DEPARTMENT OF CHEMISTRY& PHARMACEUTICAL SCIENCES
MAHATMA GANDHI UNIVERSITY, NALGONDA

M.Sc. Chemistry I &II Semester (CBCS) Syllabus

Blow up 2017-18

Semester-I

Paper-I: CH 101T (INORGANIC CHEMISTRY)

IC 01: Symmetry of molecules
IC 02: Bonding in Metal Complexes - I
IC 03: Coordination equilibria
IC 04: Ligational aspects of diatomic molecules

INORGANIC CHEMISTRY		
Lecture No.	**IC-01: UNIT – 1 Symmetry of Molecules (17 Hrs.)**	**Remarks**
Lecture No. 1	Concept of Symmetry in Chemistry - Symmetry Operations	
Lecture No. 2	Symmetry Elements : Rotational Axis of Symmetry and Types of Rotational Axes	
Lecture No. 3	Plane of Symmetry and Types of Planes	
Lecture No. 4	Improper Rotational Axis of symmetry	
Lecture No. 5	Inversion Center & Identity Element	
Lecture No. 6	More about Symmetry Elements	
Lecture No. 7	Molecular Point Groups: Definition and Notation of Point Groups	
Lecture No. 8	Classification Molecules in to C_1 group	
Lecture No. 9	Classification of Molecules in to C_s , C_i groups	
Lecture No. 10	Classification of Molecules in to C_n ,C_{nv} groups	
Lecture No. 11	Classification of Molecules in to C_{nh} , $C_{\infty v}$ groups	
Lecture No. 12	Classification of Molecules in to D_n & D_{nh} groups & D_{nd} & $D_{\infty h}$ groups	
Lecture No. 13	Classification of Molecules in to S_n (n=even) T, T_h & T_d groups	
Lecture No. 14	Classification of Molecules into O & O_h groups I, I_h & K_h groups	
Lecture No. 15	Descent in Symmetry with Substitution & Exercises in Molecular Point Groups	
Lecture No. 16	Symmetry and Dipole moment	
Lecture No. 17	Symmetry criteria for Optical activity	

IC-02: UNIT-II : Bonding in metal complexes – I (16 Hrs.)

Lecture No.	Topic	Remarks
Lecture No. 1	Crystal Field Theory - Salient features of CFT	
Lecture No. 2	d-orbital splitting patterns in regular Octahedral	
Lecture No. 3	d-orbital splitting patterns in Tetragonally distorted octahedral	
Lecture No. 4	Jahn-Tellar theorem-, Tetrahedral & Square planar	
Lecture No. 5	Jahn-Tellar theorem-, trigonal planar, and linear geometries.	
Lecture No. 6	Factors influencing the magnitude of crystal field splitting in octahedral complexes	
Lecture No. 7	Factors influencing the magnitude of crystal field splitting in octahedral complexes	
Lecture No. 8	Concept of weak field and strong fields	
Lecture No. 9	Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate complexes.	
Lecture No. 10	Calculation of crystal field stabilization energies (CFSE's) in four coordinate complexes.	
Lecture No. 11	Types of magnetic behaviour	
Lecture No. 12	magnetic susceptibility – calculation of magnetic moment from magnetic susceptibility spin only formula	
Lecture No. 13	Quenching of orbital angular momentum	
Lecture No. 14	Determination of magnetic moment from Guoy's method	
Lecture No. 15	Applications of magnetic moment data for the determination of oxidation states & bond type	
Lecture No. 16	Applications of magnetic moment data for the determination of stereochemistry	

IC-03: UNIT-III - Coordination Equilibria (15 Hrs.)

Lecture No.	Topic	Remarks
Lecture No. 1	Solvation of metal ions- Binary complexes	
Lecture No. 2	Formation of binary Metal Complexes and their stability	
Lecture No. 3	Types of Stability Constants – relation between them- trends in Step-wise Stability Constants	
Lecture No. 4	Factors influencing the stability constants : (i) Ligand effects: Basicity , Substituent, Steric, Chelate(size and number of chelate rings)	
Lecture No. 5	Factors influencing the stability constants : Steric, Chelate(size and number of chelate rings)	
Lecture No. 6	Macrocyclic and Cryptate effects	
Lecture No. 7	(ii) Metal ion effects: Ionic potential ,Effective Nuclear charge and Atomic Number (Irving-William's Order, geometry of Metal ion and Ligand)	
Lecture No. 8	Chelate effect and its Thermodynamic origin	
Lecture No. 9	Jahn-Tellar effect on Stability constants of Metal complexes	
Lecture No. 10	Pearson's Theory of Hard and Soft Acids and Bases (HSAB)	
Lecture No. 11	Applications of HSAB, Electronegetivity Vs Hardness and Softness.	
Lecture No. 12	Symbiosis – Methods used for the determination of Stability constants (Basic Principles only): pH metric	
Lecture No. 13	Methods of determination of stability constants : Spectrophotometric and Polarographic methods.	
Lecture No. 14	Ternary Metal Complexes – definition – Formation of ternary metal complexes – Stepwise and simultaneous equilibria with simple examples.	
Lecture No. 15	Ternary Metal Complexes Stepwise and simultaneous equilibria with simple examples.	

IC-04: UNIT-IV : Ligational Aspects of Diatomic molecules (15 Hrs.)

Lecture No.	Topic	Remarks
Lecture No. 1	**Metal Carbonyls**:- Carbon monoxide as a ligand	
Lecture No. 2	Molecular orbitals of CO - Donor and Acceptor molecular orbitals of CO	
Lecture No. 3	Bonding modes of CO- Terminal and Bridging	
Lecture No. 4	Evidence for multiple bonding from Bond lengths and Stretching frequencies	
Lecture No. 5	18 Valence electron rule and its application	
Lecture No. 6	**Metal Nitrosyls**: - NO as a ligand – Molecular orbitals of NO – Donor and Acceptor components	
Lecture No. 7	Bonding modes of NO – Terminal (Linear, Bent) and Bridging	
Lecture No. 8	Structural aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$	
Lecture No. 9	Structural aspects of $[RuCl(PPh_3)_2(NO)_2]^+$.	
Lecture No. 10	Stereo chemical control of valence in $[Co(diars)_2(NO)]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$.	
Lecture No. 11	**Metal Dinitrogen complexes:** - N_2 as aligand – Molecular orbitals of N_2	
Lecture No. 12	Bonding modes – Terminal and Bridging; Stretching frequencies	
Lecture No. 13	Structures of Ru (II) and Mo (0)	
Lecture No. 14	Dinitrogen complexes	
Lecture No. 15	Chemical fixation of dinitrogen	

References:

1. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London (2000).
2. Molecular Symmetry and Group Theory, Robert L.Carter, John Wiley & Son (1998).
3. Symmetry and Spectroscopy of Molecules. K.Veera Reddy, New Age International (P) Limited (1999).
4. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6 th Edition, Wiley Interscience, N.Y (1999
5. Inorganic Chemistry, J.E.Huheey , K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
6. Homogeneous Catalysis by Metal complexes Vol I, M M Taqui Khan and A E Martell, Academic Press NY (1974).
7. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).

Paper-II: CH 102 T(ORGANIC CHEMISTRY)
OC-01: Stereochemistry
OC-02: Reaction mechanism-I
OC-03: Carbohydrates and Proteins
OC-04: Heterocyclic compounds

OC-01: Stereochemistry

Sl.No.	Name Of the topic	Remarks
Lecture-1	**Molecular representations:** Wedge, Fischer, Newman and Saw-horse formulae, description and inter conversions.	
Lecture-2	**Molecular Symmetry & Chirality:** Symmetry operations and symmetry elements (Cn &Sn). Criteria for Chirality. Desymmetrization.	
Lecture-3	Symmetry operations	
Lecture-4	symmetry elements (Cn &Sn)	
Lecture-5	**Axial, planar and helical chirality**: Configurational nomenclature:Axially chiral, allenes,spiranes,alkylidene	
Lecture-6	cycloalkanes, chiral biaryls, atropisomerism. Planar chiral ansa compounds	
Lecture-7	Chirality of Trans-Cycloocatene, Helically chiral compounds	
Lecture-8	**Relative and absolute configuration**: Determination of absolute configuration by chemical correlation methods.	
Lecture-9	**Relative and absolute configuration**: Determination of absolute configuration by chemical correlation methods.	
Lecture-10	**Racemisation, racemates and resolution techniques**: Resolutions by direct crystallization	
Lecture-11	**Racemisation, racemates and resolution techniques**: Resolutions by direct crystallization	
Lecture-12	diastereoisomer salt formation chiral chromatography and asymmetric transformation.	
Lecture-13	**Determination of configuration in E,Z-isomers:** Spectral and Chemical methods of configuration determination of E,Z isomers.	
Lecture-14	Determination of **E, Z-** Examples.	
Lecture-15	Determination of configuration in aldoximes and ketoximes	

OC-02: Reaction mechanism-I

Lecture.No.	Name Of the topic	Remarks
Lecture-1	**Electrophilic addition to carbon carbon double bond**	
Lecture-2	Stereoselective addition to carbon carbon double bond	
Lecture-3	Anti addition of Bromin to bromime to double bond	
Lecture-4	*anti* addition- Bromination and epoxidation followed by ring opening. *Syn* addition of OsO_4 and $KMnO_4$.	
Lecture-5	Addition of KMnO4 to Alkenes examples	
Lecture-6	**Elimination reactions** Elimination reactions E2, E1, E1CB mechanisms. Orientation	
Lecture-7	Elimination reactions E1	
Lecture-8	Elimination reactions E1CB	
Lecture-9	stereoselectivity in E2 eliminations. Pyrolytic *syn* elimination and α-elimination,	
Lecture-10	Elimination Vs substitution.	
Lecture-11	**Determination of reaction mechanism:** Determination of reaction mechanism: Energy profiles	
Lecture-12	**Determination of reaction mechanism:** Determination of reaction mechanism: Energy profiles	
Lecture-13	Energy profiles of addition and elimination reactions, transition states, product isolation and Use of IR	
Lecture-14	Structure of intermediates, use of isotopes, chemical trapping, crossover experiments.	
Lecture-15	NMR in the investigation of reaction mechanism	

OC-03: Carbohydrates and Proteins

Lecture.No.	Topic	Remarks
Lecture-1	Determination of the relative and absolute configuration in D (+) glucose	
Lecture-2	Determination of the relative and absolute configuration in D (-) fructose	
Lecture-3	Proof for the chair conformation of D (+) glucose.	
Lecture-4	Occurrence of monosaccharides containing functional groups such as amino, halo and sulphur.	
Lecture-5	Importance of monosaccharides containing functional groups such as amino, halo and sulphur.	
Lecture-6	Synthesis of monosaccharides containing functional groups such as amino, halo and sulphur.	
Lecture-7	Structure elucidation of sucrose.	
Lecture-8	Synthesis of sucrose.	
Lecture-9	Conformational structures of D(+)ribose, 2-deoxyD-ribose, sucrose, lactose maltose and cellobiose. Structural features of starch, cellulose and chitin.	
Lecture-10	Conformational structures of sucrose, maltose and cellobiose. Structural features of starch, cellulose and chitin.	
Lecture-11	**Proteins:** Acid and enzymatic hydrolysis of proteins.	
Lecture-12	Determination of the amino acid sequence in polypeptides by end group analysis.	
Lecture-13	Chemical synthesis of di and tripeptides.	
Lecture-14	Merrifield's solid phase synthesis.	

OC-4: Heterocyclic compounds

Lecture. No	Content	
Lecture 1	Importance of heterocyclic compounds as drugs	
Lecture 2	Nomenclature of heterocyclic systems based on ring size,number and nature of hetero atoms.	
Lecture 3	Synthesis of Indole	
Lecture 4	Reactivity of Indole	
Lecture 5	Synthesis and reactivity of benzofuran,	
Lecture 6	Synthesis and reactivity of benzothiophene,	
Lecture 7	Synthesis of quinoline,	
Lecture 8	Reactivity of quinoline,	
Lecture 9	Synthesis of isoquinoline,	
Lecture 10	Reactivity of isoquinoline	
Lecture 11	Synthesis and reactivity of coumarin,	
Lecture 12	Synthesis and reactivity of chromone,	
Lecture 13	Synthesis and reactivity of carbazole	
Lecture 14	Synthesis of acridine.	
Lecture 15	Reactivity of acridine.	

