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- Yates, P. Chemical calculations. 2nd Ed. CRC Press (2007).
- Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de. How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. Physical chemistry on a Microcomputer. Little Brown & Co. (1985).
- Venit, S.M. Programming in BASIC: Problem solving with structure and style. Jaico Publishing House: Delhi (1996).

Semester-IV

Chemistry MAJOR

Paper code: CHEM4011 (3 and 4 Years)

Paper title: Organic Chemistry (Theory)

Credit: 5

Course objective

- Development of knowledge for several basic and advanced topics of organic chemistry

Course outcome

- The course will help the students to develop a complete knowledge on stereochemistry, reaction mechanism and others of organic chemistry.

Theory

Credit: 3

Stereochemistry II

18 Hours

Chirality arising out of stereoaxis: stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkylidenecycloalkanes and biphenyls; related configurational descriptors (R_a/S_a and P/M); atropisomerism; racemisation of chiral biphenyls; buttressing effect.

Concept of prostereoisomerism: prostereogenic centre; concept of (pro)n-chirality: topicity of ligands and faces (elementary idea); pro-R/pro-S, pro-E/pro-Z and Re/Si descriptors; pro-r and pro-s descriptors of ligands on propseudoasymmetric centre.

Conformation: conformational nomenclature: eclipsed, staggered, gauche, syn and anti; dihedral angle, torsion angle; Klyne-Prelog terminology; P/M descriptors; energy barrier of rotation, concept of torsional and steric strains; relative stability of conformers on the basis of steric effect, dipole-dipole interaction and H-bonding; butane gauche interaction; conformational analysis of ethane, propane, n-butane. 2-methylbutane and 2,3-dimethylbutane; haloalkane, 1,2-dihaloalkanes and 1,2-diols (up to four carbons); 1,2-halohydrin; conformation of conjugated systems (*s*-cis and *s*-trans).

Chemistry of alkenes and alkynes

15 Hours

Addition to C=C and C≡C: Mechanism (with evidence wherever applicable), reactivity, regioselectivity (Markownikoff and anti-Markownikoff additions) and stereoselectivity; reactions: hydrogenation, halogenations, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, ozonolysis; epoxidation, syn and anti-hydroxylation, iodolactonisation, addition of singlet and triplet carbenes (for alkenes); electrophilic addition to diene (conjugated dienes and allene); radical addition: HBr addition; use of NBS for allylic and benzylic bromination with mechanism, competition with brominations across C=C;; Birch reduction of benzenoid aromatics; interconversion of *E*- and *Z*-alkenes. dissolving metal reduction of alkynes (Birch); reactions of terminal alkynes by exploring its acidity.

Aromatic Substitution

10 Hours

Electrophilic aromatic substitution: mechanisms and evidences in favour of it; orientation and reactivity; reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction; one-carbon electrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Houben-Hoesch, Vilsmeier-Haack, Reimer-Tiemann, Kolbe-Schmidt); Ipso substitution.

Nucleophilic aromatic substitution: addition-elimination mechanism and evidences in favour of it; cine substitution (benzyne mechanism), structure of benzyne and unimolecular mechanism.

Carbonyl and Related Compounds

24 Hours

Addition to C=O: structure, reactivity and preparation of carbonyl compounds; mechanism (with evidence), reactivity, equilibrium and kinetic control; Burgi-Dunitz trajectory in nucleophilic additions; formation of hydrates, cyano hydrins and bisulphite adduct; nucleophilic addition-elimination reactions with alcohols, thiols and nitrogen-based nucleophiles; reactions: benzoin condensation, Cannizzaro and Tischenko reactions, reactions with ylides: Wittig reaction; oxidations and reductions: Clemmensen, Wolff-Kishner, LiAlH_4 , NaBH_4 , MPV, Oppenauer, Bouveault-Blanc, acyloin condensation; oxidation of alcohols with PDC and PCC; periodic acid and lead tetraacetate oxidation of 1,2-diols.

Exploitation of acidity of α -H of C=O: formation of enols and enolates; kinetic and thermodynamic enolates; reactions (mechanism with evidence): halogenation of carbonyl compounds under acidic and basic conditions, Hell-Volhard-Zelinsky (H. V. Z.) reaction, nitrosation, SeO_2 (Riley) oxidation; condensations (mechanism with evidence): Aldol, Tollens', Knoevenagel, Claisen-Schmidt, Claisen ester including Dieckmann, Stobbe; Mannich reaction, Perkin reaction, Favorskii rearrangement; alkylation of active methylene compounds; preparation and synthetic applications of diethyl malonate and ethyl acetoacetate; specific enol equivalents (lithium enolates, enamines) in connection with alkylation, acylation and aldol type reaction.

