

Programme Project Report (PPR)
M.Sc. Chemistry Programme (MSCCH)
Department of Chemistry
School of Sciences, Uttarakhand Open University

1. Overview :

The MSc (Chemistry) programme is conducted under the department of Chemistry, School of Sciences, Uttarakhand Open University. The Department of Chemistry shares the vision of achieving excellence in distance education and research. Uttarakhand Open University Haldwani was established in the year 2005 by Act No 23 of Uttarakhand Government. The University is fully equipped with Information and Communication Technology. Our University have the Learners support system. The current information is given on University Website (<https://www.uou.ac.in/>) and other electronic medium (SMS, whatapps group, department blog, telephonic conversation, mail etc). All learners can take admission through our university website and in some cases offline admission is also available. The learners need not to come in the university for taking the Self Learning Materials (SLM) and Examination etc. All of these facilities are provided to the learners through respective study center.

2. Contents of Programme Project Report (PPR):

The MSc (Chemistry) Programme was started in 2012 in Uttarakhand Open University Haldwani. Presently the programme is the two year Programme (Semester Mode). In the first semester four papers are compulsory and in second semester four papers are to be studied then in third semester four papers are compulsory and in forth Semester two paper are to be selected out of three optional papers and dissertation is compulsory.

The content of the programme project report is as: -

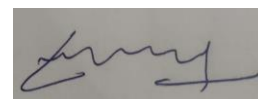
i. Programme Mission & Objectives: Uttarakhand state comprises of geographically constrained areas. A large number of learners cannot avail higher education due to the aforesaid geographical constraints. The learners can avail higher education through ODL (Open and Distance Learning) mode. The mission of the programme is to provide higher education to the learners in a way which is easily accessible. The mission of the Chemistry program parallels the



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mission of the University in its vision and purpose. The programme is committed to academic excellence and intends to provide a comprehensive study material, audio video lectures and a workshop-based learning to the learners who choose Chemistry as a subject for pursuing higher education. The department support active teaching and learning opportunities that prepare students for productive careers within a broad range of scientific and Chemistry-related professions.

ii. Relevance of the Programme with HEI's Mission and Goals: In Uttarakhand large number of students are interested in Science subject i.e. Chemistry as it opens up job opportunities in the various field such as academics, research and the courses available in higher education open up a wide spectrum of job opportunities in different types of industries such as chemical and Pharmaceutical and also laboratory related jobs. Thus the Graduate and Post graduate chemistry programme are useful for the students.

iii. Nature of Prospective Target group of Learners: The target groups of learners are all Science graduate and undergraduates, the teachers, those who want to enhance their education and also the people those who are already working in corporate section who couldn't complete their studies. In addition to this, faculties are required to teach Chemistry at Under Graduate and Post Graduate level in conventional Universities and professional/ technical Universities or Colleges

iv. Appropriateness of the Programme to be conducted in ODL mode to acquire skill competence:

The access to knowledge on the subject is not accessible easily to those aspirants who reside in far remote areas and those who belong to weaker and marginal sections of the society. Therefore, initiating such programme in Open and Distance Learning (ODL) mode will help aspirants particularly residing in far-flung areas and those who belong to weaker sections, to acquire skill and knowledge on the subject area.

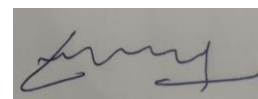
The learners those who fulfill all the requirements of the programme shall be highly trained and skilled through the year counseling and special Practical and theoretical workshop and counseling session making them at par with the learners studying in a traditional University based education system.



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v. Instructional Design:

The curriculum designed for Chemistry programmes are as per the scientific requirements. In curriculum there is a provision of two days regular weakened counseling session and a Practical session. The study is also available in different electronic mediums (Internet mobile E-portal, YouTube etc), The instructional design of Chemistry programme includes technologies those are user friendly. The details of the programme curriculum are given below:

Programme Curriculum:

Name of the Programme	:	Master of Science Chemistry (M.Sc. Chemistry)
Programme Code	:	MSCCH-21
Programme Mode	:	Semester
Eligibility	:	Graduation in concern subject
Duration Min	:	2 Years; Max: 6 Years
Self-Learning Material (SLM)	:	English
Programme Fee	:	Fee per Semester: - 9650
Total fee M.Sc. Programme	:	38950
Total Credit	:	72

First Semester:

S.N.	Course Name	Course Code	Marks			Credits	Minimum Counseling hours
			Th.	Ass.	Total		
1.	Inorganic Chemistry I	MSCCH-501	70	30	100	03	9
2.	Organic Chemistry I	MSCCH-502	70	30	100	03	9
3.	Physical Chemistry I	MSCCH-503	70	30	100	03	9

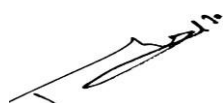
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4.	Group Theory Instrumentation Chemistry and Computer for Chemists	MSCCH-504	70	30	100	03	9
6.	Laboratory Course -I	MSCCH- 505L			200	06	18
	Total Credits					18	54

Second semester:

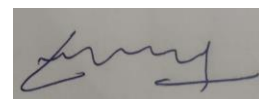
S.N.	Course Name	Course Code	Marks			Credits	Minimum Counseling hours
			Th.	Ass.	Total		
1.	Inorganic Chemistry -II	MSCCH-506	70	30	100	03	9
2.	Organic Chemistry -II	MSCCH-507	70	30	100	03	9
3.	Physical Chemistry II	MSCCH-508	70	30	100	03	9
4.	Spectroscopy I	MSCCH-509	70	30	100	03	9
5.	Lab Course II	MSCCH510 L			200	06	18
	Total Credits					18	54



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Third semester:

S.N.	Course Name	Course Code	Marks			Credits	Minimum Counseling hours
			Th.	Ass.	Total		
1.	Solid State and Materials Chemistry	MSCCH-601	70	30	100	03	9
2.	Spectroscopy II	MSCCH-602	70	30	100	03	9
3.	Bio-Inorganic and Bio-Physical Chemistry	MSCCH-603	70	30	100	03	9
4.	Photo Chemistry and Allied Chemistry	MSCCH-604	70	30	100	03	9
5.	Laboratory Course -III	MSCCH-605L			200	06	18
	Total Credits					18	54

Fourth semester (Organic Chemistry):

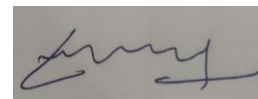
S.N.	Course Name	Course Code	Marks			Credits	Minimum Counseling hours
			Th.	Ass.	Total		
1.	*Organic Synthesis	MSCCH-606	70	30	100	03	09
2.	**Chemistry of Natural product and Heterocyclic compounds	MSCCH-607	70	30	100	03	09



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3.	**Medicinal Chemistry	MSCCH-608	70	30	100	03	09
4.	Laboratory Course-IV (Organic Chemistry)	MSCCH609 L			100	03	09
5.	Dissertation	MSCCH-610				09	Grade
Total Credits						18	54
*Compulsory Course							
**Elective Course							

Details Syllabus

M.Sc. (Chemistry) Programme

SEMESTER-I

Course – 1: MSCCH 501 Inorganic Chemistry – I

(3 Cr.)

Course outcome:

Upon successful completion of this course, the learners will be able to describe the stereochemistry and bonding in the main group elements. They will also be able to understand the bonding in inorganic molecules and know about the salient features of phosphorus-nitrogen and sulfur-nitrogen compounds, organometallic compounds of the alkali and alkaline earth metals, aryls and alkyls of transition metals. Learners will also be able to learn about the metal pi-complexes, metal clusters and metal-ligand equilibria in solution at the end of this course.

