



Department of Chemistry  
Study and Evaluation Scheme

Program: Master of Science (Chemistry)

Year: Second / Semester: Third

S. No.	Course code	Course Title	Type of Paper	Period/ hr./week			Evaluation Scheme				Subject Total	Total Credits	Attributes						United Nations Sustainable Development Goals (SDGs)	
				L	T	P	CA	TA	Total	ESE			Employability	Entrepreneurship	Skill Development	Gender Equality	Environment & Sustainability	Human Value		Professional Ethics
<b>THEORIES</b>																				
1.	CH501	Polymer Chemistry	Core	03	01	00	40	20	60	40	100	4	✓	✓	✓	✓	✓	Industry Innovation and Infrastructure		
2.	CH513	Organic reaction, Reagents and Heterocyclic Chemistry	Core	03	01	00	40	20	60	40	100	4	✓		✓	✓				
3.	CH514	Chemical Kinetics and Chemical Equilibrium	Core	03	01	00	40	20	60	40	100	4	✓		✓	✓		Zero Hunger		
4.	CH515	Inorganic Reaction Mechanism and Catalysis	Core	03	01	00	40	20	60	40	100	4	✓	✓	✓	✓		-	-	
5.	CH516	Quantum Chemistry; A Molecular Approach	Elective	03	01	00	40	20	60	40	100	4	✓		✓	✓		Clean and Affordable Energy		
6.	CH506	Bioinorganic & Supra molecular Chemistry	Elective										✓	✓	✓			Good Health and Well-being		
<b>PRACTICALS</b>																				
6.	CH517	Chemistry LabPracticals-3	Core	00	00	08	40	20	60	40	100	4	✓	✓	✓	✓		Good Health and Well-being		
<b>Total</b>				<b>15</b>	<b>05</b>	<b>08</b>	<b>240</b>	<b>120</b>	<b>360</b>	<b>240</b>	<b>600</b>	<b>24</b>								

L = Lecture, T = Tutorial, P = Practical, CA = Continuous Assessment, TA = Teacher's Assessment, ESE = End Semester Examination; Sessional = CT+TA; Subject Total =



## Integral University, Lucknow

<b>Effective from Session: 2023-24</b>							
<b>Course Code</b>	CH501	<b>Title of the Course</b>	Polymer Chemistry	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Third	3	1	0	4
<b>Pre-Requisite</b>	B.Sc. with Chemistry	<b>Co-requisite</b>	-				
<b>Course Objectives</b>	The main objective of this course is to study the mechanism of polymer preparation, their processing techniques, commercial uses, identification techniques and preparation process of vinyl polymers, polyamides, polyesters, synthetic rubbers, cellulose and copolymer resins						

Course Outcomes	
<b>CO1</b>	Evaluate the different mechanisms of polymer preparation and their classification.
<b>CO2</b>	Understand the molecular weights of polymers and characterizations techniques such as IR, NMR of polymers
<b>CO3</b>	Analyze various processing techniques of thermoplastics and thermosetting polymer.
<b>CO4</b>	Understand the degradation of polymer and mechanism of oxidative degradation of rubber.
<b>CO5</b>	Detailed study of modification and various additives of polymer and kinetics of vulcanization of rubber

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Polymer & Polymerization	Monomers, functionality, degree of polymerizations, classification of polymers, glass transition, melting transition, polymerization methods: kinetics of addition and polycondensation polymerization (non-catalyzed and acid catalyzed); copolymerization, monomer reactivity ratios and its significance, , random, alternating, block and graft copolymers	8	1
2	Molecular weights and Characterizations of polymers	Concept of molecular weight distribution and its significance, concept of average molecular weight, determination of number average, weight average, viscosity average and Z-average molecular weights, analysis of polymers using IR, XRD UV-visible spectroscopy and microscopic techniques, polymer crystallinity, crystallites, Degree of polymerization.	8	2
3	Thermoplastics and Thermosetting polymers	Commodity and general-purpose thermoplastics: PE, PP, PS, PVC, Acrylic plastics. Condensation plastics: PET, PEAK PBI, PTFE, Polyvinyl Fluoride and Polyvinylidene fluoride, Epoxy Polymers and Silicon Polymers Thermosetting polymers: Elastomers and Resin, Biopolymers: Cellulose, Chitin and Chitosan	8	3
4	Polymer Degradation	Types of Degradation (Chain end and random degradation), Thermal Degradation, Mechanical degradation, Degradation by Ultrasonic Waves, Photodegradation, Oxidative Degradation and Hydrolytic degradation, Mechanism of oxidative degradation of rubber, Ozone Degradation.	8	4
5	Modifications and Additives of Polymers	Polymer Blends, Blending, Fiber-reinforced polymer (FRP), Polymer composites, Additives for Polymers: Types of Additives, Antioxidants, Light stabilizers, UV stabilizers, Lubricants, Process aids, Impact Modifiers, Flame retardant, antistatic agents. PVC stabilizers and Plasticizers), use of carbon black, cross-linking and vulcanization,	8	5

<b>Reference Books:</b>	
Principles of polymer chemistry: A Ravve, 2nd Edition, Kluwer Academic publications; Polymer Science: V R Gowariker, II edition.	
Polymer science and technology: Joll.R..Fried,Prentice-Hall.	
Principles of polymer systems: F. Rodriguez, Claude Cohen, C.K. Ober, L.A. Archer, Vth Edition, Taylor & Francis	
Introduction to polymer :R.J Young and P.A.Lovell.2nd Edition,Newton Thrones publication	
<b>e-Learning Source:</b>	
<a href="https://nptel.ac.in/content/storage2/courses/103103029/pdf/mod7.pdf2">https://nptel.ac.in/content/storage2/courses/103103029/pdf/mod7.pdf2</a> .	
<a href="https://www.e-education.psu.edu/matse202/node/712">https://www.e-education.psu.edu/matse202/node/712</a> <a href="https://nptel.ac.in/content/storage2/nptel_data3/html/mhrd/ict/text/113105028/lec20.pdf">https://nptel.ac.in/content/storage2/nptel_data3/html/mhrd/ict/text/113105028/lec20.pdf</a>	
<a href="http://eacharya.inflibnet.ac.in/data-server/eacharya_documents/55daa452e41301c73a2cb5ac_INFIEP_208/806/ET/lec%20-3.pdf">http://eacharya.inflibnet.ac.in/data-server/eacharya_documents/55daa452e41301c73a2cb5ac_INFIEP_208/806/ET/lec%20-3.pdf</a>	
<a href="https://nptel.ac.in/content/storage2/courses/103103029/pdf/mod7.pdf">https://nptel.ac.in/content/storage2/courses/103103029/pdf/mod7.pdf</a>	

