PROGRAMME AND COURSE STRUCTURE WITH CREDIT DISTRIBUTION

FOR

UG Degree Programmes with Single Major

IN

CHEMISTRY

(*w.e.f.* 2023-2024)

BANKURA UNIVERSITY
BANKURA
WEST BENGAL
PIN - 722155

STRUCTURE IN CHEMISTRY

SEMESTER-VII

Category of Course	Course Code	Course Title	Credit	Marks			No. of Hours		
				I.A.	ESE	Total	Lec.	Tu.	Lab.
1. Major :: DSC	S/CHEM/701/MJC-17	Inorganic Chemistry V	3 (Th.) + 1 (Lab.) = 4	10	25 (Th.) 15 (Lab.)	50	45		30
2. Major :: DSC	S/CHEM/702/MJC-18	Organic Chemistry V	3 (Th.) + 1 (Lab.) = 4	10	25 (Th.) 15 (Lab.)	50	45		30
3. Major :: DSC	S/CHEM/703/MJC-19	Physical Chemistry V	3 (Th.) + 1 (Lab.) = 4	10	25 (Th.) 15 (Lab.)	50	45		30
4. Major :: DSC	S/CHEM/704/MJC-20	Green Chemistry	3 (Th.) + 1 (Lab.) = 4	10	25 (Th.) 15 (Lab.)	50	45		30
5. Minor Stream	S/CHEM/705/MN-7	Physical Chemistry II	3 (Th.) + 1 (Lab.) = 4	10	25 (Th.) 15 (Lab.)	50	45		30
Total credits = 4+4+4+4+4 = 20				Total no. of courses = 5					

N.B.: S = Science, CHEM = Chemistry, MJ = Major, MN = Minor, ACS = Arts Commerce Science, C = Core Course, AEC = Ability Enhancement Course, SEC = Skill Enhancement Course, DSC = Discipline Specific Core, DSE = Discipline Specific Elective, VAC = Value Added Course, MD = Multidisciplinary, INT = Internship, I.A. = Internal Assessment, ESE = End-Semester Examination, Lec. = Lecture, Tu.= Tutorial, and Lab. = Laboratory

SEM VII

Major (MJC - 17)

(Credits - 3 + 1)

Core T-17-Inorganic Chemistry V (3 Credits) (45 Lectures)

Chemical Bonding - A Quantum Chemical Approach (10 Lectures)

The Born-Oppenheimer approximation, MO of homo and heteronuclear diatomic molecules, MO of polynuclear AB_n type molecules, Koopmans' theorem, Walsh diagram, isolobal analogy, molecular term symbols, Huckel method of π-MO calculation in ethylene, allyl system etc.

Coordination Chemistry: Bonding, Stereochemistry and Structure (10 Lectures)

Tanabe-Sugano diagram, molecular orbital, spectral properties, vibronic coupling, band broadening, spin-orbit coupling, spin-forbidden transition, intensity stealing, magnetic properties, lowering of symmetry, electronic, steric, Renner-Teller effects on energy levels, conformation of chelator/congregator, structural equilibrium and implication, correlation of CFSE with spectroscopy.

Organometallic Chemistry II (10 Lectures)

Overview and striking differences among related pi-acids, alkyl, alkene, alkyne, π-allyl, polyene and cyclopolyene compounds; metal carbenes and carbynes, hydride and dihydrogen complexes; isolobal analogy; Dewar-Chatt Duncanson model; oxophilicity; agostic interaction; metal-carbon bonded compounds (σ bonded).

Cluster compounds (7 lectures)

Introduction, clusters in elemental states, cluster classification, skeletal electron (Elm) counting, higher boron hydrides structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, chevrel compounds, infinite metal chains, multidecker molecules, cluster-surface analogy.

Bioinorganic Chemistry (8 Lectures)

Blue copper proteins, biological fixation of nitrogen; urease, xanthine oxidase, sulphite oxidase, nitrate reductase; study of metalloprotein and metalloenzyme: superoxide dismutase, catalase, peroxidase, cytochrome P-450, cytochrome oxidase, carbonic anhydrase, carboxy peptidase, catechol oxidase, metallothionine; vitamin B12 and B12-enzyme.