References:

1. Stereochemistry of carbon compounds by Ernest L.Eliel and Samuel H. Wilen
2. Stereochemistry of organic compounds- Principles and Applications by D. Nasipuri
3. Heterocyclic Chemistry, T.L. Gilchrist, Longman UK Ltd, London (1985).
4. Benzofurans A. Mustafa, Wiley-Interscience, New York (1974).
5. Heterocyclic Chemistry, 3rd Edn J.A.Joule, K.Mills and G..F.Smith, Stanley Thornes Ltd,UK, (1998)
6. The Chemistry of Indole, R.J. Sunderberg, Academic Press, New York (1970).
7. An introduction to the chemistry of heterocyclic compounds, 2nd Edn.R.M.Acheson, Interscience Publishers, New York, 1967.
8. Advanced Organic Chemistry by Jerry March
9. Mechanism and Structure in Organic Chemistry S. Mukerjee
10. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes.
11. Organic Chemistry by Graham Solomous and Craig Fryhle.
12. Organic Chemistry by RT Morrison and RN Boyd.
13. Organic Chemistry, Vol. 2 by I.L. Finar.
14. Organic Chemistry: Structure and Reactivity by Seyhan Ege.

Paper-III: CH 103 T(PHYSICAL CHEMISTRY)
PC-01: Thermodynamics-I
PC-02: Electrochemistry-I
PC-03: Quantum Chemistry-I
PC-04: Chemical Kinetics-I

PC-01: Thermodynamics-I

Lecture	Topic	Remarks
Lecture 1	Brief review of concepts of I and II laws of thermodynamics. Concept of entropy.	
Lecture 2	Entropy is a state function. Calculation of entropy changes in various processes. Entropy changes in an ideal gas.	
Lecture 3	Entropy changes on mixing of ideal gases. Entropy as a function of V and T.	
Lecture 4	Entropy as a function of P and T. Entropy change in isolated systems- Clausius inequality.	
Lecture 5	Entropy change as criterion for spontaneity and equilibrium. Third law of thermodynamics.	
Lecture 6	Evaluation of absolute entropies from heat capacity data for solids, liquids and gases.	
Lecture 7	Standard entropies and entropy changes of chemical reactions.	
Lecture 8	Helmholtz and Gibbs free energies (A and G). A and G as criteria for equilibrium and spontaneity. Physical significance of A and G.	
Lecture 9	Driving force for chemical reactions- relative signs of ΔH and ΔS. Thermodynamic relations. Gibbs equations.	
Lecture 10	Maxwell relations. Temperature dependence of Gibbs- Helmholtz equation. Pressure dependence of G.	
Lecture 11	Chemical potential: Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibium.	
Lecture 12	Clapeyron equation and Clausius-Clapeyron equation .	
Lecture 13	Conditions for equilibrium in a closed system. Chemical potential of ideal gases.	
Lecture 14	Ideal-gas reaction equlibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.	

PC-02: Electrochemistry- I

Lecture	Topic	Remarks
Lecture 1	Electrochemical Cells: Derivation of Nernst equation – problems.	
Lecture 2	Chemical cells (with and without transference).	
Lecture 3	Concentration cells (with and without transference).	
Lecture 4	Liquid junction potential – derivation of the expression for LJP – its determination and elimination.	
Lecture 5	Applications of EMF measurements: Solubility product,	
Lecture 6	Potentiometric titrations	
Lecture 7	Determination of transport numbers, equilibrium constant measurements	
Lecture 8	Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration over potential.	
Lecture 9	Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient.	
Lecture 10	Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law(derivation not required).	
Lecture 11	Calculation of mean ionic activity coefficient.	
Lecture 12	Limitations of Debye-Huckel theory. Extended Debye-Huckel law. Theory of electrolytic conductance.	
Lecture 13	Derivation of Debye-Huckel-Onsager equation – its validity and limitations.	
Lecture 14	Concept of ion association – Bjerrum theory of ion association (elementary treatment) -ion association constant –	
Lecture 15	Debye-Huckel-Bjerrum equation.	

PC-03: Quantum Chemistry- I

Lecture	Topic	Remarks
Lecture 1	Black body radiation-Planck's concept of quantization	
Lecture 2	Planck's equation, average energy of an oscillator (derivation not required).	
Lecture 3	Wave particle duality and uncertainty principle significance of these for microscopic entities.	
Lecture 4	Emergence of quantum mechanics. Wave mechanics and Schroedinger wave equation.	
Lecture 5	Operators-operator algebra. Commutation of operators	
Lecture 6	linear operators. Complex functions. Hermitian operators.	
Lecture 7	Operators ∇ and ∇^2 . Eigenfunctions and eigenvalues. Degeneracy.	
Lecture 8	Linear combination of eigen functions of an operator. Well behaved functions.	
Lecture 9	Normalized and orthogonal functions.	
Lecture 10	**Postulates of quantum mechanics**. Physical interpretation of wave function. Observables and operators. Measurability of operators.	
Lecture 11	Average values of observables. The time dependent Schrodinger equation.	
Lecture 12	Separation of variables and the time-independent Schrodinger equation.	
Lecture 13	**Theorems of quantum mechanics**. Real nature of the eigen values of a Hermitian operator. significance.	
Lecture 14	Orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality. Expansion of a function in terms of eigenvalues.	
Lecture 15	Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.	

PC-04:Chemical Kinetics- I

Lecture	Topic	Remarks
Lecture 1	Theories of reaction rates: Collision theory, steric factor. 1hr	
Lecture 2	Transition state theory. Reaction coordinate activated complex and the transition state. Thermodynamic formulation of transition state theory.	
Lecture 3	Activation parameters and their significance. The Eyring equation.	
Lecture 4	Unimolecular reactions	
Lecture 5	Lindeman's theory.	
Lecture 6	Complex reactions- Opposing reactions, parallel reactions and consecutive reactions (all first order type).	
Lecture 7	Complex reactions- Opposing reactions, parallel reactions and consecutive reactions (all first order type	
Lecture 8	Chain reactions-general characteristics, steady state treatment. Example- H_2-Br_2 reaction. Derivation of rate law.	
Lecture 9	Effect of structure on reactivity- Linear free energy relationships.	
Lecture 10	Hammett and Taft equations-substituent (σ and σ^*) and reaction constant (ρ and ρ^*)with examples.	
Lecture 11	Deviations from Hammett correlations. Reasons- Change of mechanism, resonance interaction. Taft four parameter equation.	
Lecture 12	Correlations for nucleophilic reactions. The Swain – Scott equation and the Edward equation.	
Lecture 13	The reactivity-selectivity principle and the iso-selectivity rule.	
Lecture 14	The intrinsic barrier and Hammond's postulate.	

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon,Viva Books Pvt. Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Chemical Kinetics, K.J. Laidler, McGraw Hill
8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan
9. Introduction to Electrochemistry, S. Glasstone
10. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
11. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford& IBH
12. The Physical Basis of Organic Chemistry by Howard Maskill, Oxford University Press (New York)
13. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
14. Physical Organic Chemistry, N. S. Isaacs, ELBS

Paper-IV: CH 104 T (ANALYTICAL TECHNIQUES and SPECTROSCOPY- I)
ASP 01: Techniques of Chromatography
ASP 02: NMR spectroscopy-I (^{1}H NMR)
ASP 03: Rotational and Vibrational spectroscopy
ASP 04: Electronic spectroscopy

ASP-01: Techniques of Chromatography

Lecture No.	Topic	Remarks
Lecture No. 1	Introduction of Chromatography	
Lecture No. 2	Classification of chromatographic techniques	
Lecture No. 3	Differential migration rates, partition ratio, retention time	
Lecture No. 4	Relation between partition ratio and retention time, Capacity factor, Selectivity Factor	
Lecture No. 5	Efficiency of separation- resolution, diffusion, plate theory and rate theory.	
Lecture No. 6	GC:Principle, Instrumentation	
Lecture No. 7	Detectors- TCD, FID, ECD	
Lecture No. 8	Derivatisation techniques	
Lecture No.9	PTGC	
Lecture No.10	HPLC:Principle, Instrumentation	
Lecture No. 11	Detectors- UV detectors, Photodiode array detector, Fluorescence detector.	
Lecture No. 12	Applications: Methods of quantitation for GC. GC analysis of hydrocarbons in a mixture	
Lecture No. 13	GC assay of methyl testosterone in tablets	
Lecture No. 14	GC assay of atropine in eye drops.	
Lecture No. 15	HPLC assay of Paracetamol in tablets.	
Lecture No. 16	HPLC assay of Asprin in tablets.	

ASP 02: NMR spectroscopy-I ($_1$H NMR)

Lecture No	Topic	Remarks
Lecture No. 1	Magnetic properties of nuclei, Principles of NMR.	
Lecture No. 2	Instrumentation	
Lecture No. 3	CW and pulsed FT instrumentation,	
Lecture No. 4	Equivalent and non equivalent protons, enantiotopic and diastereotopic protons	
Lecture No. 5	Chemical shifts its properties of ^{1}H NMR	
Lecture No. 6	Factors affecting the chemical shifts such as electronegativity, IE etc., of ^{1}H NMR	
Lecture No. 7	Anisotropy of ^{1}H NMR	
Lecture No. 8	shielding and deshielding effects, and Signal integration	
Lecture No.9	Spin-spin coupling: vicinal, germinal	
Lecture No.10	Spin-spin coupling: long range, Coupling constants	
Lecture No. 11	Spin-spin coupling: factors affecting coupling constants.	
Lecture No. 12	Reaction mechanisms (cyclic bromonium ion,electrophilic and nucleophilic substitutions, carbocations and carbanions)	
Lecture No. 13	E,Z isomers conformation of cyclohexane and decalins keto-enol tautomerism	
Lecture No. 14	hydrogen bonding proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Magnetic resonance imaging(MRI). ethyl acetate,	
Lecture No. 15	mesitylene, paracetamol,asprin,	
Lecture No. 16	ethylbenzoate, benzyl acetate, 2- chloro propionic acid	
Lecture No. 17	[HNi(OPEt3)4]+, [HRh(CN)5] Rh *I*=1/2, [Pt(acac)2].	

ASP 03 :Rotational and Vibrational spectroscopy

Lecture No.	Topic	Remarks
Lecture 1	**a). Microwave Spectroscopy:** Classification of molecules based on moment of inertia.	
Lecture 2	Diatomic molecule as rigid rotator and its rotational energy levels.	
Lecture 3	Selection rules microwave spectroscopy. Calculation of bond lengths from rotational spectra of diatomic molecules.	
Lecture 4	Isotope effect on rotational spectra.	
Lecture 5	Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer.	
Lecture 6	**b). Vibrational Spectroscopy**. Vibrational energy levels of diatomic molecules, selection rules (derivation not required).	
Lecture 7	Calculation force constant from vibrational frequency	
Lecture 8	Anharmonic nature of vibrations.Fundamental bands, overtones and hot bands, Fermi Resonance.	
Lecture 9	Vibration-rotation spectra diatomic molecules. Vibrations of poly atomic molecules.	
Lecture 10	Normal modes of vibration, concept of group frequencies.	
Lecture 11	Characteristics of vibrational frequencies of functional groups;	
Lecture 12	Stereochemical effects on the absorption pattern in carbonyl group,	
Lecture 13	cis-trans isomerism and hydrogen bonding.	
Lecture 14	Isotopic effect on group frequency.	
Lecture 15	IR spectra of metal coordinated NO_3^-, SO_4^{2-} and CO_3^{2-} ions.	
Lecture 16	**Raman Spectroscopy-** Quantum theory of Raman effect,	
Lecture 17	Rotational raman and Vibrational Raman spectra, Stokes and anti-Stokes lines. Complementary nature of IR and Raman spectra.	

ASP 04:Electronic spectroscopy

Lecture No.	Topic	
Lecture 1	**Electronic spectroscopy:** Electronic spectra:	
Lecture 2	Elementary energy levels of molecules-selection rules for electronic spectra;	
Lecture 3	types of electronic transitions in molecules.	
Lecture 4	Chromophores: Congugated dienes,	
Lecture 5	trienes and polyenes,	
Lecture 6	unsaturated carbonyl compounds,	
Lecture 7	benzene and its derivatives,	
Lecture 8	Woodward-Fieser rules.	
Lecture 9	Polynuclear aromatic hydrocarbons	
Lecture 10	diketones.	
Lecture 11	Solvent and structural influences on absorption maxima, stereochemical factors.	
Lecture 12	Cis-trans isomers, and cross conjugation	
Lecture 13	Beer's law application to mixture analysis and	
Lecture 14	dissociation constant of a weak acid.	

References:

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
2. Introduction to Molecular Spectroscopy, G.M. Barrow.
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer.
4. Biochemistry: Hames and Hooper.
5. Introduction to Spectroscopy, Pavia Lampman Kriz.
6. Pharmaceutical analysis, Watson
7. NMR in Chemistry- A multinuclear introduction, William Kemp.
8. Organic Spectroscopy, William Kemp.
9. Spectroscopy of organic compounds, P.S. Kalsi.
10. Structural methods n Inorganic chemistry, E.A.V Ebsworth.