Course Articulation Matrix: (Mapping of COs with POs and PSOs)																		
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO4	PSO5	PSO6	PSO7
<b>CO1</b>	3	-	2	-	-	2	2	3	-	2	-	-	3	2	2	2	2	2
<b>CO2</b>	1	-	2	-	-	2	2	3	-	3	-	-	2	2	2	1	3	3
<b>CO3</b>	3	-	2	-	-	2	2	3	-	3	-	-	3	2	2	2	2	2
<b>CO4</b>	3	-	2	-	-	2	2	3	-	3	-	-	3	2	2	2	1	3
<b>CO5</b>	3	-	2	-	-	2	2	3	-	2	-	-	3	2	2	2	1	3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

<b>Name &amp; Sign of Program Coordinator</b>	<b>Sign &amp; Seal of HoD</b>
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## Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH513	<b>Title of the Course</b>	Organic reaction, reagents & heterocyclic chemistry	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Third	<b>3</b>	<b>1</b>	<b>0</b>	<b>4</b>
<b>Pre-Requisite</b>	BSc. with Chemistry	<b>Co-requisite</b>					
<b>Course Objectives</b>	To understand organic name reaction, rearrangement and its mechanism, Use of reagents in organic synthesis, preparation and chemical reactions of heterocyclic compounds.						

Course Outcomes				
<b>CO1</b>	Mechanistic concept of some name reactions such as Mannich reaction, Stork Enamine reaction, Shapiro reaction, Perkin reaction, Sharpless Asymmetric Epoxidation, Dieckmann condensation and Knoevenagel condensation			
<b>CO2</b>	Explain the mechanism of some important rearrangement like Pinacol-pinacolone rearrangements, Benzil-Benzilic acid rearrangements, Curtius rearrangements, Schmidt reaction, Lossen rearrangements, Baeyer Villiger reaction and Favorskii rearrangements			
<b>CO3</b>	Analyze and compare the uses of some important reagents in organic transformation like oxidation, reduction, dehydration, alkylation, acylation etc.			
<b>CO4</b>	Evaluate the methods for the synthesis of some important five membered heterocyclic compounds and its chemical reaction.			
<b>CO5</b>	Comprehension for the synthesis of some important six membered heterocyclic compounds and its chemical reaction.			
Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Name reactions	Mannich reaction, Stobbe condensation, Stork Enamine reaction, Shapiro reaction, Perkin reaction, Woodward hydroxylation, Prevost hydroxylation, Robinson annulations, Sharpless Asymmetric Epoxidation, Ullmann reaction, Benzoin condensation, Dieckmann condensation and Knoevenagel condensation	8	1
2	Rearrangements	Pinacol-pinacolone rearrangements, Wagner-Meerwein rearrangements, Benzil-Benzilic acid rearrangements, Sommelet Hauser rearrangements, Curtius rearrangements, Schmidt reaction, Lossen rearrangements, Neber rearrangements, Baeyer Villiger reaction and Favorskii rearrangements	8	2
3	Reagents	Use of following reagents in organic synthesis: Dicyclohexylcarbodiimide (DCC), Gilman's reagent (lithium dimethyl cuprate), Lithium aluminium hydride (LiAlH <sub>4</sub> ), Sodium borohydride (NaBH <sub>4</sub> ), Lithium diisopropylamide (LDA), trimethylsilyl iodide, Wilkinson's catalyst, Pyridinium Chlorochromate (PCC), Perbenzoic acid	8	3
4	Introduction to condensed five membered heterocycles	Introduction of petroleum refining, cracking, application of cracking, synthetic petrol, Bergius process, Fischer-Tropsch process, octane number, flash point, determination of flash point, synthesis of pure chemicals from petrochemicals.	8	4
5	Introduction to condensed six membered heterocycles	Methods of synthesis with special reference to Knorr synthesis, Pall-Knorr synthesis and Hantzsch synthesis, chemical reactions of pyrrole, furan and thiophene, mechanism of electrophilic substitution reactions of pyrrole, furan and thiophene	8	5

### Reference Books:

Advanced Organic Chemistry (Reactions, Mechanisms and Structure): Michel B. Smith and Jerry March, 4th Edition, Wiley Interscience Publication.

A Guidebook to Mechanism in Organic Chemistry by Peter Sykes, Six edition, Pearson publication.

Organic Chemistry by Robert Thornton Morrison, Robert Neilson Boyd, and Saibal Kanti Bhattacharjee, Seventh edition, Pearson publication.

Organic Chemistry by Jonathan Clayden, Nick Greeves, and Stuart Warren, Second edition, Oxford Publication.

### e-Learning Source:

<https://www.organic-chemistry.org/namedreactions/beckmann-rearrangement.shtm>

[https://www.youtube.com/watch?v=F\\_xKfs4gzLg](https://www.youtube.com/watch?v=F_xKfs4gzLg)

<https://nptel.ac.in/courses/104/103/104103111/>

<https://www.youtube.com/watch?v=IG-4TJsAwGY>

### Course Articulation Matrix: (Mapping of COs with POs and PSOs)

PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	3	2	2	-	1	3	3	3	-	-	-	-	-
<b>CO2</b>	3	2	2	-	1	2	2	2	-	-	-	-	-
<b>CO3</b>	3	2	3	-	1	3	2	3	-	-	-	-	-
<b>CO4</b>	3	2	3	-	1	3	3	2	-	-	-	-	-
<b>CO5</b>	3	2	1	-	1	3	2	1	-	-	-	-	-

**1-Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation**

<b>Name &amp; Sign of Program Coordinator</b>	<b>Sign &amp; Seal of HoD</b>
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## Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH514	<b>Title of the Course</b>	Chemical Kinetics And Chemical Equilibrium	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Third	<b>3</b>	<b>1</b>	<b>0</b>	<b>4</b>
<b>Pre-Requisite</b>	B.Sc. with Chemistry	<b>Co-requisite</b>	Elementary Mathematics				
<b>Course Objectives</b>	This course is designed for postgraduate students of chemistry as a broad base introduction to chemical kinetics and chemical equilibrium. After successfully completion of course, the student will be able to understand the chemical dynamics of complex reaction and their mechanism. Interestingly, it also deals with homogeneous catalysis and its applications.						