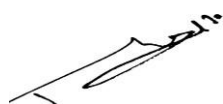
Block I Stereochemistry and Bonding

Unit 1: Stereochemistry and Bonding in Main Group Compounds

VSEPR, Walsh diagram (triatomic and penta-atomic molecules), $d\pi-p\pi$ bond, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

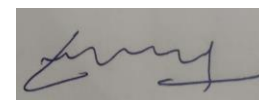
Unit 2: Phosphorus-Nitrogen and Sulfur-Nitrogen Compounds

Synthesis, structure, bonding and uses of cyclic and linear phosphonitrilic compounds, phosphorus-sulphur compounds, sulphur-nitrogen compounds, ring and chain compounds



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S₂N₂, S₄N₄, (SN)_x etc

Unit 3: Organometallic compounds of Alkali and Alkaline Earth metals

Organometallic compounds of Li, Mg, Be, Ca, Na: Synthesis, properties, structure, bonding, uses.

Unit 4: Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways, organocopper compounds in organic synthesis.

Block II Metal π -Complexes and Metal Clusters

Unit 5: Metal π Complexes-I

Metal carbonyl, preparation, properties, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

Unit 6: Metal π -Complexes-II

Alkene, alkyne, allyl, diene and cyclopentadienyl complexes. Arenes and other alicyclic ligands.

Unit 7: Metal Clusters

Higher boranes, carboranes, metalloboranes and metallocarboranes. Compounds with metal-metal multiple bonds. Isopoly and heteropoly acids and salts (or anions) with special reference to vanadium, molybdenum and tungsten. Nomenclature, classification and preparation.

Unit 8: Metal-Ligand Equilibria in Solution

Stepwise and overall formation constants and relation between them, trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Formation functions n , a_c , ϕ ; Evaluation of stepwise stability constants. Chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

Course – 2: MSCCH 502 Organic Chemistry I

(3Cr.)

Course outcome:

After successful completion of this course learners will understand delocalized chemical bond, conjugation, cross-conjugation, resonance, hyper conjugation, tautomerism, Energy levels of π orbitals, Huckel's rule, aromaticity, anti-aromaticity in the organic molecules, reactive intermediates such as



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carbene, nitrene, carbocations, carbanions, carbon radicals etc. After completing this course, they will be able to determine structure, reactivity and stereochemistry of the organic molecules.

Block 1 Nature of Bonding in Organic Molecules

1: Nature of Bonding in Organic Molecules

Delocalized chemical bonding: conjugation, cross-conjugation, resonance, hyper conjugation, tautomerism, Energy levels of π orbitals, Huckel's rule, aromaticity, anti-aromaticity and homoaromaticity, benzenoid and non-benzenoid aromatic compounds, alternant and non-alternant hydrocarbons. Annulenes. Non-covalent bonding – addition compounds, crown ether complexes, cryptands, inclusion compounds, catenanes, rotaxanes and ionic liquids.

Unit 2: Structure and Reactivity

Types of reaction mechanisms, types of reactions, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammond principle. Reaction coordinate, potential energy diagrams, transition states and intermediates. Methods of determining mechanisms, isotope effects.

Unit 3: Reactive Intermediates

Generation, structure, stability and reactivity of carbocations, carbanions, carbon radicals, singlet and triplet carbenes and nitrenes. Effect of structure on reactivity: resonance and field effects, steric effects and quantitative treatment. The Hammett equation and linear free energy relationships, substituent and reaction constants, Taft equation.

Block 2: Stereochemistry

Unit 4: Stereochemistry 1

Stereogenicity, chirality and prochirality, Enantiomerism, Diastereomerism and meso isomerism and racemic modification. Configuration and conformation. Stereochemical descriptors: D, L; R, S; E, Z; syn, anti, etc. Axial, planar and helical chirality. Stereoprojections – Fischer, Sawhorse, Newman and wedge projections and their interconversions. Absolute and relative configurations and their determination; molecules with one, two or more chiral centres. Simple chemical correlation of configurations with examples, quasisracemates. Stereochemistry and configurations of allenes, spiranes, alkylidene cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes.



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Unit 5: Stereochemistry 2

Topocity and prochirality: Topocity of ligands and faces and their nomenclature. Cram's, and Prelog's. Stereoselectivity and stereospecificity and enantiomeric diastereomeric excess, Asymmetric induction. Configuration, conformation and stability of cyclohexanes, cyclohexene (mono and disubstituted), cyclohexanones, halocyclohexanones, decalins. Qualitative correlation between conformation and reactivity, Stereochemistry of Compounds having P, N and S.

Book Suggested:

1. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S.(2007).
2. Eliel, E.L. *Stereochemistry of Carbon Compounds* Textbook Publishers (2003).
3. Finar, I. L. *Organic Chemistry* Vol. 1, Longman (1998).
4. Lowry, T. H. & Richardson, K.S. *Mechanism and Theory in Organic Chemistry* Addison –Wesley Educational Publishers, Inc. (1981).
5. Nasipuri. D. N. *Stereochemistry of Organic Compounds: Principles & Applications* SouthAsia Books (1994).
6. March, J. *Advanced Organic Chemistry* John Wiley & Sons (2004).
7. Kalsi, P.S. *Stereochemistry: Conformation and Mechanism, 7th Edition New Age International, Delhi (2008).*
8. Sengupta.

Course – 3: MSCCH 503 Physical Chemistry I

(3 Cr.)

Course outcome:

After this course learners able to the understood basic concepts of laws of thermodynamics, free energy, chemical potential and entropy under the thermodynamics. They will also able to understand the statistical thermodynamics, application of the statistical thermodynamics and different aspects of chemical kinetics, catalysis. After completing this course, they will able to the electrochemistry and its application in the chemistry..

Block I Thermodynamics

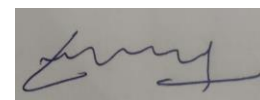
Unit 1: Classical Thermodynamics



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Brief resume of Partial molar quantities and their physical significance. Concepts of activity and fugacity.

Unit 2: Statistical Thermodynamics

Role and importance of Statistical Mechanics in Chemistry, Fundamentals of Statistical Mechanics, Concept of distribution, Thermodynamic probability and most probable distribution. Types of statistics: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac Statistics. Idea of microstates and macrostates. Thermodynamic probability (W) for the three types of statistics. Derivation of Distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance.

Unit 3 Applications of Statistical Mechanics

The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monoatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures. Specific Heat of solids-Einstein and Debye Theory of heat capacities of monatomic solids. Third Law of Thermodynamics, Residual entropy.

Block II Chemical Kinetics and Catalysis

Unit 4 Theories of Reaction Rates

Collision theory. Potential energy surfaces (basic idea). Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).

Unit 5 Solution Kinetics

Factors affecting reaction rates in solution. Effect of solvent (dielectric constant) and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

Unit 6 The Fast Reaction Kinetics

Relaxation methods, flow and flash photolysis. Preliminary ideas of molecular reaction dynamics. Kinetics of Chain reaction involving Hydrogen- Chlorine, Hydrogen- Bromine reaction and pyrolysis of acetaldehyde. Kinetics of enzyme reactions.

Unit 7 Catalysis

Gibbs adsorption isotherm, estimation of surface area (BET equation without derivation), catalytic activity at surfaces.

