



# ODISHA UNIVERSITY OF TECHNOLOGY AND RESEARCH

Techno Campus, Mahalaxmi Vihar, Ghatikia, Bhubaneswar-751029.

## Syllabus Structure (Effective from 2023-24)

School/ Department: School of Basic Sciences & Humanities

Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)

### Subject Code Format:

A1	A2	B3	C4	C5	C6
<b>School/ Dept. (Offering)</b>		<b>Level</b>	<b>0: AC</b>	<b>Serial Number (01 to 99)</b>	
<b>BH:</b> Basic Sciences and Humanities		<b>1:</b> UG/ Int. MSc. (1 <sup>st</sup> Year)	<b>1:</b> PC	01/ 03/.../ 19: Odd Sem. (CHEM)	
<b>CS:</b> Computer Sciences		<b>2:</b> UG/ Int. MSc. (2 <sup>nd</sup> Year)	<b>2:</b> PE	21/ 23/.../ 39: Odd Sem. (HUM)	
<b>EE:</b> Electrical Sciences		<b>3:</b> UG/ Int. MSc. (3 <sup>rd</sup> Year)	<b>3:</b> OE	41/ 43/.../ 59: Odd Sem. (MATH)	
<b>EI:</b> Electronic Sciences		<b>4:</b> UG/ Int. MSc. (4 <sup>th</sup> Year)	<b>4:</b> MC	61/ 63/.../ 79: Odd Sem. (PHY)	
<b>IP:</b> Infrastructure and Planning		<b>5:</b> UG/ Int. MSc. (5 <sup>th</sup> Year)	<b>5:</b> LC	81/ 83/.../ 99: Odd Sem. ()	
<b>MS:</b> Mechanical Sciences		<b>6:</b> PG (1 <sup>st</sup> Year)	<b>6:</b> PR	02/ 04/.../ 20: Even Sem. (CHEM)	
<b>BT:</b> Biotechnology		<b>7:</b> PG (2 <sup>nd</sup> Year)	<b>7:</b> SE	22/ 24/.../ 40: Even Sem. (HUM)	
<b>TE:</b> Textile Engineering		<b>8:</b> Ph.D.	<b>8:</b>	42/ 44/.../ 60: Even Sem. (MATH)	
			<b>9:</b>	62/ 64/.../ 80: Even Sem. (PHY)	
				82/ 84/.../ 98: Even Sem. ()	

### Abbreviation used:

PC:	Professional Core	IA*:	Internal Assessment	L:	Lecture
PE:	Professional Elective	EA:	End-Semester Assessment	T:	Tutorial
OE:	Open Elective	PA:	Practical Assessment	P:	Practical
MC:	Mandatory Course	PR:	Project/ Seminar/ Practical		
LC:	Lab Course	AC:	Audit course		

### 1st Semester M.Sc.

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit	Maximum Marks			
			L	T	P		IA	EA	PA	Total
PC-1	BH6101	Inorganic Chemistry-I	4	0	0	4	40	60	-	100
PC-2	BH6103	Organic Chemistry-I	4	0	0	4	40	60	-	100
PE-1	BH6201	Quantum Chemistry	3	0	0	3	40	60	-	100
PE-2	BH6203	Group Theory And Molecular Spectroscopy	3	0	0	3	40	60	-	100
PC Lab-1	BH6501	Inorganic Chemistry Laboratory-I	0	0	3	2	-	-	100	100
AECC Lab-1	CS6583	Computational Chemistry Laboratory-I	0	0	2	1	-	-	100	100
PC Lab-2	BH6503	Organic Chemistry Laboratory-I	0	0	3	2	-	-	100	100
<b>Total credit</b>			<b>14</b>	<b>0</b>	<b>8</b>	<b>21</b>	<b>160</b>	<b>240</b>	<b>300</b>	<b>700</b>



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### 2nd Semester M.Sc.

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit	Maximum Marks			
			L	T	P		IA	EA	PA	Total
PC-3	BH6102	Inorganic Chemistry-II	4	0	0	4	40	60	-	100
PC-4	BH6104	Organic Chemistry-II	4	0	0	4	40	60	-	100
PC-5	BH6106	Physical Chemistry-I	4	0	0	4	40	60	-	100
PE-3	BH6202	Biochemistry	3	0	0	3	40	60	-	100
PC Lab-3	BH6502	Inorganic Chemistry Laboratory-II	0	0	3	2	-	-	100	100
PC Lab-4	BH6504	Organic Chemistry Laboratory-II	0	0	3	2	-	-	100	100
PC Lab-5	BH6506	Physical Chemistry Laboratory-I	0	0	3	2	-	-	100	100
<b>Total credit</b>			<b>15</b>	<b>0</b>	<b>9</b>	<b>21</b>	<b>160</b>	<b>240</b>	<b>300</b>	<b>700</b>

### 3rd Semester M.Sc.

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit	Maximum Marks			
			L	T	P		IA	EA	PA	Total
PE-4	BH7201	Organic Spectroscopy	3	0	0	3	40	60	-	100
PE-5	BH7203	Elective-I	3	0	0	3	40	60	-	100
PE-6	BH7205	Elective-II	0	0	3	3	40	60	-	100
PC-6	BH7101	Physical Chemistry-II	4	0	0	4	40	60	-	100
Seminar	BH7701	Literature Review & Seminar	0	0	4	2	-	-	100	100
PC Lab-6	BH7501	Physical Chemistry Laboratory-II	0	0	3	2	-	-	100	100
PE Lab-1	BH7503	Biochemistry Laboratory	0	0	3	2	-	-	100	100
PE Lab-2	BH7505	Computational Chemistry Lab-II	0	0	3	2	-	-	100	100
<b>Total credit</b>			<b>10</b>	<b>0</b>	<b>16</b>	<b>21</b>	<b>160</b>	<b>240</b>	<b>400</b>	<b>800</b>

### 4th Semester M.Sc.

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit	Maximum Marks			
			L	T	P		IA	EA	PA	Total
PC-7	BH7102	Inorganic Chemistry-III	4	0	0	4	40	60	-	100
PC-8	BH7104	Bioinorganic And Supramolecular Chemistry	4	0	0	3	40	60	-	100
PC-9	BH7106	Organic Chemistry-III	4	0	0	3	40	60	-	100
PE-7	BH7202	Elective-III	4	0	0	3	40	60	-	100
Project	BH7602	Project	0	0	6	6	-	-	100	100
<b>Total credit</b>			<b>16</b>	<b>0</b>	<b>6</b>	<b>19</b>	<b>160</b>	<b>240</b>	<b>100</b>	<b>500</b>

Students have to opt electives either from group-A or B or C

ELECTIVE	Group-A	Group-B	Group-C
I	Spectral Techniques in Inorganic Chemistry	Natural Product Chemistry	Advanced Chemical Kinetics
II	Chemistry of Materials	Pharmaceutical Chemistry	Biophysical Chemistry
III	Nuclear And Radiochemistry	Newer Synthetic Reactions and Reagents	Advanced Electrochemistry



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### 1<sup>st</sup> SEMESTER

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-1	BH6101	INORGANIC CHEMISTRY-I	4	0	0	4

**Course Outcomes:** Upon completion of this course, the students will be able to

1. understand structure and bonding of compounds involving main group elements.
2. predict the spectral properties of coordination compounds based on crystal field theory.
3. describe the stability of metal complexes through formation constants and able to calculate thermodynamic parameters from them.
4. demonstrate the reaction mechanism of selected substitution and electron transfer reaction of co-ordination compounds.

#### Unit- I

##### **Stereochemistry and Bonding in Main Group Compounds**

Wade's rule, STYX method, application to boron compounds and carboranes.

Structure and bonding in condensed phosphates, silicates, cyclo phosphazenes and S-N cyclic compounds.

##### **Metal - Ligand Bonding**

Limitation of CFT, MOT: energy level diagram of  $\sigma$  – and  $\pi$  – bonding in octahedral, tetrahedral and square planar complexes.

#### Unit- II

##### **Electronic Spectra of Coordination Compounds:**

Spectroscopic ground states, term symbols for  $d^n$  ions, Racah parameters, selection rules and intensities of bands, Orgel diagram, correlation and Tanabe-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent metal ions ( $d^1$ - $d^6$ ), divalent (Mn, Co and Ni), Calculation of  $Dq$ ,  $B$  and  $\beta$  parameters for tetrahedral and octahedral complexes, CT spectra. Spectral properties of lanthanide and actinide metal complexes.

#### Unit- III

##### **Metal-ligand Equilibria in Solution**

Stability of metal complexes, compositions of metal complexes by Job's method. Stepwise and overall stability constant, factors affecting the stability constant, Determination of stability constants by (pHmetry and spectroscopic methods) and their applications.

#### Unit- IV

##### **Inorganic Reaction Mechanism**

Inert and labile complexes, factors affecting the reactivity of complexes, mechanisms of substitution (acid, base hydrolysis and anation) reactions of octahedral complexes, substitution reactions of square planar complexes, trans-effect – theories and applications in synthesis of metal complexes, redox reactions: mechanism of one electron transfer reaction (inner sphere and outer-sphere), Marcus theory for outer-sphere reactions.

##### **Suggested Readings:**

1. P.W. Atkins, and D.F. Shriver, Inorganic Chemistry 5<sup>th</sup> Edition, 2010, Oxford University Press.
2. N. N. Greenwood, and A. Earnshaw, Chemistry of the Elements, 2<sup>nd</sup> Edition, 1997, Butterworth-Heinemann, Elsevier.
3. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Inorganic Chemistry, 1<sup>st</sup> Indian Edition, 2006, Pearson Education.
4. F. A. Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann, Advanced Inorganic Chemistry, 6<sup>th</sup> Edition, 1999, John Wiley & Sons.
5. A. K. Das and M. Das, Fundamental Concept of Inorganic Chemistry, Vol. 4 and 5, 2<sup>nd</sup> Edition, 2014, CBS Publisher & Distributor Pvt. Ltd.
6. G. L. Miessler, P. J. Fischer and D. A. Tarr, Inorganic Chemistry, 5<sup>th</sup> Edition, 2013 Pearson Education.