Course Outcomes	
<b>CO1</b>	Students would be able to analyze theories of reaction rates by taking collision theory of bimolecular reaction and activated complex, as a reference and also understand how the concentration of inert salt affects the rate of chemical reaction.
<b>CO2</b>	Students evaluate fundamentals of Homogeneous catalysis with reference to Enzyme catalysis. They got sound insight into the effect of solvent on the rate of chemical reaction.
<b>CO3</b>	Students would develop the concept of chemical dynamics; Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theory. They got the sound insight of fast reactions by flow method, Relaxation method, and Flash photolysis and their applications in research.
<b>CO4</b>	Students would develop the concept of spontaneity; $\Delta G$ and how the Van't Hoff equations play a very important role in homogeneous as well as heterogeneous equilibrium. They got the sound insight with reference to Le-Chatelier's principle and its industrial applications.
<b>CO5</b>	Students would be able to illustrate how ionic strength affects activity coefficient and mean activity coefficient of electrolytes. They also got the concept of Debye-Huckel limiting law and its importance.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Theories of Reaction Rates	Kinetic theory of collision, Steric factor, Extension of collision theory, Conventional transition state theory, Thermodynamic aspects of CTST, Kinetic and thermodynamic control of reactions, Salt effects, Steady state kinetics, Kinetic isotopic effect.	8	1
2	Solution Kinetic	Homogeneous catalysis (acid-base catalysis), Enzyme kinetics – Michaelis-Menten kinetics, Lineweaver-Burk plot, Enzyme inhibition; competitive and noncompetitive, Factors affecting the rate reaction in solutions, Effect of solvent on reaction rates.	8	2
3	Chemical Dynamics	Unimolecular reactions and their treatments (Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theory), Complex reactions (chain reactions, and oscillatory reactions), Studies of fast reactions by flow method, Relaxation method, Flash photolysis.	8	3
4	Chemical Equilibrium	Spontaneity of chemical reactions; Gibbs energy minimum; Perfect gas equilibria; Gibbs free energy change for the reaction and chemical quotient; Expression for thermodynamic equilibrium constant; Equilibrium Calculations, Response of equilibrium to pressure, volume and temperature, The van't Hoff equation, Le-Chatelier's principle.	8	4
5	Electrochemistry	Ionic strength, Activity coefficient and mean activity coefficient of electrolytes, Debye-Hückel theory of strong electrolytes, Debye-Huckel limiting law, Electrified interfaces, Overpotential, Electrolytic conductivity.	8	5

### Reference Books:

- Physical Chemistry, P.W. Atkins and J. D. Paulo, Oxford, 2013, 10th edition New Delhi.
- Chemical Kinetics, K.J. Laidler, McGraw-Hill.
- Physical Chemistry, George Woodbury, Brooks/ Cole Publishing, 1997, Pacific Grove, USA.
- Physical Chemistry, T. Engel and P. Reid, Pearson, 2006, 1st edition, New Delhi.

### e-Learning Source:

- <https://nptel.ac.in/content/storage2/courses/122101001/downloads/lec-32.pdf>
- <https://www.youtube.com/watch?v=gN-yU0MDFzE>
- <https://www.youtube.com/watch?v=c34viSd-dVA>
- <https://www.khanacademy.org/science/chemistry/chemical-equilibrium>

Course Articulation Matrix: (Mapping of COs with POs and PSOs)													
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	3	1	-	-	-	2	1	3	3	1	2	2	2
<b>CO2</b>	3	1	-	-	-	2	2	3	3	2	3	3	3
<b>CO3</b>	3	1	-	-	-	2	2	3	2	1	2	2	2
<b>CO4</b>	3	1	-	-	-	2	1	3	2	1	2	2	2
<b>CO5</b>	3	1	-	-	-	1	3		3	2	3	2	2

**1-Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation**

Name & Sign of Program Coordinator	Sign & Seal of HoD
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## Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH515	<b>Title of the Course</b>	Inorganic Reactions, Mechanism And Catalysis	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Third	<b>3</b>	<b>1</b>	<b>0</b>	<b>4</b>
<b>Pre-Requisite</b>	B.Sc. with Chemistry	<b>Co-requisite</b>					
<b>Course Objectives</b>	To comprehend inorganic reaction mechanisms, influencing factors, and the significance of inorganic elements in context with bio-inorganic chemistry.						

Course Outcomes	
<b>CO1</b>	Explanation of the basic concepts related to stability of coordination complexes and an elementary idea will be imparted regarding the basics of reaction mechanisms.
<b>CO2</b>	Detailed study and analysis of reaction mechanisms in coordination complexes will be discussed along with the factors affecting the rate of reactions.
<b>CO3</b>	Inculcation of higher order thinking ability in students to comprehend the inner and outer sphere reactions.
<b>CO4</b>	Set the overture of Bio-inorganic chemistry along with the elucidation of the role of inorganic elements in the metabolism.
<b>CO5</b>	Comprehension of the structure, functioning and role of important bio-inorganic moieties as well as the role of metal ions in body.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Types of Mechanisms	Basic concepts as kinetic and thermodynamic stability and lability, stability constants; HSAB principle, Factors affecting the stability of complexes with special emphasis to chelate effect and macrocyclic effect.	8	1
2	Substitution Reactions in Coordination Compounds	Substitution reactions in coordination compounds: Substitution reactions in square planar complexes, Trans effect, trans series, Substitution in octahedral complexes, SN1, SN2, SNICB mechanisms, steric effects on substitutions.	8	2
3	Ligand Transfer and Electron Transfer Reactions in Coordination Compounds	Inner and outer sphere reactions, Electron Transfer reactions, Potential energy diagrams as a conceptual tool, Marcus equation, Types of and factors affecting electron transfer reactions.	8	3
4	Metal Ions in Biological Systems	Essential and trace metals. Vitamin B12, methyl cobalamine, Biomethylation. Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.	8	4
5	Important Biomolecules	Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, homocyanins and hemerythrin, model synthetic complexes of iron, and copper Electron Transfer in Biology Structure and function of metalloproteins in electron transport processes-cytochromes and ion sulphur proteins.	8	5

### Reference Books:

- Inorganic Chemistry – Principles of Structure and Reactivity”, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th edition. Harper Collins College Publ. New York.
- Mechanism of Inorganic Reactions in Solution – An Introduction”, D. Benson, McGraw –Hill.
- Mechanisms of Inorganic Reactions, by C.F.Basolo and R.G.Pearson, Wiley, New York.
- d- and f- block Chemistry, C. J. Jones, Tutorial Chemistry Texts, E. W. Abel (Ed.), Royal Society of Chemistry, Cambridge.

### e-Learning Source:

[https://www.youtube.com/watch?v=dFfv\\_jC3\\_ZY](https://www.youtube.com/watch?v=dFfv_jC3_ZY)

<https://bnmu.ac.in/DetailOnline.aspx?Id=388>

[https://link.springer.com/chapter/10.1007/978-94-011-0255-1\\_17](https://link.springer.com/chapter/10.1007/978-94-011-0255-1_17)

### Course Articulation Matrix: (Mapping of COs with POs and PSOs)

PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	3	-	-	-	-	2	-	3	3	-	3	3	-
<b>CO2</b>	3	-	-	-	-	2	-	3	2	-	3	3	-
<b>CO3</b>	3	-	-	-	-	2	-	3	3	-	3	2	-
<b>CO4</b>	3	-	-	-	-	2	-	3	2	-	3	2	-
<b>CO5</b>	3	-	-	-	-	2	-	3	2	-	3	2	-

**1-Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation**

<b>Name &amp; Sign of Program Coordinator</b>	<b>Sign &amp; Seal of HoD</b>
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## Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH516	<b>Title of the Course</b>	Quantum Chemistry: A Molecular Approach	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Third	<b>3</b>	<b>1</b>	<b>0</b>	<b>4</b>
<b>Pre-Requisite</b>	B.Sc. with Chemistry	<b>Co-requisite</b>	Elementary Mathematics				
<b>Course Objectives</b>	Quantum chemistry uses high-level mathematics as a tool to understand atomic and molecular structure, properties, energy as well as chemical reactivity. It introduces the mathematical foundations of a variety of wave functions as well as a practical, hands-on experience. The main objective of computational chemistry is to solve chemical problems by simulating chemical systems (molecular, biological, materials) in order to provide reliable, accurate and comprehensive information at an atomic level.						

Course Outcomes	
<b>CO1</b>	Apply the knowledge of matrices to solve the problems.
<b>CO2</b>	Understand the basic concepts and ideas of Quantum Mechanics.
<b>CO3</b>	Solve the time dependent Schrödinger-equation for discrete two-level systems and being able to apply this to simple problems involving electron spin and photon polarization.
<b>CO4</b>	Apply the technique of separation of variables to solve problems in more than one dimension and to understand the role of degeneracy in the occurrence of electron shell structure in atoms.
<b>CO5</b>	To understand analysis of indeterminate structures and adopt an appropriate structural analysis technique

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Elementary Mathematical Concept	Matrices (2x2, 3x3) only, Multiplication, inverse of matrix, (identity matrix) 2x2, 2x3, 3x3), commutative properties of matrices, complex number Z and its complex conjugate Z*, Expansion of series [ex, sinx, cosx, ln(1+x), ln(1-x)], stirling approximation,	8	1
2	Introductory Quantum Mechanics	Black-body radiation, Planck's radiation law, photoelectric effect, heat capacity of solids, Bohr's model of hydrogen atom (without derivation) their solution of overall solution and its defects, Compton effect, de-Broglie's hypothesis, the Heisenberg's uncertainty principle, Hamiltonian Operator.	8	2
3	Elementary Quantum Mechanics-I	Postulates of quantum mechanics, Eigen value equations & function, concept of Wave function, normalization and orthogonalization of wave function, Quantum mechanical operator, commutation of operators, Time dependent and time independent Schrödinger wave equation and its importance.	8	3
4	Elementary Quantum Mechanics-II	Particle in a one dimensional box, physical interpretation of the wave function, radial node, wave function and shape of orbital, radial probability density, Angular momentum in quantum mechanics (Lx, Ly, Lz), Harmonic oscillator, Rigid rotor.	8	4
5	Approximation Methods	The variation theorem, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory of the Hydrogen atom. Molecular Orbital Theory Huckel theory of conjugated systems, Bond order and charge density calculations, Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc.	8	5

**Reference Books:**

- Physical Chemistry, P.W. Atkins, Oxford Press. 7thEdn.
- Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
- Quantum Chemistry, Ira N. Levine, Prentice Hall.
- Modern Spectroscopy, J.M. Hollas, John Wiley.

**e-Learning Source:**

- <https://www.khanacademy.org/math/precalculus/x9e81a4f98389efdf:matrices/x9e81a4f98389efdf:mat-intro/a/intro-to-matrices>
- <https://www.youtube.com/watch?v=8JF6lvPBAzk>
- <https://nptel.ac.in/noc/courses/noc17/SEM1/noc17-ph03/>
- <https://www.youtube.com/watch?v=SQmj5jT2VLU>

Course Articulation Matrix: (Mapping of COs with POs and PSOs)													
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	3	1	-	-	-	1	1	3	3	1	2	3	2
<b>CO2</b>	3	1	-	-	-	2	1	3	3	1	2	2	3
<b>CO3</b>	3	1	-	-	-	2	1	3	3	1	2	2	2
<b>CO4</b>	3	1	-	-	-	2	1	3	3	1	2	2	2
<b>CO5</b>	3	1	-	-	-	2	1	3	3	1	2	2	3

**1-Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation**

<b>Name &amp; Sign of Program Coordinator</b>	<b>Sign &amp; Seal of HoD</b>
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## Integral University, Lucknow

<b>Effective from Session: 2023-24</b>							
<b>Course Code</b>	CH506	<b>Title of the Course</b>	Bioinorganic And Supramolecular Chemistry	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Third	3	1	0	4
<b>Pre-Requisite</b>	B.Sc. Chemistry	<b>Co-requisite</b>					
<b>Course Objectives</b>	The course aims at providing understanding of the chemistry of d-block metals in metalloproteins and of metal based bioactive compounds, use of metals in medicine, fundamentals of molecular recognition, interactions responsible for the formation of supramolecular systems and applications of supramolecular devices.						

Course Outcomes	
<b>CO1</b>	Student would be able to understand the role of metal ions in biological system.
<b>CO2</b>	Students evaluate fundamentals of enzyme reactions and metalloenzymes.
<b>CO3</b>	Students would develop the concept of metal acid reactions, metals used in diagnosis and administration of drugs.
<b>CO4</b>	Students would restate difference between different modes of molecular reactions.
<b>CO5</b>	Students would able to apply the concepts of supramolecular chemistry.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Metal ions in Biological functions	A brief introduction to bio-inorganic chemistry. Essential and trace metal ions in biological systems with special reference to Na <sup>+</sup> , K <sup>+</sup> and Mg <sup>2+</sup> ions: Na/K pump; Role of Mg <sup>2+</sup> ions in energy production. Role of Ca <sup>2+</sup> in blood clotting, stabilization of protein structures and structural role (bones).	8	1
2	Metalloenzymes	Enzyme, coenzyme, apoenzyme and holoenzyme, Zinc enzymes: carboxypeptidase, carbonic anhydrase and alcohol dehydrogenase. Iron enzymes-catalase and peroxidase. Copper enzymes -superoxide dismutase. Molybdenum enzymes –xanthine oxidase.	8	2
3	Metal-Nucleic Acid Interactions	Metal ions and metal complex interactions,–nucleic acids. Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs. cis-platin, indication and contra indications. Administration of drug and its antidote, use of antihistamine, mannitol, epinephrine and steroid	8	3
4	Supramolecular Chemistry	Concepts and language. Molecular recognition, principle, molecular receptors for different types of molecules including cationic and anionic substrates, design and synthesis of coreceptor molecules.	8	4
5	Applications of Supramolecular Species/Compounds	Supramolecular reactivity and catalysis, Transport processes and carrier design, Supramolecular devices: electronic, ionic, switching and light conversion devices, Some example of self-assembly in supramolecular chemistry.	8	5

**Reference Books:**

- New Concise Inorganic Chemistry by J.D. Lee Edition III Compton Printing Ltd London.
- Principles of Bioinorganic Chemistry, Stephen J. Lippard & Jeremy M. Berg, University Science Books.
- Bioinorganic and supramolecular Chemistry, Ajay Kumar Bhagi and G. R. Chatwal, First Edition, Himalaya Publishing House
- Bioorganic, Bioinorganic and Supramolecular Chemistry, P.S. Kalsi and J.P. Kalsi, Fourth Edition, New Age International Publishers.
- Enzymes: Biochemistry, Biotechnology and Clinical Chemistry, Trevor Palmer and Philip L. Bonner Second Edition, Woodhead Publishing
- Supramolecular Chemistry: Concepts & Perspectives, Lehn, J. M. Print ISBN:9783527293124 Wiley-VCH (2006).

**e-Learning Source:**

- <https://archive.nptel.ac.in/noc/courses/noc19/SEM2/noc19-cy27/>
- <https://www.digimat.in/nptel/courses/video/104104109/L01.html>
- <https://www.youtube.com/watch?v=mdwUnjipR28>

PO-PSO CO	Course Articulation Matrix: (Mapping of COs with POs and PSOs)												
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	2	1	2	1	-	1	1	2	2	1	2	2	2
CO2	2	1	1	1	-	1	1	2	2	1	2	2	2
CO3	2	1	2	-	1	1	2	2	2	1	2	2	2
CO4	3	1	3	-	-	1	2	3	2	2	3	1	3
CO5	3	1	1	-	1	1	2	3	2	1	2	1	3

**1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation**

<b>Name &amp; Sign of Program Coordinator</b>	<b>Sign &amp; Seal of HoD</b>
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## Integral University, Lucknow

Effective from Session: 2015-16							
Course Code	CH517	Title of the Course	Chemistry Lab Practicals-3	L	T <th style="width: 5%;">P</th> <td style="width: 5%;">C</td>	P	C
Year	Second	Semester	Third	0	0	8	4
Pre-Requisite	BSc. with Chemistry	Co-requisite					
Course Objectives	<ul style="list-style-type: none"> <li>Imparting of scientific methodology.</li> <li>Development of practical/technical skills.</li> <li>Ability to work effectively and safely in a laboratory environment.</li> <li>Developing transferable skills (team work, time management).</li> <li>Enhancing communication skill.</li> </ul>						

Course Outcomes	
<b>CO1</b>	Preparation of polymers.
<b>CO2</b>	Preparation of cosmetic products.
<b>CO3</b>	Estimation of key ingredients present in cosmetic products.
<b>CO4</b>	Analysis of food samples.
<b>CO5</b>	Estimation of food samples.

Exp. No.	Title of the Experiment	Content of unit	Contact Hrs.	Mapped CO
1	Phenol formaldehyde resin.	Preparation of Phenol formaldehyde resin.	4	1
2	Urea formaldehyde resin.	Preparation of Urea formaldehyde resin.	4	1
3	Nylon 66.	Preparation of Nylon 66.	4	1
4	Dibenzal acetone	Synthesis of Dibenzal acetone from benzaldehyde.	2	2
5	p-chlorotoluene	Sandmeyer reaction: p-chlorotoluene from p-toluidine.	2	2
6	Hydrolysis	Compare the strength of HCl and H <sub>2</sub> SO <sub>4</sub> by studying the rate of hydrolysis of methyl acetate.	2	3
7	Sugar/glucose	Determination of sugar/glucose content in the given sample of food.	2	3
8	Ascorbic acid	Estimation of ascorbic acid in the given fruit juice.	4	3
9	Cobalt (II) Chloride Complex	Observe the effect of (Temperature) on equilibrium systems on Cobalt (II) Chloride Complex	4	4
10	Solubility product	To determine the solubility product for sparingly soluble salt (e.g. lead sulphate or barium Sulfate).	2	4
11	Effect of concentration	Effect of concentration: The purpose of this part is to observe the effect of certain stresses (ion concentration) on equilibrium systems.	2	5
12	Equilibrium	The equilibrium between Fe <sup>3+</sup> and Fe(CNS) <sup>2+</sup> .	2	5

### Reference Books:

Advance Practical Chemistry: Jagdamba Singh, L.D.S Yadav, Jaya Singh, I.R. Siddiqui, Pragati Edition.

### e-Learning Source:

<https://youtu.be/r2LZxmLtdqU>

<https://youtube.com/watch?v=q8IMKft663I&feature=share>

<https://youtu.be/eA9I2MkWMW0>

<https://youtu.be/gYg2sFqkptc>

Course Articulation Matrix: (Mapping of COs with POs and PSOs)													
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	1	-	-	1	3	2	3	3	2	2	2	2
CO2	3	1	-	-	1	2	3	3	3	2	2	2	2
CO3	3	1	-	-	1	2	2	3	3	2	2	2	2
CO4	3	1	-	-	1	3	2	3	3	2	2	2	2
CO5	3	1	-	-	1	3	2	3	3	2	2	2	2

1-Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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Department of Chemistry  
Study and Evaluation Scheme

Program: Master of Science (Chemistry)

Year: Second / Semester: Fourth

S. No.	Course code	Course Title	Type of Paper	Period/ hr./week			Evaluation Scheme				Subject Total	Total Credits	Attributes						United Nations Sustainable Development Goals (SDGs)		
				L	T	P	CA	TA	Total	ESE			Employability	Entrepreneurship	Skill Development	Gender Equality	Environment & Sustainability	Human Value		Professional Ethics	
<b>THEORIES</b>																					
1.	CH518	Molecular Spectroscopy and Spectral Techniques	Core	03	01	00	40	20	60	40	100	4	✓					✓	✓	-	-
2.	CH509	Green Chemistry	Elective	03	01	00	40	20	60	40	100	4	✓	✓	✓		✓		Climate Action		
3.	CH519	Computational Methods in Chemistry	Elective										✓	✓	✓		✓	✓	✓	Good Health and Well-being	
4.	CH520	Seminar	Core	00	00	04	00	00	00	100	100	2			✓			✓	-	-	
5.	*CH521	Project Training and Evaluation	Core	00	00	00	00	00	00	300	300	10	✓	✓	✓		✓	✓	✓	-	-
<b>Total</b>				<b>06</b>	<b>02</b>	<b>04</b>	<b>80</b>	<b>40</b>	<b>120</b>	<b>480</b>	<b>600</b>	<b>20</b>									

L = Lecture, T = Tutorial, P = Practical, CA = Continuous Assessment, TA = Teacher's Assessment, ESE = End Semester Examination; Sessonal = CT+TA; Subject Total = Sessonal + ESE

\* The Evaluation scheme for the Industrial Training:

Course Title	Course Code	Dissertation	Presentation	Viva/Discussion	Total
Project Training and Evaluation	CH521	200	50	50	300



## Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH518	<b>Title of the Course</b>	Molecular Spectroscopy And Spectral Techniques	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Fourth	<b>3</b>	<b>1</b>	<b>0</b>	<b>4</b>
<b>Pre-Requisite</b>	B.Sc. with Chemistry	<b>Co-requisite</b>	Elementary Physics				
<b>Course Objectives</b>	The main aim of this course is to provide students a concept about how to commonly used molecular spectroscopy techniques work, a theoretical knowledge of each of these methods and their usage in molecular and electronic structure determination.						

Course Outcomes	
<b>CO1</b>	To understand the significance of group theory for chemistry, which allow the prediction of many molecular properties.
<b>CO2</b>	Can explain vibrating diatomic molecule, energy levels of a diatomic molecule, simple harmonic and anharmonic oscillator, Scattering of light and Raman Spectrum. rotational and vibrational Raman Spectra and PQR branches.
<b>CO3</b>	Understand rotational spectra of rigid diatomic molecules, selection rules, interaction of spectral lines.
<b>CO4</b>	To learn Basic principles, Zero field splitting and Kramer's degeneracy, Factors affecting the 'g' value, hyperfine coupling constants, hyperfine splitting, Spin, Hamiltonian, Measurement techniques.
<b>CO5</b>	Students will be able to understand the basics of Mossbauer/ NRF spectroscopy.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Concept of Group theory in Chemistry	Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups: C <sub>n</sub> , C <sub>nv</sub> , C <sub>nh</sub> , D <sub>nh</sub> etc. Character table	8	1
2	Vibrational Spectroscopy	Review of linear harmonic oscillator, energy levels of simple harmonic oscillator, selection rules, pure vibrational spectrum, intensity, determination of force constant and qualitative relation of force constant and bond energies, effect of anharmonic motion and isotope on the spectrum, idea of vibrational frequencies of different functional groups., morse potential energy diagram, Franck Condon Principle, vibrational-rotation spectroscopy, PQR branches.	8	2
3	Rotational Spectroscopy	Classification of molecules, rigid rotor model, energy levels of a rigid rotor (semi-classical principles), selection rules, spectral intensity, distribution using population distribution (Maxwell-Boltzmann distribution) determination of bond length, qualitative description of non-rigid rotor, isotope effect, stark effect and applications	8	3
4	Electron Spin Resonance Spectroscopy	Basic principles, Zero field splitting and Kramer's degeneracy, Factors affecting the 'g' value, hyperfine coupling constants, hyperfine splitting, Spin, Hamiltonian, Measurement techniques, calculation of number of signal, degeneracy, Applications.	8	4
5	Mossbauer Spectroscopy	Basic principles of Mossbauer/ NRF spectroscopy, Isomer shift and nuclear Zeeman splitting, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe <sup>2+</sup> and Fe <sup>3+</sup> compounds including those of intermediate spin, (2) Sn <sup>2+</sup> and Sn <sup>4+</sup> compounds-nature of M-L bond, coordination number, structure	8	5

### Reference Books:

Physical Chemistry, P.W. Atkins, ELBS

Quantum Chemistry, By I.R.N. Levine, Private, Hall of India Ltd.