Block III Electrochemistry

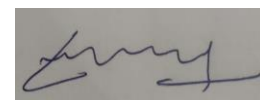
Unit 8 Electrochemistry-I



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Debye-Huckel theory theory for electrolytic solution, recall of activity, activity coefficients and their determination including ionic strength, electrochemistry of solution, Debye-Huckel treatment of dilute solutions.

Unit 9 Electrochemistry-II

Determination of activity coefficient, Debye-Huckel theory of strong electrolytes with derivation, ionic atmosphere and thickness of ionic atmosphere, Debye-Huckel-Onsagar theory, theory of conduction, Onsagar equation including mathematical deduction, overvoltage and decomposition potential.

Course-4: MSCCH-504 Group Theory and Instrumentation Chemistry (3 Cr.)

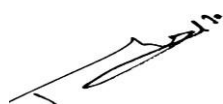
Course outcome :

Upon successful completion of this course, the learners will be able to understand symmetry elements and symmetry operations, definitions of group and subgroup and their characteristics, character of a representation. They gain knowledge about the great orthogonality theorem and its importance, character tables and their use in spectroscopy. They will also learn about X-ray diffraction methods, different chromatographic technique which used in molecule identification, radioanalytical methods and radio analytical method. After successful completion of this course, the learners should be able to types of errors, propagation of errors, accuracy and precision, least square analysis, average standard deviation and the history of the development of computers. They will learn the Basic structure and functioning of computers, computer programming involving in the chemistry, The learners will learn how to operate a PC and how to run standard programme.

Block I Symmetry and Group Theory in Chemistry:

Unit 1 Symmetry and Group Theory

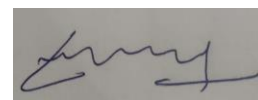
Symmetry elements and symmetry operations, definitions of group and subgroup and their characteristics, similarity transformation, product of symmetry operations, equivalent atoms and equivalent symmetry elements, relation between symmetry elements and operation, relation between orders of a finite group and its subgroup. Conjugacy relation and classes of symmetry operations, point symmetry (or group) and its classification, Schonfliess symbols, representation of group by matrices (representation for the C_n , C_{nv} , C_{nh} , D_{nh} etc. groups to be worked out explicitly), products of symmetry operations. Character of a representation. The great orthogonality



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theorem (without proof) and its importance. Character tables and their use in spectroscopy.

Unit 2 X-ray Diffraction Methods

Bragg condition, Miller indices, Laue's method, Bragg's method, Debye- Scherrer method of X-ray structural analysis of crystals. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules. Ramchandran diagram. General Introduction of Electron Diffraction : Scattering intensity vs scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules.

Block II Chromatographic and Radioanalytical Methods

Unit 3 Chromatographic methods

Principle, instrumentation and applications of gas and liquid chromatography. Principle and application of TLC, paper, column and HPLC. Ion Exchange chromatography: Cationic, anionic exchangers and their applications.

Unit 4 Gas Chromatography

Theory of gas chromatography, parts of gas chromatograph, detectors (TCD, FID, ECD), Van-Deemter equation (no derivation), concept about HEPT- plate theory and rate theory. Applications.

Unit 5 Radio Analytical Methods

Basic principles and types of measuring instrument, isotope dilution techniques.

Block III Computer

Unit 5 Data Analysis

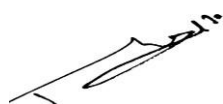
Types of errors, propagation of errors, accuracy and precision, least square analysis, average standard deviation.

Unit 6 History of development of computers

Main frames, Mini, Micro and Super Computer systems. General awareness of computer hardware i.e CPU and other peripheral devices.

Unit 7 Introduction to Computers and Computing

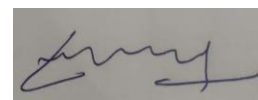
Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/Q devices, Secondary storage. Computer languages. Operating system with DOS as an example.



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Introduction to WINDOWS. Data Processing, principles of programming. Algorithms and flowcharts.

Unit 8 Programming in Chemistry

Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data.

Unit 9 Use of Computer Programmes

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot. Further, the students will operate one or two of the packages such as MATLAB, EASYPLOT, DBASE, and Word Processing software such as MS-WORD and CHEMDRAW.

Course -5: MSCCH-505L Chemistry Lab-I:Inorganic and organic (3 Cr.)

Course outcome :

Upon completion of this course, the learners will have the knowledge and skills to understand the laboratory methods and tests related to inorganic mixture analysis and preparation of inorganic compounds. They will also separate and identification of components of binary mixtures.

Block I Inorganic Chemistry Unit 1 Qualitative Analysis

Qualitative analysis of mixtures of salts containing not more than eight radicals including Rare-earth element salts (two rare element ions), Interfering radicals, Other anions, which have not been done in under graduate practical, Insolubles and simple salts.

Unit 2 Preparations

Preparation of selected inorganic compounds such as:

[Ni(dmg)₂], Prussian Blue, Turnbull's Blue,
[Cu(NH₃)₄]SO₄.H₂O, Co[NH₃]₆[[Co(NO₂)₆],
cis-K[Cr(C₂O₄)₂(H₂O)₂], *cis*-[Co(trien)(NO₂)₂]Cl.H₂O,
Na[Cr(NH₃)₂(SCN)₄], Hg [Co(SCN)₄],
[Mn(acac)₃], [Co(py)₂Cl₂],
K₃[Fe(C₂O₄)₃], [Ni(NH₃)₆]Cl₂

Unit 3 Quantitative Estimations

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Quantitative estimation of metal ions by complexometric titration, direct and / or back titration, use of masking agents.

Block II Organic Chemistry

Unit 4 Separation and Identification of components of Binary Mixtures

Separation and identification of components of binary mixtures with water, aqueous solutions of sodium bicarbonate, sodium hydroxide, hydrochloric acid and ether separation.

Unit 5 Quantitative Estimations

1. Determination of the percentage of number of hydroxyl groups in an organic compound by acetylation method.
2. Estimation of amines/ phenols using bromate-bromide solution/ or acetylation method.
3. Determination of Iodine and Saponification values of an oil sample.
4. Determination of DO, COD and BOD of water sample
5. Spectrophotometric (UV/VIS) Estimations of :
 - (i) Amino acids
 - (ii) Proteins
 - (iii) Carbohydrates
 - (iv) Cholesterol
 - (v) Ascorbic acid
 - (vi) Aspirin
 - (vii) Caffeine

Note: Inorganic exercise	:	60
Organic exercises	:	60
Record(including test)	:	30
Attendance	:	30
Viva	:	20

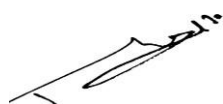
SEMESTER-II

Course –6 : MSCCH-506 Inorganic Chemistry II

(3 Cr.)

Course outcome :

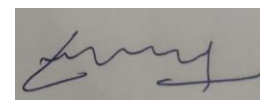
Upon successful completion of this course, the learners will be able to reaction mechanism of transition metal complexes, Redox reaction, electron transfer reactions, Marcus-Hush theory, inner sphere type reactions, crystal field theory, electronic spectra and magnetic properties of coordination compounds. They will be able to understand about the Orgel and Tanabe-Sugano diagrams for



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transition metal complexes (d^1-d^9 states).

Block I: Reaction Mechanism

Unit 1: Reaction Mechanism of Transition Metal Complexes - I

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, A, D and I mechanisms for metal complexes, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage.

Unit 2: Reaction Mechanism of Transition Metal Complexes - II

Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reactions. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Block II Electronic Spectra

Unit 3: Metal-Ligand Bonding

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, Jahn Teller effect, pi-bonding and molecular orbital theory, spectrochemical series, low spin and high spin complexes, crystal field stabilization energy, spectrochemical series, weak and strong field complexes, thermodynamic and related aspects of crystal fields, ionic radii, heats of ligation, lattice energies, site preference energies.