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Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-2	BH6103	ORGANIC CHEMISTRY-I	4	0	0	4

**Course Outcomes:** Upon completion of this course students will be able to

1. comprehend the organic reaction mechanism through the knowledge of structure, reactivity and rearrangement in organic molecules.
2. understand the basic mechanism of various organic substitution reactions and their application towards preparation of different organic compounds.
3. reveal the structural features of organic compounds and the genesis of the optical activity of chiral substances.
4. familiarize with some well-known organic reaction and its applications

### Unit- I

#### Stereochemistry

Conformational analysis of cycloalkanes, decalin, effect of conformation on reactivity, conformation of sugars, Elements of symmetry, chirality, molecules with more than one chiral center, threo- and erythro- isomers, methods of resolution. Optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape.

### Unit- II

#### Reaction Mechanism (Structure, Reactivity and Rearrangements)

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes, benzyne. Types of mechanisms:  $S_N2$ ,  $S_N1$ , mixed  $S_N1$  and  $S_N2$ ,  $S_N$  at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity: effects of substrate, structure, attacking nucleophile, leaving group and reaction medium, ambient nucleophile and regioselectivity. Kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates. Methods of determining reaction mechanisms, isotope effects. Quantitative treatment, Hammett equation and linear free energy relationships, substituent and reaction constants, Taft equation. The NGP mechanism, NGP by  $\pi$  and  $\sigma$  bonds, anchimeric assistance. Classical and nonclassical carbocations, norbornyl systems.

### Unit- III

#### Aromatic Electrophilic Substitution Reactions

The arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction. The  $S_NAr$ ,  $SRN1$  mechanisms, reactivity effect of substrate structure, leaving group and attacking nucleophile. Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance, reactivity of aliphatic and aromatic substrates at bridgehead, reactivity in the attacking radicals, effects of solvents on reactivity.

### Unit- IV

#### Molecular rearrangements

General mechanistic considerations-nature of migration, Migratory aptitude, A detailed study of the following rearrangements: Pinacol-Pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Ester synthesis, The von Richter, Sommelet-Hauser and Smiles rearrangements, Neber, Beckmann, Hoffman, Curtius, Schmidt, Bayer-Villiger, Fries rearrangement, Shapiro reaction.

#### Suggested Readings:

1. M. B. Smith, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7<sup>th</sup> Edition, 2013, John Wiley & Sons.
2. F. A. Carey, and R. J. Sundberg, Advanced Organic Chemistry Part A & B: Structure and Mechanisms, 5<sup>th</sup> Edition, 2007, Springer International Edition.
3. P. Sykes, A Guide Book to Mechanism in Organic Chemistry, 6<sup>th</sup> Edition, 1985, John Wiley & Sons Inc.
4. H. O. House, Modern Organic Reactions, 2<sup>nd</sup> Edition, 1972, Addison Wesley.



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5. R. O. C. Norman, and J.M. Coxon, Principles of Organic Synthesis, 3<sup>rd</sup> Edition, 1993, Academic Press.
6. P.S. Kalsi, Stereochemistry of Organic Compounds, 8<sup>th</sup> Edition, 2015, New Age International Publication.
7. J. Clayden, N. Greeves, and S. Warren, Organic Chemistry, 2<sup>nd</sup> Edition, 2000, Oxford University Press.
8. S. N. Ege, Organic Chemistry: Structure and Reactivity, 5<sup>th</sup> Edition, 2001, Prentice Hall Macmillan.



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			L	T	P	
PE-1	BH6201	QUANTUM CHEMISTRY	3	0	0	3

**Course Outcomes: The students will be able to**

1. Utilize the mathematical methods for quantum mechanical calculations.
2. Derive the selection rules of electronic transitions based on postulates of quantum mechanics.
3. Design significance of quantum numbers based upon solutions of Schrodinger equation.
4. Predict the molecular properties of small molecules based on quantum mechanical concepts.

### Unit-I

**Matrix Algebra:** Matrices, determinants, matrix rank, orthogonal and unitary transformations, eigenvalues and eigenvectors, diagonalization of matrices. **Vectors and Tensors:** Introduction to vectors; vector operations; coordinate system transformation; Vector spaces, inner products, linear independence, bases. **Ordinary Differential Equations:** Linear first and second order ODEs, homogeneous and inhomogeneous ODEs with constant coefficients, system of linear ODEs, power series solution of differential equations and special functions.

### Unit-II

**Operators in Quantum mechanics:** Linear, Hermitian and Angular Momentum operators, Eigenvalue problem, particle in 3-dimensional box, degeneracy and tunneling. Derivation of selection rules for electronic transitions, Solution of the Schrodinger equation for hydrogen and hydrogen-like atoms, significance of n, l and m quantum numbers.

### Unit-III

Approximation methods (variation method and perturbation theory), multielectron atoms (Helium and  $\text{Li}^+$  ion), spin quantum number, ground and excited state of helium atom. Born-Oppenheimer approximation, Hückel Molecular Orbital Theory, Molecular term symbols, Homonuclear and heteronuclear diatomic molecules (HF, CO, NO).

**Suggested Readings:**

1. G. Doggett, M. Cockett, and E. Abel, Maths for Chemists: RSC (Tutorial Chemistry Texts), 1<sup>st</sup> Edition, 2012, RSC.
2. P. Tebbutt, Basic Mathematics for Chemists, 1<sup>st</sup> Edition, 1998, Wiley-Blackwell.
3. D.A. McQuarrie, and J.D Simon, Physical Chemistry: A Molecular Approach, 2<sup>nd</sup> Edition, 2015, Viva Books.
4. Quantum Chemistry. D.A. McQuarrie and J.D Simon, 2<sup>nd</sup> Edition, 2015, Viva Books.
5. A. Szabo, and N. S. Ostlund, Modern Quantum Chemistry, 1<sup>st</sup> Edition, 1996, Dover Books.
6. I. N. Levine, Quantum Chemistry, 4<sup>th</sup> Edition, 2000, Prentice Hall India Pvt. Ltd.
7. A. K. Chandra, Introductory Quantum Chemistry, 4<sup>th</sup> Edition, 2009, Tata McGraw Hill.
8. P. W. Atkins, and R. S. Friedman, Molecular Quantum Mechanics, 3<sup>rd</sup> Edition, 1997, Oxford University Press.



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Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-2	BH6203	GROUP THEORY AND MOLECULAR SPECTROSCOPY	3	0	0	3

**Course Outcomes: Upon completion of this course, the students will be able to**

1. acquire the fundamental knowledge on symmetry, point groups and their properties; construct the character tables and predict their applications.
2. predict the rotational, vibrational and Raman spectra of complex systems; apply symmetry considerations to vibrational and Raman spectra.
3. understand the theories of magnetic resonances and apply these to predict the structure of molecules/compounds/ions etc.
4. understand the functioning of Mossbauer spectra and their application to ascertain the oxidation states of Fe and Sn systems.

### Unit-I

#### Group Theory

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup, conjugacy relation and classes, generators, Point group. Representations of group operators, The great orthogonality theorem (without proof) and its explanation, irreducible and reducible representation, bases of a representation, character of a representation, character table and its meaning, reduction formula, symmetry and selection rules for transitions between rotational, vibrational and electronic states, Symmetry and normal modes of vibration. Determination of normal modes from Symmetry for AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub> and AB<sub>6</sub> systems, symmetry of overtones and combination bands.

### Unit-II

**Rotational and Infrared Spectroscopy:** Rotational spectra of simple polyatomic molecules (linear, non-linear- symmetric top and spherical top, prolate and oblate types) Stark effects on rotational spectrum. Fundamental and overtone bands. Isotope effects.

### Unit-III

#### Spin Based Spectroscopy

**Nuclear Magnetic Resonance Spectroscopy:** Nuclear spin; nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A<sub>2</sub>B<sub>2</sub> etc.), spin decoupling; basic ideas about instrument, 1-D NMR studies of nuclei other than proton- <sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

**Electron Paramagnetic (Spin) Resonance (EPR or ESR) Spectroscopy:** Basic principles, zero field splitting and Kramer's rule, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship.

#### Suggested Readings:

1. C. N. Banwell, and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Edition, 1995, Tata McGraw Hill.
2. G. M. Barrow, Molecular Spectroscopy, 4<sup>th</sup> Edition, 1995, McGraw Hill.
3. P. F. Bernath, Spectra of Atoms and Molecules, 2<sup>nd</sup> Edition, 2005, Oxford University Press.
4. F. A. Cotton, Chemical Applications of Group Theory, 3<sup>rd</sup> Edition, 2003, John Wiley & Sons.
5. A. M. Lesk, Introduction to Symmetry and Group Theory for Chemists, 1<sup>st</sup> Edition, 2004, Springer.
6. A. Vincent, Molecular Symmetry and Group Theory, A Programmed Introduction to Chemical Applications, 2<sup>nd</sup> Edition, 2013, John Wiley & Sons.
7. R. L. Carter, Molecular Symmetry and Group Theory, 2<sup>nd</sup> Edition, 1997, John Wiley & Sons.
8. K. V. Reddy, Symmetry and Spectroscopy of Molecules, 2<sup>nd</sup> Edition, 2009, New Age International Publications.
9. J. M. Hollas, Modern Spectroscopy, 4<sup>th</sup> Edition, 2004, John Wiley & Sons.



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10. D.C. Haris, and M.D. Bertolucci, Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, 1<sup>st</sup> Edition, 1989, Dover Publications Inc.
11. J. A. Weil, J. R. Bolton, and J. E. Wertz, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, 1<sup>st</sup> Edition, 1994, Wiley-Interscience.





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			L	T	P	
PC Lab-1	BH6501	INORGANIC CHEMISTRY LABORATORY-I	0	0	3	2

**Course Outcomes:** Upon completion of this course, the students will be able to

1. Identify the acid and basic radicals in a mixture of inorganic salts based on the principles of qualitative analysis.
2. Carry out synthesis of various types of simple inorganic complexes.
3. learn the basic characterization of the synthesized complexes by spectroscopic technique (UV-Visible and IR).

### Syllabus

- I. Semi micro qualitative analysis of inorganic mixtures containing anions, common cations, less familiar element (W, Mo, Ce, Th, Zr, V and U), insoluble (sulphate, oxides, halide).
- II. Preparation and characterization (UV-Visible and IR spectra) of complexes
  - Hexaamminenickel (II) chloride
  - Sodium tris-(oxalate)iron(III)
  - Tris(thiourea) copper(I) complex
  - Ammonium tetrathiocyanatocobaltate(II)
  - Chrome alum

### Suggested Readings:

1. G. Svehla, Vogel's Qualitative Inorganic Analysis, 6<sup>th</sup> Edition, 1987, Orient Longman.
2. A. J. Elias, A Collection of Interesting General Chemistry Experiments, 1<sup>st</sup> Edition, 2002, Universities Press (India) Pvt. Ltd.



