Department of Chemistry
Government Degree College, Baramulla (Autonomous)

Semester 4th **Major/Minor Course**

Subject: Chemistry

Course Title: Chemistry-IV **Course Code: BCH22C401**
Credit: Theory: 04; Practical: 02 **Contact Hours: (64 Th + 64 Pr)**

Course Objectives:

- *To understand the concept of rate of change associated with chemical change, to determine rate law of chemical change based on experimental data, understand the laws of absorption light by molecules and deactivation processes, and to characterize the kinetics of deactivation process and their role in photochemistry*
- *To understand the, nomenclature, isomerism and chemistry of coordination complexes. To understand theories of bonding, geometric shapes and distortion in shapes of coordination complexes.*
- *To understand the chemistry of Aldehydes, Ketones and Carboxylic acids.*
- *To understand the chemistry of Amines, Nitriles, Isonitriles and Nitro compounds*

Learning outcomes:

After the successful completion of the course the student shall be able to;

- *Be able to identify the order of a reaction and apply integrated rate equations to know the mechanism of a chemical reaction. The student shall comprehend reaction intermediates and use of energy profile diagram. The student shall be able to differentiate between the thermal and photochemical process, know various chemical process and fate of excited electron*
- *Name the different coordination complexes, the knowledge of stability, colour, magnetic properties and isomerism. The student shall learn CFSE calculations, Isomerism in complex compounds.*
- *To understand the synthesis of carbonyl and carboxylic compounds, recognise their properties and comprehend the mechanism of the reactions involved.*
- *To understand the synthesis of nitrogen compounds, recognise their properties and comprehend the mechanism of the reactions involved.*

Unit I: Chemical Kinetics and Photochemistry *(16 Contact hours)*

Order of reaction; derivation of rate equations for second (two reactants) and third order reactions. Determination of order of reaction by differential rate, integration, half-life period and isolation methods. Temperature dependence of reaction rates:-Arrhenius equation, concept of activation energy. Theories of chemical kinetics: Simple collision theory based on hard sphere model, evaluation of rate constants of atomic reactions, limitations. Brief idea of transition state theory (equilibrium hypothesis).

Photochemistry: Introduction, Laws of photochemistry; Grothus-Drapper law, Stark-Einstein law, Jablonski diagram: Description quantum yield, photosensitized reactions, energy transfer processes (simple examples).

Kinetics of photochemical reactions: hydrogen iodide and hydrogen-bromine.

Unit II: Coordination Chemistry of Transition Elements *(16 Contact hours)*

IUPAC nomenclature of coordination compounds, isomerism structural isomers (ionization isomers, coordination isomerism, hydrate/solvate isomerism, linkage isomerism), geometric and optical isomerism.

Bonding theories in coordination compounds: Werner's theory, valence bond theory and its limitations. Crystal field theory, crystal field splitting in octahedral, tetrahedral, and square planar complexes. Spectrochemical Series; Crystal field splitting energy (CFSE) in weak and strong fields, pairing energies, calculation of energies, factors effecting the magnitude of splitting. Jahn-Teller distortions.

Unit III: Aldehydes, Ketones and carboxylic Acids *(16 Contact hours)*

Preparation of aldehydes and ketones (Aliphatic and aromatic) from alkenes, alkynes, acid chlorides, nitriles, toluene and benzene. Reactions – Reaction with HCN, ROH, $NaHSO_3$ ammonia-derivatives. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation, Clemenson reduction and Wolff Kishner reduction. Meerwein-Pondorff Verley reduction.

Preparation of Carboxylic acids, Reactions: Anhydrides, Esters and Amides and their inter conversion. Reaction: Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

Unit IV: Amines, Nitriles, Isonitriles and Nitro compounds *(16 Contact hours)*

Amines (Aliphatic and Aromatic): Preparation from nitro compounds, nitriles and isonitriles, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction. Reactions: Electrophilic substitution of Aniline: nitration, bromination, sulphonation. Carbylamines reaction, Hinsberg test, Alkylation and acylation reactions

Diazonium salts: Preparation from aromatic amines. Sandmeyer and Gattermanns reactions; Synthetic application of diazonium salts.