Quantum Chemistry, By R.K. Prasad, new age International.

Banwell C. N.; McCash, E. M., Fundamentals of Molecular Spectroscopy, 4th Ed., Tata McGraw Hill, New Delhi (2017).

### e-Learning Source:

<https://www.youtube.com/watch?v=WukUvN721Ag>

<https://study.com/academy/lesson/vibrational-spectroscopy-definition-types.html>

<https://www.youtube.com/watch?v=dU38K-5-j1g>

<https://www.youtube.com/watch?v=eZ-Vnj0sS2M>

Course Articulation Matrix: (Mapping of COs with POs and PSOs)													
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	3	1	-	-	-	3	1	3	3	1	3	3	2
<b>CO2</b>	3	1	-	-	-	3	3	3	3	3	3	3	3
<b>CO3</b>	3	1	-	-	-	3	2	3	3	3	3	3	2
<b>CO4</b>	3	1	-	-	-	3	2	3	3	3	3	3	2
<b>CO5</b>	3	1	-	-	-	3	2	3	3	3	3	3	3

**1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation**

Name & Sign of Program Coordinator	Sign & Seal of HoD
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## Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH509	<b>Title of the Course</b>	Green Chemistry	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Fourth	<b>3</b>	<b>1</b>	<b>0</b>	<b>4</b>
<b>Pre-Requisite</b>	BSc. with Chemistry	<b>Co-requisite</b>	-				
<b>Course Objectives</b>	This course is designed for postgraduate students of chemistry and industrial chemistry as a broad base introduction to analytical instrumentation techniques for the measurement of different chemical and physical properties of compounds and materials (composition, structure, etc.). After successfully completion of course, the student will be able to understand the working principle and applications of various modern analytical techniques as well as their operation.						

Course Outcomes	
<b>CO1</b>	Students would be able to create new routes for the synthesis of useful compounds without consuming harmful solvents.
<b>CO2</b>	Students would be able to understand the principles of green chemistry
<b>CO3</b>	Students would be able to apply the important tools for the synthesis of useful compounds without harming the environment.
<b>CO4</b>	Students would restate the difference between different modes of chromatographic separation; apply knowledge of qualitative and quantitative analysis in various fields of chemical, pharmaceutical industry etc.
<b>CO5</b>	Students would be able to illustrate the future of green chemistry

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Introduction	Definition and concept of Green Chemistry, Need for Green Chemistry, Goals of Green Chemistry, Emergence of green Chemistry, Limitations/Obstacles in the pursuit of the goals of Green Chemistry.	8	1
2	Principles of Green Chemistry and Designing a Chemical synthesis	Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes..	8	2
3	Green Synthesis/Reactions -I	1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, disodium iminodiacetate (alternative to strecker synthesis), citral, ibuprofen, paracetamol, furfural. 2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzoic acid), Oxidation (of toluene, alcohols). Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels Alder Reaction, Decarboxylation. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine derivatives; benzimidazoles.	8	3
4	Green Synthesis/Reactions -II	1. Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizzaro reaction, Strecker synthesis, Reformatsky reaction. 2. Selective methylation of active methylene group using dimethylcarbonate: Solid-state polymerization of amorphous polymers using diphenylcarbonate; Use of "Clayon", a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in Organic Syntheses; Biocatalysis in Organic Syntheses.	8	4
5	Future Trends in Green Chemistry	Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; oncovalent derivatization; Green chemistry in sustainable development.	8	5

### Reference Books:

- V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers (2005).  
 P.T. Anastas & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).  
 M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).  
 M.A. Ryan & M. Timmesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

### e-Learning Source:

- <https://www.acs.org/content/acs/en/greenchemistry/principles/12-principles-of-green-chemistry.html>  
[https://www.youtube.com/watch?v=SvRe\\_wc0w3Q](https://www.youtube.com/watch?v=SvRe_wc0w3Q)  
<https://extension.harvard.edu/blog/green-chemistry-and-the-future-of-sustainability/>

<b>Course Articulation Matrix: (Mapping of COs with POs and PSOs)</b>													
<b>PO-PSO CO</b>	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	3	1	2	3	1	2	-	-	3	-	3	3	3
<b>CO2</b>	3	1	2	3	1	2	-	-	3	-	3	3	3
<b>CO3</b>	3	1	2	3	1	2	-	-	3	-	3	3	3
<b>CO4</b>	3	1	2	3	1	2	-	-	3	-	3	3	3
<b>CO5</b>	3	1	2	3	1	2	-	-	3	-	3	3	3

**1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation**

<b>Name &amp; Sign of Program Coordinator</b>	<b>Sign &amp; Seal of HoD</b>
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# Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH519	<b>Title of the Course</b>	Computational Methods In Chemistry	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Fourth	<b>3</b>	<b>1</b>	<b>0</b>	<b>4</b>
<b>Pre-Requisite</b>	BSc. with Chemistry	<b>Co-requisite</b>					
<b>Course Objectives</b>	The objective of this course is to provide introduction to chemo-informatics, Molecular modeling for drug designing and other area of chemistry, informatics and biology.						