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Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC Lab-2	BH6503	ORGANIC CHEMISTRY LABORATORY-I	0	0	3	2

**Course Outcomes:** Upon completion of this course students will be able:

1. identify various functional group present in an organic-compounds by qualitative analysis and confirmation by various analytical techniques.
2. synthesize some organic compounds.
3. separate the organic compounds by adopting various separation techniques.

### Syllabus

1. Qualitative Analysis: Identification of organic compounds.
2. Separation, purification and identification of compounds of binary mixture using TLC and column chromatography.
3. Preparation of Picric acid.
4. Interpretation of IR spectra for functional group identification.
5. Structure Drawing of various organic building blocks using ChemDraw software.

### Suggested Readings:

1. D. J. Pasto, C. R. Johnson, and M. J. Miller, Experiments and Techniques in Organic Chemistry, 6<sup>th</sup> Edition, 1992, Prentice Hall India Pvt. Ltd.
2. H. Middleton, Systematic Qualitative Organic Analysis, 2<sup>nd</sup> Edition, 1982, Rupa Publishing House.
3. H. T. Clarke, Hand Book of Organic Analysis, Qualitative & Quantitative, 2<sup>nd</sup> Edition, 1967, E. Arnold Publication.
4. A. I. Vogel, Text book of Practical Organic Chemistry, 5<sup>th</sup> Edition, 1989, ELBS (London).
5. K. L. Williamson, Macro-scale and Micro-scale Organic Experiments, 2<sup>nd</sup> Edition, 1994, D. C. Heath & Co.



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### 2<sup>nd</sup> SEMESTER

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-3	BH6102	INORGANIC CHEMISTRY-II	4	0	0	4

**Course Outcomes:** Upon completion of this course, the students will be able to

1. derive the magnetic properties of coordination, lanthanide and actinide compounds.
2. employ concepts to comprehend presence of para, Ferro, Anti-Ferro magnetism *etc.* in various inorganic complexes.
3. get knowledge on organometallic and fluxional compounds, their classifications, bonding and structures.
4. realize the reactions and catalytic properties of organometallic compounds.

#### Unit-I

##### Magnetic properties of coordination compounds

Types of magnetic behaviour, magnetic susceptibility and its determination by Gouy, Faraday and VSM method, Pascal's constants and constitutive corrections, paramagnetism, Curie-Weiss law, van Vleck's equation (derivation excluded) and its applications, spin-orbit coupling, ferro- and anti-ferromagnetism coupling, super paramagnetism, high and low spin equilibria. Anomalous magnetic moments, magnetic exchange coupling and spin crossover. Magnetic properties of Lanthanide and Actinide metal complexes.

#### Unit-II

##### Organometallic Chemistry-I

Stability and 18 electron rules (covalent and ionic), Alkyls/aryl and hydrides: alkyls and aryls (metal alkyls stabilized carbanion,  $\beta$ -elimination, stable alkyls, Agostic alkyls, reductive elimination, preparation of metal allyls). Metal hydrides: synthesis, characterization, reactions, bridging hydrides.

#### Unit-III

##### Organometallic Chemistry-II

Synthesis, bonding, properties of Pi-complexes and applications of alkenes and alkynes, allyls, diene, cyclopentadiene, Dienyl, arenes. Introductory idea on transition metal-carbon multiple compounds: carbenes and carbyne.

##### Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as  $\eta^2$ -olefin,  $\eta^3$ -allyl and Dienyl complexes.

#### Unit-IV

##### Organometallic chemistry-III

Reactivity of organo-transition metal complexes: Coordinative unsaturation, substitution reactions (nucleophilic and electrophilic addition and abstraction), oxidative addition and reductive elimination, insertion reactions (insertion of CO, SO<sub>2</sub> and alkenes). Catalysis by organo-transition metal complexes: Alkene isomerization, hydrogenation and hydroformylation; Zeigler-Natta polymerization of ethylene, reduction of carbon monoxide by hydrogen (Fischer-Tropsch reaction).

##### Suggested Readings:

1. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 1<sup>st</sup> Edition, 2014, John Wiley & Sons.
2. J. F. Hartwig, Organo-transition Metal Chemistry: From Bonding to Catalysis, 1<sup>st</sup> Edition, 2009, University Science Books.
3. A. F. Hill, Organo-transition Metal Chemistry, 1<sup>st</sup> Edition, 2002, Royal Society of Chemistry.



# ODISHA UNIVERSITY OF TECHNOLOGY AND RESEARCH

Techno Campus, Mahalaxmi Vihar, Ghatikia, Bhubaneswar-751029.

## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

4. C.H. Elshebroich, and A Salzer, Organometallics: A Concise Introduction, 3<sup>rd</sup> Edition, 2006, John Wiley & Sons.
5. S. G. Davies, Organo-transition Metal Chemistry: Applications to Organic Synthesis, 1<sup>st</sup> Edition, 1982, Pergamon Inc.
6. A.K. Das and M. Das, Fundamental Concept of Inorganic Chemistry, Vol. 4 and 5, 2<sup>nd</sup> Edition, 2016, CBS Publisher & Distributor Pvt. Ltd.
7. R. C. Mehrotra, and A. Singh Organometallic Chemistry, 2<sup>nd</sup> Edition, 2000, New Age International Publishers.
8. R. L. Dutta, and A. Samal, Elements of Magnetochemistry, 2<sup>nd</sup> Edition, 2004, S. Chand & Company Ltd.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-4	BH6104	ORGANIC CHEMISTRY-II	4	0	0	4

**Course Outcomes:** Upon completion of this course, students will be able:

1. To comprehend the science behind the creation of diverse natural products.
2. To grasp the reactivity pattern and fundamental reaction mechanism of distinct reducing and oxidizing agents.
3. To understand the utility of retrosynthesis towards formation of various organic species, selectively protecting and deprotecting organic functionalities.
4. To comprehend the use of coupling reaction in the creation of carbon-carbon and carbon-hetero atom bonds.

### Unit- I

**Organic transformations and reagents:** Functional group interconversions including oxidations and reduction and stereochemistry.

**Reductions:** Catalytic hydrogenation, reduction by dissolving metals, Bio-reduction. Hydride transfer reagents: Sodium borohydride, Sodium cyanoborohydride, Lithium aluminium hydride, alkoxy substituted LAH reducing agents, DIBAL, Application of Hydroboration. Diborane, Disiamylborane, 9-Borabicyclo [3.3.1] nonane (9-BBN), isopinocampheyl and diisopinocampheylborane. Homogeneous hydrogenation: Mechanism and applications using Rh, Ru and other metal complexes.

**Oxidations:** Scope of the following oxidizing agents with relevant applications and mechanism: DDQ, DCC, Chromium (VI) oxidants, Osmium tetroxide, Selenium dioxide, KMnO<sub>4</sub>, tertiary-Butyl hydro peroxide. Manganese (IV) oxidants, Swern oxidation, Oxidation with per-acids. Oxidation with hypervalent organoiodines.

### Unit- II

**Coupling Reactions:** Carbon-carbon bond formation through coupling reactions (Heck, Suzuki, Stille and Sonogashira, Negishi), Carbon-hetero atom bond forming reactions using transition metals (Cu, Pd, Rh, Ru, Ni, Fe etc.), Buchwald- Hartwig reaction, C-C bond forming reaction; Wittig reaction, Julia-Kocienski olefination, Peterson olefination, Metathesis reaction (Cross or ring closure).

### Unit-III

**Disconnection Approach:** An introduction to synthon and synthetic equivalents, disconnection approach, functional group inter conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemo-selectivity.

**Reversal polarity & protecting group:** Umpolung approach, cyclisation reactions, amine synthesis. Protecting Groups: Principle of protection and deprotection of alcohol, amine, carbonyl and carboxyl groups and their application in organic synthesis.

### Unit-IV

**One Group -C Disconnection:** Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

**Two Group C-C Disconnections:** Diels-Alder reaction, 1, 3-difunctionalised compounds,  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds, control in carbonyl condensations, 1, 5-difunctionalised compounds. Michael addition and Robinson annulation.

**Ring Synthesis:** Saturated heterocycles, synthesis of 3-, 4-, 5- and 6- membered rings, aromatic heterocycles in organic synthesis.

**Synthesis of Some Complex Molecules:** Application of the above protocols in the synthesis of following compounds: Camphor, Vitamin D and Cortisone.

### Suggested Readings:

1. G. S. Zweifel, M. Nantz, P. Somfai, Modern Organic Synthesis and Introduction, 2<sup>nd</sup> Edition, 2014, John Wiley & Sons.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

2. J. Fuhrhop, and G. Penzlin, Organic Synthesis: Concepts, Methods and Starting Materials, 2<sup>nd</sup> Edition, 1993, Wiley-VCH.
3. W. Carruthers, Some Modern Methods of Organic Synthesis, 4<sup>th</sup> Edition, 2004, Cambridge University Press.
4. H. O. House, Modern Synthetic Reactions, 2<sup>nd</sup> Edition, 1972, W. A. Benjamin & Co.
5. M. B. Smith, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7<sup>th</sup> Edition, 2013, John Wiley & Sons.
6. R.O.C. Norman, and J. M. Coxon, Principles of Organic synthesis, 3<sup>rd</sup> Edition, 1993, CRC Press.
7. F. A. Carey, and R. J. Sundberg, Advanced Organic Chemistry Part B: Structure and Mechanism, 5<sup>th</sup> Edition, 2008, Springer.
8. S. Warren, and P. Wyatt, Organic Synthesis: The Disconnection Approach, 2<sup>nd</sup> Edition, 2008, Wiley India Pvt. Ltd.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-5	BH6106	PHYSICAL CHEMISTRY-I	4	0	0	4

### Course Outcomes: The students will be able to

1. Utilize basics of classical thermodynamics to explain real systems.
2. Employ phase rule to explain processes of industrial importance.
3. Acquired knowledge on statistical mechanics and their application in chemistry.
4. Describe kinetics of complex reactions.

### Unit- I

**Classical Thermodynamics:** Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient. Standard States for Gases, Liquids and Solids and its Applications. Free Energies, Enthalpies and Entropies of Ions in Solutions. Debye Hückel theory of activity coefficient. Activity, fugacity and mean Activity coefficients of Electrolytes and their Determinations, Debye-Hückel Limiting Law. Thermodynamics of Mixing–Mixtures of Volatile Liquids– ideal and Real Solutions and -Excess Functions.