Unit 4: Electronic Spectra of Transition Metal Complexes

Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Racah parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, Inter-valence, Charge-transfer spectra, R-S coupling of d^n system.

Unit 5: Magnetic Properties of Transition Metals

Origin of magnetic moment, Spin contribution, Orbital Contribution, Derivation of Van Vleck equation, Methods for magnetic susceptibility measurements, Ferromagnetism and Antiferromagnetism, mechanism of anti-ferromagnetic interaction, spin cross over and anomalous magnetic moments. Applications of magnetic measurement for structural elucidation

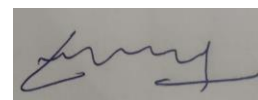
Course – 7: MSCCH-507 Organic Chemistry II (3 Cr.)



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Course outcome:

Upon completion of this course, the learners will be able to understand the basic knowledge of the aliphatic and aromatic nucleophilic substitution, aliphatic and aromatic electrophilic substitution reactions of the organic compounds. Learners also able to know about the elimination reactions, addition to carbon-carbon multiple bonds, addition to carbon-hetero atom multiple bonds, free radical reactions and pericyclic reaction in the organic chemistry.

Block I: Nucleophilic Substitution

Unit 1 Aliphatic Nucleophilic Substitution

The S_N2 , S_N1 , mixed S_N1 and S_N2 , S_Ni and SET mechanism. Neighboring group participation by sigma and pi- bonds, anchimeric assistance. Classical and non-classical carbocations, arenium ions, norbornyl systems, common carbocation rearrangements. The S_Ni mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium. HSAB principle. Ambident nucleophiles.

Unit 2 Aromatic Nucleophilic Substitution

The S_NAr , S_Ni , benzyne and S_{NRi} mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangements.

Block II: Electrophilic Substitution

Unit 3 Aliphatic Electrophilic Substitution

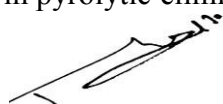
Bimolecular mechanisms, S_E2 , S_{Ei} , S_{E1} mechanism, electrophilic substitution accompanied by double bond shifts. Addition-elimination mechanism. Effect of substrates, leaving groups and the solvent polarity on the reactivity.

Unit 4 Aromatic Electrophilic Substitution

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, Gatterman – Koch reaction.

Unit 5 Elimination Reactions

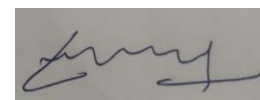
The $E2$, $E1$, $E1cB$ and $E2c$ mechanisms. Orientation of the double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination-Saytzeff, Hoffman and Cope elimination.



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Block III: Addition and free Radical Reactions

Unit 6 Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals; region- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration and related reactions, Michael addition, Sharpless asymmetric epoxidation.

Unit 7 Addition to Carbon-Hetero Atom Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid esters and nitriles. Addition of Grignard reagents, Reformatsky reaction and related reactions. Mechanism of Wittig reaction, Knoevenagel, Claisen, Mannich, Stobbe reactions. Stork enamine reaction. Concept and applications of Umpolung and sulfur ylides.

Unit 8 Free Radical Reactions

Types of free radical reactions, mechanism of free radical substitution, reactions on aromatic substrates, neighboring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead carbon. Reactivity of the attacking radicals. The effect of solvents on reactivity. Allylic halogenations (NBS). Oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Block IV Pericyclic Reactions

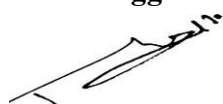
Unit 9 Electrocyclic Reactions

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 motions, $4n$, $4n+2$ and allyl system.

Unit 10 Cycloadditions and Sigmatropic Reaction

Introduction, antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, $1,3$ -dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, $3,3$ - and $5,5$ sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Fluxional tautomerism, Ene reaction.

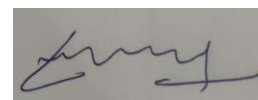
Books Suggested:



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1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, M. B. Smith and Jerry March, John Wiley 2001.
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum Publishers.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
6. Principles of Organic Synthesis, R.O.C. Norman and J. M. Coxon, Blackie Academic & Professional.
7. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
8. Organic Reaction Mechanism by Ahluwalia and R. K. Parashar, Narosa Book Distributor Pvt. Ltd.

Course –8: MSCCH-508 Physical Chemistry-I

(3Cr.)

Course outcome :

After completing this course, learners will gain basic and fundamental knowledge about the surface and polymer chemistry. Learning the Quantum Mechanics will help them to praise the beauty of behavior of fundamental particles. They will be able to Schrodinger's wave equation, general and brief discussion on the applications of Schrodinger's wave equation to some model systems and concept of Cartesian and spherical coordinates.

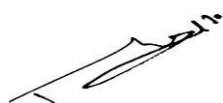
Block I Surface and Polymer Chemistry

Unit 1 Surface Chemistry

Gibb's adsorption isotherm, Freundlich and Langmuir adsorption isotherms, determination of free energy of adsorption, BET theory for multilayer adsorption with derivation, determination of surface area using BET method, catalytic activity at surfaces.

Unit 2 Polymer Chemistry

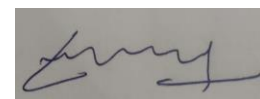
Macromolecules, polymers and their general applications, classification of polymers, chain configuration of polymers, liquid crystals and their applications. Molecular mass, number and mass average molecular mass, molecular mass determination using osmometry, viscometry, diffusion and light scattering methods.



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Block II Quantum Chemistry-I

Unit 3 Quantum Chemistry I

de-Broglie concept and de-Broglie equation, postulates of quantum mechanics, physical interpretation and properties of wave functions, Linear, Laplacian, Linear-momentum and Hamiltonian operators, eigen values, eigen functions, normalization and orthogonalization,

Unit 4 Quantum Chemistry II

Derivation of the Schrodinger's wave equation, general and brief discussion on the applications of Schrodinger's wave equation to some model systems viz. particles in a box, harmonic oscillator, rigid rotator

Unit 5 Quantum Chemistry III

Hydrogen atom. concept of cartesian and spherical coordinates.

Course – 9 : MSCCH-509 Spectroscopy I

(3Cr.)

Course outcome :

The prime aim of this course is to characterize and identify the organic molecule with the help of the spectroscopic techniques. In this course learners will be able to the fundamentals of spectroscopy and concept of the atomic spectroscopy, XPS and UPS and basic of the different type of the spectroscopy viz. rotational, vibrational, electronic spectroscopy. They will be able to in this course, fundamentals of raman spectroscopy and application of the raman spectroscopy in the physical chemistry.

Block 1: Atomic spectroscopy

Unit 1 Fundamentals of Spectroscopy

Recapitulation and role of Quantum Mechanics and its importance to the understanding of spectroscopy in chemistry. Characterization of electromagnetic radiation. Heisenberg's Uncertainty Principle and line width. Basic elements of spectroscopy. Einstein coefficients. Lambert-Beer's law. Integrated absorption coefficients. Oscillator strengths. Transition dipole moments and general selection rules based on symmetry ideas.

Unit 2: Atomic spectroscopy, XPS and UPS

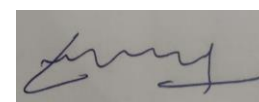
Characterization of atomic states. Microstates and spin factoring methods. Hund's rules. Derivation



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of spin and orbital selection rules (based on recursion relations of Legendre polynomials). Spectra of complex atoms. Zeeman and Stark effects. Atomic photoelectron spectroscopy.

Block 2: Molecular Spectroscopy-I

Unit 2: Rotational Spectroscopy

Recapitulate Rotational spectra of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and/or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules and applications.

Unit 3: Vibrational Spectroscopy-I : Diatomic Molecules

Basic principles of vibrational spectroscopy of homonuclear and heteronuclear diatomic molecules. Selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones and combination bands. Dissociation energies from Vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation, Nuclear spin effect.

Unit 4: Vibrational Spectroscopy-II : Polyatomic Molecules

Extension to polyatomic molecules, fingerprint region, Group frequencies, Interpretation IR spectra: IR region, molecular vibrations, the molecule spring analogy, Hooke's law. Bond stretching frequencies effect of increasing atomic weight and bond energy, IR active and inactive frequencies, obtaining IR spectra, FTIR, Region of IR spectra, Compound comparison, and a general survey of different regions for detection of different functional groups. Factors influencing vibrational frequencies: Symmetry Conjugation lowering C=O and C=C frequencies, electronic effects (inductive and mesomeric effects) Hydrogen bonding, Ring strain, Fermi resonance and coupled vibrations Interpretation of spectra of some classes of compounds.

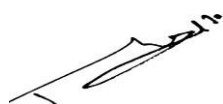
Unit 5: Raman spectroscopy

Mechanism of Raman excitations, Stokes and anti-Stokes lines, Polarizability ellipsoids, Rotational and Vibrational Raman spectroscopy, Selection rules, Polarization of Raman lines, Rule of mutual exclusion.

Block 3: Molecular Spectroscopy-II

Unit 6: Electronic Spectroscopy-I

Diatomic molecules, Selection rules, Breakdown of selection rules. Franck-Condon principle.



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(Dr. Vinod Kumar)

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Deep
(Dr. Deep Prakash)

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Coarse and Fine structure in electronic spectra of diatomic molecules. Dissociation energies. Transitions in simple polyatomic molecules, Photoelectron spectroscopy of diatomic (N_2) and simple polyatomic molecules (H_2O , formaldehyde). Adiabatic and vertical ionization energies, Use of Free Electron Model. Qualitative aspects of solvent effects- viscosity, polarity, hydrogenbonding.

Unit 7: Electronic Spectroscopy-II: applications of UV-VIS Spectrometry

Absorption of UV- vis; electromagnetic radiation, electronic transitions and energy level; Isolated chromophores ($C=C$ and $C=O$), Beer-Lambert law; Effect of conjugation on UV Spectra; Terminology of UV Spectroscopy; Selection rules (allowed and for forbidden transitions) Solvent and their effect on different transitions. Measurement of UV spectra General application of spectroscopy (extent of conjugation, comparison of different compounds with the same chromophore, study of strain, study of geometrical isomerism and steric effects, study of tautomerism, effect of S-cis and S-trans conformations, effect of alkyl substitution and exocyclic double bond, Woodward Fieser rules for conjugated dienes and enones, identification of aromatic systems, Trans annular conjugation. Influence of constituents ring size and strain on UV Spectra.

Book Suggested:

1. Practical NMR Spectroscopy, M. L. Martin. J. J. Deepish and G. J. Martin, Heyden.
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley.
3. Introduction to NMR spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
4. Application of Spectroscopy of Organic Compounds, J. R. Dyer Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry D. H. Williams, I. Fleming, Tata McGraw-Hill.
6. W. Kemp, Organic Spectroscopy, 3rd edition, Wiley, 1995.
7. Introduction to Spectroscopy: Donald L. Pavia, Thompson, 2009.
8. Modern NMR techniques for Chemistry Research, A. E. Derome, Pergamon.
9. Physical Methods in Chemistry, R. S. Drago, Saunders College.
10. Chemical Applications of Group Theory, F. A. Cotton.

Course – 10: MSCCH-510 L Lab Organic/Physical Chemistry Lab Course (3Cr.)

Course outcome:

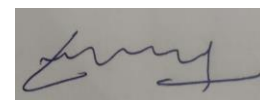
Upon completion of this course, the learners will have the knowledge and skills to determination of



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the velocity constant of acid catalyzed hydrolysis of an ester and activation energy of a reaction. After completing this course, the learners will be able to study of the adsorption of an acid by charcoal and validity of Freundlich's adsorption isotherm. Test the use of organic reagent and may involve purification of the products by cinematographic techniques. They will be able to the enzyme reduction and separation and identification of the sugars present in the given mixture by the paper and thin layer chromatography techniques.

Block I: Physical Chemistry

Unit 1 Kinetic Studies

Determination of the velocity constant of acid catalyzed hydrolysis of an ester. Determination of activation energy of a reaction.

Determination of Frequency factor of a reaction by kinetic studies. Validity of Arrhenius equation.

Determination of the effect of change in temperature on rate constant of a reaction.

Determination of the effect of change in concentration of the reactants on rate constant of a reaction.

Determination of the effect of change in concentration of the catalyst on rate constant of a reaction.

Determination of the effect of change in ionic strength on the rate constant of a reaction.

Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide.

Unit 2 Surface Chemistry

Flowing Clock reactions (Ref. Experiments in Physical Chemistry by Showmaker). Study of the adsorption of an acid by charcoal.

Validity of Freundlich's Adsorption isotherm. Determination of Partition Coefficients.

Determination of molecular surface energy of a liquid by Stalagmometer method. Determination of association factor of the given liquid by drop-pipette method.

Note: The candidates shall have to do a minimum of 05 experiments.

Block II Organic Chemistry

Unit 3 Multi-step Synthesis of Organic Compounds

The exercises should illustrate the use of organic reagent and may involve purification of the products by chromatographic techniques.

Photochemical reaction:



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Shahin

Deep
(Dr. Deep Prakash)

Benzophenone Benzopinacol Benzpinacolone Beckmann rearrangement: Benzanilide from benzene.

Benzene Benzophenone Benzophenoneoxime Benzanilide. Benzilic acid rearrangement: Benzilic acid from benzoin Benzoin Benzil Benzilic acid

Synthesis of heterocyclic compounds

Skraup synthesis: Preparation of quinoline from aniline.

Fischer indol synthesis: Preparation of 2-phenyl indole from phenylhydrazine. Enzymatic Synthesis

Unit 4 Enzymatic reduction:

Reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S(+)-ethyl-3-hydroxybutanoate and determine its optical purity.

Biosynthesis of ethanol from sucrose Synthesis using microwaves

Alkylation of diethyl malonate with benzyl chloride.

Synthesis using phase transfer catalyst

Alkylation of diethyl malonate or ethylacetoacetate with an alkyl halide.

Unit 5 Paper Chromatography/Thin Layer Chromatography

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose etc. By Paper chromatography, thin layer chromatography and determination of R_f values.

Note: Organic exercise	:	60
Physical exercise	:	60
Record(including test)	:	30
Attendance	:	30
Viva	:	20

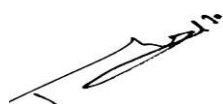
SEMESTER-III

Course – 11: MSCCH-601 Solid State and Materials Chemistry

(3 Cr.)

Course outcome :

The course will also strengthen the knowledge of learners regarding complete picture of states of



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matter that includes recapitulation of fundamental principles of solid states, solid state reactions, crystal defects and non-stoichiometry, Organic solids, fullerenes, and molecular devices. They will be able to the different diffraction techniques to identify the molecular structure viz. ray diffraction-Laue and Bragg method, Debye-Scherrer method of X-ray structure analysis of crystals index reflections and end of the this course know about the liquid crystal and surface active agents.