Books Recommended:

1. Concise Inorganic Chemistry; J.D. Lee; 5thEdn., OUP/Wiley India Pvt. Limited, 2008
2. Chemistry of the Elements; N. N. Greenwood, A. Earnshaw; 2nd Edn., Elsevier India, 2010.
3. Principles of Inorganic Chemistry; B.R. Puri, L.R. Sharma and K.C. Kalia; 33rdEdn., Milestone Publishers & Distributors/ Vishal Publishing Co., 2017
4. Advanced General Organic Chemistry: A Modern Approach; S.K. Ghosh; 3rd Revised Edn., New Central, 2010.
5. Organic Chemistry; R.T. Morrison, R.N. Boyd, S. K. Bhattacharjee; 7th Edn, Pearson India, 2011.
6. Organic Chemistry; P.Y. Bruice; 8th Edn, Pearson Education, 2017.
7. Advanced Organic Chemistry; Dr. Jagdamba Singh and LDS Yadav; Pragati edition, 2017.
8. Principles of Physical Chemistry; B.R. Puri, L.R. Sharma and L.S. Pathania; 47th Edn., Vishal Pubs & Co, 2017.
9. Physical Chemistry; T. Engel, P. Reid, 3rd Edn. Pearson India, 2013.
10. Atkins Physical Chemistry, Peter Atkins, Julio de Paula, James Keeler; 11th Edn, Oxford University Press, 2018
11. Chemical Kinetics, Keith J. Laidler, 3rd Edition, Pearson Education, 1987

Part 2: Laboratory Course (2 Credits)

Course Objectives:

- *To understand the estimation of metal in complexes.*
- *To understand the process of purification organic compounds by different methods and to synthesise the organic molecules*
- *To determine change in pH of different solutions.*

Learning outcomes:

On completion of the course, the student should be able to:

- *Estimate the metal concentration in coordination complexes.*
- *Synthesize and process of organic molecules*
- *Learn methods for determination of pH metry and use of technique.*

Inorganic Chemistry

Gravimetry (Any Three)

1. Estimation of Copper as CuSCN.
2. Estimation of Nickel as $[Ni(dmg)_2]$.
3. Estimation of Silver as AgCl.
4. Estimation of Barium as $BaSO_4$.

Organic Chemistry

1. Separation of mixture of organic mixtures by TLC / Column chromatography.
2. Preparation of nitro and m-dinitrobenzene from Benzene
3. An education/Industrial Tour

Physical Chemistry

1. To determine the concentration of a strong acid solution by titration with a strong base Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures (pH metry)
2. To determine pKa of a weak acid by pH metry.
3. Determination of specific rotation by polarimetry.
4. Kinetics of inversion of cane sugar by polarimetry.

Books Recommended

1. Advanced Practical Physical Chemistry, J. P. Yadav, Krishna Publications, 2022
2. Advanced Practical Organic Chemistry, N. K. Vishnoi, 3rd Edn. Vikas Publication House, 2009
3. Vogel's Textbook of Practical Organic Chemistry, Brain S. Furniss, Antony J. Hannaford, Peter W. G. Smith and Austin R. Tatchel; 5th Edn. Pearson 2003

Department of Chemistry
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Semester 4th **Major only**

Subject: Chemistry

Course Title: Chemistry-V **Course Code: BCH22C402**
Credit: Theory: 04; Practical: 02 **Contact Hours: (64 Th + 64 Pr)**

Course Objectives:

- *To understand the classical mechanism and complex numbers, functions, operators, and mathematical foundations of quantum chemistry. To comprehend size and shape of a box, and the mass of a particle in it, influence the allowed energy states; calculate realistic energies for particle-in-a-box (PIB) systems.*
- *An introduction to the broad field of heterocyclic organic chemistry by reviewing the major classes of heterocyclic compounds in terms of nomenclature, structure, properties, preparations and reactions. The syntheses of several physiologically important heterocyclic compounds are given.*
- *To impart advanced knowledge on nature of bonding in organic molecules, structure & reactivity, intermediate formation and reaction mechanism.*
- To understand the role and importance of metal ions in biological system.

Learning outcomes:

After the successful completion of the course the student shall be able to;

- *Explain the reason for failure of classical mechanics for experimental observations and predict the agreement of quantum mechanics to such observations. The student shall carry out simple calculations involving complex numbers functions and operators.*
- *Understand the major classes of heterocyclic compounds. Specifically, the student will learn nomenclature, structure, properties, syntheses, and reactions of 3, 4, 5 and 6-membered ring heterocycles, the benzene ring fused ring heterocycles, the pyridine group, and the quinoline and isoquinoline groups.*
- *Understand the fundamental concept of delocalized chemical bonding, conjugation in organic molecules and role of electronic effects. The student shall understand the reaction mechanism, kinetics, energetics, structure, stabilities and reactivity's of various reactive intermediates. The chemistry of various chemical rearrangement and mechanism of important reaction mechanisms.*
- *To understand the essential, non-essential and trace elements and their biological system. The student shall learn about the diseases caused by their deficiencies.*

Unit I: An introduction to Quantum Chemistry (16 Contact hours)

Limitation of Classical mechanics: Black-body radiation and Planck's radiation law, photoelectric effect, heat capacity of solids Classical wave equation, Schrodinger wave equation and its importance. Eigen function and Eigen values. Introduction to operators, Algebra, Rules for setting operators (position and linear momentum), Hamiltonian operator.