Reference Books

• F. A. Cotton. Chemical Applications of Group Theory, 3rd Edn. John Wiley & Sons, New York, 1999.

• F. A. Cotton, G. Wilkinson, C. M. Murillo, M. Bochmann. Advanced Inorganic Chemistry, 6th Edn. John Wiley & Sons, New York, 1999.

• B. Douglas, D. McDaniel, J. Alexander. Concepts and Models of Inorganic Chemistry, 3rd Edn. John Wiley & Sons, New York, 2001.

• J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi. Inorganic Chemistry: Principles of Structures and Reactivity, 4th Edn. Pearson, New Delhi, 2006.

• H. E. White. Introduction to Atomic Spectra, McGraw-Hill Kogakusha Ltd, Tokyo, 1934.

• B. N. Figgis. Introduction to Ligand Field Theory, Interscience, New York, 1966.

• C. J. Ballhausen. Molecular Electronic Structure of Transition Metal Complexes, McGraw Hill, London, 1979.

• R. McWeeney. Coulsons' Valence, 3rd Edn. Oxford University Press, Oxford, 1979.

• A. B. P. Lever. Inorganic Electronic Spectroscopy, Elsevier, New York, 1984.

• B. E. Douglas, C. A. Hollingsworth. Symmetry in Bonding and Spectra; an Introduction, Academic Press, New York, 1985.

• T. A. Albright, J. K. Burdett, M. H. Whangbo. Orbital Interactions in Chemistry, Wiley, New York, 1985.

• V. Heine. Group Theory in Quantum Mechanics: An introduction to its present usage, Dover publication, New York, 1991.

• P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong. Shriver & Atkins Inorganic Chemistry, 4th Edn. Oxford, 2006.

• P. Powell. Principles of Organometallic Chemistry, 2nd Edn. Chapman and Hall, London, 1988.

• J. D. Atwood. Inorganic and Organometallic Reaction Mechanisms, 2nd Edn. VCH, New York, 1997.

• R. H. Crabtree. The Organometallic Chemistry of the Transition Metals, 4th Edn. Wiley, New York, 2005.

• C. Elschenbroich. Organometallics, 3rd Edn. Wiley-VCH, Weinheim, 2006.

• R. A. Van Santen, M. Neurock. Molecular Heterogenous Catalysis, Wiley-VCH, Weinheim, 2006.

• G. O. Spessard, G. L. Miessler. Organometallic Chemistry, 2nd Edn. Oxford University Press, Oxford, 2010.
• J. F. Hartwig. Organotransition Metal Chemistry: from bonding to catalysis, University Science Books, Sausalito, CA, 2010.
• S. J. Lippard, J. M. Berg. Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, CA, 1993.
• W. Kaim, B. Schwederski. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, Wiley, New York, 1994.
• I. Bertini, H. B. Gray, S. J. Lipperd, J. S. Valentine. Bioinorganic Chemistry, Viva books (P) Ltd. New Delhi, 1998.
• A. Das, G. N. Mukherjee. Elements of Bioinorganic Chemistry, 2nd Edn. U. N. Dhur & Sons, Kolkata, 2002.
• A. K. Das. Bioinorganic Chemistry, Books & allied (P) Ltd. Kolkata, 2007.
• E. Ochiai, Bioinorganic Chemistry: A Survey, Academic press, Elsevier, 2009.
• R. R. Crichten. Biological Inorganic Chemistry: A New Introduction to Molecular Structure, 2nd Edn. Elsevier, New York, 2012.
• R. M. Roat-Malone. Bioinorganic Chemistry: A Short Course, 2nd Edn. Wiley, New York, 2013.