### Unit-II

**Equilibrium Thermodynamics:** Thermodynamic Derivations of Gibbs equation Phase Rule, Applications to two component (eutectic) & three component systems involving solids and liquids (Acetic Acid – Chloroform - Water, NaCl-Na<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O, NH<sub>4</sub>NO<sub>3</sub>-(NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O.

**Non Equilibrium Thermodynamics:** Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the properties of and forces, non-equilibrium stationary states, phenomenological equations.

### Unit- III

**Statistical Thermodynamics:** Distribution Laws: Maxwell-Boltzmann, Bose-Einstein, Fermi-Dirac model, Most probable configuration and concept of entropy. Principle of equipartition of energy, partition functions: Molecular partition functions-translational, rotational, vibrational and electronic partition functions. Derivation of thermodynamic functions (energy, enthalpy, entropy and free energy) for ideal monoatomic and diatomic gases.

### Unit-IV

**Chemical Kinetics:** Complex reactions: opposing, parallel and consecutive reactions. Chain reactions (linear), branching chains–explosion limits; Rice Herzfeld scheme for photochemical reactions. Theories of reaction rates: Collision theory, Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment.

**Solution Kinetics:** Factors affecting reaction rates in solution, effect of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effect, isotope effect, Kramer's theory. Diffusion limited reactions. Study of fast reactions using stopped flow and relaxation techniques (T-jump and P-jump).

### Suggested Readings:

1. D. A. McQuarrie, and J. D. Simon, Molecular Thermodynamics, 1<sup>st</sup> Edition, 2015, Viva Books.
2. R. S. Berry, S. A. Rice, and J. Ross, Physical Chemistry, 2nd Edition, 2000, Oxford University Press.
3. D. A. McQuarrie, and J. D. Simon, Physical Chemistry: A Molecular Approach, 1<sup>st</sup> Edition, 2015, Viva Books.
4. R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Physical Chemistry, 4<sup>th</sup> Edition, 2005, John Wiley & Sons Inc.
5. P.W. Atkins, Physical Chemistry, 8<sup>th</sup> Edition, 1998, Oxford University Press.
6. A. W. Adamson, Physical Chemistry of Surfaces, 2<sup>nd</sup> Edition, 2012, Wiley (India) Pvt. Ltd.
7. D. A. McQuarrie, Statistical Mechanics, 2<sup>nd</sup> Edition, 2000, University Science Books.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-3	BH6202	BIOCHEMISTRY	3	0	0	3

### Course Outcomes

1. Understand the structure and function of selected biomolecules.
2. Get the knowledge on working of bioenergetics and metabolism of glucose.
3. Identify the ion-channel and transport phenomena on biosystem.
4. Get comprehensive knowledge on the enzymes, their functions and kinetics.

### Unit- I

**Introduction to Biomolecules:** Structure and Function: Carbohydrates (Monosaccharide, oligosaccharides, polysaccharides (starch, Glycogen, Cellulose); Lipids: Saturated and unsaturated fatty acids, triacylglycerols, phosphoglycerides, sphingolipids, waxes and sterol; amino acids and peptides, proteins - hierarchy of protein architecture, Ramachandran plot; nucleic acids: DNA, RNA, double helix model of DNA, denaturation and renaturation of DNA; replication, transcription and translation of DNA; hormones and vitamins.

### Unit- II

**Principle of Bioenergetics:** Bioenergetics and Thermodynamics; Phosphoryl group transfer and energy currency-ATP; Biological Oxidation and reduction reactions  
Metabolic processes: Introduction to metabolism of carbohydrates: Glycolysis, TCA Cycle, Gluconeogenesis.

### Unit- III

**Transport Mechanism:** Introduction to ion-channel,  $\text{Na}^+/\text{K}^+$  transport (Ion pump);  $\text{O}_2$  transport by hemoglobin,  $\text{CO}_2$  transport by carbonic anhydrase.

**Enzymes:** Properties of enzyme, classification of enzymes, mechanism of enzyme action, kinetics of enzyme action, activation energy, enzyme inhibition, coenzyme, apoenzyme and holoenzyme.

### Suggested Readings:

1. D. L. Nelson, and M. M. Cox, Lehninger Principles of Bio-Chemistry, 7<sup>th</sup> Edition, 2017, W. H. Freeman & Co. Ltd.
2. J. M Berg, J. L. Tymoczko, and L. Stryer, Biochemistry, 9<sup>th</sup> Edition, 2019, W. H. Freeman & Co. Ltd.
3. D. Voet, J. G. Voet, and C.W. Pratt, Fundamentals of Biochemistry, 2<sup>nd</sup> Edition, 2011, John Wiley & Sons.
4. C. B. Powar, & G. R. Chatwal, Biochemistry, 5<sup>th</sup> Edition, 2017, Himalaya Publishing House.
5. S. C. Rastogi, Biochemistry, 3<sup>rd</sup> Edition, 2010, Tata McGraw Hill.





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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC Lab-3	BH6502	INORGANIC CHEMISTRY LABORATORY-II	0	0	3	2

**Course Outcomes:** Upon completion of this course, the students will be able to

- 1 To carry out synthesis of simple complexes and pursue the quantitative analysis of metals or the ligands in those complexes.
- 2 To carry out volumetric analysis of metals in a mixture of their salts.
- 3 Quantitatively analyze the metals in a mixture of their salts by volumetric methods.

I. Preparation and quantitative analysis of complexes

- Preparation of Pentaamminechlorocobalt (III) chloride.
- trans- Dichlorobis (ethylenediamine) cobalt (III) chloride
- sodium tris-(oxalate)iron(III)
- Tris(thiourea) copper(I) complex
- ammonium tetrathiocyanatocobaltate(II)
- Potassium tris-(oxalato)aluminate(III)
- Tetraaminecopper (II) sulphate.

II. Volumetric analysis

- Volumetric estimation of Fe & Cu in their mixture.
- Volumetric estimation of Zn & Cu in their mixture.
- Volumetric estimation of Ni and Zn in their mixture.

**Suggested Readings:**

1. J. Mendham, A. I. Vogel's Quantitative Chemical Analysis, 6<sup>th</sup> Edition, 2009, Pearson.
2. G. Svehala, and B. Sivasankar, Vogel's Qualitative Inorganic Analysis, 7<sup>th</sup> Edition, 2012, Pearson.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC Lab-4	BH6504	ORGANIC CHEMISTRY LABORATORY-II	0	0	3	2

**Course Outcomes:** Upon completion of this course, students will be able to

1. practice standard synthesis procedure for synthesis of some organic compounds.
2. estimate organic compounds using standard methods.
3. isolate some pharmaceuticals from a given mixture by distillation.

### Syllabus

1. Application of steam distillation in isolation of essential oil (clove) and perfume (rose).
2. Preparation of paracetamol, aspirin, and some dyes and indicators.
3. Preparation of (i) o-iodobenzoic acid from anthranilic acid, furoic acid from furfural, (ii) Thiamine catalyzed benzoin condensation and (iii) benzil from benzoin.
4. Estimation of (i) phenol, aniline, ascorbic acid and glucose by Fehling's method & Bertrand's method.

### Suggested Readings:

1. D. J. Pasto, C. R. Johnson and M. J. Miller, Experiments and Techniques in Organic Chemistry, 6<sup>th</sup> Edition, 1992, Prentice Hall.
2. H. Middleton, Systematic Qualitative Organic Analysis, 2<sup>nd</sup> Edition, 1982, Rupa Publishing House.
3. A. I. Vogel, Text book of Practical Organic Chemistry, 5<sup>th</sup> Edition, 1989, ELBS (London).
4. K. L. Williamson, Macro-scale and Micro-scale Organic Experiments, 2<sup>nd</sup> Edition, 1994, D. C. Heath & Co.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC Lab-5	BH6506	PHYSICAL CHEMISTRY LABORATORY-I	0	0	3	2

### Course Outcomes: The students will be able to

1. Utilize basics of electrochemistry to explain titrations.
2. Experience operation of spectrophotometers and related data analysis
3. Acquire proficiency in handling various optical instruments

### Syllabus

1. pHmetry / conductometric / potentiometric and precipitation titrations.
2. Determination of acid dissociation constant by spectrophotometric technique.
3. Determination of inversion of sucrose using polarimeter.
4. Determination of critical micellar concentration (CMC) of surfactants.
5. Determination of polarizability from refractive index measurements.
6. Determination of composition of a complex by Job's method.
7. Determination of polarity of solvent by dye absorption.

### Suggested Readings:

1. D. P. Shoemaker, C. W. Garland, and J. W. Nibber, Experiments in Physical Chemistry, 5<sup>th</sup> Edition, 1989, McGraw Hill.
2. B. D. Khosla, V. C. Garg, and A. Gulati, Senior Practical Physical Chemistry, 18<sup>th</sup> Edition, 2020, R. Chand & Co.
3. C. W. Garland, J. W. Nibler, and D. P. Shoemaker, Experiments in Physical Chemistry, 8<sup>th</sup> Edition, 2003, McGraw-Hill Education.
4. A. M. Halpern, and G. C. McBane, Experimental Physical Chemistry, 3<sup>rd</sup> Edition, 2003, W.H. Freeman & Co.



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**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

### 3<sup>rd</sup> SEMESTER

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-4	BH7201	ORGANIC SPECTROSCOPY	3	0	0	3

**Course Outcomes:** Upon completion of this course students will be able to

1. gain knowledge on principles of various spectroscopic techniques and mass spectrometry.
2. envisage the spectral data for various organic and inorganic compounds based on these principles.
3. deduce the structure of organic and inorganic compounds based on various spectral data.

#### Unit-I

Introduction to spectroscopic techniques for structure elucidation. Electromagnetic radiation, absorption of energy by organic compounds, types of spectroscopic methods for structural elucidation of organic and inorganic molecules.

**IR – Spectroscopy:** Basic principles, characteristic frequencies of common functional groups.

**UV-Visible Spectroscopy:** Basic principles. Born-Oppenheimer approximation, Frank Condon principle, laws of photochemical equivalence. Application of UV – Visible spectroscopy to organic structure elucidation, Woodward – Fisher rules.

#### Unit-II

**Nuclear Magnetic Resonance (NMR) Spectroscopy:** JJ coupling, vicinal and germinal coupling and, Applications of  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy in the structural determination of organic compounds. One-dimensional NMR of common heteroatoms present in organic compounds (N, F and P).

