemical process related to elements like carbon, nitrogen, phosphorous and silicon in the estuarine environments and their cycles. Nutrient and trace gas biogeochemistry in the mangrove dominated estuaries: blue carbon, carbon sequestration in the coastal systems, contribution to the global carbon budget.

Learning Outcomes

After completion of the course, the students will be able to:

1. Describe the origin, nature and fate of organic compounds in the sea and the processes that influence the organic compounds in the ocean in the context of recent literature.

2. Discuss the material transfer from land to sea through geochemical processes and also within the sediment column in the oceans.
3. Identify processes that control the biomass, growth, and productivity of organisms in the marine environment.
4. Explain different chemical cycles in the ocean and how these cycles are influenced by biogeochemical processes such as ocean circulation, biological processes, riverine input etc.
5. Identify the chemical processes taking place in coastal waters, including estuaries, and how and to what extent these chemical processes could be affected by other geological, physical and biological processes, and also a special reference to blue carbon and carbon sequestration.

References

1. M.J.R. Fasham, Ocean Biogeochemistry: The role of the ocean carbon cycle in global change, Springer, 2003.
2. R. James, Marine Biogeochemical Cycles, Open University, 2005
3. J.P. Riley and R. Chester, Introduction to Marine Chemistry, Academic Press, 1971
4. H.D. Schulz, Marine Geochemistry, Springer, 2000
5. K.A. Sverdrup and V. Armbrust, Introduction to the World’s Oceans, Science, 2008
6. K.B. Krauskopf, Introduction to geochemistry, Mc.Graw-hill, 1967
7. B. Mason, B. and Moore, Principles of Geochemistry, John Wiley & Sons, 1956
8. J.P. Riley and G. Skrirow, Chemical oceanography (Vol. 1 & 3), Academic Press, 1975.
9. T. S. Balanchi, Biogeochemistry of Estuaries, Oxford University Press, London, 2007.
10. D. McLusky, Treatise on Estuarine and Coastal Science, Academic Press, 2012
11. J.D. Burton and P.S. Liss, Estuarine Chemistry, Academic Press, 1976
12. The Open University, Ocean Chemistry and Deep-Sea Sediments, Oceanography Series, Pergamon, 1989.
13. K.K. Turekian, Marine Chemistry and Geochemistry, Academic press, 2010.
14. J. Middelburg. Introduction to Marine Carbon Biogeochemistry, Springer, 2019

20-304-0017 – Marine Geochemistry

Unit I - Introduction

Components of marine sediments and their origin. Sedimentary environments and facies-sediment texture, weathering and transportation. Benthic fluxes and their distribution – coastal, continental shelf and pelagic sedimentary characteristics. Suspended matter – component composition, particle flux and their spatial and temporal variation, settling rates. Physicochemical factors in sedimentation – ionic potential, hydrogen ion concentration, redox potential and colloids.

Unit II – Radioactive Isotopes

Introduction and scope of isotope geochemistry, isotopes, isobars and isotones, stable and radioactive isotopes. Radioactive decay schemes. Decay constant, half-life, parent-daughter relations. Rb-Sr and Sm-Nd systematics and their use in geochemistry. Short-lived isotopes. Determination of sedimentation rates using radioisotopes, radiocarbon method. Basics of stable isotope mass spectrometry Dating of sediments and corals: 210-Pb, C-14, U-Th.

Unit III - Stable Isotopes

Isotope fractionation, δ-notation for C, H, O, N and S isotopes, fractionation factor. Water isotopes – O, H fractionation in the hydrologic cycle and applications. Applications of stable isotopes in climate studies, paleoclimate reconstruction, paleo-temperatures reconstruction using Mg/Ca in foraminifera. Uses of isotopes in productivity studies.

Unit IV - Geochemical Processes

Distribution of major, minor, trace elements and nutrients in marine sediments. Pore water composition, sediment interstitial water interaction. Mineralization of oxygen. Nitrification and denitrification. Pathways of iron input into marine sediments and early diagenesis, iron as a limiting nutrient. Silica preservation in the ocean. Carbonate distribution and preservation in the ocean. Hydrothermal processes and mineralization – black smokers and massive sulfide formation.

Unit V - Organic Geochemistry

Composition of organic carbon in marine sediments, reactivity and budgets, major reservoirs. Pathways of organic matter degradation and role of oxygen and nitrate, the role of anoxia in OC burial, models for OC degradation and preservation, relationships between dissolved and particulate (sinking and suspended) OC, methods for characterization of sedimentary organic matter, application of biological markers as tools in oceanography. Diagenesis of hydrocarbons, porphyrins, steroids and terpenes. Theories of petroleum formation (an outline only).