Course Outcomes

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

1. Apply quantum chemical concepts and molecular orbital theory to explain bonding in homo- and heteronuclear molecules.
2. Interpret electronic spectra and magnetic properties of coordination compounds using Tanabe–Sugano diagrams and ligand field theory.
3. Analyze structure, bonding, and reactivity of organometallic compounds using models such as the Dewar–Chatt–Duncanson model and isolobal analogy.
4. Perform electron counting and structural analysis of cluster compounds using PSEPT/Wade–Mingos rules and related theoretical approaches.
5. Explain the structure and function of biologically important metal-containing enzymes and proteins.
6. Integrate concepts from quantum chemistry, coordination chemistry, organometallic chemistry, and bioinorganic chemistry to interpret advanced chemical structures and mechanisms.

Core P-17-Inorganic Chemistry V Lab (1 Credit) (30 Lectures)

Synthesis and characterization of inorganic and co-ordination compounds: selected simple salts, double salts and co-ordination compounds with some available inorganic and organic ligands.

1. $NiCO_3$
2. $CuSO_4.5H_2O$
3. $ZnSO_4.7H_2O$
4. Mohr's salt
5. Potash alum
6. $[Cr(acac)_3]$
7. $[Cu(oxin)_2]$
8. [Fe(salen)Cl]
9. $[Co\ (NH_3)_6]Cl_3$
10. $[Cu(en)_2]SO_4$

Reference Books

• Svehla & Sivasankar, Vogel's Qualitative Inorganic Analysis, 7th Ed. Pearson, 2012.

• Maji, S. K. Practical Inorganic Chemistry Books & Allied (P) Ltd.

• Mendham, J. A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

• G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney. Vogel's Textbook of Quantitative Chemical Analysis. 5th Edn. John Wiley & Sons, New York, 1989.

• G. N. Mukherjee. Advanced Experiments in Inorganic Chemistry, 2nd Edn. U. N. Dhur & Sons Pvt. Ltd. 2018.

• Dr. L. R. Sharma. Practical Inorganic Chemistry, Evincepub Publishing, 2021.

Course Outcomes

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

1. Successfully synthesize and isolate inorganic salts and coordination complexes using appropriate laboratory procedures.
2. Apply experimental techniques such as crystallization, filtration, and drying for purification and preparation of coordination compounds.
3. Interpret experimental observations and basic characterization results to confirm the formation and properties of synthesized inorganic and coordination compounds.

Major (MJC - 18)

(Credits - 3 + 1)

Core T-18-Organic Chemistry V (3 Credits) (45 Lectures)

Bonding in Organic Molecules & Structure-Reactivity Relationship (6 Lectures)

Linear free energy relations, Hammett equation; equilibria and rates in organic reactions; separation of polar, steric and resonance effects: Taft equation, Grunwald-Winstein equation.

Conformation and Reactivity of Acyclic and Cyclic Systems (9 Lectures)

Determination of relative configuration: Prelog's rule, Cram's rule, Sharpless rule; conformations of acyclic and cyclic systems (3 to 8 membered rings), fused (5/5 and 6/6), spiro and bridged bicyclo-systems; stability, reactivity and mechanism; allylic strain; reactions of 5 and 6-membered ring containing one or more trigonal carbon(s).

Asymmetric Synthesis-I (9 Lectures)

1. Introduction to asymmetric synthesis, preliminary idea about different methods of asymmetric synthesis with special reference to the chiral pool strategy, chiral auxiliaries

2. Stereoselective and stereospecific reactions; diastereoselectivity and enantioselectivity, Stereochemistry of nucleophilic addition reactions to carbonyl compounds: Felkin-Anh and Zimmermann-Traxler models.

Organic Name Reactions and Reagents (12 Lectures)

1. Barton reaction; McMurry reaction; Luche reduction; Yamaguchi esterification; hydride transfer reagent: Boranes, trialkyl borohydrides, Diimide, Baker's yeast, trialkyl tin hydride; DIBAL-H, $Na(CN)BH_3$, Red-Al; Selectrides; Woodward and Prévost hydroxylation; Mn(IV) oxide; RuO_4 (TRAP); Moffat oxidation; Swern oxidation; Dess-Martin Periodinane; Shapiro reaction; Peterson reaction; OsO_4.

2. Nucleophilic catalyst: Examples of nucleophilic catalysis reaction: aza-Baylis-Hillman reaction (DABCO), Steglich Esterification (DMAP), Appel Reaction.

3. Cross-coupling reaction: Heck reaction, Suzuki reaction.

The Logic of Organic Synthesis (9 Lectures)

1. Retrosynthetic analysis: Disconnections; synthons (donor and acceptor); natural reactivity and umpolung; latent polarity in bifunctional compounds: consonant and dissonant polarity; Lagical and illogical electrophiles and nucleophiles; synthetic equivalents; functional group interconversion and

addition (FGI and FGA); C-C disconnections and synthesis: one-group and two-group (1,2- to 1,5-dioxygenated compounds), reconnection (1,6-dicarbonyl); protection-deprotection strategy (alcohol, amine, carbonyl, acid). Synthesis of some organic molecules by disconnection approach.

2. Strategy of ring synthesis: Thermodynamic and kinetic factors; synthesis of large rings, application of high dilution technique.

Reference Books:

- Anslyn, E. V.; Dougherty, D. A. Modern Physical Organic Chemistry, University Science Books, 2006.
- Shaik, S.; Hiberty. P. C. Valence Bond Theory, its History, Fundamentals and Applications: a Primer, Reviews in Computational Chemistry, Volume 20 (Eds. K. B. Lipkowitz, R. Larter, T. R. Cundari), John Wiley & Sons, Hoboken, NJ, USA, 2004.
- Caroll, F. A. Perspectives on Structure and Mechanism in Organic Chemistry, 2nd Edn. Wiley-VCH, 2011.
- Lowry, T. H.; Richardson, K. S. Mechanism and Theory in Organic Chemistry, (Harper Row Publishers, New York)
- Eliel, E. L. Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London.
- Nasipuri. D. Stereochemistry of Organic Compounds (Principles and Applications), 2nd Edn. Wiley astern Limited, New Delhi, 1994.
- Juaristi. E. Stereochemistry and Conformational Analysis, John Wiley & Sons, 1991.
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Pal, S. C. Principles of Stereochemistry and their Application in Organic Reactions.
- Hassner, A.; Namboothiri, I. Organic Syntheses based on Name Reactions, 3rd Edn. Elsevier, 2012.
- Kürti, L.; Czakó. B. Strategic Applications of Name Reactions in Organic Synthesis: Background and Detailed Mechanisms, Elsevier Academic Press, 2005.
- Wang, Z. Comprehensive Organic Name Reactions and Reagents, Wiley-VCH, 2009.
- Brahmachari, G. Organic Name Reactions: A Unified Approach, Narosa Publishing House Pvt. Ltd. New Delhi, 2012.
- Gawley, R. E.; Aubé, J. Principles of Asymmetric Synthesis (2nd Ed)
- Warren, S. Organic Synthesis the Disconnection Approach, John Wiley and Sons.

- Carruthers, W. Modern methods of Organic Synthesis, Cambridge University Press, 4th Edn. 2012.
- Willis, C. A.; Wills, M. Organic Synthesis, Oxford Chemistry Primer, Oxford University Press.
- Carey, F. A. Sundberg, R. J. Advanced Organic Chemistry Part B: Reaction and Synthesis, Springer, 5th Edition, 2010.
- Clayden, J., Greeves, N., Warren, S., Organic Chemistry, Second edition, Oxford University Press 2012.
- R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee. Organic Chemistry, 7th Edn. Pearson Education, 2013.
- M. B. Smith, J. March. March's Advanced Organic Chemistry (Reactions, Mechanisms and Structure), 5th Edn. John Wiley & Sons, 2001.

Course Outcomes

1. To impart knowledge on bonding in organic molecules & structure-reactivity relationship.

2. To acquire the concepts in conformation and reactivity of acyclic and cyclic systems to understand stereochemical outcome in a reaction.

3. To identify, understand, and apply different organic name reactions and reagents for strategic organic synthesis and functional group manipulations.

4. To make it possible to use the logic of organic synthesis disconnection approaches (retrosynthetic analysis) to create effective synthetic routes, comprehend reactivity, and predict the feasibility of chemical reactions.