#### Unit-III

**Mass spectrometry:** Basic principles of mass spectrometry, fragmentation and rearrangements (including McLafferty rearrangement) of organic molecules, basics of high resolution mass spectrometry, ionization potential and isotopic distribution, experimental setup, application of mass spectrometry to organic and inorganic compounds in structural determination.

#### Unit-IV

Problem solving exercises involving UV, IR, NMR & MS data: Problems involving interpretation of spectral details of organic compounds.

#### Suggested Readings:

1. E. A. O. Ebsworth, Structural Methods in Inorganic Chemistry, 2<sup>nd</sup> Edition, 1991, Blackwell Scientific Publications.
2. R. S. Drago, Physical Methods in Chemistry, 2<sup>nd</sup> Edition, 1992, Saunders Co.
3. R. M. Silverstein, and F. X. Webster, Spectrometric Identification of Organic Compounds, 6<sup>th</sup> Edition, 1997, John Wiley & Sons. Inc.
4. W. Kemp, Organic Spectroscopy, 3<sup>rd</sup> Edition, 1994, MacMillan.
5. L. Pavia, and V. Kriz, Introduction to Spectroscopy, 3<sup>rd</sup> Edition, 2000, Cengage Learning.
6. D. H. Williams, and I. Fleming, Spectroscopic Methods in Organic Chemistry, 6<sup>th</sup> Edition, 2014, Tata McGraw Hill.
7. P. S. Kalsi, Spectroscopy of Organic Compounds, 6<sup>th</sup> Edition, 2006, New Age International Publishers.
8. J. A. Weil, J. R. Bolton, and J. E. Wertz, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, 1<sup>st</sup> Edition, 1994, Wiley Interscience.
9. H. Friebolin, Basic One and Two Dimensional NMR Spectroscopy, 1<sup>st</sup> Edition, 1991, Wiley-VCH.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-5	BH7203	ELECTIVE-I (SPECTRAL TECHNIQUES IN INORGANIC CHEMISTRY)	3	0	0	3

**Course Outcomes: Upon completion of this course, the students will be able to**

1. learn about the applications of various spectroscopic techniques.
2. gain fundamental of operation and interpretation of spectra of inorganic compounds for their structural characterization.
3. describe the fundamental requirement to interpret the electronic spectra of metal complexes for prediction of their properties.

### Unit-I

**Vibrational spectroscopy:** Vibrational spectra and symmetry, selection rules, symmetry of an entire set of normal vibrations, F and G matrix. Raman spectra and selection rules, polarized and depolarized Raman lines, resonance Raman spectroscopy, use of symmetry to determine the number of active infrared and Raman lines, Non-resonance overtones and difference bands. Application of Raman and Infrared selection rules to the determination of inorganic structures, bond strength frequency shift relations, changes in spectra of donor molecules on coordination, change in symmetry on coordination.

### Unit-II

**Electronic spectroscopy:** Nephelauxetic effect, effect of  $\sigma$  and  $\pi$  bonding on the energy of  $t_{2g}$  orbitals and  $Dq$ , spectrochemical series, effect of distortion on the  $d$  orbital energy level ( $T_d$ ,  $D_{2d}$ ,  $D_{4h}$ ), *cis*- and *trans*- isomers and bonding parameters from spectra of tetragonal complexes, bonding parameters, calculation of  $Dq$ ,  $Ds$  and  $Dt$  for tetragonal complexes, intervalence electronic transition, structural evidence from electronic spectra.

**Mossbauer spectroscopy:** Basic principles, spectral line shape and natural line width, characteristics of Mossbauer nuclides, Doppler's effect, parameters to evaluate Mossbauer spectra: chemical shift or isomer shift and its interpretation, quadruple interaction, Magnetic field interaction. Application of Mossbauer spectra to Fe and Sn system with respect to oxidation states, Recoil energy, Partial quadrupole splitting and geometry of the complexes.

### Unit-III

**Nuclear Magnetic Resonance (NMR) spectroscopy:** Effect of fast chemical reactions, coupling to quadrupole nuclei, NMR of paramagnetic substances in solution, nuclear and electron relaxation time, the expectation value of  $\langle S_z \rangle$ , contact shift, pseudo contact shift, factoring contact and pseudo contact shift for transition metal ions. Contact shift and spin density,  $\pi$  delocalization, simplified M.O. diagram for Co(II) and Ni(II). Application to planar tetrahedral equilibrium, Contrast agents.

**Nuclear Quadrupolar Resonance (NQR) Spectroscopy:** Quadrupolar moment, energy bands of a Quadrupolar nucleuse and effect of asymmetry parameters and energy lends. Effect of an external magnetic field, selected examples for elucidation of structural aspects of inorganic compounds using NQR spectroscopy.

### Suggested Readings:

1. S. F. A. Kettle, Physical Inorganic Chemistry: A Coordination Chemistry Approach, 1<sup>st</sup> Edition, 1996, Springer.
2. R.S. Drago, Physical Methods for Chemists, 2<sup>nd</sup> Edition, 2016, East West Press Pvt. Ltd.
3. F. E. Mabbs, and D. J. Machin, Magnetism and Transition Metal Complexes. 2<sup>nd</sup> Edition, 2008, Dover Publications.
4. E. A. O. Ebsworth, Structural Methods in Inorganic Chemistry, 2<sup>nd</sup> Edition, 1991, Blackwell Scientific Publications.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-6	BH7205	ELECTIVE-II (CHEMISTRY OF MATERIALS)	3	0	0	3

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

1. Learn the basic properties of materials & nanomaterials, role of size and shape in nanomaterials.
2. Acquire concepts on the dramatic changes in properties that occur by reducing the size and shape of materials.
3. impart knowledge on how to perform the synthesis of such small sizes and shapes of materials.
4. learn about the several characterization techniques for the elucidation of molecular structure and their composition.

### Unit-I

**Introduction:** Properties of materials & nanomaterials, role of size and shape in nanomaterials.

**Electronic Properties:** Classification of materials: Metal, Semiconductor, Insulator, Band structures, Brillouin zones, Mobility, Resistivity.

**Magnetic Properties:** Superparamagnetism, blocking. Important properties in relation to nano magnetism.

**Optical Properties:** Photoconductivity, Optical absorption & transmission, Photoluminescence, Fluorescence, Phosphorescence, Electroluminescence. Thermal and Mechanical Properties.

### Unit-II

**Chemical Methods:** Metal nanocrystals by reduction, Solvothermal synthesis, Photochemical synthesis, Electrochemical synthesis, Nanocrystals of semiconductors and other materials by arrested precipitation, Thermolysis routes, Sonochemical routes, Post synthetic size-selective processing, Sol-gel route, Micelles and microemulsions.

**Biological Methods of Synthesis:** Use of bacteria, fungi, Actinomycetes for nanoparticles synthesis, Magnetotactic bacteria for natural synthesis of magnetic nanoparticles; Mechanism of formation; Viruses as components for the formation of nanostructured materials; Synthesis process and application, Role of plants in nanoparticle synthesis.

### Unit-III

**Characterization Techniques:** X-ray diffraction, Scanning Probe Microscopy, SEM, TEM, Optical microscope, UV-Vis spectrophotometers, IR Spectrophotometers and their description, operational principle and application for analysis of nanomaterials.

### Suggested Readings:

1. C. Dupas, P. Houdy, and M. Lahmani, Nanoscience: Nanotechnology and Nanophysics, 1<sup>st</sup> Edition, 2004, Springer.
2. K. J. Klabunde, Nanoscale Materials in Chemistry, 1<sup>st</sup> Edition, 2001, Wiley Interscience.
3. S. K. Kulkarni, Nanotechnology: Principles and Practices, 1<sup>st</sup> Edition, 2007, Capitol Publishing Company.
4. M. Wilson, K. Kannangara, G. Smith, M. Simmons, and B. Raguse, Nanotechnology: Basic Science and Emerging Technologies, 1<sup>st</sup> Edition, 2005, Overseas Press.
5. C. P. Poole Jr., and F. J. Ovens, Introduction to Nanotechnology, 2<sup>nd</sup> Edition, 2003, Wiley Interscience.
6. A. S. Edelstein, and R.C. Cammarata, Nanomaterials: Synthesis, Properties and Applications, 1<sup>st</sup> Edition, 1996, Institute of Physics Publishing.



# ODISHA UNIVERSITY OF TECHNOLOGY AND RESEARCH

Techno Campus, Mahalaxmi Vihar, Ghatikia, Bhubaneswar-751029.

## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-5	BH7203	ELECTIVE-I (ADVANCED CHEMICAL KINETICS)	3	0	0	3

**Course Outcomes:** The students will be able to

1. Utilize concepts of thermodynamics to explain phenomenological behavior of complex reactions.
2. Attain ideas of kinetics of biomolecules and its significance.
3. Develop essentials of sophisticated instruments for kinetics measurement.

### Unit-I

**Statistical theories of kinetics:** Attractive and repulsive forces, potential energy surfaces. Lindemann's theory of unimolecular reactions- energy transfer, fall-off region and its limitations. Rice-Ramsperger and Kassel (RRK) model, and Marcus refinement of RRK model (RRKM) for the calculation of rate constants of simple unimolecular (isomerization) reactions.

**Complex reactions:** Chain reactions and oscillatory reactions, photochemical reactions, Homogeneous catalysis.

### Unit-II

**Enzyme kinetics:** Michaelis-Menten mechanism - single and double intermediates. King-Altman method for working out the kinetics of complex enzyme reactions. Enzyme inhibition- reversibility and products inhibition. Computer simulation in chemical kinetics.

### Unit-III

**Reaction Dynamics:** Molecular beams, principle of crossed-molecular beams. Molecular encounters and principal parameters, *e.g.* Impact parameter, Collision cross-section, Reaction cross-section and relation between reaction cross-section and reaction rate (single velocity). Dependence of collisional cross-section on translational energy. Probing the transition state, Dynamics of barrier less chemical kinetics in solution, dynamics of unimolecular reactions.

### Suggested Readings:

1. M. J. Pilling, and P.W. Seakins, Reaction Kinetics, 1<sup>st</sup> Edition, 1997, Oxford University Press.
2. K. J. Laidler, Chemical Kinetics, 3<sup>rd</sup> Edition, 1997, Pearson Education.
3. P. L. Houston, Chemical Kinetics and Reaction Dynamics, 1<sup>st</sup> Edition, 2006, Dover Publication.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-6	BH7205	ELECTIVE-II (BIOPHYSICAL CHEMISTRY)	3	0	0	3

### Course Outcomes: The students will be able to

1. Implement basics of thermodynamics to understand biological systems.
2. Gain available techniques and methodology for separation of different biomolecules.
3. Acquire knowledge on various tools for determination of macromolecules.

### Unit-I

**Physical basis of biological systems:** Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; polypeptide chain geometries and internal rotational angles; Ramachandran plots; Structures of nucleic acids. Protein structure and function. Properties of nucleosides and nucleotides; composition of nucleic acids.

### Unit-II

**Separation techniques of Biomolecules:** General principles, including Chromatography; Sedimentation, Moving Boundary Sedimentation, Zonal Sedimentation, Electrophoresis, Isoelectric focusing, Capillary electrophoresis, MALDI-TOF.

### Unit-III

#### Structural Determination of Biomolecules:

**Physical methods:** Ultracentrifugation and other hydrodynamic techniques; Light scattering, fundamental concepts, scattering from a number of small particles: Rayleigh scattering, scattering from particles that are not small compared to the wavelength of radiation; Dynamic light scattering; Low angle X-Ray scattering; Neutron scattering; Raman scattering

**Optical methods:** Optical techniques in biological systems: Absorption spectroscopy, Fluorescence spectroscopy, Linear and Circular Dichroism, Single and multidimensional NMR spectroscopy. Single molecule spectroscopy of biomolecules.

#### Suggested Readings:

1. A. Cooper, Biophysical Chemistry, 2<sup>nd</sup> Edition, 2015, RSC.
2. D. L. Nelson, and M. M. Cox, Lehninger Principles of Bio-Chemistry, 7<sup>th</sup> Edition, 2017, W. H. Freeman & Co. Ltd.
3. J. M Berg, J. L. Tymoczko, and L. Stryer, Biochemistry, 9<sup>th</sup> Edition, 2019, W. H. Freeman & Co. Ltd.
4. D. Voet, J. G. Voet, and C.W. Pratt, Fundamentals of Biochemistry, 2<sup>nd</sup> Edition, 2011, John Wiley & Sons.





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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-5	BH7203	ELECTIVE-I (NATURAL PRODUCT CHEMISTRY)	3	0	0	3

**Course Outcomes:** Upon completion of this course students will be able

1. To acquire knowledge on classification and importance of various natural products.
2. To understand the isolation and structure elucidation of natural products
3. To gain a broad spectrum about total synthesis and characterization of various natural products

### Unit-I

**Terpenes and steroids:** Classification and biosynthesis of mono- sesqui-, di- and tri-terpenoids and steroids. Acetyl CoA, Mevalonic acid, Acetoacetyl- CoA, squalene to lanosterol, lanosterol to Cholesterol, Cholesterol to estradiol and progesterone, diosgenin and its utility in hormone synthesis. General chemistry of the following compounds- Cholesterol, Artemisinin, Gibberellic acid, Azadirachtin.

### Unit-II

**Alkaloids:** Isolation and structure elucidation of alkaloids, Biosynthesis of alkaloids using thiokinase, mixed function oxygenase, methyl transferase, amino acid decarboxylases. Total synthesis of morphine, reserpine and ergotamine.

### Unit-III

**Polyphenols:** Biosynthesis of flavonoids and related polyphenols. Synthesis of apigenin, luteolin, quercetin, Daidzein, myricetin, genistein, naringenin and bioflavonoids.

### Suggested Readings:

1. I. L. Finar, Organic Chemistry Vol. 2: Stereochemistry and the Chemistry of Natural Products, 5<sup>th</sup> Edition, 2002, Pearson Education.
2. A. Puszati, Plant Lectins (Chemistry and Pharmacology of Natural Products), 1<sup>st</sup> Edition, 2008, Cambridge University Press.
3. N. R. Krisnaswamy, Chemistry of Natural Products: A Laboratory Handbook, 2<sup>nd</sup> Edition, 2012, Universities Press.



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**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-6	BH7205	ELECTIVE-II (PHARMAEUTICAL CHEMISTRY)	3	0	0	3

**Course/Learning Outcome:** The students will acquire knowledge of

1. Drug designing and development, their SAR and QSAR.
2. Mode of action of different drugs.
3. Role of drugs to inhibit the particular enzymes and treatment of disease.
4. Drug delivery and pharmaceutical technologies development.

### Unit-I

**Drug Delivery:** Importance of Targeted Drug Delivery, Efficacy, Safety and Toxicity Issues. Molecular basis of targeted drug delivery. Drug Release and Uptake Phenomenon.

**Drug Encapsulation:** Characterization, generation, efficacy, toxicity and release profile of nanomaterials (metal-based, metal oxide based and polymeric) in drug encapsulation and drug delivery. Factors affecting drug loading and drug release. Techniques to measure degree of loading and release efficiency. Metabolism and excretion of drug delivery carriers.

### Unit-II

**Drug Delivery Systems:** Methods of preparations, characterization and applications of liposomes, ionosomes, erythrocytes, nanoparticulate systems, solid-liquid nanoparticles, dendrimers, organogels, multiple emulsions and nanoemulsions. Overview and application of aquasomes, pharmacosomes, liquid crystalline systems, protein and peptide-based drug delivery systems.

### Unit-III

**Polymers in drug encapsulation and drug delivery:** Classification, synthesis and applications of biodegradable and natural polymers in formulation of controlled drug delivery systems.

### Suggested readings:

1. E. Mathiowitz, Encyclopaedia of Controlled Drug Delivery, 1<sup>st</sup> Edition, 1999, Wiley India Pvt.Ltd.
2. J. R. Robinson and Vincent H. L. Lee, Controlled Drug Delivery: Fundamentals and Applications, 2<sup>nd</sup> Edition, 1987, CRC Press.
3. W. M. Saltzman, Drug Delivery: Engineering Principles for Drug Therapy, 2<sup>nd</sup> Edition, 2022, Oxford University Press.



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**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-6	BH7101	PHYSICAL CHEMISTRY-II	4	0	0	4

### Course Outcomes: The students will be able to

1. Apprehend ideas on surface science to explain various processes.
2. Develop theoretical understanding of electrochemistry.
3. Extend concepts of electrochemistry in technologies of commercial importance.
4. Impart basics of photochemistry to various applications (LASER, LED, etc.).

### Unit-I

**Surface Chemistry: (a) Adsorption:** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation). Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electrokinetic phenomenon), catalytic activity at surfaces.

**(b) Micelles:** Surface active agents, classification of surface-active agents, ionic and non-ionic micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants counter ion binding to micelles, thermodynamics of micellization, phase separation and mass action models, Solubilization, micro emulsion, reverse micelles.

### Unit-II

**Electrochemistry: Ionics-** Non-structural treatment of ion solvent interaction, quantitative measure of ion solvent interactions. The Born model, Electrostatic potential at the surface of a charged sphere. The electrostatics of charging and discharging spheres. The Born expression for the free energy of ion-solvent interactions, the interaction of a single ionic species with the solvents and solvent, limitation of Born theory. Structural treatment of the ion-solvent interactions, structure of water near an ion, Ion dipole model of ion solvent interaction, limitation of ion-dipole theory of solvation, water molecule as electrical quadrupole, ion-quadrupole model of ion-solvent interaction, Ion-induced dipole interactions, primary and secondary solvation, Limitation of ion-quadrupole theory.

### Unit-III

**Electrodeics:** Thermodynamics of electrified interface equations. Derivation of electrocapilarity; Lippmann equations (surface excess), methods of determination, Structure of electrified interfaces. Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot, Interfaces-theory of double layer at semiconductor-electrolyte solution interfaces. Effect of light at semiconductor solution interface. Electrocatalysis-influence of various parameters. Diffusion layer. The limiting current density and its practical application. Corrosion, Battery and Fuel cell.

### Unit-IV

#### Advanced Photochemistry:

Bimolecular Photophysical Processes: Photo-induced electron-transfer and charge transfer processes, excimer and exiplex, fluorescence quenching. Radiative, Forster type and Dexter type energy transfer.

#### Suggested readings:

1. P. W. Atkins, and J. D. Paulo, Physical Chemistry, 10<sup>th</sup> Edition, 2014, Oxford University Press.
2. T. Engel and P. Reid, Physical Chemistry, 1<sup>st</sup> Edition, 2006, Pearson Education.
3. A.W. Adamson and A.P. Gast, Physical Chemistry of the Surfaces, 6<sup>th</sup> Edition, 1997, John Wiley & Sons.
4. D.K. Chakraborty, Adsorption and Catalysis, 1<sup>st</sup> Edition, 1992, Narosa (India) Pvt. Ltd.
5. K. Holmberg, B. Jonsson, B. Kronberg and B. Lindman, Surfactants and Polymers in aqueous solution, 1<sup>st</sup> Edition, 2002, John Wiley & Sons.
6. J. Rajaraman and J. Kuriacose, Kinetics and Mechanism of Chemical Transformations, 3<sup>rd</sup> Edition, 2010, McMillan.
7. J.O.M. Bockris, and A. K. N. Reddy, Modern Electrochemistry Vol. I and II, 3<sup>rd</sup> Edition, 1997, Plenum Press.



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**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC Lab-6	BH7501	PHYSICAL CHEMISTRY LABORATORY-II	0	0	3	2

**Course outcomes: The students will be able to**

1. Develop expertise for performing experiments to determine the physical properties/parameters of surfactants, solvents, acids etc.
2. Learn experimental techniques to validate photochemical laws.
3. Study thermo gravimetric analysis and fast reactions.

**Syllabus**

1. Determination of CMC of surfactants by different methods.
2. Adsorption isotherm studies.
3. pKa determination of tribasic acid by pH titration method
4. Iodination of acetone by spectrophotometric method
5. Fluorometry studies of naphthalene/anthracene.
6. Study of fast reactions by Stopped flow Spectrophotometry (reaction of Fe(III)thiocyanate and ascorbic acid).
7. Thermogravimetric analysis of calcium oxalate and copper sulphate.
8. Determination of surface tension by tensiometer.
9. Cyclicvoltametric study of Ferri-Ferrocyanide system

**Suggested Readings:**

1. D. P. Shoemaker, C. W. Garland, and J. W. Nibber, Experiments in Physical Chemistry, 5<sup>th</sup> Edition, 1989, McGraw Hill.
2. B. D. Khosla, V. C. Garg, and A. Gulati, Senior Practical Physical Chemistry, 18<sup>th</sup> Edition, 2020, R. Chand & Co.
3. C. W. Garland, J. W. Nibler, and D. P. Shoemaker, Experiments in Physical Chemistry, 8<sup>th</sup> Edition, 2003, McGraw-Hill Education.
4. A. M. Halpern, and G. C. McBane, Experimental Physical Chemistry, 3<sup>rd</sup> Edition, 2003, W.H. Freeman & Co.