Learning Outcomes

After completion of the course, the students will be able to:

1. Discuss the origin and components of marine sediments and the physicochemical processes that regulate the transportation, sedimentation and fluxes of suspended loads in the marine environment.
2. Explain the fundamental principles and concepts of isotope geochemistry and its scope in the field of marine geochemistry
3. Explain the applications of stable isotopes in oceanography like dating of sediments and corals, paleo-oceanographic studies, foraminifera studies, productivity studies, hydrologic cycles etc.
4. Illustrate the sedimentary processes involved in the distribution of major, minor, trace elements and nutrients in marine sediments, and with special emphasis on iron, silica and carbonate chemistry.
5. Explain the fate of marine organic matter from its formation through its transformation and destruction during depositional, diagenetic (remineralization) and catagenic processes.

References

1. R. Chester and T. D. Jickells, Marine Geochemistry 3rd ed., Wiley-Blackwell, 2012
2. H. D. Schulz and M. Zabel, Marine Geochemistry 2nd ed., Springer, 2006
3. J. Hoefs, Stable isotope geochemistry, Springer, 2009
4. G. Faure, Principles of Isotope Geology, Wiley & Sons, 2004
5. H. Elderfield, H. D. Holland and K. K. Turekian, The Oceans and Marine Geochemistry, Elsevier, 2006
6. W. M. White, Isotope Geochemistry, Wiley-Blackwell, 2015
7. H. Jochen, Stable Isotope Geochemistry, Springer, 2015
8. T. E. Dawson and R.T.W. Seigwolf, Stable Isotopes as Indicators of Ecological Change, Academic Press, 2007
9. M. Baskaran, Handbook of Environmental Isotope Geochemistry, Springer, 2011
10. R. James, Marine Biogeochemical Cycles, Open University, 2002
11. K, B. Krauskopf and D.K. Bird, Introduction to geochemistry, Mc.Graw-hill, 1995.

12. S.M. Libes, Introduction to Marine Biogeochemistry. Elsevier, 2009
13. William H. Schlesinger and Emily S. Bernhardt, Biogeochemistry: An Analysis of Global Change 3rd ed., Academic Press, 2013.
14. F.J. Millero. Chemical Oceanography, 4th ed., CRC Press, 2013.
15. S. B. Libes, An Introduction to Marine Biogeochemistry 2nd ed., Wiley, 2009
16. The Open University. Ocean Chemistry and Deep-Sea Sediments, Oceanography Series, 1989
17. J. Jiao and V. Post. Coastal Hydrogeology, 2019

20-304-0018 – Marine Natural Products

Unit I - Marine Natural Products

Introduction and general classification. Isolation techniques - Introduction, different extraction methods, purification by solvent extraction, chromatographic techniques (like size exclusion, ion exchange, counter-current – general principle only). Commercial potential and development of marine natural products. Marine bio-sensor and transgenic marine organisms.

Unit II - Phycochemicals

Seaweeds and its economic importance. Polysaccharides of seaweeds. Structure and uses of agar, alginates, carrageenan and furcellaran. Storage products (structural characteristics and occurrence): α (1,4) linked glucans - floridean starch, and other mycophycen and chlorophyce starches; β(1,3)linked glucans – laminorin, chrysolaminarin and paramylon starches. Introduction to bioactive compounds isolated from seaweed sources. Introduction and general chemical features of chitosan.

Unit III - Nitrogenous Compounds

Amides, (symbioramide, mycalamide – A), tyrosine based metabolites (aeroplysinin – 1), indoles (herbindoles), imidazole (girolline), pyridine (theonelladines) **(**Source, structure and general chemistry only**)**. Bioactive peptides - isolation of seafood peptides- Functional value – calcium binding, antibacterial and anti-oxidant activity. Examples and applications of marine enzymes, anti-freeze proteins, cold adapted enzymes.

Unit IV – Non-Nitrogenous Compounds

Source, Structure and General chemistry: polyketides (ficulinic acids-A and B, aliphatic esters, peroxides), marine prostanoides and prostaglandins (clavulone–II punaglandin-1). Polyethers (hemibrevitoxin B, lokadaicacid), Terpenoides (kalihinol, manoalide, geranyl hydroquinone, avarol and avarone, curcuphenol). General overview of biosynthetic pathways.

Unit V – Marine Drugs

Introduction and importance of marine drugs. Chemical and pharmacological aspects – examples (name, structure, chemical classification and sources only) of antibiotic, anti-tumour, anti-inflammatory, analgesic, cytotoxic, anti-viral and anti-fouling compounds of marine origin. Examples of drugs isolated from the main groups of marine organisms - sponges, corals, algae, fungus, cone snails, dogfish and tunicates (four examples each with nomenclature, structure, chemical group and the specific activity). Introduction to marine cosmetic products.

Learning Outcomes

After completion of the course, the students will be able to:

1. Discuss the chemistry is involved in the area of marine natural products and marine bioprospecting globally
2. Explain the phycochemical aspects of various polysaccharides and bioactive compounds isolated from marine seaweeds and their economic potentials.
3. Identify the marine resources of nitrogenous compounds including bioactive peptides, and marine enzymes
4. Discuss and identify non-nitorgenous compounds from marine sources like polyketides, polyethers, terpenoids etc.
5. Review the chemical and pharmacological aspects of marine drugs isolated from the main groups of marine organisms - sponges, corals, algae, fungus, cone snails, dogfish and tunicates.