Course Outcomes	
<b>CO1</b>	The student is expected to achieve a good grasp of the concepts and applications of chemoinformatics.
<b>CO2</b>	Explain the various stages of drug discovery. Explain various structure-based drug design methods, define molecular modeling. the student is expected to achieve a better understanding of in-silico drug designing, and the factors influencing drug discovery Explain various structure-based drug design methods, bioinformatics in drug development.
<b>CO3</b>	Understand, algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzman velocity, duration of the MD run etc.
<b>CO4</b>	The student is expected to achieve a good grasp of the concepts and applications of chemoinformatics.
<b>CO5</b>	Explain the various stages of drug discovery. Explain various structure-based drug design methods, define molecular modeling. the student is expected to achieve a better understanding of in-silico drug designing, and the factors influencing drug discovery Explain various structure-based drug design methods, bioinformatics in drug development.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Introduction to cheminformatics	Evolution of cheminformatics, history of chemical information science, use of cheminformatics, prospectus of cheminformatics, and history of medicinal chemistry. Prodrugs and soft drugs, drug target, drug solubility, natural resources of lead compounds, pharmacokinetics and drug metabolism. Molecular modeling using computer	8	1
2	Occupational Safety; Molecular modeling	Introduction, force field, quantum chemistry, Schrödinger equation, potential energy functions, energy minimization, local and global minima, saddle point, grid search. Semi-empirical methods (ZDO, MNDO, AM1, PM3). Molecular mechanics; Definition, balls and springs, force fields, bond-stretching, bond-bending, dihedral motions, out of plane angle potential, non-bonded interaction, coulomb interactions. Derivative methods; Steepest descent, conjugate gradient and Newton-Raphson method.	8	2
3	Drug design and discovery (DDD)	Introduction drug design and discovery, principles of drug development. Bioinformatics in drug development, cheminformatics and pharmacoinformatics. Applications of drug discovery, in-silico drug designing, area influencing drug discovery. Introduction of two and three-dimensional quantitative structure–activity relationship (QSAR) and its role in DDD.	8	3
4	Structure-based drug designing (SBDD)	Introduction, target identification and validation, homology modeling, receptor mapping, active site analysis, pharmacophore mapping and grid maps. Ligand-based drug designing (LBDD); Introduction, lead designing, combinatorial chemistry, high throughput screening (HTS), database generation and chemical libraries, ADME property. Introduction to docking, methods of docking, docking with AutoDock, Vina, Dock etc.	8	4
5	Molecular dynamics (MD)	Introduction, Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, MD methodology, algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzman velocity, duration of the MD run. Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions.	8	5

### Reference Books:

- Chapman, Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York (2006).  
 V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi (1997).  
 W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press (1996).  
 R. L. Schwartz, T. Christiansen, L. Wall, Learning Perl Second Edition, O'Reilly Media (1997). 5. Foy, Mastering Perl First Edition, O'Reilly Media (2007)

### e-Learning Source:

- [https://www.youtube.com/watch?v=yX\\_nPzmTpi8](https://www.youtube.com/watch?v=yX_nPzmTpi8)  
<https://www.youtube.com/watch?v=Y3utQZIPJ-4>  
<https://www.jubilantbiosys.com/integrated-drug-discovery-services>

Course Articulation Matrix: (Mapping of COs with POs and PSOs)													
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	3		2		2	3	3	3	3	3	3	2	2
<b>CO2</b>	3				2	2	3	2	3	3	3	2	3
<b>CO3</b>	3		2		2	3	2	3	3	3	3	3	3
<b>CO4</b>	3	2	2		2	3	2	2	3	2	3	3	3
<b>CO5</b>	3	2	2		2	3	2	2	3	2	3	3	3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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## Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH520	<b>Title of the Course</b>	Seminar	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Fourth	<b>0</b>	<b>0</b>	<b>4</b>	<b>2</b>
<b>Pre-Requisite</b>	BSc. with Chemistry	<b>Co-requisite</b>					
<b>Course Objectives</b>	<ul style="list-style-type: none"> <li>To develop students' communication and discussion skills</li> <li>Increase vocabulary knowledge, learn about communication style, develop learner autonomy.</li> <li>To build confidence to use English for oral presentation.</li> <li>To develop the ability to seek clarification and defend the ideas of others effectively.</li> </ul>						

Course Outcomes	
<b>CO1</b>	To develop and improve the communication skills
<b>CO2</b>	To develop discussion and leadership abilities
<b>CO3</b>	Skills for the development of demonstration abilities
<b>CO4</b>	To develop skills for effective power point presentation
<b>CO5</b>	To understand importance of gestures and body language during presentation

Course Articulation Matrix: (Mapping of COs with POs and PSOs)													
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	2	3	1	-	2	-	-	3	-	3	2	2	3
<b>CO2</b>	3	3	2	-	2	2	-	3	1	2	2	1	3
<b>CO3</b>	3	3	1	-	1	2	-	3	2	2	2	1	3
<b>CO4</b>	3	3	1	-	1	2	-	3	2	2	2	2	3
<b>CO5</b>	3	3	1	-	1	1	-	3	-	2	1	-	3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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## Integral University, Lucknow

<b>Effective from Session:</b> 2019-2020							
<b>Course Code</b>	CH521	<b>Title of the Course</b>	Project Training and Evaluation	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>Year</b>	Second	<b>Semester</b>	Fourth	<b>0</b>	<b>0</b>	<b>0</b>	<b>10</b>
<b>Pre-Requisite</b>	BSc. with Chemistry	<b>Co-requisite</b>					
<b>Course Objectives</b>	To provide the industrial exposure and enhance technical skills of students						

Course Outcomes	
<b>CO1</b>	Hands on training
<b>CO2</b>	Integrate class room theory with laboratory practice.
<b>CO3</b>	Understanding professional ethics of industry and code of conduct.
<b>CO4</b>	Essential training in laboratory safety procedures
<b>CO5</b>	Compilation of data and report writing

Course Articulation Matrix: (Mapping of COs with POs and PSOs)													
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	3	1	1	-	-	3	2	3	3	3	3	3	3
<b>CO2</b>	3	-	1	-	-	3	1	3	3	2	2	3	3
<b>CO3</b>	3	2	1	-	3	2	-	3	3	3	1	2	3
<b>CO4</b>	3	1	1	-	2	3	2	3	3	2	3	3	3
<b>CO5</b>	3	3	1	-	2	3	-	3	3	3	3	3	3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

<b>Name &amp; Sign of Program Coordinator</b>	<b>Sign &amp; Seal of HoD</b>
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