Core P-18-Organic Chemistry V Lab (1 Credit) **(30 Lectures)**

1. Qualitative Organic Analysis **(20 Lectures)**

Identification of a single liquid organic compound by physical and chemical tests and preparation of at least one suitable solid derivative after consulting literature. Functional groups include: amino (1˚, 2˚, 3˚), anilido-, nitro-, cyano-, alcoholic -OH, phenolic -OH, enols, carbonyl (aldehydo-, keto-), carboxylic acids, esters, unsaturation and hydrocarbons.

At least six experiments to be performed in class.

2. Separation of binary mixture (liquid-liquid) **(10 Lectures)**

Separation of binary mixture (liquid-liquid): based upon the chemical properties, by using common laboratory reagents like water, dil.HCl, dil. NaOH, dil. $NaHCO_3$, $NaHSO_3$ etc., determination of the

boiling point of any one of the separated components. The composition of the mixture may be of the following types: aniline and toluene; acetic acid and toluene; ethanol and acetone etc.

Reference Books

- Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell. A. R. Vogel's Textbook of Practical Organic Chemistry, 5th Edn. John Wiley & Sons. New York, 1989.
- Vogel, I. A Textbook of Practical Organic Chemistry, 3rd Edn. Longman Group Ltd., London, 1956.
- Mann, F. G.; Saunders, B. C. Practical Organic Chemistry, 3rd Edition, Longman, 1978.
- Roberts, R. M.; Gilbert, J. C.; Rodewald, L. B.; Wingrove, A. S. An Introduction to Modern Experimental Organic Chemistry, 3rd Edn. Holt, Rinehart & Winston Publishers, New York, 1969.
- Clarke, H. T. Handbook of Organic Analysis, 4th Edn. Hodder & Stoughton Educational, London, 1926.
- Middleton, H. Systematic Qualitative Organic Analysis, 2nd Edn. Hodder & Stoughton Educational, London, 1943.
- Ahluwalia, V. K., Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press, 2001.

Course Outcomes

1. To gather knowledge and skills to understand the laboratory methods and tests related to the detection of elements and functional groups in different liquid organic samples.

2. To develop practical knowledge about techniques for the separation of binary mixtures of organic compounds.

Major (MJC - 19)

(Credits - 3 + 1)

Core T-19-Physical Chemistry V (3 Credits) **(45 Lectures)**

Spectroscopy II (NMR, ESR) **(9 Lectures)**

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low-resolution spectra, different scales, spin-spin coupling and high-resolution spectra, interpretation of PMR spectra of organic molecules and instrumentation of NMR spectroscopy.

Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine splitting interaction between nuclear spin and electron spin, ESR spectra of simple radicals and instrumentation of ESR spectroscopy.

Quantum Chemistry (12 Lectures)

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component; Rigid rotator model of rotation of diatomic molecule; Schrödinger equation, transformation to spherical polar coordinates; Separation of variables. Spherical harmonics; Discussion of solution.

Qualitative treatment of hydrogen atom and hydrogen-like ions: Setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression); Average and most probable distances of electron from nucleus; Setting up of Schrödinger equation for many-electron atoms (He, Li).

Symmetry & Group Theory I (12 Lectures)

Introduction, symmetry, symmetry elements and symmetry operations, definition of a group, point symmetry groups, group multiplication tables, theorems of groups, conjugate elements and class, symmetry operators and their matrix representation.

Bio-physical Chemistry (12 Lectures)

Colloids: Lyophobic and lyophilic sols, Origin of charge and stability of lyophobic colloids, Coagulation and Schultz-Hardy rule, Zeta potential and Stern double layer (qualitative), Tyndall effect; Electrokinetic phenomena (qualitative idea only); Determination of Avogadro number by Perrin's method; Stability of colloids and zeta potential; micelles, reverse micelles, microemulsion, thermodynamics of micellization, hydrophobic hydration, interaction; stabilization and denaturation of protein.

Reference Books

- Banwell, C. N. Fundamentals of Molecular Spectroscopy, Tata-McGraw-Hill
- Brown, J. M. Molecular Spectroscopy, OUP
- Levine, I. N. Quantum Chemistry, PHI
- Atkins, P. W. Molecular Quantum Mechanics, Oxford
- Rakshit, S. C. Molecular Symmetry Group and Chemistry, The New Book Stall, Kolkata, 1988.
- Cotton, F. A. Chemical Applications of Group Theory, 3rd Edn. John Wiley & Sons. New York, 1999.

- Bishop, D. M. Group Theory and Chemistry, Oxford University Press, 1993.
- Vincent, J. Molecular Symmetry & Group Theory, John Wiley & Sons. New York, 1998.
- Van Holde, K. V., Johnson, W. C., Ho, P. S. Principles of Physical Biochemistry, Prentice Hall, 1998.
- Nelson, D. L., Cox, M. Lehninger Principles of Biochemistry, 8th Edn. Macmillan Learning, 2017.

Course Outcomes

1. To gain foundational knowledge about NMR and ESR spectroscopy.
2. To learn the basic concept of quantum chemistry and simple quantum models.
3. To identify molecular symmetry elements, assign point groups, construct character tables, and apply these concepts to predict spectroscopic properties and molecular orbitals.
4. To understand biological macromolecules (micelles, reverse micelles and proteins) and their interactions.

Core P-19-Physical Chemistry V Lab (1 Credit) (30 Lectures)

1. Determination of composition of Fe^{II}/Fe^{III} complex with salicylic acid by Job's method of continuous variation.
2. Determination of CMC of surfactants by surface tension method.
3. Spectrophotometric/Conductometric determination of CMC of surfactants.

Reference Books

- Viswanathan, B., Raghavan, P.S. Practical Physical Chemistry Viva Books (2009).
- Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson
- Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007)
- Palit, S.R., De, S. K. Practical Physical Chemistry Science Book Agency
- University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta.
- Levitt, B. P. edited Findlay's Practical Physical Chemistry Longman Group Ltd.
- Gurtu, J. N., Kapoor, R., Advanced Experimental Chemistry S. Chand & Co. Ltd.

Course Outcomes

1. To become skilled in order to determination of composition of Fe^{II}/Fe^{III} complex.
2. To become skilled in order to determination of CMC of surfactants by surface tension method.

3. To become skilled in order to determination of CMC of surfactants by Spectrophotometric or Conductometric method.

Major (MJC - 20)

(Credits - 3 + 1)

Core T-20-Green Chemistry (3 Credits) (45 Lectures)

Introduction to Green Chemistry (4 Lectures)

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

Principles of Green Chemistry and Designing a Chemical Synthesis (20 Lectures)

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:

1. Designing a Green Synthesis using these principles: Prevention of waste/ byproducts; maximum incorporation of the materials used in the process into the final products, atom economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
2. Prevention/minimisation of hazardous/ toxic products, reducing toxicity. risk = (function)hazard × exposure; waste or pollution prevention hierarchy.
3. Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilised solvents and how to compare greenness of solvents.
4. Energy requirements for reactions – alternative sources of energy: use of microwaves (MW) and ultrasonic energy.
5. Selection of starting materials; avoidance of unnecessary derivatisation – careful use of blocking/protecting groups.
6. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
7. Prevention of chemical accidents, designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal Gas Tragedy (safer route to carbaryl) and Flixiborough accident (safer route to cyclohexanol), subdivision of ISD, minimisation, simplification, substitution, moderation and limitation.

8. Strengthening/development of analytical techniques to prevent and minimise the generation of hazardous substances in chemical processes.

Examples of Green Synthesis/ Reactions and some real-world cases (15 Lectures)

1. Green Synthesis of the following compounds: adipic acid, catechol, disodiumiminodiacetate (alternative to Strecker synthesis)

2. Microwave-assisted reactions in water: Hofmann elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave-assisted reactions in organic solvents: Diels-Alder reaction and Decarboxylation reaction

3. Ultrasound-assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)

4. Surfactants for carbon dioxide – replacing smog-producing and ozone-depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.

5. Designing an environmentally safe marine antifoulant.

6. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.

7. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.

8. Healthier Fats and Oils by Green Chemistry: Enzymatic Inter-esterification for the production of no trans-Fats and Oils.

9. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting.

10. Green counterpart of common organic reactions: Aldol, Friedel-Crafts, Michael, Knoevenagel, Cannizzaro, Benzoin condensation and Dieckmann condensation, Fries rearrangement, Claisen rearrangement, Beckmann rearrangement, Baeyer-Villiger oxidation.

Future Trends in Green Chemistry (6 Lectures)

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; Co-crystal controlled solid state synthesis (C_2S_3); Green chemistry in sustainable development.

Reference Books

- Anastas, P.T. & Warner, J.K.Green Chemistry - Theory and Practical, Oxford University Press (1998).
- Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).

- Cann, M.C. Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
- Ryan, M.A.; Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
- Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.
- Mandal, S. K. Introductory Green Chemistry, 2025, Redshine Publisher, ISBN 9789358797749.
- Kumar, V. An Introduction to Green Chemistry, 2018, Vishal Publishing Co. ISBN 8188646474.
- Bandopadhyay, C. An Insight into green Chemistry, 2019, Books & Allied Pvt. Ltd. ISBN 9788193984871.

Course Outcomes

1. To gain an understanding of the principles of green chemistry, including their explanations and examples, with special emphasis on applying these principles to design environmentally friendly (green) synthesis methods.

2. To gather knowledge and skills to understand the future trends of green synthesis.

Core P-20-Green Chemistry Lab (1 Credit) (30 Lectures)

Green Organic Preparations: The following reactions are to be performed, noting the yield of the crude product:

- **Safer chemicals/starting materials**

1. Preparation and characterisation of nanoparticles of gold/silver using tea/moringa leaves.
2. Nitration of aromatic compounds (CAN/Cu-nitrate)
3. Bromination of anilides using green approach (Bromate-Bromide method/CAN-Bromide)

- **Using renewable resources**

4. Preparation of biodiesel from vegetable/ waste cooking oil.
5. Extraction of D-limonene from orange peel using the conventional method

- **Prevention of waste**

6. Solid-state synthesis of benzilic acid from benzil.

- **Use of enzymes as catalysts**

7. Benzoin condensation using thiamine hydrochloride as a catalyst instead of cyanide.
8. Thiazolium salt as a safer surrogate for the Stetter reaction.

- **Alternative Green solvents**

9. Extraction of D-limonene from orange peel using liquid CO_2 prepared from dry ice.
10. Mechanochemical solvent-free synthesis of azomethines / benzilic acid.
11. Visible light-induced 'on water' benzylic bromination with N-bromosuccinimide

- **Alternative sources of energy**

12. Solvent-free, microwave-assisted one-pot synthesis of phthalocyanine complex of copper (II).
13. Photoreduction of benzophenone to benzopinacol in the presence of sunlight / UV irradiation.
14. Visible light-induced 'on water' benzylic bromination with N-bromosuccinimide

Reference Books

- Kirchoff, M.; Ryan, M.A. Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC (2002).
- Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. Green Chemistry Experiment: A monograph, International Publishing House Pvt Ltd. New Delhi. Bangalore ISBN 978-93-81141-55-7 (2013).
- Pavia, D.L.; Lampman, G.M. Kriz, G.S. & Engel, R.G. Introduction to Organic Laboratory Techniques: A Microscale and Macro Scale Approach, W.B.Saunders, 1995.
- Manna, A. K. Practical Organic Chemistry, Books and Allied (P) Ltd.
- Mandal, S. K. Introductory Green Chemistry, 2025, Redshine Publisher, ISBN 9789358797749.

Course Outcomes

- To gain the knowledge and skills required to comprehend how to apply green chemistry concepts such as atom economy, safer solvents, and energy-efficient reactions during practical experiments.

Minor (MN-7)

(Credits - 3 + 1)

T-7-Physical Chemistry II (3 Credits) **(45 Lectures)**

Chemical Equilibrium **(10 Lectures)**

Chemical Equilibrium: Thermodynamic conditions for equilibrium, degree of advancement; Variation of free energy with degree of advancement; Equilibrium constant and standard Gibbs free energy change; Definitions of K_P, K_C and K_X and relation among them; van't Hoff's reaction isotherm, isobar and isochore from different standard states; Shifting of equilibrium due to change in external

parameters e.g. temperature and pressure; variation of equilibrium constant with addition to inert gas; Le Chatelier's principle.

Application of Thermodynamics (11 Lectures)

Partial Properties and Chemical Potential: Chemical potential and activity, relation between Chemical potential and Gibb's free energy and other thermodynamic state functions; variation of Chemical potential (μ) with temperature and pressure; Gibbs-Duhem equation; Variation of thermodynamic functions for systems with variable composition; partial molar quantities, Change in G, S H and V during mixing for binary solutions.

Chemical potential and other properties of ideal substances – pure and mixtures: Ideal solution – Definition, Raoult's law; Mixing properties of ideal solutions, chemical potential of a component in an ideal solution.

Nernst's distribution law; Application (Equilibrium constant of $KI+I_2 = KI_3$ and solvent extraction).

EMF Cell (12 Lectures)

Electromotive Force: Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry; Chemical cells, reversible and irreversible cells with examples; Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone; Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation)

Crystal Structure (12 Lectures)

Bravais Lattice and Laws of Crystallography: Types of solid, Bragg's law of diffraction; Laws of crystallography (Haüy's law and Steno's law); Permissible symmetry axes in crystals; Lattice, space lattice, unit cell, crystal planes, Bravais lattice. Packing of uniform hard sphere, close packed arrangements (fcc and hcp); Tetrahedral and octahedral voids.

Crystal planes: Distance between consecutive planes [cubic, tetragonal and orthorhombic lattices]; Indexing of planes, Miller indices; calculation of d_{hkl}; Relation between molar mass and unit cell dimension for cubic system; Bragg's law (derivation)

Determination of crystal structure: Powder method; Structure of NaCl and KCl crystals.

Reference Books:

- Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press.

- Barrow, G.M. Physical Chemistry Tata McGraw- Hill (2007).
- Castellan, G.W. Physical Chemistry 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry Cengage Learning India Pvt. Ltd., New Delhi (2009).
- Mahan, B.H. University Chemistry 3rd Ed. Narosa (1998).
- Ekambaram, S. General Chemistry, Pearson.
- Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).
- Chugh, K.L., Agnish, S.L. A Text Book of Physical Chemistry Kalyani Publishers
- Bahl, B.S., Bahl, A., Tuli, G.D., Essentials of Physical Chemistry S. Chand & Co. ltd.
- Palit, S. R., Elementary Physical Chemistry Book Syndicate Pvt. Ltd.
- Mandal, A. K. Degree Physical and General Chemistry Sarat Book House
- Pahari, S., Physical Chemistry New Central Book Agency
- Pahari, S., Pahari, D., Problems in Physical Chemistry New Central Book Agency

Course Outcomes

1. To gather in-depth knowledge about chemical equilibrium and Chemical Potential.
2. To gather detailed knowledge about the electromotive force, concentration cells etc.
3. To acquire in depth idea about crystal structure, planes and laws of crystallography.

P-7-Physical Chemistry II Lab (1 Credit) (30 Lectures)

1. Study of kinetics of acid-catalyzed hydrolysis of methyl acetate.
2. Study of kinetics of decomposition of H_2O_2.
3. Determination of Keq for $KI + I_2 = KI_3$, using partition coefficient between water and CCl_4.

References:

- University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta, 2003.
- Palit, S.R., Practical Physical Chemistry Science Book Agency.
- Mukherjee, N.G., Selected Experiments in Physical Chemistry J. N. Ghose & Sons.
- Dutta, S.K., Physical Chemistry Experiments Bharati Book Stall.
- Bhattacharyya, R. C, A Manual of Practical Chemistry.

Course Outcomes

1. To become skilled at carrying out acid catalyzed hydrolysis of ester.
2. To become skilled at carrying out the kinetics for decomposition of H_2O_2.

3. To become experienced to evaluate the equilibrium constant of any chemical reaction.