SEMESTER –II

Paper-I: CH 201T (INORGANIC CHEMISTRY)

IC 05: Reaction mechanisms of transition metalcomplexes
IC 06: Bonding in metal complexes-II
IC 07: Metal clusters
IC 08: Biocoordination chemistry

IC-05: UNIT – 1 Reaction Mechanisms of Transition Metal Complexes (18 Hrs.)		
Lecture No.	**TITLE**	**Remarks**
Lecture No. 1	Ligand substitution reactions	
Lecture No. 2	Energy profile of a reaction – Transition state or Activated Complex.	
Lecture No. 3	Types of substitution reactions (SE,SN,SN_1,SN_2)	
Lecture No. 4	Ligand substitution reactions in octahedral complexes	
Lecture No. 5	Aquation or Acid hydrolysis reactions	
Lecture No. 6	Acid Hydrolysis Reactions	
Lecture No. 7	Factors Effecting Acid Hydrolysis	
Lecture No. 8	Base Hydrolysis & Conjugate Base Mechanism	
Lecture No. 9	Evidences in favour of SN_1CB Mechanism	
Lecture No. 10	Annation reactions	
Lecture No. 11	Substitution reactions without Breaking Metal-Ligand bond	
Lecture No. 12	Ligand Substitution reactions in Square-Planar complexes	
Lecture No. 13	Mechanism of Substitution in Square-Planar complexes	
Lecture No. 14	Trans-effect & Grienberg's Polarization theory and π – bonding theory	
Lecture No. 15	Applications of Trans-effect in synthesis of Pt (II) complexes	
Lecture No. 16	Electron Transfer Reactions (or Oxidation-Reduction Reactions) in Coordination compounds	
Lecture No. 17	Mechanism of One-electron Transfer Reactions : Atom or Group Transfer or Inner Sphere Mechanism	
Lecture No.18	Direct Electron Transfer or Outer Sphere Mechanism & Marcus-Hush Theory	

IC-06: UNIT-II : Bonding in Metal Complexes – II (17 hrs.)		
Lecture No. 1	Free ion terms and Energy levels	
Lecture No. 2	Configurations, Terms, States and Microstates	
Lecture No. 3	Formula for the calculation of Microstates p^n and d^n configurations	
Lecture No. 4	Formula for the calculation of Microstates p^n and d^n configurations	
Lecture No. 5	L-S (Russel-Saunders) coupling scheme	
Lecture No. 6	j-j coupling scheme	
Lecture No. 7	Determination of terms for various p^n of metal ions	
Lecture No. 8	Determination of terms for various dn configurations of metal ions	
Lecture No. 9	Hole formalism	
Lecture No. 10	Energy ordering of terms (Hund's rules)	
Lecture No. 11	Inter – electron repulsion Parameters (Racah parameters)	
Lecture No. 12	Spin-Orbital coupling parameters	
Lecture No. 13	Effect of weak cubic crystal fields on S & P terms	
Lecture No. 14	Effect of weak cubic crystal fields on D & F terms	
Lecture No. 15	Orgel Diagrams	
Lecture No. 16	Orgel Diagrams	
Lecture No. 17	Jahn –Tellor theorem and its effects on terms	
IC-07: UNIT-III : Metal Clusters (18 Hrs.)		
Lecture No. 1	Carbonyl clusters & Factors favouring Metal-Metal bonding	
Lecture No. 2	Classification of Clusters	
Lecture No. 3	Low Nuclearity Clusters M_3 clusters & M_4 clusters	
Lecture No. 4	Structural patterns in $M_3(CO)_{12}$ (M=Fe,Ru,Os) Clusters	

Lecture No. 5	Structural patterns in $M_4(CO)_{12}$ (M=Co,Rh,Ir) Clusters	
Lecture No. 6	Metal carbonyl scrambling & High Nuclearity clusters M_5 and M_6 Clusters	
Lecture No. 7	High Nuclearity clusters M_7,M_8 and M_{10} Clusters	
Lecture No. 8	Polyhedral skeletal electron pair theory & Total Electron Count theory	
Lecture No. 9	Wades rules – Capping rule	
Lecture No. 10	Structural patterns in $[Os_6(CO)_{18}]^{2-}$ & $[Rh_6(CO)_{16}]$	
Lecture No. 11	Structural patterns in $[Os_7(CO)_{21}]$ & $[Rh_7(CO)_{16}]^{3-}$	
Lecture No. 12	Structural patterns in $[Os_8(CO)_{22}]^{2-}$, $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_5(CO)_{12}]^{2-}$	
Lecture No. 13	Metal Halide clusters & Major Structural types in Dinuclear Metal-Metal Systems	
Lecture No. 14	Edge sharing Bioctahedra & Face sharing Bioctahedra	
Lecture No. 15	Tetragonal prismatic and Trigonal antiprismatic structures	
Lecture No. 16	Structure and bonding in $[Re_2Cl_8]^{2-}$ and Octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$.	
Lecture No. 17	Trinuclear halides of Re(III).	
Lecture No. 18	Hoffman's Isolobal analogy and its Structural implications.	

IC-08: UNIT-IV : Bio Coordination Chemistry (15 Hrs.)

Lecture No. 1	Metal ions in Biological systems: Brief survey of metal ions in biological systems	
Lecture No. 2	Effect of metal ion concentration and its physiological effects	
Lecture No. 3	Basic principles in the biological selection of elements	
Lecture No. 4	Oxygen transport and storage	
Lecture No. 5	Hemoglobin & Myoglobin	
Lecture No. 6	Geometric, electronic and magnetic aspects of Dioxygen binding	
Lecture No. 7	Oxygen adsorption isotherms and cooperativity in Hemoglobin and its physiological significance	

Lecture No. 8	Role of Globin chain	
Lecture No. 9	Hemerythrin and Hemocyanin	
Lecture No. 10	Structure of deoxy forms, oxygen binding, Geometric, electronic and magnetic aspects	
Lecture No. 11	Comparison of Hemerythrin and Hemocyanin with hemoglobin.	
Lecture No. 12	Photosynthesis & Structural aspects of Chlorophyll	
Lecture No. 13	Photo system I and Photo system II	
Lecture No. 14	Vitamin B_6 model systems	
Lecture No. 15	Forms of vitamin B_6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation in presence of metal ions	

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1. Inorganic Reaction Mechanisms. M.L.Tobe and John Burgess, Addison Wesley Longman (1999).
2. Metal ions in Reaction Mechanisms. K.Veera Reddy. Golgotia Publications (P) Ltd
3. Mechanisms of Reactions in Transition Metal Sites. Richard A Henderson, Oxford Science Publications, London (1993).
4. Inorganic Reaction Mechanisms, F.Basolo and R.G.Pearson, New York (1967).
5. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6 Th Edition, Wiley Interscience, N.Y (1999
6. Inorganic Chemistry, J.E.Huheey , K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
7. Inorganic Biochemistry Edited by G.L.Eichorn, Volume 1 Elsevier (1982).
8. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
9. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
10. Bioinorganic Chemistry, I.Bertini, H.B.Gray, S.J.Lippard and S.J.Valentine, Viva Low-Priced Student Edition, New Delhi (1998).
11. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W.Kain and B.Schwederski, John Wiley and Sons, NY (1999).
12. Bioorganic Chemistry – Dugas.

Paper-II: CH 202T (ORGANIC CHEMISTRY)

OC-05: Conformational analysis (acyclic systems)
OC-06: Reaction mechanism-II
OC-07: Reactive intermediates and Molecular rearrangements.
OC-08: Natural products (Terpenoids and Alkaloids).

Unit -05 Conformational Analysis-20 Marks		
Lecture.No.	**Name of the Topic**	**Remarks**
Lecture-1	Introduction:Isomers classification , Definition of conformational Isomerism	
Lecture-2	Definition of enantiomers, diastereomers with examples	
Lecture-3	Concept of Stereo chemistry, dynamic stereo chemistry,	
Lecture-4	factors effective stability of conformations (like torsional strain vanderwall strain, hydrogen bonding, dipole dipole repulsions, hyper conjugation.	
Lecture-5	Definition of conformation with examples writing of possible conformation with potential energy order and population. Examples of Ethane, 1,2 disubstituted Ethane amino alcohols, tetra halobutanes, butane, dihalobutanes, halohydrine, ethylene glycol etc.,	
Lecture-6	Examples of Ethane, 1,2 disubstituted Ethane amino alcohols, tetra halobutanes, butane, dihalobutanes, halohydrine, ethylene glycol etc.,	
Lecture-7	Eamples and Exercise of confirmations	
Lecture-8	Explanation of Klyne-Prelog terminology for conformations	
Lecture-9	Conformations of unsaturated acylic molecules like 1-butene, acetaldehyde, propionaldehyde, Butanone.	
Lecture-10	Conformations of unsaturated acylic molecules like 1-butene, acetaldehyde, propionaldehyde, Butanone.	
Lecture-11	Use of Physical and spectral Methods in conformational analysis like dipole moments, x-ray diffraction, IR spectra, Proton NMR,	
Lecture-12	Use of Physical and spectral Methods in conformational analysis like dipole moments, x-ray diffraction, IR spectra, Proton NMR,	
Lecture-13	Factors effecting conformational stability & conformational equilibrium	
Lecture-14	Conformational effects on the stability & reactivity of acyclic dia stereo Isomers with examples	
Lecture-15	Winstein-Holness equation & Curtin-Hammett Principles explanation with examples	

OC-06: Reaction mechanism-II

Unit :06 Reaction Mechanism -II 20 Marks		
Lecture No.	**Name of the Topic**	**Remarks**
Lecture-1	Introduction-Nucleoplilic Aromatic substitution Reactions	
Lecture-2	Definition of SN1(Ar), SN2 (Ar) reactions	
Lecture-3	Benzyne mechanisms, evidence for the structure of benzyne.	
Lecture-4	Types of nucleophiles	
Lecture-5	Von Richter rearrangement, Definition and types of ambident nucleophiles.	

Lecture-6	Neighbouring group participation: Criteria for determining the participation of neighbouring group.	
Lecture-7	Neighbouring group participation: Criteria for determining the participation of neighbouring group.	
Lecture-8	Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates.	
Lecture-9	Neighbouring group participation involving Halogens,	
Lecture-10	Neighbouring group participation involving Oxygen, Aryl, Cycloalkyl groups αand II bonds.	
Lecture-11	Neighbouring group participation involving Sulphur	
Lecture-12	Neighbouring group participation involving Nitrogen	
Lecture-13	Introduction to nonclassical carbonium ions.	
Lecture-14	Electrophilic substitution at saturated carbon and single electron transfer reactions	
Lecture-15	Electrophilic substitution at saturated carbon and single electron transfer reactions	

OC-07: Reactive intermediates and Molecular rearrangements.

Unit :07 Reactive intermediates and Molecular rearrangements-20 Marks		
Sl.No.	**Name of the Topic**	**Remarks**
Lecture-1	Definition , examples of reactive intermediates,	
Lecture-2	generation detection structure stability and reactions of carbocation	
Lecture-3	Definition , examples of reactive intermediates, generation detection structure stability and reactions of carbanion	
Lecture-4	Definition , examples of reactive intermediates,	
Lecture-5	generation detection structure stability and reactions of carbene	
Lecture-6	Definition , examples of reactive intermediates, generation detection structure stability and reactions of nitrenes and freeradicals	
Lecture-7	Molecular rearrangements defination and classification - involving electron deficient carbon examples:	
Lecture-8	Wagner-Meerwein , Pinacol-Pinacolone,	
Lecture-9	Allylic and Wolf rearrangement	
Lecture-10	Electron deficient Nitrogen rearrangement examples Hoffmann, Lossen, Curtius Schmidt Beckmann rearrangements	
Lecture-11	Electron deficient Nitrogen rearrangement examples Lossen, Curtius Schmidt	
Lecture-12	Electron deficient Nitrogen rearrangement examples -Beckmann rearrangements	
Lecture-13	Electron deficient Oxygen, Baeyer-Villiger oxidation	
Lecture-14	Base catalysed rearrangements :Benzilic acid, Favourski,	
Lecture-15	Transannular, Sommlett, Hauser and Smiles rearragement	

OC-08: Natural products-I (Terpenoids and Alkaloids)

Unit :08 NATURAL PRODUCTS-20 Marks		
Sl.No.	**Name of the Topic**	**Remarks**
Lecture-1	Introduction and Importance of Natural products sources of natural products ,examples of natural products as drugs	
Lecture-2	Isolation of Natural Products by Steam distilation,	
Lecture-3	solvant extraction & chemical Methods i.e(detection anad seperation and isolation)	
Lecture-4	General methods for structural determination of alkaloids by zerwitnoffs method, zeisel method , nature of Nitrogen, Hoffman exhaustive methods	
Lecture-5	structural determination and synthesis of Papaverine	
Lecture-6	structural determination and synthesis of Papaverine	
Lecture-7	structural determination and synthesis of Quinine	
Lecture-8	structural determination and synthesis of Quinine	
Lecture-9	General methods for structure determination of Terpene, Isoprene rule	
Lecture-10	sructural determination & Synthesis of camphor	
Lecture-11	Strutural determination and Synthesis of Alpha terpeniol	
Lecture-12	Introduction to biogenesis of mono terpines	
Lecture-13	structure of determination of B-carotene	
Lecture-14	structure of determination of B-carotene	
Lecture-15	Synthesis of B-carotene	

References :

1. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
2. Stereochemistry of organic compounds – Principles and Applications by D Nasipuri
3. The third dimension in organic chemistry, by Alan Bassindale
4. Stereochemistry: Conformation and Mechanism by P S Kalsi
5. Stereochemistry by V M Potapov
6. Advanced Organic Chemistry by Jerry March
7. Mechanism and Structure in Organic Chemistry S. Mukerjee
8. Organic chemistry Vol.I and II by I.L.Finar
9. Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D..Ollis
10. Organic Chemistry, Vol. 2 by I.L. Finar.
11. Chemistry of Natural Products by Bhat, Nagasampagi and Siva Kumar.
12. Alkaloids by K.W. Bentley.
13. Steroids and Terpenoids by Bentle.