Nucleophilic addition to α , β -unsaturated carbonyl system: general principle and mechanism (with evidence); direct and conjugate addition, addition of enolates (Michael reaction), Robinson annulation.

Substitution at sp^2 carbon (C=O system): mechanism (with evidence): BAC^2 , AAC^2 , AAC^1 , AAL^1 (in connection to acid and ester); acid derivatives: amides, anhydrides and acyl halides (formation and hydrolysis including comparison).

Organometallics

8 Hours

Grignard reagent; Organolithiums; Gilman cuprates: preparation and reactions (mechanism with evidence); addition of Grignard and organo-lithium to carbonyl compounds; substitution on - COX; conjugate addition by Gilman cuprates; Corey-House synthesis; abnormal behavior of Grignard reagents; comparison of reactivity among Grignard, organo-lithium and organo-copper reagents; Reformatsky reaction; concept of umpolung and base-nucleophile dichotomy in case of organometallic reagents.

Reference Books/ Journals

Clayden, J., Greeves, N. & Warren, S. Organic Chemistry, Second edition, Oxford University Press, 2012.

Smith, J. G. Organic Chemistry, Tata McGraw-Hill Publishing Company Limited.

Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Pathak & Saha, Organic Chemistry (Volume-1 & 2), Books and Allied (P) Ltd.

Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd., (Pearson Education).

Morrison, R. T. Study guide to organic Chemistry, Pearson.

Nasipuri, D. Stereochemistry of Organic Compounds, New Age International (P) Ltd.

Sengupta, S. Basic Stereochemistry of Organic Molecules, Oxford University Press

Chemistry MAJOR

Paper code: CHEM4012 (3 and 4 Years)

Paper title: Physical Chemistry (Theory)

Credit: 5

Course objective

- Development of knowledge of theories of several experimental and theoretical aspects of chemistry

Course outcome

- The course will help to develop physical chemistry knowledge of solid, liquid and gaseous states of matter. Students will also learn to do quantum chemical calculations for various systems.

Theory

Credit: 5

Chemical Kinetics-II and Catalysis

12 Hours

Theories of reaction rate: Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment).

Homogeneous catalysis: Homogeneous catalysis with reference to acid-base catalysis; Primary kinetic salt effect; Enzyme catalysis; Michaelis-Menten equation, Lineweaver-Burk plot, turn over number, autocatalysis; periodic reactions.

Electrochemistry-I

15 Hours

Conductance and transport number: Ion conductance; Conductance and measurement of conductance, cell constant, specific conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes; Debye-Hückel theory of ion atmosphere (qualitative)-asymmetric effect, relaxation effect and electrophoretic effect; Ostwald's dilution law; Ionic mobility; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations.

Transport number, Principles of Hittorf's and Moving-boundary method; Wien effect, Debye-Falkenhagen effect, Walden's rule.

Partial molar properties and Chemical potential

12 Hours

Chemical potential and activity, partial molar quantities, 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; fugacity and fugacity coefficient; Variation of thermodynamic functions for systems with variable composition; Equations of states for these systems, Change in G, S, H and V during mixing for binary solutions.

Chemical Equilibrium

14 Hours

Thermodynamic conditions for equilibrium, degree of advancement; van't Hoff's reaction isotherm (deduction from chemical potential); 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 ; van't Hoff's reaction 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 and its derivation, Nernst Distribution law & its application-solvent extraction, steam distillation.

Specific heats of solid

5 Hours

Coefficient of thermal expansion, thermal compressibility of solids; Dulong –Petit's law; Perfect Crystal model, Einstein's theory – derivation from partition function, limitations; Debye's T^3 law – analysis at the two extremes (without derivation of T^3 law).

Thermodynamics-III

3 Hours

Third law of Thermodynamics: Absolute entropy, Planck's law, Calculation of entropy, Nernst heat theorem

Quantum Mechanics-I

14 Hours

Beginning of Quantum Mechanics: Wave-particle duality, light as particles: photoelectric and Compton effects; electrons as waves and the de Broglie hypothesis; Uncertainty relations (without proof).

Postulates of Quantum Mechanics, Wave function: Schrödinger time-independent equation; nature of the equation, acceptability conditions imposed on the wave functions and probability interpretations of wave function.