Linear and Hermitian operators, commutation of operators. Postulates of quantum mechanics, Quantum mechanical treatment of particle in a one-dimensional box.

Unit II: Heterocyclic Compounds: (16 Contact hours)

Nomenclature of Heterocyclic compounds: trivial name Hantzsch-Widman nomenclature for monocyclic, fused and bridged heterocycles. Replacement of Hanzsch-Widman nomenclature by IUPAC nomenclature. Three and four membered heterocyclic compounds (Preparation Only): Aziridine, thiirane, oxetanes and thietanes; Five membered heterocyclic compound: Properties of pyrroles, furans and thiophenes; Six Membered heterocyclic Compounds: Properties of pyridines, pyrimidine, dioxane, Mechanistic details in the preparations of indole and quinoline using Fischer-Indole and Bishlier-Napierlaski synthesis.

Unit III: Mechanistic Study of Molecular Rearrangements (16 Contact hours)

General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Nature of migration and migratory aptitude and memory effect. Rearrangement to electron deficient centers: Wagneer Meerwin, Pinacol-Pinacolon, Demyanov, Benzil-Benzilic Acid, Arndt-Eistert, Pyne, Dienone-Phenol, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Dakin, Neber; Rearrangement to electron rich centres: Stevens, Favorskii; Free Radical Rearrangement: Claisen rearrangement, Photo-Fries Rearrangement

Unit IV: Bio Inorganic Chemistry (16 Contact hours)

Metal ions present in biological systems, classification of elements according to their action in biological system. Excess and deficiency of some trace metals. Sodium-potassium pump, role of zinc in carboxypeptidase and carbonic anhydrase. Iron and its application in bio-systems; structure and function of haemoglobin, storage and transfer of iron. Toxicity of metal ions (Hg, Pb, Cd and As), and reasons for toxicity. Use of chelating agents in medicine.

Part 2: Laboratory Course (2 Credits)

Course Objectives:

- *To understand the separation techniques.*
- *To understand different methods of organic synthesis*
- *To understand the technique of potentiometry.*

Learning outcomes:

On completion of the course, the student should be able to:

- *Isolate the given mixtures of metal ions.*
- *Synthesize and process of organic molecules*

- *Apply the potentiometric titration methods.*

Inorganic Chemistry

Chromatography of metal ions: Principles involved in chromatographic separations.

Paper chromatographic separation of following metal ions:

i. Ni(II) and Co(II)

ii. Fe(III) and Al(III)

Organic Chemistry

Following organic Preparations/Reactions

1. Benzil-Benzilic acid rearrangement/Backman rearrangement.
2. Phenol formaldehyde resin.
3. Dibenzal acetone from benzaldehyde.

Physical Chemistry

Conductometry

Perform the following potentiometric titrations:

i) Strong acid vs. strong base

ii) Weak acid vs. strong base

iii) Mixture of strong and weak acid *Vs* strong base

Books Recommended:

1. Concise Inorganic Chemistry; J.D. Lee; 5thEdn., OUP/Wiley India Pvt. Limited, 2008
2. Chemistry of the Elements; N. N. Greenwood, A. Earnshaw; 2nd Edn., Elsevier India, 2010.
3. Principles of Inorganic Chemistry; B.R. Puri, L.R. Sharma and K.C. Kalia; 33rdEdn., Milestone Publishers & Distributors/ Vishal Publishing Co., 2017
4. Advanced General Organic Chemistry: A Modern Approach; S.K. Ghosh; 3rd Revised Edn., New Central, 2010.
5. Organic Chemistry; P.Y. Bruice; 8th Edn, Pearson Education, 2017.
6. Principles of Physical Chemistry; B.R. Puri, L.R. Sharma and L.S. Pathania; 47th Edn, Vishal Pubs & Co, 2017.
7. A Guidebook to Mechanism in Organic Chemistry; Peter Sykes, 6th Edn, 2003 Pearson
8. Organic Reaction Mechanism; Ash Copeland & Luke Bell, ED Tech Press 2019
9. Heterocyclic Chemistry, Thoimas L. Gilchrist, 3rd Edn, Paerson 2005
10. Heterocyclic Chemistry; Raj K Bansal, 5th Edn, New Age International Publishers, 2017
11. A Text Book of Physical Chemistry, Quantum Chemistry and Molecular Spectroscopy, Vol 4; K. L. Kapoor, 4th Edn, McGraw Hill Education, 2020
12. A Text Book of Physical Chemistry, Vol 1; Mandeep Dalal, 1st Edn, Dalal Institute, 2018

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Semester 4th **Major only**

Subject: Chemistry

Course Title: Mathematics for Chemists **Course Code: BCH22C403**
Credit: Theory: 04; Tutorial: 02 **Contact Hours: (64 Th + 32 Tu)**

Learning Objective:
The course will provide a basic understanding of mathematics mainly focused on its use in chemistry.