Paper-III: CH 203T (PHYSICAL CHEMISTRY)

PC-05: Thermodynamics-II
PC-06: Photochemistry-I
PC-07: Quantum Chemistry-II
PC-08: Solid state chemistry

PC-05:Thermodynamics-II

Lecture No.	Topic	Remarks
Lecture-1	Solutions: Specifying the Solution composition.	
Lecture-2	Partial molar properties-significance. Relation between solution volume and partial molar volume.	
Lecture-3	Measurement of partial molar volumes- slope and intercept methods.	
Lecture-4	The chemical potential. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance.	
Lecture-5	Ideal solutions. Thermodynamic properties of ideal solutions.	
Lecture-6	Mixing quantities. Vapour pressure-Raoult's law.	
Lecture-7	Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.	
Lecture-8	Non ideal systems. Concept of fugacity, fugacity coefficient. Determination of fugacity.	
Lecture-9	Non ideal solutions. Activities and activity coefficients.	
Lecture-10	Standard-state conventions for non ideal solutions.	
Lecture-11	Determination of activity coefficients from vapour pressure measurements.	
Lecture-12	Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation.	
Lecture-13	Multicomponent phase equilibrium: Vapour pressure lowering,	
Lecture-14	freezing point depression	
Lecture-15	Boiling point elevation.	

PC-06:Photochemistry –I

Lecture No.	Topic	Remarks
Lecture-1	Electronic transitions in molecules.	
Lecture-2	The Franck Condon principle.	
Lecture-3	Electronically excited molecules- singlet and triplet states.	
Lecture-4	Radiative life times of excited states-theoretical treatment.	
Lecture-5	Measured lifetimes. Quantum yield and its determination.	

Lecture-6	Actinometry-ferrioxalate and uranyl oxalate actinometers-problems.	
Lecture-7	Derivation of fluorescence quantum yields.	
Lecture-8	Derivation of phosphorescence quantum yields.	
Lecture-9	E-type delayed fluorescence- evaluation of triplet energy splitting(ΔE_{ST})	
Lecture-10	Photophysical processes photophysical kinetics of unimolecular reactions.	
Lecture-11	Calculation of rate constants of various photophysical processes-problems, State diagrams.	
Lecture-12	Photochemical primary processes. Types of photochemical reactions- electron transfer, photodissociation,	
Lecture-13	Types of photochemical reactions : addition, abstraction, oxidation and isomerization reactions with examples.	
Lecture-14	Effect of light intensity on the rates of photochemical reactions.	
Lecture-15	Photosensitization.Quenching-Stern Volmer equation.	
Lecture-16	Experimental set up of a photochemical reaction. Introduction to fast reactions- Principle of flash photolysis.	

PC-07: Quantum chemistry-II

Lecture No.	Topic	Remarks
Lecture-1	*Particle in a box*- one dimensional.	
Lecture-2	*Particle in a box*- three dimensional.	
Lecture-3	Plots of ψ and ψ^2-discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles	
Lecture-4	Calculations using wave functions of the particle in a box-orthogonality,	
Lecture-5	Measurability of energy, position and momentum, average values and probabilities.	
Lecture-6	Application to the spectra of conjugated molecules.	
Lecture-7	*Schrodinger equation for the hydrogen atom*- separation into three equations.	
Lecture-8	Hydrogen like wave functions. Radial and angular functions.	

Lecture-9	Quantum numbers n, l and m and their importance. The radial distribution functions.	
Lecture-10	Hydrogen like orbitals and their representation	
Lecture-11	Polar plots, contour plots and boundary diagrams.	
Lecture-12	*Many electron systems.* Approximate methods. The variation method-variation theorem and its proof.	
Lecture-13	Trial variation function and variation integral.	
Lecture-14	Examples of variational calculations.	
Lecture-15	Particle in a box. Construction of trial functions by the method of linear combinations.	
Lecture-16	Variation parameters. Secular equations and secular determinant.	
Lecture-17	*Bonding in molecules.* Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion.	
Lecture-18	The variation of an integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs.	
Lecture-19	Physical picture of bonding and antibonding wave functions. Energy diagram.	
Lecture-20	The MO and VB wave functions for H_2 molecule and their comparision.	

PC-08: Solid state chemistry

Lecture No.	Topic	Remarks
Lecture-1	Magnetic properties of solids- classification of magnetic materials	
Lecture-2	Magnetic susceptibility. Langevin diamagnetism,	
Lecture-3	Weiss theory of para magnetism.	
Lecture-4	Electronic properties of metals, insulators and semi conductors: Electronic structure of solids	
Lecture-5	Band theory, band structure of metals, insulators and semiconductors.	
Lecture-6	Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi conductors.	
Lecture-7	Photo conductivity and photovoltaic effect-p-n junctions.	
Lecture-8	**Superconductivity.** Occurrence of superconductivity. Destruction of superconductivity by magnetic fields-Meisner effect	
Lecture-9	Types of superconductors. Theories of super conductivity-BCS theory.	
Lecture-10	**High temperature superconductors.** Structure of defect perovskites. High T_c superconductivity in cuprates.	

Lecture-11	Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_{7-x}$.	
Lecture-12	Preparation of 1-2-3 materials. Origin of high T_c superconductivity.	

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
9. Solid state Chemistry and its aplications, A.R. West, Plenum.
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
11. Molecular Photochemistry, N.J. Turro, Benjamin
12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
16. Principles of the Solid State, H. V. Keer, New Age International

Paper-IV: CH 204 T (ANALYTICAL TECHNIQUES and SPECTROSCOPY - II)

ASP-05: Electro analytical Techniques.
ASP-06: NMR- II
ASP-07: Mass Spectroscopy
ASP-08: Photoelectron & ESR spectroscopy

ASP-05: Electro Analytical Techniques

Lecture No.	Topic	Remarks
Lecture 1	a) Types and Classification of Electro analytical Methods. i) Potentiometry- Types of electrodes, Hydrogen gas,	
Lecture 2	Calomel, Quin hydrone and glass electrodes.	
Lecture 3	Determination of pH. Potentiometric titrations.	
Lecture 4	ii) Conductometry – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions,	
Lecture 5	Conductometric titrations.	
Lecture 6	b) D.C Polarography :. Dropping mercury electrode- Instrumentation-polarogram.	
Lecture 7	Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences.	
Lecture 8	Types of limiting Currents : Adsorption, Diffusion, Kinetic.	
Lecture 9	Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures.	
Lecture 10	Application to inorganic and organic compounds. Determination of stability constants of complexes.	
Lecture 11	c) Brief account of following techniques and their advantages over conventional d.c.polargraphy. (i) A.C.polarography (ii) Square-wave polarography	
Lecture 12	(iii) Pulse polarography (iv)Differential pulse polarography	
Lecture 13	d) Amperometric titrations :Principle, Instrumentation. Types and applications of amperometric titrations.	
Lecture 14	Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances	
Lecture 15	e) Cyclic Voltammetry : Principle, instrumentation, reversible and irreversible cyclic voltammograms.	
Lecture 16	Applications. Cyclic voltammetric study of insecticide parathion.	

ASP 06: NMR spectroscopy-II (^{1}H,^{19}F and ^{31}P NMR)

Lecture No.	Topic	Remarks
Lecture 1	First order and non first order spectra e.g.,AX,AX2,AX3, A2X3,AMX and AB,ABC,	
Lecture 2	e.g.,AX,AX2,AX3,	
Lecture 3	A2X3,AMX and AB,ABC,	
Lecture 4	increased field strength deuterium exchange	
Lecture 5	Lanthanide shift reagents double resonance techniques	
Lecture 6	Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid.	
Lecture 7	Nuclear Overhauser enhancement (NOE).	
Lecture 8	**Fluxional molecules-** bullvalene, [η5-C5H5M], [η5-(C5H5)2 Ti η1-(C5H5)2] and [η4C8H8Ru(CO)3].	
	19F NMR spectroscopy:	
Lecture 9	19F chemical shifts, coupling constants.	
Lecture 10	Applications of 19F NMR Involving coupling with 19F,1H and 31P	
Lecture 11	1,2 dichloro-1,1 difluoro ethane, BrF5	
Lecture 12	SF4, PF5, ClF3, IF5, HF2.	
Lecture 13	31p chemical shifts, coupling constants.	
Lecture 14	Applications of 31P NMR Involving coupling with 19F,1H, 31P and 13C	
Lecture 15	ATP, Ph_3PSe, P4S3, P(OCH3)3	
Lecture 16	H3PO4, H3PO3, H3PO2, HPF2, PF6, PH3, [Rh(PPh3)Cl3]	
Lecture 17	Introduction to solid state NMR: Magic angle spinning (MAS). Applications of solid state NMR	

ASP 07: Mass spectrometry

Lecture No.	Topic	Remarks
Lecture 1	Origin of mass spectrum- Introduction, basic principle	
Lecture 2	Simple mass spectrometry, mass spectrum, Advantages, disadvantages	
Lecture 3	Principles of EI mass spectrometer-Inlet systems, ion production, analyzer, collector-detector and display	
Lecture 4	Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule),	
Lecture 5	Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule),	
Lecture 6	Nitrogen rule-Even and odd mass molecules with examples	
Lecture 7	Isotopic peaks-Sulfur, Halogens-Chloride and Bromide and significant peaks for fluoride and iodine	
Lecture 8	Determination of molecular formula-Mass of the compound-Molecular ion peak, Calculation of carbon atoms, significanc of $[M+2]^+$ peak, application of nitrogen rule, presence of oxygen atoms and Un-saturation number or double bond equivalent (DBE).	
Lecture 9	Metastable ion peaks-toluene, phenyl cation, benzyl cation etc	
Lecture 10	High resolution mass spectrometry- instrument, use of HRMS	
Lecture 11	β-cleavage, including Mclafferty rearrangement	
Lecture 12	Retro Diels – Alder fragmentation and Ortho effect	
Lecture 13	Salient features of fragmentation pattern of organic compounds-Alkanes, cyclo alkanes	
Lecture 14	Alkenes, alkynes, cycloalkens	
Lecture 15	Aromatic hydrocarbons, alkyl benzenes	
Lecture 16	Alcohols-1^o, 2^o, 3^o, phonols, ethers, acetols, ketols, halides	
Lecture 17	Calbonyl compounds-aldehydes, ketones, quinines	
Lecture 18	Carboxylic acids, esters, amides, anhydrides, acid chlorides	
Lecture 19	Nitriles, Nitro compounds, amines, sulphur coumpounds	
Lecture 20	Nitrogen heterocyclic	
Lecture 21	Principle of CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS),	
Lecture 22	Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods.	
Lecture 23	Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS)	
Lecture 24	Liquid chromatography-Mass Spectrometry (LC-MS) techniques	

ASP-08: Photoelectron & ESR spectroscopy

Lecture No.	Topic	Remarks
Lecture 1	**Photoelectron Spectroscopy** Principle and Instrumentation,1hr	
Lecture 2	Types of Photoelectron Spectroscopy – UPS & XPS 1hr	
Lecture 3	Binding Energies, Koopman's Theorem,1hr	
Lecture 4	Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, CO, HF, NH_3 and H_2O	
Lecture 5	Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, CO, HF, NH_3 and H_2O	
Lecture 6	Vibrational Structure of PES Bands, Potential energy curves,	
Lecture 7	Interpretation of Vibrational spectral data for ionized (M^+) species, Prediction of Nature of Molecular Orbitals..	
Lecture 8	ESCA in qualitative analysis, Principles of Auger electron spectroscopy	
Lecture 9	**Electron Spin Resonance** Introduction, principle, instrumentation,	
Lecture 10	selection rules, interpretation of Lande's factor 'g'.	
Lecture 11	Hyperfine and super hyperfine Coupling.	
Lecture 12	Anisotropy in 'g' values and hyperfine coupling constants	
Lecture 13	Zero field splitting, Kramer's degeneracy, quadrupolar interactions.	
Lecture 14	Study of free radicals and	
Lecture 15	transition metal complexes.	