Concept of Operators: Elementary concepts of operators, eigenfunctions and eigenvalues; Linear and Hermitian operators; Commutation of operators, commutator and uncertainty relation; Expectation value.

Reference Books/ Journals

Atkins, P. W. & Paula, J. de Atkins' Physical Chemistry, Oxford University Press.

Castellan, G. W., Physical Chemistry, Narosa Publishing House.

McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press.

Engel, T. & Reid, P. Physical Chemistry, Pearson.

Maron, S. & Prutton, Principles of Physical Chemistry, Collier Macmillan Ltd.

Mortimer, R. G. Physical Chemistry, Elsevier.

Ball, D. W., Physical Chemistry, Thomson Press.

Glasstone, S. & Lewis, G.N. Elements of Physical Chemistry.

Rakshit, P.C., Physical Chemistry, Sarat Book House.

Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, Tata-McGraw-Hill.

Rastogi, R. P. & Misra, R.R. An Introduction to Chemical Thermodynamics, Vikas Publishing House.

Clauze & Rosenberg, Chemical Thermodynamics: Basic concepts & Methods, John Wiley & Sons, 2008.

Sharma, K. K. & Sharma, L. K., A Textbook of Physical Chemistry, Vikas Publishing House.

Chatterjee Hrishikesh, Physical Chemistry (Volume-1), Platinum Publisher

Kapoor, K.L., Textbook of Physical Chemistry (Volume 1 and Volume-2), McGraw Hill Education

Ghoshal, A. Numerical problems & short questions on Physical Chemistry, Books and Allied (P) Ltd.

Bajpai, D. N., Advanced Physical Chemistry, S. Chand Publication.

Levine, I. N. Physical Chemistry, Tata McGraw-Hill.

Chemistry MAJOR

Paper code: CHEM4013 (3 and 4 Years)

Paper title: Organic Chemistry (Practical)

Credit: 5

Course objective

- Detection of several elements in organic molecules
- Detection of functional group in organic molecules
- Organic preparations

Course outcome

- Students will have a hands-on training for detection of elements (N, S, Cl, Br, etc) and synthesis/derivatization of several organic compounds.

Practical

Credit: 5

A. Qualitative Analysis of single solid organic compound

- 1) Detection of special elements (N, S, Cl, Br) by Lassaigne's test
- 2) Solubility and classification (solvents: H₂O, 5% HCl, 5% NaOH and 5% NaHCO₃)
- 3) Detection of the following functional groups by systematic chemical tests:

- 4) Aromatic amino ($-\text{NH}_2$), aromatic nitro ($-\text{NO}_2$), amido ($-\text{CONH}_2$), anilide ($-\text{CONHAr}$), phenolic $-\text{OH}$, carboxylic acid ($-\text{COOH}$), ester ($-\text{COOR}$), carbonyl ($-\text{CHO}$ and $>\text{C}=\text{O}$)
- 5) Melting point of the given compound
- 6) Preparation of one suitable derivative of the given sample, crystallization and determination of melting point.

Each student, during laboratory session, is required to carry out qualitative chemical tests for all the special elements and the functional groups with relevant derivatisation in known and unknown (at least six) organic compounds.

B. Organic Preparations

The following reactions are to be performed, noting the yield of the crude product with melting point:

- 1) Nitration of acetanilide
- 2) Condensation reactions: Synthesis of 7-hydroxy-4-methylcoumarin
- 3) Hydrolysis of amides/imides/esters
- 4) Acetylation of phenols/aromatic amines (using Zn-dust/Acetic Acid)
- 5) Benzoylation of phenols/aromatic amines
- 6) Side chain oxidation of toluene and p-nitrotoluene
- 7) Diazo coupling reactions of aromatic amines
- 8) Bromination of acetanilide using green approach (Bromate-Bromide method)
- 9) Selective reduction of m-dinitrobenzene to m-nitroaniline
- 10) Students must also calculate percentage yield, based upon isolated yield (crude) and theoretical yield.

Purification of the crude product is to be made by crystallisation from water/alcohol, crystallization after charcoal treatment, or sublimation, whichever is applicable.

Reference Books/ Journals

Vogel, A. I. Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis, CBS Publishers and Distributors.

Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)

Clarke, H. T., A Handbook of Organic Analysis (Qualitative and Quantitative), Fourth Edition, CBS Publishers and Distributors (2007).