References

1. D.H. Attaway and O.R. Zaborsky, Marine Biotechnology. Vol. I. Pharmaceutical and Bioactive Natural Products, Plenum Press, 1993.
2. D.S. Bhakuni and D.S. Rawat, Bioactive Marine Natural Products, Springer, 2005
3. P.J. Scheuer, Marine Natural Products-Diversity and Biosynthesis. Current Chemistry Vol.167, 1993
4. D. J. Faulkner, Marine Natural Products Reviewing the literature, Natural Product Report 12, 1995
5. D. J. Faulkner, Highlights of Marine Natural Products Chemistry (1972-1999), Natural Products Report, 17, 2000
6. D. J. Faulkner and A. van Leeuwenhoek, Marine Pharmacology, 2000
7. B. S. Moore, Biosynthesis of Marine Natural Products: Microorganisms and Macroalgae, Natural Products Report, 1999
8. M. Fingerman, R. Nagabhushanam, and M. Thompson, Recent Advances in Marine Biotechnology, Vol. 2, Oxford & IBH Publishing, 1998.
9. Jean Michel Kronprobst, Encyclopedia of Marine Natural Products. Wiley Blackwell Publ., 2011.
10. V.J. Chapman and D.J. Chapman, Seaweeds and their uses, Methuen and Co. Ltd., 1980.
11. C.D. Amsler, Algal Chemical Ecology, Springer-Verlag Berlin, 2008.
12. Se-Kwon Kim, Handbook of Marine Macroalgae: Biotechnology and Applied Phycology,

John Wiley & Sons, 2011.

13. D.J. Faulkner and W.H. Fenical, Marine Natural Product Chemistry, Springer, 1977
14. C.W. Jefford, K.L. Rinehart and L.S. Shield. Pharmaceuticals and the Sea, Technomic Publ. Co. , 1988
15. E. Fatturosso, W. H. Gerwick and O. Taglialatela-Scafati (Eds.). Handbook of Marine Natural Products, Springer, 2012.
16. V. Venugopal. Marine products for health care. Functional and Bioactive nutraceutical compounds from the ocean, CRC Press, 2009.
17. J.B. McClintock and B.J. Baker. Marine Chemical Ecology, CRC Press, 2001
18. M. P. Puglisi and M. A. Becerro. Chemical Ecology – The Ecological Impact of Natural Products, Tylor and Francis,
19. R. Urbatzka and V. Vasconcels. Marine Natural Products and Obesity, Mdpi AG, 2019.
20. P.H. Rampelotto and A. Trincone. Grand Challenges in Marine Biotechnology, Springer, 2018.

20-304-0019 – Marine Organic Chemistry

Unit I - Marine Carbon

Types and classification – inorganic and organic carbon, size continuum fractions (dissolved/colloidal/particulate phases), blue carbon, carbon sequestration, marine carbon pumps - solubility pump, carbonate pump and biological pump, carbon sequestration potential in the Indian Sundarbans.

Unit II – Dissolved Organic Matter

Sources – terrestrial, atmospheric and other inputs. Primary and bacterial production in the ocean; Phytoplankton and their role in primary, new and export production. Molecular constituents of dissolved organic matter in the ocean - carbohydrates, amino acids and proteins, hydrocarbons, carboxylic acids, humic substances, steroids and other low oxidation products. Physical properties and molecular complexity of DOM. Ecological effects and fate of DOM in seawater, distribution pathways and the organic carbon cycle. Photo-oxidation of dissolved organic compounds. Organic gases and volatiles in the marine environment (An introductory nature only)

Unit III – Particulate And Colloidal Organic Matter.

Sources, nature and composition of POM. Vertical flux of POM - particle sinking velocity, aggregation and disaggregation, biological particle consumption and transformation, and potential mineral interaction. Colloidal and gel organic matter – origin and nature (physical, chemical, and biological attributes). Role in biological productivity and microbial degradation (metabolic hotspots)

Unit IV- Sediment Organic Matter

Origin, sources and composition of sediment organic carbon. Diagenesis – aerobic to anaerobic, role of diagenesis in hydrocarbon generation. Organic biomarker proxies – amino acid dating, lipid biomarkers. Organic matter in eolian dusts. Organic matter preservation in marine sediments - kerogen and bitumen (introductory nature only).

Unit V - Marine Macromolecules

Introduction, sources of important biomaterials. Chemical and biological properties of macromolecular organic matter. Marine proteins – collagen, elastin and gelatin; marine polysaccharides – chitosan, agar, carrageenan and alginate (basic structural features only). Applications of marine macromolecules.

Learning Outcomes

After completion of the course, the students will be able to:

1. Describe the chemical structures and nature of several different organic substances usually found in the ocean
2. Discuss the basic mechanisms of production and degradation of dissolved organic matter in the ocean along with physical properties and molecular complexity of DOM.
3. Explain the sources, nature and composition of particulate and colloidal organic matter and the main biotic and abiotic reaction pathways that take place and influence their distributions/partitioning in the oceanic system.
4. Explain the origin, sources and composition of sediment organic carbon along with the relevance of diagenesis and preservation of organic matter in the sediment.
5. Summarize the recent findings in marine macromolecular organic matter like polysaccharides and proteins, and their applications.

References

1. S. Libes, An Introduction to Marine Geochemistry, 2nd ed., Wiley, 2009
2. E.K. Duursma and R. Dawson, Marine Organic Chemistry Vol. 31, Elsevier, 2000
3. R. Chester, Marine Geochemistry, Blackwell Science, 2002
4. J. P. Riley and G. Skirrow, Chemical Oceanography, Vols. I to III, Academic Press, 1975
5. N. R. Andersen. Concepts in Marine Organic Chemistry, Marine Chemsitry, 1977
6. R. A. Daumas and A. Saliot, The inventory in marine organic chemistry, Elsevier, 1977
7. S. R. Emerson and J. I. Hedges, Chemical Oceanography and the Marine Carbon Cycle, Cambridge, 2008
8. R.P. Schwarzenbach, P.M. Gschwend and D.M. Imboden D.M., Environmental Organic Chemistry, John Wiley & Sons, 2002
9. P.J. Wangersky, Marine Chemistry, Springer, 2000
10. R. Chester and T. Jickelles, Marine Geochemisty, Wiley, 2012
11. J.B. McClintock and B.J. Baker, Marine Chemical Ecology, CRC Press, 2001

20-304-0020 – Nanomaterials and Supramolecular Chemistry

Unit I – Introduction

Nanostructured materials. The density of states in one, two, three, and zero-dimensional nanostructures. Surface plasmon resonance. Optical properties of nanoparticles-explanation based on Mie theory. Corney-penning model of electrons in solids. Quantum confinement effect. Types of nanoparticles (semiconductor, metal and organic nanoparticles), properties and applications.

Unit II – Synthesis

Chemical reduction methods: citrate reduction, borohydride reduction. Self-assembly of organic and inorganic molecules (organic-inorganic hybrids), polymerization (emulsion polymerization for core-shell nanomaterials, microgels and polymer nanoparticles) and Sol-gel methods (silica nanoparticles). Fullerenes molecules, carbon nanotubes and graphene synthesis via chemical vapour deposition methods. Nanomaterial's by thermolysis route, polylol synthesis, solvothermal synthesis, photochemical synthesis, electrochemical synthesis and sonochemical methods.

Unit III - Characterization Techniques

Optical microscopy, fluorescence microscopy, scanning near field optical microscopy and confocal microscopy. Electron microscopies (Transmission electron microscope and scanning electron microscope), scanning probe microscopies (Scanning tunnelling microscope and atomic force microscope), diffraction methods (X-ray diffraction, electron diffraction and neutron diffraction) and light scattering (dynamic light scattering, small-angle light scattering) techniques.

Unit IV – Catalysis Using Nanomaterials

C-C coupling reactions catalyzed by metallic nanoparticles (Heck C-C coupling, Suzuki C-C coupling, Sonagashira C-C coupling, Negishi C-C coupling), hydrogenation catalyzed by metal nanoparticles (hydrogenation of simple olefins and dienes, selective hydrogenation of unsaturated aldehydes, hydrogenation of conjugated dienes into mono-olefines), and oxidation of carbon monoxide to carbon dioxide by gold nanoparticles.

Unit V - Supramolecular Chemistry

Thermodynamics of self-assembly. Non-covalent interactions and supramolecular preparation of nanomaterial's. Self-assembly in biological systems (tobacco mosaic virus and collagen fibres). Self-assembled synthetic supramolecular systems; organo-gelators such as OPVs and crown ether appended pthalocyanine, dendrimers. Molecular switches and molecular machines. Applications of self-assembled nanomaterials.

Learning Outcomes

After completion of the course, the students will be able to:

1. Obtain an extensive understanding of the nanostructured materials, which include the density of states, optical properties and quantum confinement effect.
2. Acquire a fundamental idea on the synthesis of organic, inorganic and organic-inorganic hybrid nanomaterials.
3. Analyze size, shape, crystal structure, zeta potential, and absorption and fluorescence behaviour of various classes of nanomaterials.
4. Create a fundamental idea on novel organic reactions recently applied to generate nanostructured materials.
5. Investigate the role of non-covalent interactions and self-assembly to generate versatile nanostructures with multifunctional properties

References

1. E. L. Wolf, Nanophysics and Nanotechnology: An Introduction to Modern Concepts in Nanoscience, 3rd ed., Wiley-VCH, 2015
2. T. Pradeep, NANO: The Essentials: Understanding Nanoscience and Nanotechnology, 1st ed., McGraw Hill Education, 2017
3. A. K. Das, M. Das, An introduction to nanomaterials and nanoscience, CBS Publishers and distributers Pvt. Ltd., 2020
4. D. M. Kane, A. Micolich, P. Roger, Nanomaterials: Science and Applications, Jenny Stanford Publishing; 1st ed., 2016
5. D. Vollath, Nanomaterials: An Introduction to Synthesis, Properties and Applications, Wiley-VCH; 2nd ed., 2013
6. G. Cao, Y. Wang, Nanostructures and Nanomaterials: Synthesis, Properties, and Applications, World Scientific Publishing Company; 2nd ed., 2010

7. R. Tantra, Nanomaterial Characterization: An Introduction, Wiley,1st ed., 2016
8. K. C. Priydarsh, Nanotechnology: Fabrication & Characterization of Nanomaterial, 007; 1st ed., 2018
9. S. M. Bhagyaraj, O. S. Oluwafemi N. Kalarikkal, S, Thomas, Characterization of Nanomaterials: Advances and Key Technologies, Elsevier, Woodhead Publishing, 1st ed., 2018.
10. P. Serp, K. Philippot, G. A. Somorjai, B. Chaudret, Nanomaterials in Catalysis, Wiley-VCH, First ed., 2012.
11. J. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley India Exclusive (CBS), 1st ed., 2018
12. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, Wiley, 2nd ed., 2013.

20-304-0021 – Organometallic Chemistry

Unit I – Introduction

Organometallic compounds: History, overview, definition, and classification. Organometallic compounds with 18-electron and 16-electrons. Concept of 'Hapticity' of a ligand, effective atomic number rule (EAN), and 18-electron rule, Structure predictions of organometallic compounds by 18-electron rule. Isolobal concepts, isoelectronic concepts, isolabel relationships, STYX number, Wade's and polyhedral skeletal electron pair theory (Mingos rules). Stereochemistry, spectroscopic identification, and catalysis.

Unit II – Organometallic Complexes

Mononuclear, binuclear, and trinuclear metal carbonyl complexes with and without bridging, Metal carbonyls anions, metal carbonyl hydrides, metal carbonyl halides, metal carbonyl clusters-Structure, synthesis, bonding and reactivity. σ-bonded, and π-bonded organo transition metal compounds: structure, bonding and reactivity. Metal-olefin, metal-alkyl, metal nitrosyl, metal cyanide, metal di-nitrogen, metal di-oxygen, metal-carbene complexes and metallocenes-Structure, synthesis, bonding and reactivity. Structure and bonding in Carbene and carbyne complexes. Important main group elements in organometallics: Organo-lithium, beryllium and magnesium compounds.

Unit III – Organometallic Clusters and Cages

Carbonyl clusters: Low Nuclearity Carbonyl clusters and High Nuclearity Carbonyl clusters. Cluster valence electrons, total electron count (TEC) and metal-metal bonds. Cluster compounds of *d*-block elements. Poly-oxo metallates of Ru, Os, Mo. Structure prediction of organometallic clusters. Structure, synthesis, and bonding in boranes, borazines, boron nitride, carboranes, metallo carboranes, S-N, S-P, and P-N compounds. Isopoly and heteropoly acids.

Unit IV – Organometallic Reactions and Stereochemistry

Reactions and reaction requirements of organometallic compounds: Substitution, oxidative addition, reductive elimination, migratory insertion, de-insertion, elimination reactions and β-hydride elimination reactions. Stereo chemically non-rigid molecules, and fluxional isomerism.

Unit V – Spectroscopic Identification and Catalysis

IR spectroscopy: Characterization of metal carbonyls. ^{1}H, ^{13}C, ^{31}P, dynamic NMR spectroscopy and spectrometry: Identify fluxional difference of organometallic compounds at high and low temperature, and characterize the structure and non-rigidity of organometallic compounds. Organometallic catalysts, Homogeneous catalysis: Hydrogenation, hydroformylation of olefins, Monsanto process and Wacker process. Heterogeneous catalysis: Fischer-Tropsch reaction, Ziegler-Natta polymerization and C-C coupling reactions. Reaction steps in the aforementioned catalytic processes.

Learning Outcomes

After completion of the course, the students will be able to:

1. Discuss primary concepts and different electron counting rules to predict the shape/geometry of organometallic compounds.
2. Explain the structure, synthesis, bonding and reactivity's of cages, clusters, and the organometallic compounds based on transition metals and main group elements.
3. Explain Homogeneous and Heterogeneous catalytic processes
4. Recognize the mechanism of various organometallic reactions and implement such concepts to describe different catalytic reactions.
5. Apply knowledge on spectroscopic identification of organometallic compounds in unknown compounds to determine structure and stereochemistry.

References

1. M. Bochmann, Organometallics and Catalysis: An Introduction, Oxford, UK, 2014
2. C. Elschenbroich, Organometallics: A Concise Introduction, Wiley, 3rd ed., 2016
3. R. B. King, Transition-Metal Organometallic Chemistry: An Introduction, Academic Press, 2012
4. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Blackwell, 6th ed., 2014
5. B. G. Luisa and I. Bernal, Stereochemistry of Organometallic and Inorganic Compounds, Elsevier Science, 2012
6. P. S. Pregosin, NMR in Organometallic Chemistry, Wiley, 1st ed., 2013
7. P. Powell, Principles of organometallic Chemistry, Springer, 2nd ed., 2009.
8. F. A Cotton, G. Wilkinson, Advanced Inorganic Chemistry, Wiley, 6th ed., 2007
9. J. D. Lee, Concise Inorganic Chemistry, Oxford University Press, 5th ed., 2008
10. P. J. Perez. Advances in Organometallic Chemistry. Academic Press,1st ed., 2020
11. R. Whyman, Applied Organometallic Chemistry and Catalysis, Oxford chemistry primers, 1st ed., 2001

20-304-0022 Polar Sciences

Unit I – Introduction

Antarctic, Arctic and Himalayan glaciers. Response of polar oceans on deep ocean circulation and modern climate changes, type of glaciers (Ice sheets, ice caps, tidal and mountain glaciers).

Unit II - Polar Cryospheric Studies

Mass balance, snow accumulation rates and its measurements in glaciers. Snow, firn, ice formations and Ice cores as achieves of global climate changes. Indian polar initiatives.

Unit III - Polar Oceanography

Introduction to Arctic and Southern (Antarctic) ocean and its role on modern climate changes. Sea ice, formation of sea ice and role in climate changes.

Unit IV - Southern Ocean

HNLC conditions, iron fertilization; Acidification of Southern Ocean, and role on global carbon budget.

Unit V – Polar Studies in India.

Indian initiatives on polar ocean studies. Major expeditions. Resarch stations. Scope and career perspectives.

Learning Outcomes

After completion of the course, the students will be able to:

1. Explain southern ocean and deep circulation.
2. Describe the importance glaciers in modern climate regulation.
3. Calculate snow accumulation rates and its measurements in glaciers.
4. Discuss the HNLC conditions and iron fertilisation experiments.
5. Discribe the initiatives of polar studies in india.

References:

1. W. Richard Peltier: Ice in the Climate System: Springer-Verlag Berlin Heidelberg 1993.
2. Ramesh Chandra Pathak and Priya Ranjan Trivedi: Glaciology Handbook, Jnanada Prakashan, 2019.
3. Joy McCann, Wild Sea: A History of the Southern Ocean. University of Chicago Press, 2019.

4. Turner, J. and Marshall, G. J., Climate Change in the Polar Regions. Cambridge University Press, 2011.
5. Veronika Meduna, Science on Ice: Discovering the Secrets of Antarctica, Auckland University Press, 2013.
6. Committee on Future Science Opportunities in Antarctica and the Southern Ocean, Future Science Opportunities in Antarctica and the Southern Ocean, The National academy Press, 2011.
7. Mark Serreze and Roger Barry, The Arctic Climate System, Cambridge University Press, 2009.
8. Rajiv Sinha and Rasik Ravindra. Earth System Processes and Disaster Management. Springer-Verlag Berlin Heidelberg 2013.

20-304-0023 – Solid State Chemistry

Unit I - Crystal Structure

Crystalline and amorphous solids. Crystal systems, crystal symmetry, point groups and space groups. Miller indices and Bravais Lattices. Methods of characterizing crystal structure, powder x-ray diffraction, electron and neutron diffraction. Close packed structures: BCC, FCC and HCP. Voids, coordination number, packing efficiency and radius ratios. Structure of compounds: AX (zinc blende, wurtzite), AX_2 (rutile, fluorite and antifluorite), AmX_2 (Nickel arsenide) ABX_3 (perovskite, Ilmenite), Normal Spinel structures and Inverse spinel structures.

Unit II – Electrical Properties

Band theory of solids: metal and their properties. Semiconductors: extrinsic and intrinsic. Hall Effect. Thermodynamic effects (Thomson, Peltier and Seebeck). Insulators: dielectric, ferroelectric, pyroelectric and piezoelectric properties. Ionic conductors. Applications of ferro, piezo and pyroelectrics.

Unit III - Magnetic Properties

Dia, para, ferro, ferri, and anti ferri magnetic types. Soft and hard magnetic materials. Select magnetic materials such as spinels, garnets, perovskites, hexa ferrites and lanthanides. Transition metal compounds. Magnetoresistance.

Unit IV - Imperfection in Solids

Point defects: stoichiometric defects and nonstoichiometric defects. Line defects: edge dislocations and screw dislocations. Plane defects: stacking faults, grain boundaries and twin boundaries. Solid state reactions: mechanisms of migration of ions, solid electrolytes, thermal decomposition of solid-Type 1 and Type II reactions.

Unit V - Superconductivity

Superconductors, Meissner effect, Levitation, Specific heat of superconductors, Theories of superconductivity, High temperature superconductors (HTSCs), Applications of high temperature superconductors

Learning Outcomes

After completion of the course, the students will be able to:

1. Discuss the fundamentals of crystal structure and characterization methods.
2. Identify the thermodynamic effects, electrical properties of solids and its application in the field of electronics.

3. Explain the various kinds of magnetic materials, its properties and importance.
4. Discuss the various types of defects recognized in the crystal systems and its role in the solid-state reactions.
5. Explain the theoretical idea of superconducting materials and its application in various disciplines.

References

1. E. A. Moore, L. E. Smart, Solid State Chemistry: An Introduction, CRC Press, 4th ed., 2019
2. R. J. D. Tilley, Crystals and Crystal Structures, Wiley, 2nd ed., 2020
3. M. Ladd, Bonding, Structure and Solid-State Chemistry, Oxford, 1st ed., 2016
4. A. R. West, Solid State Chemistry and its Applications, Wiley-Blackwell, 2nd ed., 2014
5. G. N. Gurtu, A. Gurtu, Solid State Chemistry, Pragati Prakashan, 3rd ed., 2017
6. J. A. Hernandez, Solid State Chemistry: An Introduction, Delve Publishing, 2016
7. C. N. R. Rao, J. Gopalakrishnan, New Directions in Solid State Chemistry, Cambridge University Press, 2nd ed., 1997
8. U. Schubert, N. Hüsing, Synthesis of Inorganic Materials, Wiley, 4th ed., 2019
9. D. Jiles, Introduction to Magnetism and Magnetic Materials, CRC Press; 3rd ed., 2015.
10. R. E. Hummel, Electronic Properties of Materials, Springer; 4th ed., 2011
11. U. Muller, Inorganic Structural Chemistry, Wiley-Blackwell, 2nd ed., 2006
12. A. Kelly, K. M. Knowles, Crystallography and Crystal Defects, Wiley, 3rd ed., 2020

20-304-0024 – Water Management

Unit I - Environment Management

Ecosystem – organisms, species, population, community, ecosystem and biosphere ecology. Forest, freshwater, estuarine, marine, agro and urban ecosystems. International standards, introduction to ISO 9000, 14000 series standards.

Unit II - Sustainable Development

Economic growth and sustainability, GNP, GDP, cost-benefit analysis, environmental valuation.

Unit III - Hydrologic Cycle

Inter-relationship of surface and ground water. Stream hydrograph, Streamflow groundwater relationships. Hydrological processes and the water budget of lakes and rivers – the interaction of lakes with surface and subsurface water. Influence of geology on groundwater – porosity, specific retention and specific yield.

Unit IV - Aquifer Characteristics

Springs and wells, Darcy's law, groundwater exploitation and management, groundwater quality, physical, biological and chemical properties, Safe yield and artificial recharge, groundwater pollution and salinity intrusion, water conservation and budgeting, modification of hydrological regimes.

Unit V - Waste Water Management

Waste management approaches, waste reduction, recycling, disposal. Wastewater treatment options, municipal and industrial discharges

Learning Outcomes

After completion of the course, the students will be able to:

1. Explain the various definitions and protocols related to environment and how amendments are made according to present status and future requirements.
2. Discuss the concept of sustainable developments and its various aspects.
3. Explain the water cycle, factors influencing it and the importance of each component of the water cycle.
4. Discuss aquifers, its importance, laws related to it, the importance of its management
5. Discuss the theoretical aspect of waste management.

References

1. R.F. Dasmann, Environmental conservation, 5th ed., John Wiley, 1984
2. R. Menaria, Environmental conservation and planning, Ashish Publ., 1989
3. W. Viesmann and Gary L. Lewis, Introduction to hydrology, 5th ed., Prentice Hall, 2002
4. Ven Chow, David Maidment and Larry Mays. Applied hydrology, 2nd ed., McGraw-Hill, 2013.
5. A. Srivastava, Wastewater treatment and water management, Notion Press, 2018.
6. S. Liehr, J. Kramm, A. Jokisch, K., Müller, Integrated water resources management in water-scarce regions: Water harvesting, groundwater desalination and water reuse in Namibia, IWA Publishing, 2018
7. J. Holden. Water resources: an integrated approach, Routledge, 2019.

Audit Courses

20-304-0025 – Good Laboratory Practice and safety

Unit I - Good Laboratory Practice

Quality control in analysis - Laboratory notebook and recording of operations - Standard Operating Procedures (SOP) - Instrumentation Validation - Criteria for selecting instrumental methods - precision, sensitivity, selectivity, and detection limits. Experimental Error - Significant figures- Statistics and Quality Assurance - Statistical treatment- standard deviation, variance, confidence limits, application of statistics to data treatment and evaluation, student-t and f tests, detection of gross errors, rejection of a result-Q test, estimation of detection limits. Least square method, correlation coefficient and its determination. Multi variant analysis, ANOVA, PCA. Metrological Traceability - Reagent/ Materials Certification.

Unit II - Laboratory Safety

Laboratory Protocol - Emergency Response - Fire Emergencies- Chemical Spills - First Aid - Chemical Spills: Containment and Cleanup - Routes of Exposures to Hazards - Language of Safety: Signs, Symbols, and Labels - Material Safety Data Sheets (MSDS) - Globally Harmonized System of Classification and Labelling of Chemicals (GHS) - Chemical Hygiene Plans - Recognizing Laboratory Hazards - Acute Toxicity - Chronic Toxicity – Carcinogens- Biological Hazards and Biosafety - Corrosive Hazards- Flammables - Fire and Explosions – Incompatibles - Gas Cylinders and Cryogenic Liquid Tanks –Peroxides - Hazards from Low or High-Pressure Systems - Electrical Hazards - Nonionizing Radiation and Electric And Magnetic Fields - Ionizing Radiation Hazards - Cryogenic Hazards – Runaway Reactions - Hazards of Catalysts -Risk Assessment - Safety Planning for New Experiments – Personal Protective Equipments (PPEs) - Chemical Hoods - Containment and Ventilation - Biological Safety Cabinets - Chemical Management: Inspections, Chemical Inventories, Storage, Wastes, and Security. Safety Legal Framework.

Learning Outcomes

After completion of the course, the students will be able to:

6. Practice suitable laboratory protocols in the chemical lab.
7. Expertise in handling hazardous chemicals.
8. Apply statistical tools to interpret data.

7. Safety in Academic Chemistry Laboratories, 8th ed., Best Practices for First- and Second-Year University Students, American Chemical Society, 2017.
8. E. Dittrich, The Sustainable Laboratory Handbook - Design, Equipment, Operation -, Wiley-VCH Verlag GmbH & Co.
9. Guidelines for Chemical Laboratory Safety in Academic Institutions- American Chemical Society, 2016.
10. Richard P. Pohanish, Stanley A. Greene, Wiley guide to chemical incompatibilities-. - 3rd ed. John Wiley & Sons, Inc., 2009
11. Identifying and Evaluating Hazards in Research Laboratories, American Chemical Society, 2015.
12. A. Keith Furr, Boca Raton, CRC Handbook of Laboratory Safety, 5th ed., CRC Press LLC,2000.
13. Hazardous Chemicals in Human and Environmental Health - a resource book for school, college and university students, World Health Organization, 2000
14. Richard P. Pohanish, Sittig's Handbook of Toxic and Hazardous Chemicals and Carcinogens, 6th ed., Elsevier Inc. 2012
15. Indian Standard, Chemical Laboratories - Code of Safety IS 4209, Bureau of Indian Standards (Second Revision) 2013
16. Laboratory Safety Manual, National Centre for Biological Sciences (NCBS), Revised July 2016.
17. National Disaster Management Guidelines, Chemical Disasters (Industrial), National Disaster Management Authority, Government of India, 2007.

20-304-0026 – Research Methodology

Unit I - Introduction

Meaning, objectives, purpose, significance of research. Types of research – descriptive vs analytical; applied vs fundamental; qualitative vs quantitative; conceptual vs empirical. Hypothesis – characteristics, formulation, modification etc. Criteria of good research – systematic, logical.

Unit II - The Research Problem

Literature review, selection, concept, design, approaches.

Unit III - Sampling and Methods

Site selection, periodicity, modes, environmental/ ecological considerations, precautions, tools, equipment, vessels, sampling protocols, analytical techniques, etc.

Unit IV - Ethics in Research

Honesty, objectivity, integrity, plagiarism spectrum, confidentiality, IPR, collaborative work, respect for peers.

Unit V - Scientific Writing

Review, research proposal, MS; thesis vs dissertation. Essentials of successful scientific writing – precision, clarity, objectivity. Superior research writing. General format of a research paper, first author/ co-authors, MS- review, revision, resubmission, rejection.

Learning Outcomes

After completion of the course, the students will be able to:

1. Describe different type of research in the field of chemistry.
2. Describe the ethics in research
3. Explain the sampling methods and protocols.

References:

1. Research methodology – methods and techniques, C. R. Kothari, New Age International (P) Ltd. Publishers New Delhi, 2004.
2. The student's guide to research ethics, Paul Oliver, Second edition, Maidenhead, Berkshire, England: Open University Press, McGraw-Hill Education, 2010.
3. The Craft of Scientific Writing, Michael Alley, 3rd ed., Springer, 1996.
4. Intellectual Property Rights In India : General Issues And Implications, Prankrishna Pal,
5. Deep Publications Pvt. Ltd, 2008.