References:

1. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
2. Organic spectroscopy by William Kemp
3. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W. Johnstone
4. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming
5. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake
6. Biological Mass Spectrometry by A.L. Burlingame
7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
8. Spectrscopic identification of organic compounds by R.M.Silverstein. G.C.Bassler and T.E.Morrill
9. NMR-A multinuclear introduction by William Kemp
10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
11. Principles of Polarography, Heyrovsky.

12. Principles of Polarography, Kapoor.
13. Modern Electroanalytical methods, edited by C.Charlot, Elsevier Company.
14. Principles of Instyrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
15. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
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18. Sructural methods in inorganic chemistry, E.A.V. Ebsworth.

Blow up 2017-18

III SEMESTER SYLLABUS

Paper 1- CH 301T: Conformational Analysis, Asymmetric Synthesis and Biomolecules

OC09: Conformational Analysis (cyclic systems)
OC10: Principles of Asymmetric synthesis
OC11: Methodologies in asymmetric synthesis
OC12: Biomolecules

OC 09- Conformational analysis (Cyclic systems)

Lecture No.	Topic	Remarks
Lecture 1	Study of conformations of cyclopentane, cyclobutene,	
Lecture 2	Study of conformations cyclohexane	
Lecture 3	Conformations of mono, di and polysubstitutedcyclohexanes,	
Lecture 4	excercises	
Lecture 5	cyclohexene, cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones,	
Lecture 6	Stereochemistry of bicyclo [3,3,0] octanes, hydrindanes,	
Lecture 7	Stereochemistry of decalins and perhydroanthracenes.	
Lecture 8	Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine.	
Lecture 9	Conformational structures of pseudotropine, decahydroquinoline and quinolizidine	
Lecture 10	Conformational effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereoelectronic factors – examples.	
Lecture 11	Conformational effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereoelectronic factors – examples.	
Lecture 12	excercises	
Lecture 13	Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.	
Lecture 14	Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.	
Lecture 15	excercises	
	OC l0- Principles of asymmetric synthesis	
Lecture 1	Introduction and terminology: Topicity in molecules,	
Lecture 2	Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria.	
Lecture 3	Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria.	
Lecture 4	excercises	
Lecture 5	Prochirality nomenclature: Pro-R, Pro-S, Re ii	
Lecture 6	examples	
Lecture 7	Stereoselective reactions: Substrate stereoselectivity,	

Lecture 8	product stereoselectivity	
Lecture 9	enantioselectivity and diastereoselectivity	
Lecture 10	Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control	
Lecture 11	Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio.	
Lecture 12	Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio.	
Lecture 13	Techniques for determination of enantiomeric excess, specific rotation, Chiral NMR;	
Lecture 14	Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.	
Lecture 15	Techniques for determination of enantiomeric excess, specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.	
	OC 11- Methodologies in asymmetric synthesis	
Lecture 1	**Chiral Substrate controlled asymmetric synthesis:** Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule.	
Lecture 2	Felkin-Anh model	
Lecture 3	Examples	
Lecture 4	**Chiral auxiliary controlled asymmetric synthesis:** α-Alkylation of chiral enolates, aza enolates, imines and hydrazones.	
Lecture 5	1, 4-Asymmetric induction and Prelog's rule	
Lecture 6	Use of chiral auxiliaries in Diels-Alder reaction.	
Lecture 7	**Chiral reagent controlled asymmetric synthesis:** Asymmetric reductions using BINAL-H.	
Lecture 8	Asymmetric hydroboration using IPC_2BH and $IPCBH_2$.	
Lecture 9	Asymmetric hydroboration using IPC_2BH and $IPCBH_2$.	
Lecture 10	**Chiral catalyst controlled asymmetric synthesis:** Sharpless and Jacobsen asymmetric epoxidations...	
Lecture 11	Sharpless asymmetric dihydroxylation	
Lecture 12	Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalyst	
Lecture 13	Enzyme mediated enantioselective synthesis	
Lecture 14	**Asymmetric aldol reaction:** Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes)	
Lecture 15	Explanation by Zimmerman-Traxel model.	
	OC-12 Biomolecules	
Lecture 1	Definition. Classification based on mode of action.	
Lecture 2	Mechanism of enzyme catalysis. Lock and Key model and Induced- Fit model.	
Lecture 3	Enantiomer discrimination by three point contact model. Factors affecting enzyme catalysis.	
Lecture 4	Factors affecting enzyme catalysis.	
Lecture 5	Enzyme inhibition- reversible and irreversible inhibition. Enzymes in	

	organic synthesis.	
Lecture 6	Enzymes in organic synthesis	
Lecture 7	Immobilised enzymes.	
Lecture 8	**Nucleic acids:** Primary structure of DNA	
Lecture 9	secondary and tertiary structure of DNA	
Lecture 10	Types of mRNA, tRNA and rRNA	
Lecture 11	Replication, transcription and translation.	
Lecture 12	Genetic code. Protein biosynthesis.	
Lecture 13	Chemical synthesis of nucleosides and nucleotides.	
Lecture 14	**Lipids:** Lipid structure- acyl glycerols, phosphoglycerides and sphingolipids.	
Lecture 15	Biosynthesis of Lipids and chemical synthesis of lipids	

Recommended Books:

1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. The third dimension in organic chemistry, by Alan Bassendale
5. Stereoselectivity in organic synthesis by R S Ward.
6. Asymmetric synthesis by Nogradi
7. Asymmetric organic reactions by J D Morrison and H S Moscher
8. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffry Aube
9. Stereodifferentiating reactions by Izumi
10. Modern methods of organic synthesis by W Carruthers
11. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
12. Organic synthesis by Michael B Smith
13. Enzyme structure and mechanism by Fersht and Freeman
14. Bio-Organic chemistry by Hennan Dugas
15. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
16. Lehninger Principles of Biochemistry by D L Nelson and M M Cox
17. Outlines of Biochemistry by Conn and Stumpf
18. Biotransformations in Organic Chemistry by K Faber.
19. Principles of biochemistry by Horton & others.
20. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.

Paper 2– CH (OC) 302T: Modern Organic Synthesis

OC13- Synthetic Reagents I
OC 14- Synthetic Reagents II
OC 15- New Synthetic reactions
OC 16- New techniques and concepts in organic synthesis

OC-13 Synthetic Reagents I

Lecture No	Topic	Remarks
	OC-13 Synthetic Reagents I	**15 h**
Lecture -1	Protecting groups introduction: Protection of alcohols by ether: MOM-Cl, MEM-Cl, TPHP, Benzyl ether	
Lecture -2	Protection of alcohols by silyl ether: TMS, TBDMS, TIPS	
Lecture -3	Protection of 1,2-diols by acetal, ketal and carbonate formation	
Lecture -4	Protection of amines by acetylation, benzoylation, benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenylmethyl groups	
Lecture -5	Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups.	
Lecture -6	Protection of carboxylic acids by ester and ortho ester (OBO) formation.	
Lecture -7	Oxidation reactions : Introduction; Oxidation of active C-H functions: DDQ and SeO_2.	
Lecture -8	Oxidation of Alkenes to diols: Prevost and Woodward oxidation	
Lecture -9	Oxidation of Alcohol to carbonyls; Cr VI oxidants (Jones reagent, PCC,PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation	
Lecture -10	Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.	
Lecture -11	Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction.	
Lecture -12	Non-metallic reductions: Diimide reduction, Dissolving metal reductions: Birch reduction.	
Lecture -13	Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications.	
Lecture -14	Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL, Hydrogenolysis	
Lecture -15	Radical reductions: use of tri-n-butyl tin hydride;	

OC-14: Synthetic Reagents-II (17 hrs)

Lecture	Topic	Remarks
Lecture 1	**i) Organometallic Reagents: a)** Preparation and application of the following in organic synthesis**:** 1) Grignard	
Lecture 2	Grignard	
Lecture 3	2) Organo lithium	
Lecture 4	Organo lithium	
Lecture 5	3) Organo copper reagents	
Lecture 6	Organo copper reagents	

Lecture 7	**b)** Organo boranes in C-C bond formation:	
Lecture 8	Organo boranes in C-C bond formation:	
Lecture 9	**c).** Organo silicon reagents: reactions involving β -carbocations,	
Lecture 10	α -carbanions, utility of trimethyl silyl halides,	
Lecture 11	cyanides, triflates	
Lecture 12	**ii) Carbonyl methylenation: a)** Phosphorous ylide mediated olefination: 1) Wittig reaction	
Lecture 13	Wittig reaction	
Lecture 14	2) Horner-Wadsworth-Emmons reaction	
Lecture 15	**b)** Titanium- Carbene mediated olefination**:** 1) Tebbe reagent,	
Lecture 16	2) Petasis reagent	
Lecture 17	**c)** Olefination by Nysted reagent	

302: OC-15: New Synthetic reactions (22 hrs)

Lecture	Topic	Remarks
Lecture 1	**Metal mediated C-C and C-X coupling reactions:** Suzuki, Heck	
Lecture 2	Stille, Sonogashira cross coupling	
Lecture 3	Buchwald-Hartwig, Negishi-Kumada coupling reactions	
Lecture 4	**C=C Formation Reactions:** Shapiro, Bamford-Stevens	
Lecture 5	McMurry reactions, Julia-Lythgoe olefination	
Lecture 6	Peterson's stereoselective olefination	
Lecture 7	**Multi component Reactions:** Ugi,	
Lecture 8	Passerini,	
Lecture 9	Biginelli,	
Lecture 10	Hantzsch,	

Lecture 11	Mannich reactions	
Lecture 12	**Ring Formation Reactions:** Pausan-Khand reaction,	
Lecture 13	Bergman cyclisation,	
Lecture 14	Nazerov cyclisation	
Lecture 15	**Click Chemistry:** Criteria for Click reaction,	
Lecture 16	Sharpless azides cycloadditions	
Lecture 17	**Metathesis:** Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM),	
Lecture 18	Ring closing metathesis(RCM), Ring opening metathesis (ROM), applications	
Lecture 19	**Other important synthetic reactions:** Baylis-Hilman reaction	
Lecture 20	Eschenmoser-Tanabe fragmentation,	
Lecture 21	Mitsunobu reaction, Stork-enamine reaction	
Lecture 22	Michael reactions	

OC-16: New techniques and concepts in organic synthesis **15 Hrs**

L. No.	Topic	Remarks
Lecture No.1.	Techniques in peptide synthesis: Introduction, Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin) structures,	
Lecture No.2.	flow chart for the solid phase peptide synthesis	
Lecture No.3.	synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.	
Lecture No.4.	Solid phase oligodeoxynucleotide synthesis: Triester pathway and phosphoramidite pathway.	
Lecture No.5.	Oligosaccharide synthesis**:** Protection of hydroxyl groups, cylic oxocarbenium ion, glycosyl donors and glycosyl acceptors,	
Lecture No.6.	Kahne glycosidation	
Lecture No.7.	convergent and linear oligosaccharide synthesis-synthetic strategies	
Lecture No.8.	Phase Transfer catalysis: Onium ions as PTC- General mechanism of the reaction. Applications	

Lecture No.9.	Phase Transfer catalysis: Introduction for crown ethers as PTC-applications	
Lecture No.10.	Tandem synthesis: Introduction for Tandem reactions; conjugate addition-aldol reaction, polymerization cyclisation, elctrocylic-Diels Alder reaction with mechanisms	
Lecture No.11.	Baldwin Rules- Emperical rule, Explanation for Exo and Endo cyclisation, tetrahedral, favoured and disfavoured cyclisations	
Lecture No.12.	Baldwin Rules- Emperical rule, Explanation for Exo and Endo cyclisation, trigonal systems and diagonal , favoured and disfavoured cyclisations	
Lecture No.13.	Chiron approach in organic synthesis- Nature's chiral pool, carbohydrates, amino acids, hydroxy acids	
Lecture No.14.	Definition for chiral precursors, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanomycin from D-glucose, S-(-)-ipsenol from S-leucine	
Lecture No.15.	Determination of absolute configuration: Mosher's methods.	