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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE Lab-1	BH7503	BIOCHEMISTRY LABORATORY	0	0	3	2

**Course Outcomes:** Upon completion of this course students will be able to

- Estimate proteins, DNA and RNA by spectroscopic techniques.
- Learn separation techniques for separating different biomolecules.
- Understand the enzyme activity and enzyme kinetics.

### Syllabus

1. Spectroscopic/Colorimetric estimation of protein using Lowry's and Bradford methods.
2. Spectroscopic estimation of DNA using DPA method
3. Spectroscopic estimation of RNA using Orcinol method
4. Estimation of Iodine number and saponification value of fatty acids
5. Separation of amino acids by paper chromatography
6. Separation of sugars by thin layer chromatography
7. Separation of proteins by SDS-PAGE.
8. Assay of Enzyme activity: Protease from bacteria.
9. Assay of enzyme activity: Amylase from plant tissue & saliva.
10. Determination of  $K_m$  and  $V_{max}$  of enzyme catalyzed reaction.

### Essential Readings:

1. P. Mu, and D. T. Plummer, Introduction to Practical Biochemistry, 3<sup>rd</sup> Edition, 2008, Tata McGraw-Hill Education,



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**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE Lab-2	BH7505	COMPUTATIONAL CHEMISTRY LABORATORY-II	0	0	3	2

**Course Outcomes:** Upon completion of this course, the students will be able to

- Develop expertise on drawing the structures uniformly using ChemDraw software.
- Project molecular properties based on different quantum mechanical theories using Gaussian9 software.
- Perform molecular modelling studies using Gaussian9 software.

### Syllabus

1. Practicing ChemDraw software to draw the structures.
2. Use of Gaussian9 software to predict the energies, bond angle, bond length, spectral properties of some small molecules using different methods and basis sets.

### Essential Readings:

1. F. Jensen, Introduction to Computational Chemistry, 2<sup>nd</sup> Edition, 2007, John Wiley & Sons Ltd.
2. C. J. Cramer, Essentials of Computational Chemistry, 2<sup>nd</sup> Edition, 2004, Wiley & Sons Ltd.
3. D. C. Young, Computational Chemistry, 1<sup>st</sup> Edition, 2001, Wiley-Interscience.



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**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
Seminar	BH7701	LITERATURE REVIEW & SEMINAR	0	0	4	2

### Course Objectives:

- To develop the attitude and to build confidence for presenting scientific facts and or theories etc.
- To get the opportunities to explore own potentials on creative thinking through learning and writing skill.

### Course Outcomes:

- Attain proper attitude and confidence for presenting scientific facts and or theories etc.
- Determine own potentials on creative thinking through learning and writing skill.



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**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

### 4<sup>th</sup> SEMESTER

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-7	BH7102	INORGANIC CHEMISTRY-III	4	0	0	4

**Course Outcomes: After completion of this course, the students will be able to**

1. Distinguish the structure of solids, their classification and the significance of lattice energy.
2. Basic idea about the bonding involved in different types of solids.
3. Define the electronic properties of solids and various types of defects in solids.
4. Characterize the structure of solids by different characterization techniques such as optical and electron microscopy and X-ray diffraction methods.

#### Unit-I

**Chemical crystallography:** Introduction, Space lattice, Crystal point groups, space group (working knowledge), packing in solids, Crystal structures of representative systems, Silicates and Zeolites, Spinel, Cements, Glasses, Quasicrystals, Nanostructures.

**Bonding in solids and Crystal energetics:** Crystal classifications, Madelung constant and Lattice energy.

#### Unit-II

**Electronic properties and Band theory of solids:** Metals, insulators and semiconductors, electronic structure of solids- Band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, *p-n* junctions, super conductors (Low temperature superconductor, BCS theory, High temperature superconductor).

**Defects, Nonstoichiometry and Diffusion:** Perfect and imperfect crystals, intrinsic and extrinsic defects–point defects–vacancies Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centers, non-stoichiometry defects, line defect- edge dislocation and Screw Dislocation and Plane defects- Grain boundaries, Tilt boundaries, Diffusion mechanisms, Fick's law, Kirkendall effect.

#### Unit-III

**Characterization techniques:**

**Optical Microscopy:** Optical microscope - Basic principles and components, Different examination modes (Bright field illumination, Oblique illumination, Dark field illumination, Phase contrast, Polarized light, Hot stage, Interference techniques), Stereomicroscopy, Photo microscopy, Colour metallography, Specimen preparation, Applications.

**Electron Microscopy:** Interaction of electrons with solids, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Scanning Transmission Electron Microscopy (STEM), Energy Dispersive Spectroscopy (EDS), Wavelength Dispersive Spectroscopy (WDS).

#### Unit-IV

**X-ray Diffraction Methods:** Generation of X-rays, Properties of X-rays: Continuous spectrum, characteristic spectrum, Filters, Bragg condition, Miller indices, Structure factor and its relation to intensity, identification of unit cells from systematic absences in diffraction pattern. Structure factor calculation for NaCl and KCl. Description of the procedure for an X-ray structure analysis, Laue method, Bragg method, Debye-Scherrer's method of X-ray structural analysis of crystals, indexing of crystals.

**Surface Analysis:** Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM), X-ray Photoelectron Spectroscopy (XPS).

**Essential Readings:**

1. S. Zhang, L. Li, and A. Kumar, Materials Characterization Techniques, 2<sup>nd</sup> Edition, 2009, CRC Press.
2. B.D. Cullity, and R.S. Stock, Elements of X-Ray Diffraction, 3<sup>rd</sup> Edition, 2001, Prentice-Hall.
3. A. R. West, Solid State Chemistry and Its Applications, 2<sup>nd</sup> Edition, 2014, John Wiley & Sons.
4. L. Smart, and E. Moore, Solid State Chemistry: An Introduction, 4<sup>th</sup> Edition, 2012, Chapman & Hall Co.
5. C. N. R. Rao, and J. Gopalkrishanan, New Directions in Solid State Chemistry, 2<sup>nd</sup> Edition, 2010, Cambridge University Press.





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## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-8	BH7104	BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY	3	0	0	3

**Course Outcomes: After completion of this course, the students will be able to**

1. Understand the role of metal ions in living system and depict their storage and transport mechanisms.
2. Describe various types of metalloenzymes and their roles in biological systems.
3. Demonstrate pathways of biological systems like nitrogen fixation and photosynthesis and explain the mechanism of oxygen transport and its storage.
4. Illustrate supramolecular chemistry, molecular recognition and enumerate some selected building blocks referred in supramolecular chemistry.

### Unit-I

**Metal ions in biological systems and its storage transport and bio-mineralization:** Essential and trace elements, siderophores.

**Calcium in Biology:** Transported regulation, Intracellular  $\text{Ca}^{2+}$  transport,  $\text{Ca}^{2+}$ -ATPase,  $\text{Na}^+/\text{Ca}^{2+}$  exchange, mitochondrial influx and efflux. Inositol triphosphate,  $\text{Ca}^{2+}$  regulated intracellular processes: Calmodulin, Troponin C.

**Metalloenzymes:** Zinc enzymes: Carboxypeptidase and carbonic anhydrase; Iron enzymes: catalase peroxidase and cytochromes, Cytochrome P450 (P450s or CYPs); Copper enzymes: Superoxide dismutase; Molybdenum oxotransferase enzymes: xanthine oxidase. Coenzyme vitamin  $\text{B}_{12}$ , Sulphur proteins.

### Unit-II

**Nitrogen fixation:** Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenase model systems.

**Photosynthesis:** Chlorophylls, photo system I and photo system II in cleavage of water.

**Transport and storage of dioxygen:** Heme proteins and oxygen uptake, structure and function of hemocyanin and hemerythrin, model synthetic complexes of iron, cobalt and copper.

### Unit-III

**Supramolecular Chemistry:** Introduction, meaning of supramolecular chemistry, phenomenon of molecular recognition and their quantification.

**Building blocks of supramolecular chemistry:** acyclic receptors for neutral and charged guests, macrocycles and crown ethers, macrobicycles and cryptands, macropolycycles, cucurbiturils and cyclodextrins.

#### Suggested Readings:

1. S.J. Lippard, and J. M. Berg, Principles of Bioinorganic Chemistry, 1<sup>st</sup> Edition, 1994, University Science Books.
2. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valenting, Bioinorganic Chemistry, 2<sup>nd</sup> Edition, 2002, University Science Books.
3. A. K. Das, Bioinorganic Chemistry, 2<sup>nd</sup> Edition, 2007, Allied Books.
4. J. W. Steed, and J. L. Atwood, Supramolecular Chemistry, 2<sup>nd</sup> Edition, 2009, Willey India Pvt. Ltd.
5. P. S. Kalsi, and J. P. Kalsi, Bioinorganic and Supramolecular Chemistry, 2<sup>nd</sup> Edition, 2012, New Age International Publishers.
6. J.M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, 1<sup>st</sup> Edition, 1995, Wiley-VCH.
7. H. J. Schneider and A. Yatsimirsky, Principles and Methods in Supramolecular Chemistry, 2<sup>nd</sup> Edition, 2000, John Wiley & Sons Inc.



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**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PC-9	BH7106	ORGANIC CHEMISTRY-III	3	0	0	3

**Course Outcomes:** Upon completion of this course students will be able:

1. To understand the molecular origin of pericyclic reactions.
2. To comprehend the mechanism of photochemistry of various organic compounds.
3. To acquire knowledge on spatial arrangement of atom and basic factors influence selectivity in organic synthesis.
4. Synthetic strategies towards carbon-carbon bond forming reactions through enolates.

### Unit-I

**Pericyclic Reactions and Photochemistry:** Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions: Conrotatory and disrotatory motion,  $4n$ ,  $4n+2$  and allyl systems.

**Cycloadditions:** Antarafacial and suprafacial additions,  $4n$  and  $4n+2$  systems,  $2+2$  addition of ketenes, 1, 3- dipolar cycloadditions and cheletropic reactions.