Block I Solid-State

Unit 1 Recapitulation of fundamental principles of solid states

Characteristics of solids: Crystal Symmetry: Unit cell, crew axis, glide plane on unit cell, crystal lattice, space lattice, stereographic projectors. Examples of crystallographic planes, cubic planes, Miller indices, Bravais lattices.

Unit 2 Solid State Reactions, Crystal Defects and Non-stoichiometry

General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions, Perfect and imperfect crystals, intrinsic and extrinsic defects- point defects, line and plane defects, vacancies- Schottky defects and Frenkel defects.

Unit 3 Organic solids, fullerenes, molecular devices

Electrically conducting solids, organic charge transfer complexes, organic metals, new superconductors, magnetism in organic materials, fullerenes- doped fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches, sensors.

Unit 4 Diffraction techniques

X-ray diffraction-Laue and Bragg method, Debye-Scherrer method of X-ray structure analysis of crystals index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density.

Block II Soft Materials

Unit 5 Liquid Crystals

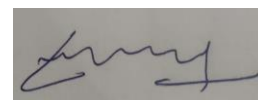
Mesomorphic behavior, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases, smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular rearrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric



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susceptibility and dielectric constants, Lyotropic phases and their description of ordering in liquid crystals

Unit 6 Surface Active Agents

Classification of surface active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Kraft temperature, Factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization, solubilization, micro emulsions, reverse micelles, surface films (electrokinetic phenomena), catalytic activity at surfaces. Electrode/electrolyte interface; electrical double layer, electrode kinetics.

Course – 12: MSCCH-602 Spectroscopy II (3Cr.)

Course outcome:

Learners will gain an understanding of how to determine the structure of organic molecules using ^1H NMR and C^{13} NMR spectroscopic techniques. Learners will be able to the two dimensional NMR spectroscopy – principles; DEPT, APT, COSY, HSQC, HMBC, NOESY,INADEQUATE techniques for structure of small molecules. After completion of this course, the learners will be able to understand the other spectroscopic technique which used to identification of the organic molecules such as spin resonance spectroscopy, mossbauer spectroscopy and mass spectrometry.

Block I Spin Resonance Spectroscopy-I

Unit 1: ^1H NMR Spectroscopy-I

Introduction to NMR; isotope ratios, nuclear spin; chemical shifts, coupling constants and integration; Fourier transform technique. Chemical shifts, coupling constants and correlation with structure and stereochemistry. Long range coupling; magnetic and chemical shift equivalence; first and second order spectra; dynamic process; simplification of spectra by shift reagents and decoupling experiments; stereochemistry by NOE measurements.

Unit 2: ^1H NMR Spectroscopy-II

Nuclear Spin states and Larmor precession, spin-spin and spin-lattice relaxations Selection rules and relative intensities of lines Treatment of Chemical Shift and spin-spin coupling in AX, AMX and AB proton NMR, Multinuclei NMR with special reference to C-13 and relative abundances and intensities, Spin-decoupling methods, Origin of NMR chemical shift, and spin-spin coupling. Factors Affection Chemical Shifts, Chemical exchange, Pulsed FT-NMR- Time and Frequency



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Domain Spectra.

Unit 3: Carbon -13 NMR Spectroscopy:

General considerations, chemical shift (aliphatic, olefinic, alkyne and aromatic hetero aromatic and carbonyl carbon). Coupling constants.

Unit 4: 2D NMR Spectroscopy

Two dimensional NMR spectroscopy – principles; DEPT, APT, COSY, HSQC, HMBC, NOESY, INADEQUATE techniques for structure of small molecules.

Block II Spin Resonance Spectroscopy-II

Unit 5 Basic Principles of ESR spectroscopy

Electron Spin and its Characteristics, Treatment of ESR of hydrogen atom with spin levels, g-value and hyperfine interaction in hydrogen atom and free radicals, Mechanism of proton splitting in organic molecules; McConnell Equation. Basic introduction to anisotropic g- and A- tensors from transition ions, Energy levels in many electron spin systems and zero-field splitting.

Unit 6 Basic Principles of Mossbauer spectroscopy

Mossbauer effect and Mossbauer Spectroscopy and Mossbauer energy levels with isomer shift, Quadrupole splitting and hyperfine interaction with special reference to Fe57, and Sn119.

Block III Mass Spectrometry

Unit 7 Mass Spectrometry-I

Introduction, ion production-EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule, example of Mass fragmentation of organic compounds with respect to their structure determination. Problems based on spectroscopic techniques.

Unit 8: Mass Spectrometry-II

Mass spectral fragmentation of organic compounds with common functional groups; molecular ion peak; metastable peaks, McLafferty rearrangement; nitrogen rule. High resolution mass spectrometry – ESIMS and MALDI-TOF. Examples of mass spectral fragmentation of organic compounds.

Books Suggested:

1. Practical NMR Spectroscopy, M. L. Martin. J. J. Deepish and G. J. Martin, Heyden.



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2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and U. C. Morrill, John Wiley.
3. Introduction to NMR spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
4. Application of Spectroscopy of Organic Compounds, J. R. Dyer Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry D. H. Williams, I. Fleming, Tata McGraw-Hill.
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8. Modern NMR techniques for Chemistry Research, A. E. Derome, Pergamon.
9. Physical Methods in Chemistry, R. S. Drago, Saunders College.
10. Chemical Applications of Group Theory, F. A. Cotton.

Course-13: MSCCH-603 Bio-Inorganic, Bio-Organic and Bio-Physical Chemistry (3 Cr.)

Course outcome:

After completion of this course, the learners will be able to understand the chemistry of bio-inorganic molecules and how bio-inorganic pigment is helpful for the metal storage and transportation in the human body and role of the metalloenzymes and metal-nucleic acid interactions. In this course learners will be able to the basic introduction of the bio-organic chemistry, about enzyme & mechanism of enzyme action, kinds of reactions catalyzed by enzymes, basic knowledge of co-enzyme chemistry and the biotechnological applications of enzymes. And end of the this course learners able to biopolymer interactions, thermodynamics of biopolymer solutions.

Block I Bioinorganic Chemistry

Unit 1: Metal Storage and Transport

Ferritin, transferrin, and siderophores, Hemoglobin and myoglobin – Perutz mechanism models of oxygen carriers, photosynthesis PSI and PSII systems, nitrogen fixation.

Unit 2: Metalloenzymes

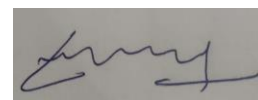
Zinc enzymes - carboxypeptidase and carbonic anhydrase, Iron enzymes - catalase, peroxidase and cytochrome P-450, copper enzymes - superoxide dismutase, Molybdenum oxotransferase



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enzymes-xanthine oxidase, Coenzyme vitamin B₁₂.

Unit 3: Metal-Nucleic Acid Interactions

Metal complex – nucleic acid interaction modes of binding to DNA, DNA cleavage, Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

Block II: Bioorganic Chemistry

Unit 4 Introduction

Basic considerations, chemical background of biomolecules (protein, lipids, carbohydrates and nucleic acids). Proximity effects and molecular adaptation.

Unit 5 Enzyme & Mechanism of Enzyme action

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed, mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition. Transition state theory, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Unit 6 Kinds of Reactions catalysed by Enzymes

Nucleophilic displacement on phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, β -cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalysed carboxylation and decarboxylation.

Unit 7 Co-Enzyme Chemistry:

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, lipoic acid, vitamin B₁₂. Mechanisms of reactions catalysed by the above cofactors.

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Unit 8 Biotechnological Applications of Enzymes:

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Block III Biophysical Chemistry

Unit 9 Bioenergetics:

Standard free energy change in Biological Reaction. Hydrolysis of ATP, Synthesis of ATP from ADP.

Unit 10 Biopolymer Interactions ,Thermodynamics of Biopolymer Solutions:

Forces involved in biopolymer interactions. Electrostatic charge and molecular expansion, hydrophobic forces, osmotic pressure, membrane equilibrium. Biopolymers and their Molecular Mass Size, shape and molecular mass of biopolymers, determination of molecular mass of biopolymers by various experimental techniques.

Course – 14: MSCCH-604 Photo Chemistry and Allied Chemistry (Cr. 3)

Course outcome:

The course is intended to impart basic knowledge about the photochemistry and photo-physical reactions. After completion of this course, the learners will be able to understand the photochemistry of the unsaturated, carbonyl and aromatic compounds. They will become acquainted in the field of data analysis. The new frontiers green chemistry are the part of syllabi of this course which boost the knowledge of the learners in these fields.

Unit 1 Basics of photochemistry:

Absorption, excitation, photochemical laws, electronically excited states-life times, measurements of the times. Flash photolysis, Stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, Photochemical stages- primary and secondary processes.

Unit 2 Photo-physical reactions:

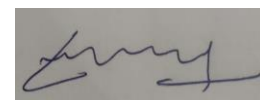
Jablonskii diagram, photosensitization, 4. Quantum yield and its determination, reactions of high and low quantum yields with suitable examples, fluorescence, phosphorescence and



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chemiluminescence with suitable examples.

Unit 3 Photochemistry of organic compounds

Photochemistry of alkenes; cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3- and 1,4-dienes; dimerisation.

Unit 4 Photochemistry of carbonyl compounds:

Norrish type I & II reactions (cyclic and acyclic); α,β unsaturated ketones; β,γ -unsaturated ketones; cyclohexenones (conjugated); cyclohexadienones (cross-conjugated & conjugated); Paterno-Buchi reactions; photoreductions.

Unit 5 Photochemistry of aromatic compounds:

Isomerisation, skeletal isomerisations, Dewar and prismanes in isomerisations. Singlet oxygens reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffmann-Loeffler-Freytag reaction.

Unit 6 Green Chemistry:

Basic principles of Green chemistry. Designing a green reagents: green catalyst phase transfer catalysis for green synthesis, choice of starting materials, Organic synthesis in solid phase reagents, and Versatile ionic liquids as Scherrer method.

Course – 15: Lab Course III MSCCH-605L (Inorganic/Physical Chemistry Lab Course) (6 Cr.)

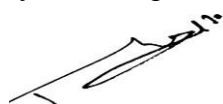
Course outcome:

Upon completion of this course, the learners will have the knowledge and skills to determine order of reaction by isolation method, order of reaction by half life period method, order of the reaction by Integration method and determination entropy of activation of a reaction. They will be able to determination of pH by electrical conductivity method and estimate different metal ions through gravimetric exercise. Chromatographic exercise will train them to interpret the chromatograms of organic compounds and will make them job ready for suitable industries.

Block I Physical Chemistry Practicals

Unit 1 Thermodynamics

Determination of the order of reaction by isolation method
Determination of the order of reaction by half life period method



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Determination of the order of the reaction by Integration method. Determination of the entropy of activation of a reaction.

Determination of free energy change of a reaction. Determination of the equilibrium constant of a reaction.

Unit 2 Electrochemistry

Determination of pH by electrical conductivity method. Hydrolysis of the salts by electrical conductivity method. Hydrolysis of the salts by EMF.

Determination of the dissociation constant of a weak acid by conductivity method. Determination of the equivalent conductivity of a strong electrolyte conductrometrically. Determination of the equivalent conductivity at infinite dilution of weak electrolyte Conductrometrically.

Validity of Ostwald's dilution law.

Determination of the degree of dissociation/ association conductrometrically.

Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO_4 , BaSO_4) conductrometrically.

Note: The candidates shall have to do a minimum of 05 experiments

Block II Inorganic Chemistry

Unit 3 Quantitative analysis

Quantitative analysis of binary mixture of metal ions involving volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis.

Unit 4 Chromatography

Separation of cations and anions by paper/TLC/Ion Exchange chromatography

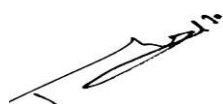
Note: Inorganic exercise 30; Physical 30; Record (including test) 15; attendance 10; viva 15

SEMESTER -IV

Course-16 : (MSCCH -606) Organic Synthesis

(Cr. 3)

Course outcome:



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Upon successful completion of this course, the students will be able to gain basic idea of the organometallic reagents and their application in field of the organic synthesis. They will also able to understand the oxidation and reduction in the organic molecules with different type oxidizing and reducing reagent. They take salient features of protecting group of the alcohol, carbonyl and carboxyl functional groups and the ring opening reaction of 3,4 and 5 member cyclic organic compounds.

Unit 1 Organometallic Reagents

Principle, preparations, properties and applications of the following in organic synthesis: Group I and II metal organic compounds Li, Hg and Zn compounds. Transition metals, Pd, Ni, Fe, Ti, Cu, Rh and Cr compounds; Other elements, S, Si and B compounds. Metallocenes, Nonbenzenoid Aromatics and Polycyclic Aromatic Compounds General considerations, synthesis and reactions of some representative compounds.

Unit 2 Oxidation:

Introduction. Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated & unactivated). Alcohol, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines and sulphides. Oxidation with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate.

Unit 3 Reduction:

Introduction, Different reductive processes. Hydrocarbons-alkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Epoxides, Nitro, nitroso, azo and oxime groups. Hydrogenolysis.

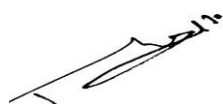
Unit 4 Disconnection Approach

An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions and amine synthesis. One group and two group C-C disconnections. Alcohol and carbonyl compounds, regioselectivity, alkene synthesis and aliphatic nitro compounds in organic synthesis.

Unit 5 Protecting group.

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

Unit 6 Ring Synthesis:



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Saturated heterocyclic, synthesis of 3-,4-,5- and 6-membered rings, aromatic heterocyclic in organic synthesis.

Course-17: (MSCCH-607) Chemistry of Natural Products & Heterocyclic Compounds

(Cr.3)

course outcome:

After completing this course, the learners will be able to basic idea of the terpenoids and carotenoids and biosynthesis of the menthol, santonin and β -carotene. Apart from this, basic knowledge about the Structure, stereochemistry, synthesis and biosynthesis of Morphine and Reserpine. After completing this course, learners will gain basic and fundamental knowledge about the steroids, different type of plant pigments. They will be able to the about the 3, 4, 5 and 6 member hetero-cyclic compound and their applications in the chemistry.

Block I Chemistry of Natural Products

Unit 1 Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representativemolecules: Menthol, Santonin and β -Carotene.

Unit 2 Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, classification, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of Morphine and Reserpine.

Unit 3 Steroids

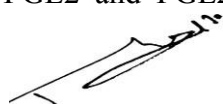
Occurrence, nomenclature, basic skeleton, Diel's Hydrocarbon and stereochemistry. Isolation, structure determination synthesis and biosynthesis of Cholesterol, Testosterone and Estrone.

Unit 4 Plant Pigments / Porphyrins

Occurrence, extraction, classification, chemical characterization and functions of anthocyanins, flavonoids, xanthophylls and porphyrins. Chemistry and structure of cyanins, flavones, flavonol, quercetin. Biosynthesis of flavonoids: Acetate and Shikimic acid pathway. Structure and synthesis of porphyrin skeleton, haemin and chlorophyll.

Unit 5 Prostaglandins/ Pyrethroids and Rotenones

Occurrence, nomenclature, classification, biogenesis, and physiological effects. Synthesis of PGE2 and PGE2 α . Synthesis and reactions of Pyrethroids and Rotenones. Note: In structure



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elucidation, emphasis is to be laid on the use of spectral parameters, wherever possible.

Block II Heterocyclic Chemistry

Unit 6 Nomenclature of Heterocycles / Aromatic and Non-aromatic Heterocycles

Systematic nomenclature (Hantzsch-Widman System) for monocyclic, fused, and bridged heterocycles. Tautomerism in aromatic heterocycles. Strain-bond angle, torsional strains, and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction.

Unit 7 Heterocyclic Synthesis

Three membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes. Benzo-Fused Five-membered Heterocycles Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.

Unit 8 Small Ring Heterocycles

Heterocyclic Systems Containing Phosphorus Heterocyclic rings containing phosphorus: Introduction, nomenclature, synthesis and characteristics of 5- and 6-membered ring systems phosphoranes, phospholanes and phospholes.

Course -18 :MSCCH-608 Medicinal Chemistry

(Cr.3)

Course outcome:

This course intends to acquaint the learners about development of drugs, procedures of drug design and concepts of prodrugs and soft drug, It would add to their knowledge regarding the basic concept of drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition. Also they will know the Antineoplastic Agents and Cardiovascular Drugs.

Unit 1 Drug Design

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drug, structure-activity relationship (SAR), factors affecting bioactivity. Theories of drug activity: general discussion. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: Lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and

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redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded).

Unit 2. Pharmacokinetics & Pharmacodynamics

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process. Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

Unit 3. Antineoplastic Agents

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotic and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melaphalan, uracil, mustards and 6- mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

Unit 4. Cardiovascular Drugs

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, verapamil, atenolol. Course 17 MSCCH -609 Laboratory Course IV Block I Qualitative Analysis

Course -19: MSCCH -609L Laboratory Course IV

(3 Cr.)

Course outcome:

Upon completion of this course, the learners will have the knowledge and skills to understand the separation, purification and identification of the components of a mixture of three organic compounds by the TLC, IR, PMR and mass spectral data. Also, they can easily learn extract the organic compounds from natural sources. It would add to their knowledge regarding the basic concept of isolation of caffeine from tea leaves, isolation of casein from milk and isolation of limonene from citrus fruits.

Block I Physical Chemistry Practicals

Unit 1 Thermodynamics

Determination of the order of reaction by isolation method

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Determination of the order of reaction by half life period method

Determination of the order of the reaction by Integration method.

Determination of the entropy of activation of a reaction.

Determination of free energy change of a reaction.

Determination of the equilibrium constant of a reaction.

Unit 2 Electrochemistry

Determination of pH by electrical conductivity method.

Hydrolysis of the salts by electrical conductivity method

Hydrolysis of the salts by EMF.

Determination of the dissociation constant of a weak acid by conductivity method.

Determination of the equivalent conductivity of a strong electrolyte conductrometrically.

Determination of the equivalent conductivity at infinite dilution of weak electrolyte

Conductrometrically.

Validity of Ostwald's dilution law.

Determination of the degree of dissociation/ association conductrometrically.

Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO_4 , BaSO_4) conductrometrically.

Note: The candidates shall have to do a minimum of 05 experiments

Block II Inorganic Chemistry

Unit 3 Quantitative analysis

Quantitative analysis of binary mixture of metal ions involving volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis.

Unit 4 Chromatography

Separation of cations and anions by paper/TLC/Ion Exchange chromatography

Note: Inorganic exercise : 30

Physical exercise : 30

Record (including test) : 15

Attendance : 15

Viva : 10

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vi. Procedure for Admission curriculum transaction and evolution:

The admission process in the programme of M.Sc. (Chemistry) is available on-line (Twice in a year). The learners may apply in the course run by the University by getting themselves enrolled in the various study centers run by the university. The criteria to be met by the learner intending to take admission in M.Sc. Chemistry courses run by the University are as follows:

For M.Sc. (Chemistry): B.Sc. with chemistry as one of the major/one of the subject at UG level .

Examination is conducted in the various examination centers decided by the University. Further, the examination copy is to be evaluated by various evaluators of the concern subject approved by Hon'ble Vice-Chancellor.

A learner will be evaluated through continuous evaluation (Assignments) and term end evaluation (Term end examination) at the end of semester. Continuous evaluation will carry 30% weightage whereas term end evaluation will carry 70% weightage.

vii. Requirement of laboratory support and Library Resource:

In order to carry out laboratory exercises, laboratory is compulsory requirement of the programme and in order to meet this requirement, the laboratory facilities of study centres will be utilized. She/he will be provided laboratory manual as per the need of the programme. Similarly for library, a learner may utilize the resources available at the designated study centre. The Department of Chemistry teachers always give the guidance to books selection in the library. Eight regional centres and study centres also give the library facility to learners. A comprehensive soft copy of the study material is provided to the learners through the online library in the University website and the learners can also avail the facility of the books available in the University Library and different e-books are provided by central library of the Uttarakhand open university.

viii. Cost Estimate for development of the Programme :

The approximate cost of development of study material

19 courses = 124 units

Cost of development of 1 unit = Rs 6000/-

Cost of development of 124 units = Rs 744,000/-

Total expenditure for Editing (approximately) =372,000/-

Number of learners getting admission each year = nearly 300 (approximated)

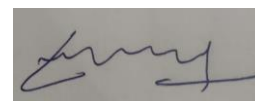
Annual Fee deposited by each M.Sc. learner = 19300/-




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Total fee deposited by all learners (300) = Rs. 5790,000/-

ix. Quality assurance mechanism and expected programme outcomes:

The M.Sc. (Chemistry) Programme is of 72 credits. The expert and department teaching staff updated the Self Learning Material (SLM) from time to time. The Self Learning Material (SLM) prepared in such a manner in which the learner feels as if the learner is being taught by a teacher in the class room. We focused in our programme in following strategies :

- Be simple
- Be flexible
- Be authentic
- Be familiar with new digital technique
- Be organized
- Be concise

The programme will help in the development of professionally skilled, in general, and in corporate sector, in particular. The programme will be implemented through only those Government Degree Colleges/ Universities / Institutions which have facilities for conducting laboratory counseling. In addition to this University will organize Laboratory workshop in designated places once (year/semester) for additional back up to the students so that competent and skilled human resource is produced.

x. Programme outcomes:

Learners residing in far flung rural hilly areas will be benefited. Marginalized and economically backward communities will get opportunity to learn Chemical science education. In-service learners will have opportunity to pursue their higher education in science disciplines.

- Further, working professionals in Govt. Organizations and Community based Organizations or other Institutions may also comprise of the target group of learners.
- The master degree (M.Sc. Chemistry) will provide learners with the advanced knowledge and skills required to further their careers and conduct meaningful scientific research.
- Candidates can look for employment in the field of Chemistry.
- They can also join the education sector (as a teacher or professor), government sector, R&D, ONGC sector and chemical industry.




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C. Dr. Deep Prakash