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Total synthesis of natural products: the Chiron approach by S. Hanesian
9. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren

Paper 3: CH (OC) 303T: Organic Spectroscopy and Pericyclic reactions.

OC-17: ^{13}C NMR spectroscopy
OC-18: 2D NMR techniques and ORD
OC-19: Pericyclic reactions I
OC-20: Pericyclic reactions II

OC-17: ^{13}C NMR spectroscopy 16 Hrs

S. No.	Topic	Remarks
Lecture No.1.	CW and PFT techniques-Instrumentaion	
Lecture No.2.	Applications of ^{13}C NMR spectra, nonequivalent sets of carbon atoms, (n+1) rule, Spliting pattern for methane, methylene carbons etc., ^{13}C chemical shift values of organic compounds, Types of ^{13}C NMR	

	spectra	
Lecture No.3.	Applications of ^{13}C NMR spectra, nonequivalent sets of carbon atoms, (n+1) rule, Spliting pattern for methane, methylene carbons etc., ^{13}C chemical shift values of organic compounds, Types of ^{13}C NMR spectra	
Lecture No.4.	Undecoupled ^{13}C NMR spectra- salient features, Spliting pattern for methane, methylene carbons etc., solving of examples.	
Lecture No.5.	Proton- decoupled ^{13}C NMR spectra- salient features, Spliting pattern for methane, methylene carbons etc., solving of examples.	
Lecture No.6.	Off resonance decoupled (ORD) spectra - salient features, Spliting pattern for methane, methylene carbons etc., solving of examples.	
Lecture No.7.	^{13}C chemical shifts, factors affecting the chemical shifts	
Lecture No.8.	Homonuclear (^{13}C, ^{13}C J) and heteronuclear (^{13}C, ^{1}H J and ^{13}C- ^{2}H J) coupling- factors affecting the coupling interactions	
Lecture No.9.	Calculation of chemical shifts of alkanes examples	
Lecture No.10.	Calculation of chemical shifts of alkanes examples	
Lecture No.11.	Calculation of chemical shifts of alkenes and alkynes- examples	
Lecture No.12.	Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry	
Lecture No.13.	Applications of ^{13}C-NMR spectroscopy: reaction mechanisms and dynamic processes in organic molecules	
Lecture No.14.	^{13}C-NMR spectral editing techniques: principle and applications of DEPT	
Lecture No.15.	^{13}C-NMR spectral editing techniques: principle and applications of INEPT	
Lecture No.16.	^{13}C-NMR spectral editing techniques: principle and applications of APT	

OC-18 2D NMR techniques and ORD 15 Hrs

L. No.	Topic	Remarks
Lecture No.1.	Principles of 2D NMR- while comparing with 1D NMR, 2D plot,	

	Explanation of Grid, Classification of 2D-experiments	
Lecture No.2.	Homonuclear and Heteronuclear 2D-J-resolved spectroscopy with examples	
Lecture No.3.	Correlation spectroscopy (COSY) HOMO COSY (^{1}H-^{1}H COSY)- contours, diagonal line, diagonal peaks, off diagonal peaks, with examples of 2-nitropropane, ethyl acetate etc.	
Lecture No.4.	Example s of HOMOCOSY- of 2-nitropropane, ethyl acetate etc.	
Lecture No.5.	TOCSY (Total Correlation Spectroscopy) with example	
Lecture No.6.	Hetero COSY (^{1}H,^{13}C COSY,HMQC)- contours, with examples of 2-nitropropane, ethyl acetate etc.	
Lecture No.7.	Example s of HETROCOSY- of 2-nitropropane, ethyl acetate etc.	
Lecture No.8.	^{1}H,^{13}C COSY,HMQC, long range ^{1}H,^{13}C COSY (HMBC) with examples	
Lecture No.9.	NOESY and 2D-INADEQUATE experiments with examples	
Lecture No.10.	Optical Rotatory Dispersion (ORD)- Optical rotation, circular birefringence, circular dichroism	
Lecture No.11.	Cotton effect- Definition and explanation of graph, Plain curves and anomalous curves	
Lecture No.12.	The octant rule- empirical rule, explanation using the cyclohexanone system	
Lecture No.13.	Octant rule- examples	
Lecture No.14.	The axial haloketone rule, with examples	
Lecture No.15.	Helicity rule with examples	

OC 19 & OC 20 2units Pericyclic Reactions I and Pericyclic Reactions II **31 hrs**

L. No.	Topic	Remarks
Lecture No.1.	Criteria for aromaticity- Theile's Theory- Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.	
Lecture No.2.	Criteria for aromaticity- craig's rule, - Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.	

Lecture No.3.	Criteria for aromaticity- Frost-Muslin diagrams- Cyclopropenium ion, cyclopentadienyl ion.	
Lecture No.4.	Criteria for aromaticity- Frost-Muslin diagrams- cycloheptatrienium ion, azulene and annulenes.	
Lecture No.5.	Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds such as Cyclopropenium ion, cyclopentadienyl ion	
Lecture No.6.	Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds such as cycloheptatrienium ion, azulene and annulenes	
Lecture No.7.	Introduction, definition of pericyclic reactions - Characteristics and classification of pericyclic reactions	
Lecture No.8.	Electrocyclic reactions—4ne and 4n+2e type examples	
Lecture No.9.	Cycloaddition & cycloreversions reactions—4ne and 4n+2e type examples	
Lecture No.10.	Sigmatropic reactions—4ne and 4n+2e type examples	
Lecture No.11.	Molecular orbital theory and their symmetry- molecular orbitals of C-C, molecular orbitals of C=C	
Lecture No.12.	Molecular orbital theory and their symmetry-molecular orbitals for conjugated systems	
Lecture No.13.	Molecular orbitals and their symmetry of 1,3-butadiene	
Lecture No.14.	Molecular orbitals and their symmetry of 1,3,5-hexatriene	
Lecture No.15.	Molecular orbitals of conjugated systems- allylic systems	
Lecture No.16.	Approaches for the interpretation of mechanisms for pericyclic reactions-PMO method- Electrocyclisations and selection rules	
Lecture No.17.	Approaches for the interpretation of mechanisms for pericyclic reactions-PMO method- Electrocyclisations and selection rules	
Lecture No.18.	FMO method - Electrocyclisations and selection rules	
Lecture No. 19.	FMO method - Electrocyclisations and selection rules	
Lecture No. 20.	Orbital symmetry correlation diagram method- Electrocyclisations and selection rules	
Lecture No. 21.	Orbital symmetry correlation diagram method- Electrocyclisations	

	and selection rules	
Lecture No. 22.	Cyclo Addition Reactions- PMO method- selection rules	
Lecture No. 23.	Cyclo Addition Reactions- PMO method- selection rules	
Lecture No. 24.	Cyclo Addition Reactions- FMO method- selection rules	
Lecture No. 25.	Cyclo Addition Reactions- FMO method- selection rules	
Lecture No. 26.	Cyclo Addition Reactions- Orbital symmetry correlation diagram method - selection rules	
Lecture No. 27.	Cyclo Addition Reactions- Orbital symmetry correlation diagram method - selection rules	
Lecture No. 28.	Sigmatropic reactions- PMO method- selection rules	
Lecture No. 29.	Sigmatropic reactions- PMO method- selection rules	
Lecture No. 30.	Sigmatropic reactions- FMO method- selection rules and sigmatropic reactions cannot be explained by Orbital symmetry correlation diagram method	
Lecture No. 31.	Sigmatropic reactions- FMO method- selection rules and sigmatropic reactions cannot be explained by Orbital symmetry correlation diagram method	

Recommended Books :

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
9. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
10. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
11. Optical rotatory dispersion by C Djerassi
12. Optical rotatory dispersion and circular dichroism by P Crabbe
13. Mechanism and Structure in Organic chemistry by S Mukherjee
14. Advanced Organic Chemistry: Reactions, Mechanisms & Structure by Michael B Smith & Jerry March
15. Pericyclic Reactions by Mukherjee S M

16. Conservation of Orbital Symmetry by Woodward and Hoffmann
17. Organic Reactions and Orbital Symmetry, Gilchrist and Storr
18. Pericyclic Reactions — a problem solving approach, Lehr and Merchand
19. The Nature of Chemistry — Units 17-19 - Aromaticity — Open University, U K. Publications
20. The aromaticity III level, units 17-19 British open university volumes
21. Aromatic character and aromaticity by G.M.Badger
22. Non-benzenoid aromatic compounds by D.Ginsberg
23. Nonbenzenoid compounds by Lloyds

Paper-4 CH 304T: Photochemistry, synthetic strategies and Green Chemistry

OC-21 Photochemistry
OC-22 Synthetic strategies - I
OC-23 Synthetic strategies - II
OC-24 Green Chemistry

Unit 21: Photo Chemistry -20 Marks

Sl.No.	Name Of the topic	Remarks
Lecture-1	Introduction, Photochemistry of (π , π *) transitions:	
Lecture-2	Excited states of alkenes, cis-trans isomerization	
Lecture-3	Photostationary state, electrocyclisation and sigmatropic rearrangements,	
Lecture-4	di- π methane rearrangement. Intermolecular reactions, photocycloadditions,	
Lecture-5	Photodimerisation of simple and conjugated olefins,	
Lecture-6	Addition of olefins to α , β -unsaturated carbonyl compounds.	
Lecture-7	Excited states of aromatic compounds, Photoisomerisation of benzene,	
Lecture-8	Photochemistry of (n- π *) transitions: Excited states of carbonyl compounds	
Lecture-9	Homolytic cleavage of α - bond, Norrish type I reactions in acyclic and cyclic ketones and	
Lecture-10	strained cycloalkanediones	
Lecture-11	Intermolecular abstraction of hydrogen: photo reduction - influence of temperature, solvent, nature of hydrogen donor and structure of the substrate Intramolecular abstraction of hydrogen:	
Lecture-12	Photo reduction factors -influencing	
Lecture-13	Norrish type II reactions in ketones, Esters and 1, 2- diketones,	
Lecture-14	Norrish type II reactions- Exercise	
Lecture-15	Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.	

Unit 22: Synthetic Strategies I -20 Marks

Sl.No.	Name Of the topic	Remarks
Lecture-1	Synthetic Strategies; Introduction, Terminology: target, synthon, synthetic equivalent with examples.	
Lecture-2	Functional group interconversion (FGI), functional group addition	
Lecture-3	Functional group elimination	
Lecture-4	Criteria for selection of target.	
Lecture-5	Linear and convergent synthesis, explanation with examples.	
Lecture-6	Retrosynthetic analysis and synthesis involving chemoselectivity,	
Lecture-7	Guidelines	
Lecture-8	Regioselectivity, explanation with examples.	
Lecture-9	Reversal of polarity and cyclizations.	
Lecture-10	Order of events in synthesis by retrosynthetic approach, explanation with examples Salbutamol.	
Lecture-11	Propoxycaine.	
Lecture-12	Dinocap.	
Lecture-13	Introduction to one group C-C - examples	
Lecture-14	C-X disconnections - examples	
Lecture-15	One group C-C disconnections, Alcohols and carbonyl compounds, ethers and sulphides.	