Learning outcomes:

After the successful completion of the course the student shall be able to;

- *apply mathematics in order to solve problems in chemistry*
- *Understand the areas of chemistry, largely based upon mathematics such as physical chemistry.*
- *develop skills for career in theoretical/computational chemistry*

Unit I: Functions and their Differentiation (16 contact hrs)
Functions, single valued and multiple valued, domain and range of a function. Algebraic & transcendental functions, trigonometric, logarithmic, experimental & hyperbolic functions. Even and odd functions, continuous and discontinuous functions.
Differentiation: Limits δ–ε rotation, derivative of a function, the differential operator. Derivatives of functions like ax^n, $(ax+b)^n$, lnx, e^x, a^x, Sin x, Cos x , Tan x, $Sin^{-1}x$, Cos^{-1} x, Tan^{-1} x.
Rules for differentiation, physical significance of the derivative, maxima & minima, higher order derivatives.

Unit II: Partial Differentiation & Integration (16 contact hrs)
Functions of multiple variables. Partial differentiation, total differential, exact and inexact differentials (examples from thermodynamics). Integration as a sum and area under a curve. Integration as inverse of differentiation, definite and indefinite integral. Table of integrals of common functions. Basic rules of integration; integration by substitution, by parts and by partial factions.

Unit III: Elementary Differential equations: (16 contact hrs)
Variable separated and variable separable differential equations. Order and degree of a differential equations, Homogenous and Heterogeneous Differential equations. First order linear differential equation and its solution. Second order homogenous differential equations and its solution by auxiliary equations method. Applications in Kinetics

Unit IV: Matrices (16contact hrs)
Definition, rectangular, square, diagonal, triangular, column and row matrices. Trace of matrix. Addition and multiplication of matrices. Zero matrix and identity or unit matrix.

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Determinant of a matrix, properties of determinants. Solutions of simultaneous equations by use of determinants. Transpose, complex conjugate, adjoint and inverse of a matrix. Solutions of simultaneous equations by matrix method.
Special matrices: Symmetric, skew symmetric, Hermitian, skew Hermitian and unitary matrices.

Unit V: Tutorial-1 (16 contact hrs)

Plot graphs of the functions $y = f(x)$ as given below:

I. $y = 3x^2 + 2x - 1; at\ x = -4, -3, -1, 0, 1, 2, 3, 4$

II. $y = cos\theta, \theta\ varying\ between - 180° to + 180°$

III. $y = tan\theta;\ -180° \leq \theta \leq +180°$

IV. $y = logx; x\ varying\ from\ 0\ to\ 100$

V. $y = e^x, y = e^{-x}\ and\ y = e^{x^2}\ for\ x = 0 - 10$

Find deviation of the functions at a given point in the range and also draw a target to the graph at the same point. Compare the slop with the derivative.

Find the value of the function $y = \int_{-1}^{+1} e^x dx$ and also find the area under the curve between the same limits.

Plot $y = sin\theta$ with the range $-180° \leq \theta \leq +180°$ find the value of θ at which $^{dy}/_{dx} = 0$ and verify that the points correspond to maxima & minima.

Unit V: Tutorial-II (16 contact hrs)

I. Solve the differential equations

i. $ydx = xdy$

ii. $(1 + x)ydx + (1 - y)xdy = 0$

iii. $-{}^{dN}/_{dt} = \lambda T$

iv. ${}^{x^2 dy}/_{dx} - 2xy = {}^{1}/_{x}$

II.

i. Given A = $\begin{pmatrix} 3 & i \\ 0 & 2 \end{pmatrix}$ & B = $\begin{pmatrix} 2 & 0 \\ -3 & -i \end{pmatrix}$

Find A+B, AB, BA, [A, B]

ii. Determine the value of the determinant

$$\begin{vmatrix} 2 & -1 & 3 \\ 6 & 8 & 9 \\ 5 & 0 & 1 \end{vmatrix}$$

iii. Solve the equation $\begin{vmatrix} x & 1 & 0 & 0 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 0 & 0 & 1 & x \end{vmatrix} = 0$

iv. Solve the equation by matrix method

$$x + iy = 3$$

v. Given $A = \begin{pmatrix} 1 & i & 0 \\ 0 & 1 & -i \\ i-1 & 0 & 1 \end{pmatrix}$ find A*, A^-, A^+

$$ix + y = 3i$$

Books Recommended

1. G. B. Thomas and R. L. Finney, Calculus, 9th edition, Pearson Education Delhi, 2005
2. H. Anton, I. Bivens and S. Davis, Calculkus, John Wiley and Sons (Asia) P. Ltd. 2002
3. Shepley L. Ross, Differential Equations, 3rd Edition, John Wiley & Sons, 1984
4. Sneddon, Elements of partial differential equations, McGraw Hill, International Edition, 1967