### Unit-II

**Sigmatropic rearrangements:** Suprafacial and antarafacial shifts of H, Sigmatropic shifts involving carbon-carbon moieties, [3, 3] and [5, 5] Sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements, fluxional tautomerism, Ene reaction. Norrish Type-I and Type-II reactions. Paterno-Buchi reaction.

### Unit-III

**Synthetic Strategies:** Umpolung reactivity – formyl and acyl anion equivalents. Selectivity in organic synthesis; chemo-, regio- and stereoselectivity. Concepts of asymmetric synthesis; resolution (including enzymatic), desymmetrization and use of chiral auxiliaries. Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silyl enol ether, Michael addition reaction. Stereoselective addition to C=O groups (Cram and Felkin-Ahn models).

### Suggested Readings:

1. F. A. Carey and R.J. Sundberg, Advanced Organic Chemistry: Part A & B, 5<sup>th</sup> Edition, 2007, Springer International.
2. R. O. C. Norman and J.M. Coxon, Principles of Organic Synthesis, 3<sup>rd</sup> Edition, 2002, CRC Press.
3. J. Clayden, N. Greeves, and S. Warren, Organic Chemistry, 2<sup>nd</sup> Edition, 2012, Oxford University Press.
4. J. Singh, Photochemistry and Pericyclic Reactions, 3<sup>rd</sup> Edition, 2012, New Age International, Publishers.
5. I. Fleming, Pericyclic Reactions, 1<sup>st</sup> Edition, 2002, Oxford Chemistry Primer, Oxford University Press.



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Techno Campus, Mahalaxmi Vihar, Ghatikia, Bhubaneswar-751029.

## Syllabus Structure (Effective from 2023-24)

**School/ Department: School of Basic Sciences & Humanities**

**Course: M. Sc., Programme: Chemistry, Duration: 2 years (Four Semesters)**

Subject Type	Subject Code	Subject Name	Teaching Hours			Credit
			L	T	P	
PE-7	BH7202	ELECTIVE-III (NUCLEAR AND RADIOCHEMISTRY)	3	0	0	3

**Course Outcomes: Upon completion of this course, the students will be able to**

1. Encompass various types of radioactive decay and detectors.
2. Illustrate the fundamental theories of nucleus and different types of nuclear reactions.
3. Explain the principles of functioning of nuclear reactors and processes followed for nuclear waste management.
4. Understand radiation chemistry and describe the wide-spread applications of radioisotopes.

### Unit-I

**General Aspects of Nuclear Chemistry:** Discovery, Types of decay, Decay kinetics; Decay constant, half-life period, mean life, Parent daughter decay, growth relationships, Secular and transient equilibrium, Units of radioactivity, Alpha, beta and gamma decay, Theory of decay, energies and properties; Artificial radioactivity- Detectors, Ionization chamber, electron pulse counters, scintillation detectors, semiconductor, detectors, thermo luminescence detectors and neutron detectors. Bethe notation, Types of nuclear reactions; The compound nucleus theory, Reaction cross section, Transmutation reactions, elastic and inelastic scattering, spallation, fragmentation, stripping and pick-up, fission, fusion, photonuclear reactions, Thermonuclear reactions.

### Unit-II

**Nuclear Disintegration and Reactors:** The fission energy, Reproduction factor, Classification of reactors- Based on Moderators, Coolant, Phase of Fuel and Generation, Principle of Thermal nuclear Reactors: The four factor formula, Reactor power, Critical size of a thermal reactor, Excess reactivity and control, Breeder reactor, Reprocessing of spent fuels, Nuclear waste management, Safety culture; Active and passive safety, containment building, nuclear criticality safety, ionizing radiation protection, enforcement agencies.

### Unit-III

**Radiation Chemistry:** Passage of radiation through matter, Units for measuring radiation absorption, Radiation dosimetry, Radiolysis of water, Free radicals in Water Radiolysis, Chemical dosimetry, Radiolysis of Fricke Dosimeter Solution.

**Application of radioisotopes:** probing by isotopes, reactions involved in the preparation of radioisotopes, The Szilard-Chalmers Reaction, Radiochemical principles in the use of Tracers, Applications of radioisotopes as tracers, Chemical investigations, analytical applications, agricultural and industrial applications, Neutron Activation Analysis Carbon and Rock Dating, Use of nuclear reactions, Radioisotopes as source of electricity, Nuclear medicines.

### Suggested Readings:

1. H. J. Arnikaar, Essentials of Nuclear Chemistry, 4<sup>th</sup> Edition, 1995, New Age International Publishers Ltd.
2. K. H. Lieser, Nuclear and Radiochemistry, 2<sup>nd</sup> Edition, 2001, Wiley-VCH.
3. G. Choppin, J. O Liljenzin and J. Rydberg, Radiochemistry and Nuclear Chemistry, 3<sup>rd</sup> Edition, 2002, Butterworth-Heinemann,
4. W. D. Loveland, and D. J. Morrissey, Modern Nuclear Chemistry, 2<sup>nd</sup> Edition, 2006, Wiley India Pvt. Ltd.



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			L	T	P	
PE-7	BH7202	ELECTIVE-III ADVANCED ELECTRO CHEMISTRY)	3	0	0	3

### Course Outcomes: The students will be able to

1. Attain working fundamentals on of electrode kinetics such as constant potential Chronoamperometry, constant current Chronoamperometry impedance methods *etc.*
2. Implement concepts of electrochemical principles in various applications *i.e.*, energy storage/conversion, electrocatalysis, corrosion, electrodeposition and bioelectrochemistry
3. Conversant with the phenomenon of Bioelectrochemistry.

### Unit-I

#### Experimental Electrochemical Techniques:

**Constant Potential Chronoamperometry:** Reversible and quasi-reversible charge transfer, Cottrell equation, Influence of uncompensated solution resistance, Application of cyclic voltammetry for characterization of various electrochemical processes.

**Constant Current Chronopotentiometry:** Reversible and quasi-reversible charge transfer, Sand equation.

**Impedance Methods:** Reversible and quasi-reversible charge transfer, Warburg equation, Influence of uncompensated solution resistance, Equivalent circuit's models.

### Unit-II

**Conversion and storage of electrochemical energy:** Fuel cells, Supercapacitors and Li- ion batteries.

**Electrocatalysis:** Influence of various parameters on water splitting, HER and OER.

**Corrosion:** Introduction to corrosion, forms of corrosion, Corrosion monitoring and prevention methods.

**Semiconductor interfaces:** Structure of double layer at the semiconductor-solution interface, Effect of light at semiconductor-solution interface. Dye sensitized solar cells.

**Electro crystallization:** Electro-growth of metals on electrode- Nucleation, Growth, Surface Diffusion, Underpotential deposition, Variety of shapes formed in electrodeposition.

### Unit-III

**Bioelectrochemistry:** Nerve impulses, Membrane potentials, Nernst-Planck equation, Hodgkin-Huxley equations, Core conductor model.

Electrochemical instrumentations and scanning probe techniques.

#### Suggested Reading:

1. A.J. Bard, and L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2<sup>nd</sup> Edition, 2002, John Wiley & Sons.
2. K. B. Oldham, J. C. Myland, and A. M. Bond, Electrochemical Science and Technology: Fundamentals, 1<sup>st</sup> Edition, 2011, Wiley Interscience.
2. J.O.M. Bockris, and A. K. N. Reddy, Modern Electrochemistry Vol. I and II, 3<sup>rd</sup> Edition, 1997, Plenum Press.



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			L	T	P	
PE-7	BH7202	ELECTIVE-III (NEWER SYNTHETIC REACTIONS AND REAGENTS)	3	0	0	3

**Course Outcome:** The students will acquire knowledge of

1. Application of modern synthetic reactions and reagents in organic synthesis
2. Nomenclature and reactivity and synthesis of different heterocyclic compounds.
3. Organic reactions involving green Chemistry.

### Unit-I

Principles and applications of phase transfer catalysis, crown ethers and polymer- supported reagents in organic synthesis.

**Enzymes in Synthesis:** Classification of enzymes, advantages and disadvantages, Artificial enzymes, applications in organic synthesis; Principles of ultrasound and microwave assisted organic synthesis. Reactions in ionic liquids.

### Unit-II

**Five membered rings with two heteroatoms:** Pyrazole, imidazole, oxazole, thiazole, isothiazole and benzofused analogs. Benzofused five membered heterocycles with one heteroatom, *e.g.* indole, benzofuran, benzothiophene.

**Chemistry of bicyclic compounds containing one or more heteroatoms:** benzopyrans, quinoline, isoquinoline, quinoxalines, acridines, phenoxazines, phenothiazines, benzotriazines, pteridines.

**Seven and large membered heterocycles:** azepines, oxepines, thiepinines. Chemistry of porphyrins and spiro heterocycles.

### Unit-III

**Green Chemistry:** Principles, green solvents, concepts of atom economy, Domino and multi component reactions. Principle and applications to green synthesis of pharmaceuticals and industrial chemicals.

**Green methods of synthesis:** microwave, sonication, PTC, ball milling with principle, working and instrumentation

#### Suggested Readings:

- 1) F. A. Carey and R.J. Sundberg, Advanced Organic Chemistry: Part A & B, 5<sup>th</sup> Edition, 2007, Springer International.
- 2) W. Carruthers, Some Modern Methods of Organic Synthesis, 4<sup>th</sup> Edition, 2004, Cambridge University Press.
- 3) R. M. Acheson, Introduction to the Chemistry of Heterocyclic Compounds, 1<sup>st</sup> Edition, 1976, John Wiley & Sons.
- 4) P. Anastas, and J. C. Warner, Green Chemistry- Theory and Practical, 1<sup>st</sup> Edition, 2005, Oxford University Press.
- 5) R. A. Sheldon, I. Arends, and U. Hanefeld, Green Chemistry and Catalysis, 1<sup>st</sup> Edition, 2007, Wiley-VCH.



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			L	T	P	
Project	BH7602	PROJECT	0	0	6	6

### Course Outcomes:

- Create interest on R&D activities.
- Get experience in handling of instruments for their practical applications.
- Garner knowledge on scientific advances in a particular field of research.
- Improve upon the technical writing skills on presenting the research outcomes

A student has to carry out an original and innovative research work according to his/her area of interest in applied chemistry under the guidance of faculty member of OTR and or in collaboration with expert(s) from other institutes. He/she has to submit a report of the findings and present the outcome of the research work.