Unit 23: Synthetic Strategies II-20 Marks

Sl.No.	Name Of the topic	Remarks
Lecture-1	Introduction to two group C-C and C-X disconnections, Two group C-X disconnections;	
Lecture-2	Two group C-X disconnections;	
Lecture-3	1, 1- difunctionalised, 1, 2-difunctionalised and 1, 3-difunctionalised compounds.	
Lecture-4	Two group C-C disconnections; Diels-Alder reaction, 1,3-difunctionalised compounds,	
Lecture-5	1,5- difunctionalised compounds, Michael addition	
Lecture-6	1,5- difunctionalised compounds , Robinson annulation.	
Lecture-7	Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid.	
Lecture-8	Strategic bond: definition, choosing disconnection/guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection,	
Lecture-9	Guidelines for disconnections.	
Lecture-10	Disconnection corresponding to known reliable reaction, high yielding steps and	

	recognizable starting materials.	
Lecture-11	Other approaches to retrosynthesis – biomimetic approach (Johnsons polyene cyclisation),	
Lecture-12	retro mass spectral fragmentation	
Lecture-13	Application of the strategies to the synthesis of (+) Disparlure,	
Lecture-14	Retronecene,	
Lecture-15	Longifoline	

Unit 24: Green Chemistry -20 Marks

Sl.No.	Name Of the topic	Remarks
Lecture-1	Introduction. Principles, atom economy and scope.	
Lecture-2	Introduction to alternative approaches.	
Lecture-3	**1.** Solvent free reactions-principle, scope, utility of solvent free condition reactions..	
Lecture-4	Organic Synthesis in solid state (without using any solvent): Michael addition, Beckmann rearrangement, Synthesis of aziridines; solid supported organic synthesis: Synthesis of aziridines, pyridines, chromenes and flavones	
Lecture-5	**2.** Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation, Dihydroxylation (Syn- & Anti-)	
Lecture-6	**3.** Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects:	
Lecture-7	a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions	
Lecture-8	.. b) Microwave assisted reactions in water -Hoffmann elimination, hydrolysis, oxidation, saponification reactions.	
Lecture-9	c) Microwave assisted reactions in organic solvents- Esterification reactions, Fries rearrangement, Orthoester Claisen rearrangement, Diels- Alder reaction, decarboxylation.	
Lecture-10	d) Microwave assisted reactions under PTC conditions	
Lecture-11	**4.** Ultrasound assisted reactions: introduction,	
Lecture-12	substitution reactions, addition, oxidation, reduction reactions.	
Lecture-13	**5.** Organo-catalysis:Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker's Yeast.	
Lecture-14	Solid state synthesis	
Lecture-15	**6.** Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).	

Recommended Books

1. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
2. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
3. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.
4. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH.
5. Molecular Reactions and Photo chemistry by Depuy and Chapman
6. Photochemistry by C W J Wells
7. Organic Photochemistry by Turro
8. Molecular Photochemistry by Gilbert & Baggo

9. Organic Photochemistry by D Coyle
10. Organic Synthesis-The disconnection approach by S Warren
11. Organic Synthesis by C Willis and M Willis
12. Problems on organic synthesis by Stuart Warren

M.Sc. CHEMISTRY(ORGANIC CHEMISTRY)
IV SEMESTER SYLLABUS, blow up 2017-18

Paper-1 CH (OC) 401T: Drug Design and Drug Discovery
OC-25: Principles of Drug design and drug discovery
OC-26: Lead modification and SAR Studies
OC 27: QSAR studies
OC 28: Combinatorial Synthesis

Lecture No	TOPIC	Remarks
	OC- 25: Principles of Drug design and drug discovery	
Lecture-1	Introduction to drug discovery. Folklore drugs, stages involved in drug discovery	
Lecture-2	Drug targets, bioassay	
Lecture-3	Discovery of lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs).	
Lecture-4	Pharmacokinetics to pharmacokinetics: absorbtion and Distribution	
Lecture-5	Pharmacokinetics: Metabolism and excretion	
Lecture-6	pharmacodynamics. Introduction: Nature of drug – receptor interactions and their theories – Occupancy theory,.	
Lecture-7	Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation	
Lecture-8	Pharmacophore - structure pruning technique e.g. morphine	
Lecture-9	Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine)	
Lecture-10	Principles of design of enzyme inhibitors (e.g. captopril).	
Lecture-11	Drug discovery without lead – serendipity-Penicillin and Librium as examples.	
Lecture-12	Introduction to prodrugs: Principles of prodrug design: to improve membrane permeability	
Lecture-13	Prodrugs to prolong drug activity, prodrugs to mask toxicity and side	

	effects	
Lecture-14	Introduction to drug patents	
Lecture-15	Clinical trials.	
	OC-26: Lead modification and SAR Studies	
Lecture-1	Introduction to SAR and binding role of the functional groups	
Lecture-2	Bioisosterism, lead modification strategies: variation of alkyl substituents	
Lecture-3	Variation of alkyl substituents	
Lecture-4	Chain homologation and branching	
Lecture-5	Variation of aromatic substituents, extension of structure	
Lecture-6	Extension of the structure, ring expansion and ring contraction,	
Lecture-7	Ring variation, variation and position of heteroatoms, ring fusion,	
Lecture-8	Rring expansion and ring contraction, ring variation, variation and position of heteroatoms, ring fusion,	
Lecture-9	Simplification of the lead.	
Lecture-10	Rigidification of lead	
Lecture-11	Discovery of oxamniquine	
Lecture-12	Discovery of captopril	
Lecture-13	Discovery of salbutamol, cimitidine	
Lecture-14	Structure-Activity Relationship studies in sulfa drugs, benzodiazepines	
Lecture-15	Structure-Activity Relationship studies of Taxol analogs	
	Structure- Activity Relationship (QSAR) studies	
Lecture-1	Introduction: Graphs and equations	
Lecture-2	physicochemical properties: Hydrophobicity,	
Lecture-3	Electronic effects and Hammett constants (σ)	
Lecture-4	lipophilicity constant (π),	
Lecture-5	Steric effects and Taft's constant,	
Lecture-6	linear and nonlinear relationship between biological activity and Hammett/ Lipophilicity Substituent constants	
Lecture-7	Lipinski rule of five. Hansch analysis,	
Lecture-8	Craig's plot	
Lecture-9	Topliss scheme	
Lecture-10	Free Wilson approach	
Lecture-11	cluster significant analysis. Three case studies.	
Lecture-12	cluster significant analysis. Three case studies.	
Lecture-13	Introduction to Molecular modelling: Principles of molecular modeling in drug design.	
Lecture-14	Principles of molecular modeling in drug design.	
Lecture-15	Case study	
	OC-28: Combinatorial Synthesis	
Lecture-1	Introduction. Combinatorial approach.	
Lecture-2	Combinatorial libraries, technologies.	
Lecture-3	Solid phase synthesis, techniques.	
Lecture-4	Solid phase synthesis: types of resins. Linkers.	

Lecture-5	Methods of Parallel synthesis: Haughton's tea bag procedure.	
Lecture-6	Automated parallel synthesis	
Lecture-7	Methods in mixed combinatorial synthesis: general principles.	
Lecture-8	Furkas mix and split combinatorial synthesis,	
Lecture-9	Structure determination of active compounds-Deconvolution, Methods in deconvolution.	
Lecture-10	recursive deconvolution, tagging and use of decoded sheets.	
Lecture-11	Planning and designing of combinatorial synthesis,	
Lecture-12	Examples of Combinatorial Chemistry.	
Lecture-13	Examples of Combinatorial Chemistry.	
Lecture-14	Spider like scaffolds, drug molecules	

Recommended books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11.Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishan singh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
1 6.Strategies for organic drug synthesis and design By Daniel Ledneicer.
1 7.Top Drugs: Top synthetic routes By John Saunders
I 8.Chirotechnoiogy By Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342–6363. http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

Paper CH (OC) 402T: Drug synthesis and mechanism of action
OC-29: Drugs acting on metabolic process, cell wall and specific enzymes
OC-30: Drugs acting on genetic material and immune system
OC-31: Drugs acting on receptors and ion channels
OC-32: Chiral drugs
OC-29: Drugs acting on metabolic process, cell wall and specific enzymes (16 hrs)

Lecture No.	Topic	
Lecture 1	**Drugs acting on metabolic process, cell wall and specific enzymes :** Basic concepts of mechanism of drug action**:** Introduction to macromolecular targets	
Lecture 2	carbohydrates, proteins, lipids and nucleic acids as possible drug targets	
Lecture 3	Classification of drugs: Enzyme inhibition and its types: **a)** Drugs acting on metabolic process: Antifolates	
Lecture 4	Discovery and mechanism of action of sulphonamides,	
Lecture 5	Synthesis of sulfomethoxazole, sulfodoxine	
Lecture 6	Sulfaguanidine, and dapsone	
Lecture 7	Diaminopyrimidine, trimethoprim	
Lecture 8	bacterial resistance to sulfonamides and drug synergism	
Lecture 9	**b)** Drugs acting on cell wall: Structure of bacterial cell wall: β-Lactam antibiotics	
Lecture 10	, mechanism of action of penicillins and cephalosporins	
Lecture 11	Synthesis of pencillin-G and cephalosporin-C	
Lecture 12	cefalexin and cycloserine, Resistance to pencillins	
Lecture 13	broad spectrum penicillins: cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin	
Lecture 14	β-Lactamase inhibitors – Structural formulae and mode of	

	action of clavulonic acid and sulbactum	
Lecture 15	**c)** Drugs acting on specific enzymes: H+/K+ -ATPase inhibitors, synthesis of Omeprazole	
Lecture 16	Carbonic anhydrase inhibitors, synthesis of Acetazolamide	

OC-30: Drugs acting on genetic material and immune system (20 hrs)

Lecture. No.	Topic	Remarks
Lecture 1	Drugs acting on genetic material: Introduction, classification and mechanism of action.	
Lecture 2	a) DNA-intercalating agents-Anticancer and antimalarial agents	
Lecture 3	Structural formulae of Daunomycin, Adriamycin, and Amsacrine	
Lecture 4	Synthesis of Amscarine, Nitracrine,	
Lecture 5	Quinacrine and Chloroquine	
Lecture 6	c) DNA- Binding and nicking agents: Antiprotozoal drugs	
Lecture 7	Synthesis of Metronidazole, Dimetridazole	
Lecture 8	and Tinidazole	
Lecture 9	DNA-Alkylators: Synthesis of Cyclophosphamide	
Lecture 10	and Bisulphan	
Lecture 11	d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir	
Lecture 12	and AZT	
Lecture 13	e) DNA-Topoisomerase inhibitors: Antibacterial agents: Synthesis of Ciprofloxacin	
Lecture 14	and Norfloxacin	
Lecture 15	Structural formulae of floxacin and Lomefloxacin	
Lecture 16	f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents	

Lecture 17	structural formulae of Rifamycins, synthesis of Rifampicin	
Lecture 18	g) Drugs interfering with translation process: Antibacterial drugs, Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin	
Lecture 19	Drugs acting on immune system: Introduction to immune system: immuno supressing agent structural formula of Cyclosporin.	
Lecture 20	Immuno enhancers- use of vaccines and strucrural formula of levamisol.	

OC-31: Drugs acting on receptors and ion channels (18 hrs)

Lecture. No.	Topic	Remarks
Lecture 1	Introduction to nervous system: structure of neuron, nerve transmission	
Lecture 2	Definition and examples of agonist, antagonist, neurotransmittersand receptors	
Lecture 3	Drugs acting on receptors: a)Adrenergic receptors: Introduction and classification: α-Adrenergic-receptor agonists and antagonists	
Lecture 4	Synthesis and biological activity of Nor-adrenaline,	
Lecture 5	Methyl L dopa, Tetrazosin	
Lecture 6	β-Adrenergic-receptor - agonists and antagonists, Structural formulae of Nicotine, Atropine and Tubocurarine.	
Lecture 7	Synthesis and pharmacological activity of Salbutamol, Tetrabutalin,	
Lecture 8	Propranolol, and Atenolol	
Lecture 9	b)Cholinergic-receptors: Introduction and classification, Cholinergic-receptor agonists and antagonists, Structural formulae of Nicotine, Atropine and Tubocurarine	
Lecture 10	Synthesis of Acetyl choline and Succinyl choline	

Lecture 11	c)Dopamine receptors:. Introduction and classification	
Lecture 12	.Dopamine- receptor agonists and antagonists- Biosynthesis of Dopamine	
Lecture 13	Synthesis of L-Dopa and Chlorpromazine	
Lecture 14	d)Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists- synthesis and pharmacological activity of Serotonin	
Lecture 15	and Metoclopramide.	
Lecture 16	e)Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists synthesis	
Lecture 17	and biological action of Histamine,	
Lecture 18	Chloropheneramine and Ranitidine	

OC-32: Chiral drugs (16 hrs)

Lecture. No.	Topic	Remarks
Lecture 1	Introduction to chiral drugs.	
Lecture 2	Three-point contact model	
Lecture 3	Eutomer, Distomer and eudesmic ratio	
Lecture 4	Pfeiffer's rule	
Lecture 5	Role of chirality on biological activity: Distomers – a) with no side effects b)with undesirable side effects	
Lecture 6	c) both isomers having independent therapeutic value d)combination products having therapeutic advantages	
Lecture 7	e) metabolic chirality inversion.	
Lecture 8	Synthesis and pharmacological activity of: S-Ibuprofen, S- Metaprolol	
Lecture 9	Ininavir sulfate, Levocetirizine,	
Lecture 10	2S-Verapamil, S,S-Ethambutol ,	

Lecture 11	(+)Lomefloxacin, Fluvastatin,	
Lecture 12	Dextropropoxyphen, (+)Ephedrine,	
Lecture 13	(+)Griseofulvin, Dexormaplatin,	
Lecture 14	R-Indacrinone, Nateglinide,	
Lecture 15	Oxybutynin hydrochloride, S,S- Captopril.	
Lecture 16	and S,S,S- Enalaprilate	