Ghoshal, A., Mahapatra, B., Nad, A. K. An Advanced Course in Practical Chemistry, New Central Book Agency (2007).

Bhattacharyya, R. C., A Manual of Practical Chemistry.

Chemistry MINOR

Paper code: CHEM4021

Paper title: General Chemistry-III

Credit: 3 + 1

Course objective

- Discussion on several general aspects of inorganic, organic and physical chemistry

Course outcome

- This course will help the students to develop advanced topics of chemistry, physics and biology. Students will learn to synthesize several coordination compounds. Students will also learn to estimate hardness of water by chemical analysis.

Theory

Credit: 3

Liquid state

6 Hours

Definition of Surface tension, its dimension and principle of its determination using stalagmometer; Viscosity of a liquid and principle of determination of coefficient of viscosity using Ostwald viscometer; Effect of temperature on surface tension and coefficient of viscosity of a liquid (qualitative treatment only).

Colligative properties

6 Hours

Raoult's law of relative lowering of vapour pressure, elevation of boiling point, depression of freezing point, osmosis and osmotic pressure, abnormal colligative property and vant Hoff factor, molecular weight determination of unknown solute

Solutions

8 Hours

Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions; Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions; Distillation of solutions; Lever rule; Azeotropes

Critical solution temperature; effect of impurity on partial miscibility of liquids; Immiscibility of liquids- Principle of steam distillation; Nernst distribution law and its applications, solvent extraction

Aromatic hydrocarbons

6 Hours

Benzene: Preparation: from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions: electrophilic substitution (general mechanism); nitration (with mechanism), halogenations (chlorination and bromination), sulphonation and Friedel-Craft's reaction (alkylation and acylation) (up to 4 carbons on benzene); side chain oxidation of alkyl benzenes (up to 4 carbons on benzene).

Synthetic uses of Grignard reagent & Active methylene compounds

6 Hours

Synthetic uses of Grignard reagent (GR), ethylacetoacetate (EAA) and diethylmalonate (DEM)

Coordination chemistry

10 Hours

Double and complex salts, Werner's theory of coordination complexes, classification of ligands, chelates, coordination numbers, IUPAC nomenclature of coordination complexes (up to two metal centers), isomerism in coordination compounds, constitutional and stereo isomerism, geometrical and optical isomerism in square planar and octahedral complexes.

Radioactivity

3 Hours

Characteristics, α , β and γ -rays, radioactive disintegration and equilibrium, decay constant, half-life and average life, artificial transmutation and artificial radioactivity, uses

Reference Books/ Journals

Lee, J. D. Concise Inorganic Chemistry ELBS, 1991.

Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic Chemistry Oxford, 1970.

Sharpe, A.G., Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005.

Mingos, D.M.P., Essential trends in inorganic chemistry. Oxford University Press (1998).

Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Sarkar, R, General and inorganic chemistry, Volume II, New central book agency, (2012).

Rakshit, P. C., Physical Chemistry, Sarat Book House.

Rastogi, R. P. & Misra, R.R. An Introduction to Chemical Thermodynamics, Vikas Publishing House.

Sharma, K. K. & Sharma, L. K., A Textbook of Physical Chemistry, Vikas Publishing House.

Bajpai, D. N., Advanced Physical Chemistry, S. Chand Publication.

Kapoor, K.L., Textbook of Physical Chemistry (Volume 1 and Volume 2), McGraw Hill Education

Ghoshal, A. Numerical problems & short questions on Physical Chemistry, Books and Allied (P) Ltd.

Practical

Credit: 1

A. Inorganic preparations

- 1) Tetraamminecarbonatocobalt(III) ion
- 2) Potassium tris(oxalato)ferrate(III)
- 3) Tris(ethylenediamine) nickel (II) chloride

B. Complexometric titration

Determination of total hardness of water by using standard EDTA solution

Reference Books/ Journals

Bhattacharyya, R. C, A Manual of Practical Chemistry.

Nad, Mahapatra, Ghosal, An Advance course in Practical Chemistry, New Central Book Agency (P) Ltd.

K. S. Mukherjee, Textbook on Practical Chemistry, New Central Book Agency (P) Ltd.

Ghosh, Das Sharma, Majumdar, Manna, Chemistry in Laboratory, Santra Publication (P) Ltd.

Poddar and Ghosh, Degree Practical Chemistry, Book Syndicate (P) Ltd.

Semester-V

Chemistry MAJOR
Course code: CHEM5011 (3 and 4 Years)