Recommended Books:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foye etal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishan singh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotecchnology By Roger A. Sheldon

Paper-3 CH (OC) 403T: Advanced Heterocyclic Chemistry

OC-33: Non aromatic heterocyclics
OC-34: Five and six membered heterocyclics with two hetero atoms
OC-35: Heterocyclics with more than two hetero atoms
OC-36: Larger ring and other heterocycles

OC-33: Nonaromatic heterocyclics **17 Hrs**

L. No.	Topic	Remarks
Lecture No.1.	Introduction: Definition, Heterocyclic compounds- Aromatic and Non-aromatic heterocycles, Classification based on the number of atoms: Small, medium and large	
Lecture No.2.	Heterocycles: containing 0ne hetero atom, containing two hetero atoms- same and different, containing more than two hetero atoms- same and different.	
Lecture No.3.	Types of strains: repulsive forces and attractive forces, steric hinderence, interactions and confirmationsal aspects- cis- & trans- and E- & Z- isomers of non aromatic heterocycles.	
Lecture No.4.	Introduction to three membered heterocycles and stability compared with cyclo propane molecule, Azirines-structure, synthesis, reactivity and importance.	
Lecture No.5.	Azirines- reactivity and importance	
Lecture No.6.	Aziridines- structure, synthesis, reactivity and importance	
Lecture No.7.	Aziridines- reactivity and importance	
Lecture No.8.	Oxiranes- structure, synthesis, reactivity: in comparision with aziridines and importance	
Lecture No.9.	Thiiranes- structure, synthesis, reactivity: in comparision with aziridines and importance	
Lecture No.10.	Diazirines- structure, synthesis	
Lecture No.11.	Diaziridines - structure, synthesis	
Lecture No.12.	Diaziridines - reactivity and importance	
Lecture No.13.	Oxaziridines - structure, synthesis	
Lecture No.14.	Oxaziridines - reactivity: in comparision with diaziridines and importance	

Lecture No.15.	Introduction to four membered heterocycles and stability compared with cyclo butane molecule, Azetidines -structure, synthesis, reactivity and importance	
Lecture No.16.	Oxetanes- structure, synthesis, reactivity and importance	
Lecture No.17.	Thietanes- structure, synthesis, reactivity and importance	

OC-34: Five and six membered heterocyclics with two hetero atoms 16 Hrs

L. No.	Topic	Remarks
Lecture No.1.	Introduction to five membered heterocyces: one hetero atom and two hetero atoms, Pyrazole - structure, aromatic character,synthesis	
Lecture No.2.	Pyrazole - reactivity and importance	
Lecture No.3.	Imidazole - structure, aromatic character, synthesis, reactivity and	
Lecture No.4.	Imidazole – Reactivity and comparing the reactivity with pyrazole and importance	
Lecture No.5.	Oxazole - structure, aromatic character, synthesis, reactivity and comparing the reactivity with imidazole and importance	
Lecture No.6.	Thiazoles- structure, aromatic character, synthesis, reactivity and comparing the reactivity with imidazole and importance	
Lecture No.7.	Isoxazole - structure, aromatic character, synthesis	
Lecture No.8.	Isoxazole-reactivity and comparing the reactivity with pyrazole and importance	
Lecture No.9.	Isothiazole - structure, aromatic character, synthesis,	
Lecture No.10.	Isothiazole-reactivity and comparing the reactivity with pyrazole and importance	
Lecture No.11.	Pyridazine - structure, aromatic character, synthesis, reactivity and importance	
Lecture No.12.	Pyrimidine - structure, aromatic character, synthesis, reactivity and comparing the reactivity with pyridazine and importance	
Lecture No.13.	Pyrazine - structure, aromatic character, synthesis, reactivity and comparing the reactivity with pyridazine and importance	

Lecture No.14.	Oxazine- structure, aromatic character,synthesis, reactivity and importance	
Lecture No.15.	Thiazine- structure, aromatic character,synthesis, reactivity and importance	
Lecture No.16.	Benzimidazole, Benzoxazoleand Benzthiazole - structure, aromatic character,synthesis	

OC-35: Heterocyclics with more than two hetero atoms **20 Hrs**

L. No.	Topic	Remarks
Lecture No.1.	1,2,3-triazoies- Synthesis, aromatic character	
Lecture No.2.	1,2,3-triazoies- reactivity and importance	
Lecture No.3.	1,2,4-triazoles- Synthesis, aromatic character	
Lecture No.4.	1,2,4-triazoles- reactivity and importance	
Lecture No.5.	Tetrazoles- Synthesis, reactivity, aromatic character and importance	
Lecture No.6.	1,2,4-oxadiazole- Synthesis, aromatic character	
Lecture No.7.	1,2,4-oxadiazole- reactivity and importance	
Lecture No.8.	1 ,3,4-oxadiazole- - Synthesis, aromatic character	
Lecture No.9.	1 ,3,4-oxadiazole- - reactivity and importance	
Lecture No.10.	1,2,5- oxadiazole Synthesis, aromatic character	
Lecture No.11.	1,2,5- oxadiazole- - reactivity and importance	
Lecture No.12.	1,2,3-thiadiazoles- Synthesis, reactivity, aromatic character and importance	
Lecture No.13.	1,3,4- thiadiazoles- Synthesis, reactivity, aromatic character and importance	
Lecture No.14.	1,2,5- thiadiazoles- Synthesis, reactivity, aromatic character and importance	
Lecture No.15.	1,2,3-triazine- Synthesis, reactivity, aromatic character and importance	
Lecture No.16.	1,2,4- triazine- Synthesis, reactivity, aromatic character and importance	

Lecture No.17.	1,3,5- triazine- Synthesis, reactivity, aromatic character and importance	
Lecture No.18.	Tetrazines- Synthesis, reactivity, aromatic character and importance	
Lecture No.19.	Synthesis and importance of purines and pteridines	
Lecture No.20.	Syntheis of Caffeine, theobromine and theophylline.	

OC-36: Larger ring and other Heterocycles **8 Hrs**

L. No.	Topic	Remarks
Lecture No.1.	Introduction to larger ring heterocycles, Azepines- Synthesis, structure, stability and reactivity	
Lecture No.2.	Oxepines- Synthesis, structure, stability and reactivity	
Lecture No.3.	Thiepines- Synthesis, structure, stability and reactivity	
Lecture No.4.	Synthesis of Diazepines rearrangements of 1,2 - diazepines	
Lecture No.5.	Synthesis of Benzoazepines, Benzodiazepines	
Lecture No.6.	Synthesis of Benzooxepines, Benzothiepines	
Lecture No.7.	Synthesis of Azocines and Azonines	
Lecture No.8.	Synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.	

Recommended Books:

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule & K.Mills
4. Principles of Modern Heterocyclie Chemistry, A.Paquette
5. Heterocyclic Chemistry, J,A.Joule & Smith
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky

Paper-4 – CH404T(CB1): Advanced Natural Products

OC(CB_1)-1: Biosynthesis of natural products

OC(CB_1)-2-: Structure determination and stereochemistry of natural products by chemical methods.

OC(CB_1)--3: Structure determination and stereochemistry of natural products by spectral methods.

OC(CB_1)--4: Total stereo selective synthesis of natural products.

Lecture No	Topic	Remarks

	OC(CB_1)-1: Biosynthesis of natural products	
Lecture 1	Biosynthesis of secondary metabolites: Introduction	
Lecture 2	Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism	
Lecture 3	Methods for determination of biosynthetic mechanism	
Lecture 4	Isolation and identification of Biosynthetic precursors	
Lecture 5	Feeding experiments – use of radioisotopes	
Lecture 6	Feeding experiments – use of radioisotopes	
Lecture 7	Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods	
Lecture 8	Identification of the position of labels in labeled natural products by chemical degradation and spectral methods	
Lecture 9	Acetate-Malonate pathway: Biosynthesis of aromatic compounds,	
Lecture 10	Shikimic acid pathway; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan,	
Lecture 11	carboxylic acid derivatives, flavonoids and morphine alkaloids	
Lecture 12	Biosynthesis of terpenes – mono, sesqui, di, tri (β -amyrin)	
Lecture 13	Biosynthesis of terpenes – mono, sesqui, di, tri (β -amyrin)	
Lecture 14	carotenoids, steroids – cholesterol.	
Lecture 15	carotenoids, steroids – cholesterol.	

OC(CB_1)-2-: . Structure determination and stereochemistry of natural products by chemical methods

Lecture No.	Topic	Remarks
Lecture 1	**Determination of structure and stereochemistry of:** Morphine-Introduction	
Lecture 2	Morphine-Structure elucidation	
Lecture 3	Morphine-Stereo Chemistry	
Lecture 4	Morphine-Total synthesis	
Lecture 5	Reserpine- Introduction	
Lecture 6	Reserpine- Structure elucidation	
Lecture 7	Reserpine- Stereo Chemistry & Synthesis	
Lecture 8	Abietic acid-Introduction	
Lecture 9	Abietic acid- Structure elucidation	
Lecture 10	Abietic acid- Stereo Chemistry & Synthesis	

Lecture 11	Cholesterol-Introduction	
Lecture 12	Cholesterol-Structure elucidation	
Lecture 13	Cholesterol-Stereo Chemistry	
Lecture 14	Cholesterol-Total synthesis	
Lecture 15	Rotenone-Introduction	
Lecture 16	Rotenone-Structure elucidation	
Lecture 17	Rotenone-Stereo Chemistry	
Lecture 18	Rotenone-Total synthesis	

OC(CB_1)-3: Structure determination and stereochemistry of natural products by spectral methods **16 Hrs**

L. No.	Topic	Remarks
Lecture No.1.	IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, 2D INADEQUATE and MS of Flavones-Chrysin	
Lecture No.2.	IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, 2D INADEQUATE and MS of Isoflavones-Diadzein	
Lecture No.3.	IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, 2D INADEQUATE and MS of Flavanones-2,3-dihydroflavone	
Lecture No.4.	IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, 2D INADEQUATE and MS of Coumarin- Umbelliferone	
Lecture No.5.	IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, NOESY, 2D INADEQUATE and MS of Biflavones-Taxus biflavone	
Lecture No.6.	IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, of Quinoline-Cusparine	
Lecture No.7.	NOESY, 2D INADEQUATE and MS of Quinoline-Cusparine	
Lecture No.8.	IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, of Isoquinolines-papaverine	
Lecture No.9.	NOESY, 2D INADEQUATE and MS of Isoquinolines-papaverine	
Lecture No.10.	IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, NOESY, 2D INADEQUATE and MS of Monoterpenes-Geraniol and Nerol- A comparative study.	

Lecture No.11.	INEPT of Menthol- $\Delta = ¼\ J_{CH}$; $^{1/2}J_{CH}$; $^{3/4}J_{CH}$	
Lecture No.12.	APT of Apparicine- Indole alkaloid	
Lecture No.13.	2DJ Resolved Spectrum of Strictcine	
Lecture No.14.	NOESY of Buxaquamarine	
Lecture No.15.	HETEROCOSY of Strictanol	
Lecture No.16.	2D INADEQUATE of α-picoline and β-methyltetrahydrafuran	

OC(CB1)--4: Total stereoselective synthesis of natural products

S. No.	Topic	Remarks
Lecture 1	Woodward's synthesis of reserpine	
Lecture 2	reserpine	
Lecture 3	Cholesterol- Total stereoselective synthesis	
Lecture 4	cholesterol -Total stereoselective synthesis	
Lecture 5	Corey's synthesis of prostaglandins (E2, F2 α)	
Lecture 6	(E2, F2 α) -Total stereoselective synthesis	
Lecture 7	paeoriflorin -Total stereoselective synthesis	
Lecture 8	paeoriflorin -Total stereoselective synthesis	
Lecture 9	Sharpless synthesis of L-hexoses	
Lecture 10	Different L-hexoses synthesis	
Lecture 11	Different L-hexoses synthesis	
Lecture 12	Nicolaous synthesis of taxol	
Lecture 13	Nicolaous synthesis of taxol	
Lecture 14	Nicolaous synthesis of taxol	
Lecture 15	Danishefsky synthesis of indolizomycin	
Lecture 16	Takasago synthesis of menthol	

Lecture 17	Hoffmann-LaRoche synthesis of Biotin.	
Lecture 18	Biotin synthesis	

Recommended books:

1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser arid Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo
11. Alkaloids by Pelletier
12. Total synthesis of Natural Products by Apsimon Vol 1-5
13. Biosynthesis by Geismann
14. Principles of organic synthesis 3rd Ed.R O C Norman and J M Coxen
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster