Annexure-I

Centre for Pharmaceutical Sciences and Natural Products

M.Sc. in Chemical Sciences (Medicinal Chemistry)

SEMESTER 1

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	MCL.501	Computer Applications	FC	2	-	-	2	10	15	15	10	50
2	MCP.502	Computer Applications-Practical	FC	-	-	4	2	-	-	-	-	50
3	MCL.503	Research Methodology	FC	2	-	-	2	10	15	15	10	50
4	MCL.504	Biostatistics	FC	2	-	-	2	10	15	15	10	50
5	MCL.505	Inorganic Chemistry-I	CC	4	1	-	4	25	25	25	25	100
6	MCP.506	Inorganic Chemistry-I-Practical	CC	-	-	4	2	-	-	-	-	50
7	MCL.507	Organic Chemistry-I	CC	4	1	-	4	25	25	25	25	100
8	MCP.508	Organic Chemistry-I-Practical	CC	-	-	4	2	-	-	-	-	50
9	MCL.509	Physical Chemistry-I	EC	4	1	-	4	25	25	25	25	100
	XXX	Inter-Disciplinary (ID) Course (Opt any one from other Centres)	EC	2	-	-	2	10	15	15	10	50
		Total		**20**	**3**	**8**	**26**					**650**

FC: Foundation Course, **CC**: Core Course, **EC**: Elective Course

A: Surprise Tests (minimum three): Based on Objective Type Tests

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

L: Lectures T: Tutorial P: Practical Cr: Credits

SEMESTER 2

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	MCL.510	Inorganic Chemistry-II	CC	4	1	-	4	25	25	25	25	100
2	MCP.511	Inorganic Chemistry-II - Practical	CC	-	-	4	2	-	-	-	-	50
3	MCL.512	Organic Chemistry-II	EC	4	1	-	4	25	25	25	25	100
4	MCL.513	Physical Chemistry-II	CC	4	1	-	4	25	25	25	25	100
5	MCP.514	Physical Chemistry-II Practical	CC	-	-	4	2	-	-	-	-	50
Opt any one course from following elective courses												
6	MCL.515	Chemistry of Natural Products	EC	4	-	-	4	25	25	25	25	100
	MCL.516	Quantum Chemistry										
7	MCS.599	Seminar	FC	-	-	-	2	-	-	-	-	50
8	XXX	Inter-Disciplinary Course (ID) (Opt any one from other Centres)	EC	2	1	-	2	10	15	15	10	50
		Total		**18**	**4**	**8**	**24**					**600**

FC: Foundation Course, **CC**: Core Course, **EC**: Elective Course

A: Surprise Tests (minimum three): Based on Objective Type Tests

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

L: Lectures T: Tutorial P: Practical Cr: Credits

SEMESTER 3

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	MCL.601	Inorganic Chemistry-III	EC	4	1	-	4	25	25	25	25	100
2	MCL.602	Organic Chemistry-III	CC	4	1	-	4	25	25	25	25	100
3	MCP.603	Organic Synthesis and Spectral Analysis - Practical	EC	-	-	4	2	-	-	-	-	50
4	MCL.604	Physical Chemistry-III	CC	4	1	-	4	25	25	25	25	100
5	MCL.605	Spectral Analysis	CC	4	1	-	4	25	25	25	25	100
6.	MCS.698	Seminar	FC	-	-	-	2	-	-	-	-	50
Opt any one course from following elective												
7	MCL.606	Medicinal Chemistry-I	EC	4	1	-	4	25	25	25	25	100
	MCL.607	Current Trends in Organic Synthesis										
	MCL.608	Nuclear Chemistry										
	Total			**20**	**5**	**4**	**24**					**600**

FC: Foundation Course, **CC**: Core Course, **EC**: Elective Course

A: Surprise Tests (minimum three): Based on Objective Type Tests

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks **L: Lectures T: Tutorial P: Practical Cr: Credits**

SEMESTER 4

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	MCL.610	Medicinal Chemistry - II	EC	4	1	-	4	25	25	25	25	100
2	MCD.600	Project	CC	-	-	-	20	-	-	-	-	500
		Total		**4**	**1**	**-**	**24**					**600**

CC: Core Course, **EC**: Elective Course

A: Surprise Tests (minimum three): Based on Objective Type Tests

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

F: L: Lectures T: Tutorial P: Practical Cr: Credits

Semester 1

Course Title: Computer Applications
Paper Code: MCL.501

L	T	P	Credits	Marks
2	0	0	2	50

Unit I **9 hours**

Fundamentals of Computers: Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean Algebra. Introduction to computer network and World Wide Web, Storage space, CPU and Memory.

Unit II **9 hours**

MS-Word: Introduction to Word Processing, Creating and Saving Documents, Text Formatting, Tables, Document Review Option, Mail Merge, Inserting Table of Contents, Reference Management.

Unit III **9 hours**

Applications Software: Introduction to MS Paint, Notepad, Spreadsheet applications, Presentation applications, Internet browsers and Image processing applications.

Unit IV **9 hours**

World Wide Web: Origin and concepts, Latency and bandwidth, searching the internet, Advanced web-search using Boolean logic, Networking fundamentals.

Text books:

1. Gookin, D. 2007. MS Word for Dummies. Wiley.
2. Harvey, G. 2007. MS Excel for Dummies. Wiley
3. Sinha, P.K. Computer Fundamentals. BPB Publications.

Suggested Readings:

1. Bott, E. 2009. Windows 7 Inside Out. Microsoft Press.
2. Goel, A., Ray, S. K. 2012. Computers: Basics and Applications. Pearson Education India.

Course Title: Computer Applications-Practical
Paper Code: MCP.502

L	T	P	Credits	Marks
-	-	4	2	50

1. Experimental design and analysis
2. Training on basic usage of Microsoft Word, Miscosoft Excel, Microsoft PowerPoint and Web Browsers
3. Optimizing web search: Google advanced search, Boolean operators, Literature search using Google Scholar, HighWire, Pubmed, Scifinder, etc.
4. Bibliography management and research paper formatting using reference software EndNote
5. Creating a functional website using HTML

Suggested Readings:

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley.
2. Harvey, G. (2007). *MS Excel 2007 for Dummies*. Wiley.
3. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc.
4. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley.

Course Title: Research Methodology

Paper Code: MCL.503

L	T	P	Credits	Marks
2	-	-	-	50

Unit 1 **10 hours**

General principles of research: Meaning and importance of research, Critical thinking, Formulating hypothesis and development of research plan, Review of literature, Interpretation of results and discussion.

Technical writing: Scientific writing, Writing research paper, Poster preparation and Presentation and Dissertation.

Library: Classification systems, e-Library, Reference management, Web-based literature search engines

Unit-2 **10 hours**

Entrepreneurship and business development: Importance of entrepreneurship and its relevance in career growth, Characteristics of entrepreneurs, Developing entrepreneurial competencies, Types of enterprises and ownership (large, medium SSI, tiny and cottage industries, limited, public limited, private limited, partnership, sole proprietorship), Employment, self-employment and entrepreneurship, Financial management-importance and techniques, Financial statements- importance and its interpretation,

Unit-3 **16 hours**

Intellectual Property Rights: Intellectual Property, intellectual property protection (IPP) and intellectual property rights (IPR), WTO (World Trade Organization), WIPO (World Intellectual Property Organization), GATT (General Agreement on Tariff and Trade), TRIPs (Trade Related Intellectual Property Rights), TRIMS (Trade Related Investment Measures) and GATS (General Agreement on Trades in Services), Nuts and Bolts of Patenting, Technology Development/Transfer Commercialization Related Aspects, Ethics and Values in IP.

Suggested Readings:

1. Gupta, S. (2005). *Research methodology and statistical techniques*, Deep & Deep Publications (p) Ltd. New Delhi.
2. Kothari, C. R. (2008.) *Research methodology(s)*, New Age International (p) Limited.New Delhi
3. Best J. W., Khan J. V. (Latest Edition) *Research in Education*, Prentice Hall of India Pvt. Ltd.
4. *Safe science: promoting a culture of safety in academic chemical research*; National Academic Press, www.nap.edu.
5. Copyright Protection in India [website: http:copyright.gov.in].
6. World Trade Organization [website: www.wto.org].
7. Wadedhra B.L. Law Relating to Patents, Trademarks, Copyright Design and Geographical Indications. Universal Law Publishing, New Delhi. Latest Edition.

Course Title: Biostatistics

Paper Code: MCL.504

L	T	P	Credits	Marks
2	-	-	-	50

Unit 1 **10 hours**

Overview of biostatistics: Difference between parametric and non-parametric statistics, Univariant and multivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Unit 2 **5 hours**

Experimental design and analysis: Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods.

Unit 3 **12 hours**

Comparing means of two or more groups: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal–Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, χ^2 test.

Unit 4 **9 hours**

Regression and correlation: Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

Suggested Readings:

1. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
2. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.
3. Bolton, S., & Bon, C. (2009). *Pharmaceutical statistics: practical and clinical applications*. CRC Press.

Course Title: Inorganic Chemistry-I
Paper Code: MCL.505

L	T	P	Credits	Marks
4	1	0	4	100

Total Lectures: 72

Course Objective: To introduce theories, reaction mechanism and stability of the coordination complexes, and their magnetic and electronic properties.

Unit 1 **12 Hrs**

Metal-Ligand Equilibria in Solution

Stepwise and overall formation constant and their interaction, trends in stepwise constants,factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formationconstants by spectrophotometry and Potentiometric (pH) methods.

Unit 2 **20 Hrs**

Reaction Mechanisms of Transition Metal Complexes

Introduction, Potential energy diagram and reactivity of metal complexes, ligand substitution reactions, substitution reactions mechanisms, Labile and Inert metal complexes, Acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reaction. Substitution reactions in square planar complexes, Trans effect, Mechanism of the substitution reaction Reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere. The Marcus theory, doubly bridged inner-sphere transfer, other electron transfer reactions; two electron transfers, Non-complementary reaction, Ligand exchange via electron exchange, reductions by metal complexes hydrated electrons, Berry pseudorotation.

Unit 3 **20 Hrs**

Isomerism; Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, Magnetic properties of transition metal ions and free ions presentive, Effects of L-S coupling on magnetic properties, Temperature independent paramagnetism (TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT), Quenching of orbital angular momentum by crystal fields in complexes in terms of splitting. Effect of spin-orbit coupling and A, E & T states mixing, first order and second order Zeeman effects, Spin paired and spin-free equilibria in complexes magnetic properties of polynuclear complexes involving OH, NH_2 and CN bridges.

Unit 4 **20 Hrs**

Crystal Fields Splitting

Spin-spin, orbital-orbital and spin orbital coupling, LS and J-J coupling schemes, determination of all the spectroscopic terms of p^n, d^n ions, determination of the ground state terms for pn, dn, fn ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, two type of electron

repulsion parameters, spin orbit coupling parameters (λ) energy separation between different j states, The effect of octahedral and tetrahedral fields on S, P, D and F terms (with help of the character table). Splitting patterns of and G, H and I terms. Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d^2 configuration in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d^2 configuration in octahedral field, study of energy level diagrams for higher configurations, selection rules of electronic transitions in transition metal complexes, their proof using group theory, relaxation of the selection rule in Centro symmetric and non-centro symmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, calculation of 10Dq and B with use of Orgel and Tanabe Sugano diagrams, quenching of orbitals angular momentum by ligand field. Variation of the Racah parameter, central field covalency, symmetry restricted covalency, differential radial expansion, spectrochemical series, band intensities, factors influencing band widths.

Course Outcome: The completion of this course will enable the students toacquire knowledge of

1. Reaction mechanism, formation constant and stability of the coordination complexes.
2. Interpretation of the electronic and magnetic properties.

SUGGESTED READINGS

1. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 6th edition, 2007, John Wiley& Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2nd edition, 2005 (reprinted), Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2nd edition, 1984, Elsevier Science Publishers B.V.
5. Carlin, R. L. and Van Duyneveldt, A.J. Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, Springerverlag New York Inc., 1977.
6. Miessler,G. L.and Tarr, D. A. Inorganic Chemistry, 4th edition, 2011, Pearson Education.
7. Figgis, B.N. Introduction to Ligand Field, 1966 Wiley Eastern.
8. Drago, R.S. Physical Method in Chemistry, 1965, W.B. Saunders Company.
9. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5th edition, 2010, Oxford University Press.
10. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
11. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2nd edition, 1993, Affiliated East West Press.
12. Drago, Russell S. Physical Methods for Chemists, 2nd edition, 1992, Saunders College Publishing.

Course Title: Inorganic Chemistry-1-Practical
Paper Code: MCP.506

L	T	P	Credits	Marks
-	-	4	2	50

Course Objective: To impart knowledge of various techniques for analysis of inorganic compounds.

Experiments:

Introduction to good laboratory practices in chemistry.

Gravimetric Estimation
1. Determination of Ba^{2+} as its chromate.
2. Estimation of lead as its lead sulfate.
3. Estimation of Nickel (II) as its nickel dimethyl glyoximate.
4. Estimation of Cu^{2+}as cuprous thiocyanate.

Precipitation Titrations
1. $AgNO_3$ standardization by Mohr's method.
2. Volhard's method for Cl^- determination.

Oxidation-Reduction Titrations
1. Standardization of $KMnO_4$with sodium oxalate and determination of Ca^{2+} ion.
2. Standardization of ceric sulphate with Mohr's salt and determination of Cu^{2+}, NO_2 and $C_2O_4^{-2}$ ions.
3. Standardization of $K_2Cr_2O_7$ with Fe^{2+} and determination of Fe^{3+} (Ferric alum)
4. Standardization of hypo solution with potassium iodate / $K_2Cr_2O_7$ and determination of available Cl_2 in bleaching powder, Sb^{3+} and Cu^{2+}.
5. Determination of hydrazine with KIO_3 titration.

Spectrophotometeric determination: NO_3^- in water sample, $K_2Cr_2O_7$ in the presence of$KMnO_4$ and Fe(III) using 8-hydroxyquinoline.

Flame photometric determination: Li, Na, K and Ca.

Atomic absorption Spectrometry: Estimation of certain transition metals.

Course outcome: The students will acquire knowledge of

1. Volumetric and gravimetric analysis of cations and anions.
2. Standardization and titrations of various inorganic compounds.

SUGGESTED READINGS

1. Pass, G. and Sutcliffe H. *Practical Inorganic Chemistry*, 1st edition, 1979, Chapman and Hall Ltd.
2. Jolly, W.L. *Synthetic Inorganic Chemistry*, 2nd edition, 1961, Prentice Hall, Inc.,.
3. Nakamoto, K. *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B*, 5th edition, 1997, John Wiley and Sons,.
4. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis*, 6th edition, 2000, Pearson Education Ltd.
5. Svehla, G. and Sivasankar, B. *Vogel's Qualitative Inorganic Analysis (revised),* 7th edition, 1996, Pearson Education Ltd.

6. Skoog, D.A., Holler, F.J., and Crouch, S.R., Principles of Instrumental Analysis, 6th Edition, 2007 Thomson Learning.

Course Title: Organic Chemistry-I

Paper Code: MCL.507

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **22 hours**

Stereochemistry: IUPAC nomenclature of organic molecules, Elements of symmetry, Chirality, Projection formulae [Flywedge, Fischer, Newman and Saw horse], Configurational and conformational isomerism in acyclic and cyclic compounds; Stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, Configurational notations of simple molecules, D/L, R/S, *E*/*Z* and *cis*/*trans* configurational notations, *Threo* and *erythro* isomers, Methods of resolution, Optical purity, Enantiotopic and diastereotopic atoms, groups and faces, Stereospecific and stereoselective synthesis, Asymmetric synthesis, Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape, Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus, Conformational analysis of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2-; 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, Effect of conformation on the course of rate of reactions, Effect of conformation on reactivity, Conformation of sugars, strain due to unavoidable crowding, .

Unit 2 **18 hours**

Aliphatic nucleophilic substitution reaction: The S_N2, S_N1, mixed S_N2 and S_N1 and SET mechanism, The S_Ni mechanism. Nucleophilic substitution at an allylic, aliphatic and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, competition between S_N2 and S_N1 mechanisms.

Aromatic nucleophilic substitution: The S_NAr, bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile, Vilsmeier–Haack reaction.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, *ortho/para* ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling.

Unit 3 **16 hours**

Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

Unit 4 **16 hours**

Addition to carbon-hetero multiple bonds: Reactivity of carbonyl group, homologation and dehomologation of carbonyl compounds, nucleophilic addition of hetero-atoms (N,O,S), conjugate addition reactions, acylation of carbonyl carbon, carbonyl cyclizations and cleavages, carboxylic acids and derivatives, decarboxylation reactions, addition of Grignard, organozinc and organolithium reagents to carbonyl and α,β-unsaturated carbonyl compounds, mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides, ammonolysis of esters.

Course Outcome: Students will acquire the knowledge of

1. Conformational analysis of cyclic and acyclic compounds, chirality and reactivity.
2. Mechanistic aspects in nucleophilic and electrophilic substitution.
3. Mechanistic aspects in addition and elimination reactions.

Suggested Readings:

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press, 2nd edition
2. Finar, I.L., (2012). *Organic Chemistry Vol. 1,* Pearson Education, 6th edition, UK.
3. Mc Murry J., *Organic Chemistry***,** Asian Book Pvt. Ltd, 8th edition, New Delhi
4. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
5. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism***,** Narosa Publishing House (P) Ltd., 4th edition, New Delhi-110002.
6. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
7. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
8. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., 3rd edition, New Delhi.
9. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
10. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, New York.
11. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.

12. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry.* Macmillan India Ltd., 3rd edition, New Delhi.
13. Robert and Casereo, (1977). *Basic principle of Organic Chemistry***,** Addison-Wesley, 2nd edition.
14. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10th edition.
15. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition.
16. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

Course Title: Organic Chemistry-1-Practical
Paper Code: MCP.508

L	T	P	Credits	Marks
-	-	4	2	50

(i) **Safety**: Eye, Fire and Chemicals
(ii) Glassware
(iii) Non-glass equipment
(iv) Heating devices
(v) Cleaning Glassware

A. Techniques: (At least One Practical of Each Technique)
Crystallization, Fractional Crystallization, Sublimation, Distillation, Fractional Distillation, Steam Distillation, Vacuum Distillation, Column Chromatography, Thin Layer Chromatography (Purity would be checked by m. p. and mixed m. p.).

B. Preparation of Derivatives: (Each Derivative of two Compounds) Oxime, 2, 4-DNP, Acetyl, Benzoyl, Semicarbazone, Anilide, Amide, Aryloxyacetic acid.

C. Preparations: Single Stage (Any 15)

1 Cyclohexanone to Adipic acid
2 Benzophenone to Benzhydral
3 *m*-Chlorobenzene to 2,4-Dinitrochlorobenzene
4 2,4-Dinitrochlorobenzene to 2,4-Dinitrophenol
5 Acetoacetic ester to 1-Phenyl-3-methyl-5 pyrazolone
6 Benzaldehyde to Cinnamic acid
7 Benzene to *β*-Benzoyl propionic acid
8 Benzaldehyde to Dibenzylidene acetone
9 Benzophenone to Benzpinacol
10 p-Nitrotoluene to p-Nitrobenzoic acid
11 Anisole to 2,4-Dinitroanisole
12 Phthalic anhydride to phthalimide
13 Phthalimide to Anthranilic acid
14 Acetanilide to p-Bromoacetanide
15 p-Bromoacetanide to p-Bromoaniline

16 m-Dinitrobenzene to m-Nitroaniline

17 Synthesis of Phenytoin

D. Use of Computer - Chem Draw-Sketch, ISI – Draw: Draw the structure of simple aliphatic, aromatic, heterocyclic organic compounds with substituents. Get the correct IUPAC name and predict the UV, IR and ^{1}H-NMR signals.

E. Demonstration of Stereochemical aspects of the compounds through molecular models.

ESSENTIAL BOOKS:

1. Harwood, L.M., Moody, C.J. *Experimental Organic Chemistry*, 1st edition, Blackwell Scientific Publishers, 1989.

2. Vogel, A.I. *Text Book of Practical Organic Chemistry*, ELBS, IVth edition, Longman Group Ltd.,1978.

3. Mann, F.G.; Saunders, B.C. *Practical Organic Chemistry*, 4th edition, New Impression, Orient Longman Pvt. Ltd., 1975.

4. Leonard, J.; Lygo, B. *Advanced Practical Organic Chemistry*, Chapman and Hall, 1995.

5. Armarego, W. L., & Chai, C. (2012). *Purification of laboratory chemicals*. Butterworth-Heinemann.

6. Young, J. A. (Ed.). (Latest Edition). *Improving safety in the chemical laboratory: a practical guide*. Wiley.

Course Title: Physical Chemistry-I
Paper Code: MCL.509
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Course Objective: To impart knowledge of advanced classical and statistical thermodynamics.

Unit 1 **14 Hrs**

Thermodynamics: Concepts involved in first, second and third law of thermodynamic, Helmholtz and Gibbs Energies, Maxwell relations, Equilibrium constant, Temperature-dependence of equilibrium constant, Van't Hoff equation.

Unit 2 **14 Hrs**

Partial Molar Properties and Fugacity: Partial molar properties. Chemical potential of a perfect gas, dependence of chemical potential on temperature and pressure, Gibbs- Duhem equation, real gases, fugacity, its importance and determination, standard state for gases.

Solid-Liquid Solutions: Solutions of nonelectrolytes and electrolytes. Colligative properties of solutions, such as osmotic pressure, depression of the freezing point and elevation of the boiling point.

Unit 3 **16 Hrs**

Thermodynamics of Simple Mixtures: Thermodynamic functions for mixing of perfect gases. Chemical potential of liquids. Raoult's law, Henry's law. Thermodynamic functions for mixing of liquids (ideal solutions only). Mixtures of volatile liquids, vapour pressure diagrams. Lever's rule, distillation diagrams. Real solutions and activities, standard states for solvent and solute. Stability of phases, clapeyron equation. Clausius-clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

Unit 4 **28 Hrs**

Statistical Thermodynamics: The concepts of Ensemble, Thermodynamic probability and entropy, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Partition function, Molar partition function, Thermodynamic properties in term of molecular partition function for diatomic molecules, Monoatomic gases, Rotational, Translational, Vibrational and Electronic partition functions for diatomic molecules, Calculation of equilibrium constants in term of partition function. Monoatomic solids, Theories of specific heat for solids.

Course Outcome: The students will acquire knowledge of

1. Classical thermodynamics and understanding thermodynamic phenomenon in a chemical system
2. Statistical thermodynamics and understanding thermodynamic properties in terms of partition functions,
3. Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, theories of specific heat for solids.

SUGGESTED READINGS

1. Barrow, G. M. Physical Chemistry, 5th Edition, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 2-3,5, 5th/3rd Edition, 2011, MACMILLAN,.
3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9th Edition, 2009, Oxford University Press.

4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1st edition, 1998, Viva Books.
5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 3rd edition, 1981, John Wiley and Sons.
6. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. Physical Chemistry, 4th Edition, 2004, Wiley-Interscience Publication.
7. Engel T., Reid, P. and Hehre, W. Physical Chemistry, 3rd Edition, 2012, Pearson Education.
8. Puri, B.R. Sharma L.R. and Pathania M.S. Principles of Physical Chemistry, 46th Edition, 2013, Vishal Publishing Company.
9. Rastogi, R. P. and Mishra, R. R. An Introduction to Chemical Thermodynamics 6th edition, 2013, Vikas Publishing
10. Rajaram, J. and Kuriacose, J. C. Chemical Thermodynamics, Classical , Statistical and Irreversible Thermodynamics, 2013, Pearson Education.
11. Laurendeau N. M. Statistical Thermodynamics: Fundamentals and Applications, 2005, Cambridge University Press.
12. Nash, L. K. Elements of Statistical Thermodynamics, 2nd Edition, 2012, Dover Publication Inc.
13. Hill, T. L. An Introduction to Statistical Thermodynamics, 1986, Dover Publications Inc.

Semester –II

Course Title: Inorganic Chemistry-II
Paper Code: MCL.510
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Course Objective: To introduce the concepts and importance of symmetry and group theory in solving chemical problems and clusters of boranes, orgnaometallics, inorganic chains, rings and cages.

Unit 1 **12 Hrs**

Symmetry

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination,

Unit2 **20 Hrs**

Group theory

determination of reducible and irreducible representations, character tables, construction of character tables for C_2v, C_3v, use of symmetry in obtaining symmetry of orbitals in molecules, qualitative splitting of s, p, d, f orbitals in octahedral, tetrahedral and square planar fields using character tables and without the use of character tables. Ligands symmetry orbitals and metal orbitals involved in molecular orbitals formation in octahedral complexes, MOEL diagrams for octahedral tetrahedral and square planar complexes showing σ and π bonding in transition metal complexes

Unit 3 **20 Hrs**

Metal Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls. Preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygencomplexes, tertiary phosphine as ligand.Organic-transition metal chemistry, complexes with π-acceptor and σ-donor ligands, 18-electron and 16-electron rules, isolobal analogy, structure and bonding, mettalocenes, metal cluster compounds, metal-metal bond, metal carbenes, carbonyl and non-carbonyl clusters, fluxional molecules, application of orgnaometallic compounds as catalysts in organic synthesis.

Unit 4 **20 Hrs**

Inorganic chains, rings and cages

a) **Chains:** Catenation, heterocatenation, isopolyanions and heteropolyanions.
b) **Rings:** Borazines, phosphazenes, other heterocyclic inorganic ring systems, homocyclic inorganic systems.
c) **Cages:** Cage compounds having phosphours, oxygen, nitrogen and sulphur: boron cage compounds, boranes, carboranes and metallocenecarboranes.

Course Outcome: The students will acquire knowledge of

1. Concepts to realize point group within chemical structure, character tables and projection operator techniques.
2. Application of symmetry and group theory in spectroscopy.
3. Structural properties of organometallic complexes and their uses.

SUGGESTED READINGS

1. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 6th edition, 2007, John Wiley& Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2nd edition, 2005 (reprinted), Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2nd edition, 1984, Elsevier Science Publishers B.V.
5. Carlin, R. L. and Van Duyneveldt, A.J. Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, Springerverlag New York Inc., 1977.
6. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5th edition, 2010, Oxford University Press.
7. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
8. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2nd edition, 1993, Affiliated East West Press.
9. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, 1992, Saunders College Publishing

Course Title: Inorganic Chemistry-II-Practical
Paper Code: MCP.511

L	T	P	Credits	Marks
-	-	4	2	50

Total Lectures: 72

Course objective: To teach the synthesis of inorganic complexes and their characterization with instrumental techniques.

1. Preparation of Chloropentaammine cobalt (III) Chloride and its IR measurements.
2. Preparation of $[Co(en)_2Cl_2]Cl$, $Na_2[Fe(CN)_5NH_3].H_2O$, $[UO_2(NO_3)_2Py_2]$, $Cu_2(CH3COO)_4(H_2O)_2$.
3. Preparation of $Hg[Co(CNS)_4]$ and used as standard for the magnetic moment measurement
4. Preparation of cis-and trans-$K[Cr(C_2O_4)_2(H_2O)_2$ and its IR study.
5. Preparation of bis(2,4-pentanedione)vanadium(IV) acetate and its piperidine or pyridine
   complex. Study of both the complexes with the help of infrared, UV-vis spectroscopy and magnetic susceptibility.
6. Preparation of lead tetraacetate.
7. Preparation and separation of isomers of $K_3[Fe(C_2O_4)_3]$, Cu(II) and Ni(II) complexes of Schiff base

Course Outcome: The students will acquire knowledge of

1. Preparation and purification of different inorganic complexes.
2. Application of UV-Vis, FT-IR, Magnetic moment measurement, Conductivity measurements, NMR and Thermogravimetric analysis for characterization of coordination complexes.

SUGGESTED READINGS

1. Pass, G. and Sutcliffe H. Practical Inorganic Chemistry, 1st edition, 1979, Chapmann and Hall Ltd.
2. Jolly, W.L. Synthetic Inorganic Chemistry, 2nd edition, 1961, Prentice Hall, Inc.,.
3. Nakamoto, K. Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B, 5th edition, 1997, John Wiley and Sons,.
4. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M. Vogel's Textbook of Quantitative Chemical Analysis, 6th edition, 2000, Pearson Education Ltd.
5. Kolthoff, I.M. and Sandell, E.B. Text Book of Quantitative Inorganic Analysis, Revised Edition, 1968, London Macmillan and Co. Ltd.
6. Marr, G. and Rockett, B.W. Practical Inorganic Chemistry, 1972, John Wiley & Sons.
7. Jolly,W.L. The Synthesis and Characterization of Inorganic Compounds. 1970, Prentice Hall Press.

Course Title: Organic Chemistry-II
Paper Code: MCL.512
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **14 hours**

Reactive intermediates: Generation, structure and reactions of carbocation, carbanion, free radicals, carbenes, nitrenes, benzynes, classical and non-classical carbocations, phenonium ions and norbornyl system, neighbouring group participation.

Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

Unit 2 **20 hours**

Synthetic methodologies: Synthon, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination, Criteria for selection of target, Linear and convergent synthesis, Retrosynthetic analysis and synthesis involving chemoselectivity, Regioselectivity, Reversal of Polarity (Umpolung), Synthesis of cyclic molecules, Strategic bond: Criteria for disconnection of strategic bonds, Importance of the order of events in organic synthesis. One group and two group C-X disconnections in 1,2-, 1,3-, 1,4 & 1,5- difunctional compounds, One group C-C disconnections, alcohol and carbonyl compounds, regioselectiviity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis, Two group C-C disconnections, Diels-Alder reaction, 1,3-difunctionalised compounds, Control in carbonyl condensation, 1,5-difunctionalised compounds.

Unit 3 **16 hours**

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, Mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzillic acid, Favorskii, Arndt-Eister synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction, Carroll, Claisen, Cope, Gabriel–Colman, Smiles and Sommelet–Hauser rearrangements.

Selective Name Reactions: Aldol, Perkin, Stobbe, Dieckmann Condensation, Reimer-Tiemann, Reformatsky Grignard reactions, Diels-Alder reaction, Robinson Annelation, Michael addition, Mannich reaction, Stork-enamine, Sharpless Assymetric Epoxidation, dihydroxylate, Ene, Barton, Hofmann-Loffler Fretag, Shapiro reaction, Chichibabin Reaction.

Unit 4 **22 hours**

Pericyclic chemistry:

Introduction, Main features of pericyclic reactions, Classification of pericyclic reactions. Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5- hexatriene. Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical. Thermal and photochemical pericyclic reactions.

Electrocyclic reactions: Conrotation and disrotation, Electrocyclic closure and opening in 4n and 4n+2 systems. Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by (i) symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and orbital symmetry

correlation diagrams and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Examples of electrocyclic reactions.

Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Cycloreversions. Stereochemical aspects in supra-supra, supra-antara, antara-supra and antara-antara $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Diels-Alder reaction. Woodward-Hoffmann Selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by (i) Conservation of orbital symmetry and orbital symmetry correlation diagrams (ii) Fukui Frontier Molecular Orbital (FMO) theory and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Examples of cyclo addition reactions.

Sigmatropic reactions: [1,j] and [i,j] shifts; Suprafacial and antarafacial shifts; Selection rules for [lj} shifts; Cope and Claisen rearrangements; Explanation for the mechanism of sigmatropic reactions by (i) symmetry properties of HOMO (ii) Huckel-Mobius aromatic and antiaromatic transition state method; Introduction to Cheletropic reactions and the explanation of mechanism by FMO theory.

Suggested Readings:

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3rd edition.
2. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press, 2nd edition
3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, India.
4. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
5. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
7. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
8. Finar, I. L., (2012). *Organic Chemistry Vol. 1,* Pearson Education, 6th edition, UK.
9. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, US.
10. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
11. Joule, J.A., Mills, K. (2010). *Heterocyc1ic Chemistry*, Blackwell Publishers, 5th edition, New York.
12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.

14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, US.
19. Norman, R.O.C.; Coxon, J.M. *Principles of Organic Synthesis*, Blackie Academic & Professional.
20. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John wiley & Sons, New York,
21. Warren, S., (2010). *Designing organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
22. Corey E.J., Cheng Xue-Min, *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons, (1989).

Course Title: Physical Chemistry-II
Paper Code: MCL.513
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Course objective: To impart knowledge of applications of electrochemistry, reaction kinetics, surface reaction, adsorption and catalysis.

Unit 1 **18 Hrs**

Electrochemistry: Nernst equation, Electrochemical series, Electrochemical cells, Concentration cells with and without liquid junction, Application of electrochemical cell, Thermodynamics of reversible electrodes and reversible cells. Zeta potential, Redox indicators, Activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions, Derivation of Debye-Huckel limiting law, Extended Debye-Huckel law, Photoelectrochemical cells. Conductometric and potentiometric titrations.

Unit 2 **18 Hrs**

Reaction Kinetics: Introduction, Rates of chemical reactions, Methods of determining rate laws, Mechanisms of chemical reactions and steady state approximation, Laws of photochemistry, , Kinetics of photochemical and composite reactions, Chain and oscillatory reactions, Collision and transition state theories, Stearic factor, Treatment of unimolecular reactions, Ionic reactions: salt effect.

Unit 3 **18 Hrs**

Fast Reaction: Introduction to fluorescence, phosphorescence and luminescence, Jablonski diagram, Steady state and time resolved emission, Quantum yield, Introduction to time-resolved techniques for absorption and emission measurements, Relaxation method, Study of kinetics of fast reactions by millisecond stopped-flow, Nanosecond flash photolysis techniques, Detection and kinetics of reactive intermediates, Measurement of fluorescence and phosphorescence lifetimes, Photo-induced electron transfer rates.

Unit 4 **18 Hrs**

Adsorption: Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm: estimation of surface area of solids, Langmuir and Fredulich Isotherms.

Catalysis: Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Effect of pressure on reaction rate, Kinetics of catalytic reactions, Kinetics of surface reaction.

Course Outcome: The students will acquire knowledge of

1. Redox processes in electrochemical systems, Debye-Huckel theory and determination of activity and activity coefficient.
2. Mechanism for chemical reactions for optimizing the experimental conditions,
3. Kinetics of fast reactions by ultrafast methods and techniques
4. Application of homogeneous and heterogeneous catalysis in chemical synthesis
5. Importance of adsorption process and catalytic activity at the solid surfaces

SUGGESTED READINGS

1. Barrow, G. M. Physical Chemistry, 5th Edition, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 1, 4, 5th Edition, 2011, MACMILLAN,.

3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9th Edition, 2009, Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1st edition, 1998, Viva Books,.
5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 3rd edition, 1981, John Wiley and Sons.
6. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. Physical Chemistry, 4th Edition, 2004, Wiley-Interscience Publication.
7. Engel T., Reid, P. and Hehre, W. Physical Chemistry, 3rd Edition, 2012, Pearson Education.
8. Puri, B.R. Sharma L.R. and Pathania M.S. Principles of Physical Chemistry, 46th Edition, 2013, Vishal Publishing Company.
9. Laidler, K. J. Chemical Kinetics, 3rd Edition, 1987, Pearson Education Ltd.
10. Engel T. and Reid, P. Thermodynamics, Statistical Thermodynamics, & Kinetics, 3rd edition, 2013, Pearson Education.
11. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3rd edition, 2006, Springer.
12. Raj, G. Surface Chemistry (Adsorption), 4th Edition, 2002, Goel Publishing House.

Course Title: Physical Chemistry-II-Practical
Paper Code: MCP.514

L	T	P	Credits	Marks
-	-	4	2	50

Course objective: To impart knowledge and hand-on experiences of different analytical techniques for chemical analysis

1. Determination of strength of a given base by titrating with an acid conductometrically.
2. Determination of solubility and solubility product of sparingly soluble salts (e.g., $PbSO_4$, $BaSO_4$) conductometrically.
3. Determination standard electrode potential of Fe^{2+}/Fe^{3+} system by potentiometer using potassium permanganate solution.
4. Determination of *pKa* of acetic acid and glycine by pH meter using NaOH.
5. Determination of relative and absolute viscosity of a given liquid.
6. Determination of surface tension of alcohols.
7. Determination of refractive indices of given liquids.
8. Determination of concentrations of heme proteins using spectrophotometer
9. Preparation of buffers and measurement of their pH
10. Verification of the Lambert Beer's law.
11. Structural analysis of amino acids and proteins using FTIR and CD spectrometer.
12. Determination of the T_m values of DNA and proteins.
13. Study of the thermal/cold denaturations of proteins using UV-visible and CD spectroscopic techniques.
14. Molecular weight of a non-electrolyte by cryoscopy method.
15. Determination of stability constant of Fe(III)-salicylic acid complex by spectrophotometer.

Course Outcome: The students will acquire knowledge of development of experimental skills on conductivity meter, potentiometer, pH meter, viscometer, refractometer, spectrophotometer,CD and FTIR for different applications.

SUGGESTED READINGS

1. Nad, A. K., Mahapatra, B. and Ghoshal, A. An Advanced Course in Practical Chemistry, 2014, New Central Book Agency (P) Ltd.
2. Maity S. and Ghosh, N. Physical Chemistry Practical, 2012, New Central Book Agency (P) Ltd.
3. Elias, A. J. Collection of Interesting General Chemistry Experiments, 2008, Universities Press.
4. Khosla, B.D., Garg, V.C., and Gulati A.R., Senior Practical Physical Chemistry, 2007, S. Chand & Sons.

5. Yadav, J.B. Advanced Practical Physical Chemistry, 2008, Krishna Prakasan Media.
6. Das, R.C. and Behra, B. Experimental Physical Chemistry, 1983, Tata McGraw-Hill.
7. James, A.M. and Prichard, F.E. Practical Physical Chemistry, 3rd edition, 1974, Longman, Harlow.
8. Ghosh, J.C., Experiments in Physical Chemistry, 1990, Bharati Bhavan.

Elective courses

Course Title: Chemistry of Natural Products

Paper Code: MCL.515

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 hours**

Terpenoids and carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Geraniol, Menthol and β-Carotene

Unit 2 **18 hours**

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine and Morphine.

Unit 3 **18 hours**

Steroids: Occurrence, nomenclature, basic skeleton and stereochemistry, Structure determination and synthesis of cholesterol, partial synthesis of Testosterone and Progesterone, Chemical tests for steroids

Unit 4 **9 hours**

Plant pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of anthocyanins

Unit 5 **9 hours**

Carbohydrates: Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of Glucose, conformation and anomeric effects in hexoses

Suggested Readings:

1. Bhat, S.V., Nagasampagi, B.A., Meenakshi, S. (2009). *Natural Product Chemistry & Applications*, Narosa Publishing House, New Delhi.
2. Bhat, S.V., Nagasampagi, B.A., Sivakumar, M. (2005), Chemistry of Natural Products. Narosa Publishing House, New Delhi.
3. Brahamchari, G. (2009). *Natural Product: Chemistry, Biochemistry and Pharmacology*. . Narosa Publishing House, New Delhi.
4. Cseke, L.J. (2009). *Natural Products from plants*. CRC Press, Taylor and Francis, 2nd edition, US.
5. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Willey & Sons, 3nd edition, UK.
6. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products.* Dorling Kindersley Pvt. Ltd., 6th edition, India.
7. Peterson, F., Amstutz, R. (2008). *Natural Compounds as drugs.* Birkhauser Verlay.
8. Thomson, R.H. (2008). *The Chemistry of Natural Products*, Springer, 1st edition.

Course Title: Quantum Chemistry
Paper Code: MCL.516
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Course objective: To acquire knowledge of the quantum chemical description of chemical bonding, reactivity and their applications in molecular spectroscopy and inorganic chemistry.

Unit 1 **18 Hrs**

Fundamental Background: Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor, Particle in a Ring, Hydrogen Atom.

Unit 2 **18 Hrs**

Approximate Methods: Perturbation theory for non-degenerate and degenerate states and its applications. The variation theorem and its application.

Unit 3 **18 Hrs**

Angular Momentum: Ordinary angular momentum, Eigen functions and Eigen values for angular momentum, Addition of angular momenta, Spin, Antisymmetry and Pauli exclusion principle.

Electronic Structure of Atoms: Electronic configuration, Russell-Saunders terms and Coupling Schemes, Magnetic Effects: Spin-orbit Coupling and Zeeman Splitting, the self-consistent field method, Hartree-Fock SCF method for molecules.

Unit 4 **18 Hr**

Born-Oppenheimer Approximation: LCAO-MO and VB treatments of the H_2^+ and H_2, Hybridization and valence MOs of H_2O and NH_3. Huckel Theory of acyclic and cyclic conjugated systems, Bond Order and Charge Density Calculations.

Course Outcome: The students will acquire knowledge of

1. Schrodinger equation for a particle in a box and quantum chemical description.
2. Electronic and Hamiltonian operators for molecules.
3. Quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
4. Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle.

SUGGESTED READINGS

1. Levine, I.N. Quantum Chemistry, 5th edition, 2000, Pearson Educ., Inc. New Delhi.
2. Chandra, A.K. Introductory Quantum Chemistry, 4th Edition, 1994, Tata Mcgraw Hill.
3. Prasad, R.K., Quantum Chemistry, 4th Edition, 2009, New Age Science.

4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1st edition, 1998, Viva Books.
5. Murrell, J.N. Kettle S.F.A. and Tedder, J. M. Valence Theory, 2nd edition, 1965, John Wiley.
6. Lowe, J. P. and Peterson, K. Quantum Chemistry, 3rd Edition, 2006, Academic Press.

Course Title: Seminar
Paper Code: MCS. 599

L	T	P	Credits	Marks
-	-	4	2	50

Course objective: The course would develop scientific aptitude, critical thinking, research writing and research presentation.

The seminar must include discussion on topics such as awareness about weapons of mass destruction (chemical, biological, radiological, and nuclear weapons), disarmament, peaceful uses of chemistry, International Regulation of Biological and Chemical or Weapons of Mass Destruction.

Course outcome: The student would be able to

1. Investigate various aspects related to the chemistry problem.
2. Appreciate the literature and its relevance to his topic of interest
3. Technical write and presentation the chemical problem in hand.
4. should generate interest in current topics of research and commercial worth of chemistry.

Semester –III

Course Title: Inorganic Chemistry-III
Paper Code: MCL.601

L	T	P	Credits	Marks
4	1	0	4	100

Course objective: To aware the knowledge of coordination chemistry and properties of f-block elements, role of metals in bioinorganic chemistry, and spectroscopic techniques to analyse the inorganic compounds

Unit 1 **28 Hrs**

Lanthanides, actinides and super-heavy elements

Coordination chemistry, magnetic and spectral properties, comparison of general properties of lanthanides and actinides, comparison with d-block elements, Organo lanthanides and actinides, separation of lanthanides and actinides, analytical application of lanthanides and actinides-lanthanides as shift reagents and high temperature super conductors, manmade elements-theoretical background, production, separation and predicted properties.

Unit 2 **20 Hrs**

Bioinorganic Chemistry: Heme and non-heme proteins, Haemoglobin and myoglobin as oxygen carriers, Bohr effect, Relaxed and tense (R & T) configurations of haemoglobin. Structure and functions of cytochromes, Hemerythrins and Hemocyanins. Biochemistry of iron, Iron storage and Transport, and ferritin, Transferrin, Blue copper proteins, Zinc protein (carbonic anhydrase), and Iron-sulfur proteins, Metal deficiency and disease, Toxic effects of metals.

Unit 3 **12 Hrs**

Nuclear Magnetic Resonance (NMR) and Electron Spin Resonance (ESR) Spectroscopy:

NMR: The contact and psedo contact shifts , factors affecting nuclear relaxation , some applications including biochemical systems , an overview of NMR of metal nuclides with emphasis on 195 Pt and 119 Sn NMR. **ESR**: Hyperfine coupling, spin polarization for atoms and transition metal ions, spin orbit coupling and significance of g-tensors , application of transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as PH_4 , F_2 and $[BH_3]$-

Nuclear Chemistry: Classification of nuclides, Nuclear stability, Atomic energy, Types of nuclear reactions-fission and fusion, Nuclear decay laws, Radioanalytical Techniques.

Unit 4 **12 Hrs**

Mossbauer Spectroscopy

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin , (2) Sn^{+2} and Sn^{+4} compounds- nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

Vibrational Spectroscopy

Symmetry and shapes of AB2, AB3, AB4, AB5 and AB6 mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, applications of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

Course Outcome: The students will acquire knowledge of

1. Details on f-block elements properties
2. Structure and biological functions of proteins and the role of metals in biology
3. Structural support to inorganic compounds through spectroscopic techniques

SUGGESTED READINGS

1. Drago, Russell S. Physical Methods for Chemists, 2nd edition, 1992, Saunders College Publishing.
2. Ebsworth, E.A.V., Rankin, D.W.H. and Cracock, S. Structural Methods in InorganicChemistry, 1st edition, 1987, ELBS.
3. Cotton, F.A. and Lippard, S. J. Progress in Inorganic Chemistry, Vol. 8, Vol. 15, Wiley Internationals.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2nd edition, 1984, Elsevier Science Publishers B.V.
5. Parish, R.V. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, 1st edition, 1990, Ellis Harwood.
6. Silverstein, R.M. Bassler, G.C. and Morrill, T.C. Spectrometric Identification of Organic Compounds, 6th edition, 2002, John Wiley.
7. Abraham, R.J., Fisher, J. and Loftus, P. Introduction to NMR Spectroscopy, Wiley.
8. Dyer, J.R. Application of Spectroscopy of Organic Compounds, Prentice Hall.
9. Nakamoto, K. Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B, 5th edition, 1997, John Wiley and Sons.
10. Carlin, R.I. Transition Metal Chemistry, Vol. 3, Marcell Dekker Publication
11. Martin, M.L., Delpeuch, J.J. and Martin, G.J. Practical NMR Spectroscopy, Heyden.
12. Williams, D.H. and Fleming, I. Spectroscopic Methods in Organic Chemistry, Tata McGraw-Hill.
13. Greenwood, N. N. and Earnshaw, A. Chemistry of the Elements, 1984.
14. Ozin, G. A., Arsenault, A. C. and Cademartiri L. Nanochemistry: a chemical approach to nanomaterials, 2009, Royal Society of Chemistry.
15. Klabunde, Kenneth J., and Ryan M. Richards, eds. Nanoscale materials in chemistry 2009, John Wiley & Sons.

Course Title: Organic Chemistry-III
Paper Code: MCL.602
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **16 hours**

Reaction mechanism, structure and reactivity: Types of mechanisms, types of reactions, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, Transition states and intermediates, Methods of determining mechanisms, Isotopes effects, Effect of structure on reactivity; Resonance, inductive, electrostatic and steric effect, quantitative treatment, the Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation.

Unit 2 **16 hours**

Photochemistry: Franck-Condon principle, Jablonski diagram, Singlet and triplet states, Photosensitization, Quantum efficiency, Photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Di π – methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction Singlet molecular oxygen reactions

Unit 3 **18 hours**

Metal and non-metal mediated oxidation and reductions: Mechanism, Selectivity, Stereochemistry and applications of oxidation reactions, Oppenauer, Baeyer-Villiger, Oxidation reactions using DDQ, lead tetraacetate, selenium dioxide, DCC, PCC, PDC, CAN, Cr and Mn reagents, periodic acid, Osmium tetroxide, Swern oxidations, Hydroboration, Dehydrogenation, Ozonolysis, Epoxidations using peracids, Dess–Martin periodinane.

Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Pondorff-Verley reduction, Dissolving metal reductions, metal hydride reductions using $NaBH_4$, $LiAlH_4$, DIBAL. Wilkinson's Rh catalysis, Boron in reduction, Birch reduction.

Unit 4 **22 hours**

Heterocyclic chemistry: Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles, Aromatic heterocycle, Non-aromatic heterocycle: Bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles and their synthesis

(a) Three-membered and four-membered heterocycles: synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

(b) Five membered heterocycles containing two heteroatoms (S,N,O): Diazoles, imidazole, pyrazole, oxazoles and thiazoles, trizoles, oxadiazole, oxathiazole.

(c) Benzo-fused five-membered and six membered heterocycles: Synthesis and reactions of indoles, benzofurans and benzimidazoles, benzothiazoles.

(d) Six-membered heterocycles with heteroatom: Synthesis and reactions of pyrylium salts and pyrones, coumarins, chromones, pyridine, pyrimidine *etc*.

Suggested Readings:

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3rd edition.
2. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, India.
3. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
4. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
5. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
8. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, US.
9. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
10. Joule, J.A., Mills, K. (2010). *Heterocyc1ic Chemistry*, Blackwell Publishers, 5th edition, New York.
11. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7th edition, India.
12. Kalsi P. S., (2014). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Joule, J.A., Mills, K. (2010). *Heterocyc1ic Chemistry*, Blackwell Publishers, 5th edition, New York.
19. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7th edition, India.
20. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
21. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.

22. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
23. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
24. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3rd edition, UK.
25. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.

Course Title: Organic Synthesis and Spectral Analysis-Practical

Paper Code: MCP.603

L	T	P	Credits	Marks
-	-	4	2	50

1. Demonstration of Stereochemical aspects of the compounds through molecular models.
2. Thin layer chromatography: Monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R_f values of known standards, preparative TLC for separation of mixtures.
3. Purification of a given organic compound through crystallization, fractional distillation or column chromatography.
4. **Organic Synthesis:** Single or multi- steps synthesis of organic compounds. Aspects such as conversion, yield, selectivity, effluent treatment, atom economy, etc. should be paid attention. TLC should be used to monitor the reaction. (attempt any five)
    a) Synthesis of an anticancer stilbene via Wittig reaction
    b) Synthesis of chalcones via Claisen-Schmidt condensation.
    c) Preparation of vanillyl alcohol from vanillin
    d) Reduction of 3-nitroacetophone using $NaBH_4$/$LiAlH_4$
    e) Preparation of bromohydrin from methylstyrene
    f) Preparation of aniline from nitrobenzene
    g) Synthesis of ethyl-*n*-butylacetoacetate by A.E.E. condensation
    h) Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.
    i) Preparation of Iodoxybenzoic acid (IBX) and its application in oxidation.
    j) Preparation of pyridine chlorochromate (PCC) and its application in oxidation.
    k) Multistep synthesis of phenytoin.
5. Exercises of structure elucidation of unknown compounds *via* spectral interpretation of ^1H, ^{13}C NMR, IR, UV and Mass.
6. Hands on experience with various analytical instruments such as FT-IR, UV-vis spectrophotomer, GC-MS, Microwave Synthesizer, Solvent Extractor and HPLC.

Suggested Readings:

1. Adams,R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmilan Limited, London.
2. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
5. Vogel, A.I. (latest edition). *Text book of practical organic chemistry*, Pearson
6. Williamson, K.L., Health, D.C. (1999). *Macroscale and Microscale Organic Experiments*, *Heath, D.C* and Co., Lexington, MA.
7. Armarego, W. L., & Chai, C. (2012). *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
8. Young, J. A. (Ed.). (Latest Edition). *Improving safety in the chemical laboratory: a practical guide*. Wiley

Course Title: Physical Chemistry-III
Paper Code: MCL.604
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Course objective: To impart the knowledge of electronic, rotation, vibration, laser, Mossbauer, NMR, FTIR, ESR spectroscopy and their applications.

Unit 1 **18Hrs**

Unifying Principles: Electromagnetic radiation, Interaction of electromagnetic radiation with matter, Line width, Selection rules, Intensity of spectral lines, , Rotational, Vibrational and Electronic energy levels.

Electronic Spectroscopy: Energies of atomic and molecular orbitals, UV-Visible spectra, Spectra of hydrogen atom and alkali metal atoms, Applications, Franck-Condon principle, Electronic spectra of polyatomic molecules.

Lasers and Laser Spectroscopy: Principles of laser action, pulsed lasers, Q-switching, harmonic generation, examples of lasers: He-Ne, Nd-YAG, dye lasers, Femtosecond spectroscopy.

Unit 2 **18 Hrs**

Microwave Spectroscopy: Classification of molecules, Rigid rotor model, Effect of isotopic substitution on the transition frequencies, Intensities, Non-rigid rotor, Stark effect, Applications.

Mossbauer Spectroscopy: Basic principles, Application of the technique to the studies of (1) bonding, structures and oxidation state of Fe^{+2} and Fe^{+3} compounds.

Unit 3 **18 Hrs**

Vibrational Spectroscopy: Infrared Spectroscopy– Simple harmonic oscillator, Vibrational energies of diatomic molecules, Anharmonicity, Vibration-rotation spectroscopy, P, Q, R branches, Vibrations of polyatomic molecules, Group frequencies, Overtones, Hot bands, Applications.

Raman Spectroscopy - Classical and quantum theories of Raman effect, Pure rotational, Vibrational and Vibrational-Rotational Raman spectra, Mutual exclusion principle, Coherent anti Stokes Raman spectroscopy.

Unit 4 **18 Hrs**

Nuclear Magnetic Resonance (NMR) Spectroscopy: Basic principles, Instrumentation, Magnetization vector and relaxation, NMR transitions, Bloch Equation, relaxation effects and mechanism, Shielding and Deshielding of magnetic nuclei, Chemical shift, Spin-spin interactions and coupling constant 'J', double resonance and spin tickling, effect of quadrapole nuclei, nuclear overhauser effect (NOE), Multiple pulse Methods, NMR in medical diagnostics.

Electron Spin Resonance Spectroscopy - Basic principles, Zero field splitting and Kramer's degeneracy, Factors affecting the 'g' value, hyperfine coupling constants, Instrumentation and Applications.

Course Outcome: The students will acquire knowledge of

1. Microwave, Infrared-Vibration-rotation Raman and infra-red Spectroscopy and their applications for chemical analysis
2. Mossbauer Spectroscopy and their applications
3. Electronic spectroscopy of different elements and simple molecules.
4. Nuclear Magnetic and Electron Spin Resonance Spectroscopy for organic compounds analysis, medical diagnostics.

SUGGESTED READINGS

1. Hollas, J. M. Modern Spectroscopy, 4th edition, 2004, John Wiley & Sons, Ltd.
2. Barrow, G. M. Introduction to Molecular Spectroscopy, 1988, McGraw-Hill International.
3. Banwell C. N. and McCash, E.M. Fundamentals of Molecular Spectroscopy, 4th edition, 1994, Tata McGraw Hill, New Delhi.
4. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3rd edition, 2006, Springer.
5. Carrington A. and Mc Lachlan, A. D. Introduction to Magnetic Resonance, 1979, Chapman and Hall, London.
6. Harris, R. K. Nuclear Magnetic Resonance Spectroscopy, 1986, Addison-Wesley Longman Ltd, London.
7. Windawi, H. and Floyd, F.L.H. Applied Electron Spectroscopy for Chemical Analysis, ***Chemical Analysis*** Vol. 63 : A Series of Monographs on Analytical Chemistry and Its Applications Series, 1982, John Wiley.
8. Parish, R.V., NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, 1991, Ellis Harwood.
9. Chang, R. Basic Principles of Spectroscopy, 1971, McGraw-Hill.
10. Ghosh, P.K. Introduction to Photoelectron Spectroscopy, ***Chemical Analysis*** Vol. 67 : A Series of Monographs on Analytical Chemistry and Its Applications Series, 1983, ***John Wiley***& Sons, New York.
11. Gunther, H. NMR Spectroscopy: Basic Principles, Concepts, and Application in Chemistry, 3rd Edition, 2013, Wiley Publishing.
12. Carrington, A. and MacLachalan, A.D. Introduction to Magnetic Resonance, 1967, ***Harper*** and Row, New York, USA.
13. Barrow, G. M. Physical Chemistry, 5th Edition, 2007, Tata McGraw-Hill.
14. Kapoor, K. L. Text Book of Physical Chemistry, Volume 1, 4, 5th Edition, 2011, MACMILLAN,.
15. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9th Edition, 2009, Oxford University Press.
16. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1st edition, 1998, Viva Books.
17. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. Physical Chemistry, 4th Edition, 2004, Wiley-Interscience Publication.

Course Title: Spectral Analysis
Paper Code: MCL.605
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 hours**

UV-Visible spectroscopy: Principle of UV-Visible Spectroscopy, Chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rule, solvent effects, stereochemical effect.

Infrared Spectroscopy: Infrared radiation and its interaction with organic molecules, vibrational mode of bonds, instrumentation and applications, effect of hydrogen bonding and conjugation on absorption bands, interpretation of IR spectra. FTIR.

Unit 2 **18 hours**

Nuclear magnetic resonance spectroscopy: Magnetic properties of nuclei, Field and precession, Chemical shift concept, Isotopic nuclei, Reference standards and solvents. ^{1}H-NMR spectra, Chemical shifts, Spin spin coupling, Coupling constants, Integration of signals, Interpretation of spectra, Decoupling, double resonance and shift reagent methods, Long range coupling, Resonance of other nuclei e.g. ^{19}F, ^{15}N, ^{31}P.

Unit 3 **18 hours**

Principles of FT-NMR with reference to ^{13}C NMR, Free induction decay, Average time domain and frequency domain signals, Spin-spin and spin-lattice relaxation phenomenon, Nuclear Overhauser enhanced (NOE), ^{13}C NMR spectra, their interpretation and application. APT and DEPT techniques, Principle of 2-D NMR, Correlation spectroscopy (COSY) Homo COSY (^{1}H-^{1}H COSY), Hetro COSY (^{1}H-^{13}C COSY, HMQC), long range ^{1}H-^{13}C COSY (HMBC), NOESY, DEPT and 2D INADEQUATE experiments and their application, Solid-state NMR.

Unit 4 **18 hours**

Mass spectrometry: Basic principles and brief outline of instrumentation, Ion formation, molecular ion, metastable ion, Mc Lafferty rearrangement, Nitrogen rule, fragmentation process in relation to molecular structure and functional groups. Relative abundance of isotopes, chemical ionization, FAB, ESI and MALDI other recent advances in mass spectrometry.

ESSENTIAL BOOKS:

1. Banwell, C.N.; McCash, E. M. (2000). *Fundamentals of molecular spectroscopy,* Tata McGraw-Hill, New Delhi.
2. Dyer, J.R. (2009). *Application of Absorption Spectroscopy of Organic Compounds*, Publisher: Phi Learning.
3. Kalsi, P.S. (2004). *Spectroscopy of Organic Compounds*, New Age International Ltd.
4. Kemp, W. (1991). *Organic spectroscopy*, ELBS London.
5. Khopkar, S.M. (2007). *Basic Concepts of Analytical Chemistry***,** New Age International Pvt Ltd.

6. Melinda J.D., (2010). *Introduction to solid NMR Spectroscopy***,** Wiley India Pvt Ltd
7. Mendham, J.; Denney, R.C.; Barnes, J. D.; Thomas, M. J. K. (2003). *Vogel's Textbook of Quantitative Chemical Analysis***,** Pearson Education Pvt. Ltd., New Delhi.
8. Pavia, D.L.; Lampman, G. M. (2010). *Introduction to Spectroscopy***,** G. S. Kriz, Harcourt College, NY.
9. Popov, A.I.; Halenga, K. (1991). *Modern NMR techniques and their Applications***,** Marcel Deckker.
10. Silverstein, R.M. (Latest Edition). *Spectrometric Identifications of Organic Compound***s**, John Wiley.
11. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.
12. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors.
13. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., New Delhi.

Course Title: Seminar
Paper Code: MCS. 698

L	T	P	Credits	Marks
-	-	4	2	50

Course objective: The course would develop scientific aptitude, critical thinking, research writing and research presentation.

The seminar must include discussion on topics such as awareness about weapons of mass destruction (chemical, biological, radiological, and nuclear weapons), disarmament, peaceful uses of chemistry, International Regulation of Biological and Chemical or Weapons of Mass Destruction.

Course outcome: The student would be able to

1. Investigate various aspects related to the chemistry problem.
2. Appreciate the literature and its relevance to his topic of interest
3. Technical write and presentation the chemical problem in hand.
4. should generate interest in current topics of research and commercial worth of chemistry.

Elective courses

Course Title: Medicinal Chemistry-I
Paper Code: MCL.606
Total Lectures: 72

L	T	P	Credits	Marks
72	1	0	4	100

Unit 1 18 Hours

Physicochemical and stereochemical aspects: In relation to biological activity, Drug receptor interaction, Adrenergic hormones and Drugs including biosynthesis, storage, release and metabolism of catecholamines (Andrenaline, Isoprenaline, Salbutamol, Amphetamine, Naphazoline), Cholinergics and Anticholinesterases including biosynthesis, storage and metabolism of acetylcholine (Methacholine Chloride, Neostigmine Bromide), Antispasmodic and Antiulcer Drugs (Cyclopentolate, Propantheline Bromide, Benzhexol), Antiparkinsonism Drugs (Apomorphine).

Unit 2 18 Hours

Neuromuscular blocking agents: Gallamine Triethiodide, Succinylcholine chloride, Hypoglycaemic drugs (Tolbutamide), Thyroid hormones and Antithyroid drugs (L-Thyroxine, Propylthiouracil).
Anticoagulants and haemostatic agents: Warfarin, Phenindione, Oxytocics (includes discussion on Ergot alkaloids) (Ergometrine).
Antihistamines including discussion on Sodium cromoglycate (Mepyramine, Diphenhydramine, Chlorpheniramine, Promethazine).
Non-steroidal anti-inflammatory drugs and anti–gout drugs: Indomethacin, Phenylbutazone, Allopurinol, Probenecid.

Unit 3 **18 Hours**

General Anaesthetic Agents: Introduction, medicinal aspects of anaesthetics, mode of action, gases and volatile liquid anaesthetics, intravenous anaesthetics or fixed anaesthetics, toxicity of general anaesthetics (Divinyl ether, Ethyl chloride, Cyclopropane, Thiopentone Sodium).
Local Anaesthetic Agents: Introduction, Structure-activity relationships, benzoic acid derivatives, aminobenzoic acid derivatives, lidocaine derivatives, miscellaneous, toxicity, mode of action (Benzocaine, Procaine Hydrochloride, Lidocaine Hydrochloride).

Unit 4 **18 Hours**

Sedatives-Hypnotics: Introduction, classification of sedative-hypnotics, structure-activity relationships, barbiturates, amides and imides, alcohols and their carbamate derivatives, aldehydes and their derivatives, mode of action, pharmacological properties and side effects (Barbitone, Phenobarbitone, Cyclobarbitone, Pentobarbitone Sodium, Thiopentone Sodium), non-barbiturates (Official drugs).

Anticonvulsants: Introduction, epilepsy and its types, SAR, barbiturates (official products), hydantoins, Oxazolidinediones, Succinamides; miscellaneous drugs, (Phenytoin Sodium, Troxidone), Antipsychotic agents: introduction, SAR and drugs like chlorpromazine, prochlorperazine *etc.*

Suggested Readings:

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea & Febiger, Philadelphia.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3rd edition, UK.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4th edition, US.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, 4th edition.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley & Sons, 7th edition, New York.

Course Title: Current Trends in Organic Synthesis
Paper Code: MCL.607
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 Hrs**

Free radical reactions

Types of free radical reactions, free radical substitution mechanism at an aromatic substrate, neighbouring group assistance, Reactivity for aliphatic and aromatic substrates at a bridgehead,

Reactivity in the attacking radicals,The effect of solvents on reactivity, Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation. Coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, Free Radical Rearrangement, Hunsdiecker reaction

Unit 2 **18 Hrs**

Alkylation: Enolates: Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, Effect of solvent, Counter cation and Electrophiles; Symbiotic effect; Thermodynamically and kinetically controlled enolate formations; Various transition state models to explain steroselective enolate formation; Enamines and metallo-enamines; Regioselectivity in generation, Application in controlling the selectivity of alkylation.

Unit 3 **18 Hrs**

Protection and deprotection of various functional groups:

Protection of alcohols by ether, silyl ethers and ester formations and their deprotection, Protection of 1, 2 diols- by acetal, ketal and carbonate formation and their deprotection, Protection of amines by acetylation, benzylation, benzyloxy carbonyl, t-butoxycarbonyl, fmoc, triphenyl methyl groups and their deprotection, Protection of carbonyls by acetal and ketal formation and their deprotection, Protection of carboxylic acids by ester formation and their deprotection

Unit 4 **18 Hrs**

New synthetic reactions: Baylis-Hillman reaction, Biginelli reaction, Mukaiyama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's stereoselective olefination, Buchwald-Hartwig coupling, Eishenmosher-Tanabe fragmentation and Shapiro reaction, Stork-enamine reaction Aza-Cope, Aza-Wittig reaction, BINAL and BINAP assisted reactions. Ugi reaction, Robinson–Gabriel synthesis, Strecker amino acid synthesis Vilsmeier–Haack reaction, Wohl–Ziegler reaction.

ESSENTIAL BOOKS:

1. Finar, I.L., (2012). *Organic Chemistry Vol. 1***,** Pearson Education, 6th edition, UK.
2. Finar, I.L., (2012). *Organic Chemsitry Vol. 2*: *Stereochemistry and The Chemistry of Natural Products,* Pearson Education, 6th edition, UK.
3. Fleming (1999). *Pericyclic Reactions***,** Oxford University Press, Oxford.
4. Fleming (2010). *Molecular Orbitals and Organic Chemical Reactions***,** John Wiley & Sons.

5. Jie Jack Li, (2009). *Name Reactions: A collection of Detailed Reaction Mechanisim*, Publisher: Springer-verlag
6. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Pub., 3rd edition, New Delhi.
7. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd., New Delhi.
8. Lowry, T.H., Richardson K.S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc.
9. Mc Murry, J., *Organic Chemistry***,** Asian Book Pvt Ltd, New Delhi
10. Morrison, R.T., Boyd, R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
11. Mukherjee, S.M., Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
12. Reinhard Bruckner, (2001). *Advanced organic chemistry: Reaction Mechanism***,** Academic Press.
13. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
14. Solomn, C.W.G, Fryble, C.B. (2003). *Organic Chemistry*, John Wiley & Sons, Inc., 8th edition, New York.
15. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition, US.
16. W. Carruthers, (2004). *Some Modern Methods of Organic Synthesis***,** Cambridge Uni. Press, 4th edition, UK.

Course Title: Nuclear Chemistry
Paper Code: MCL.608
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **16 hours**

Nuclear Structure and Stability

Binding energy, empirical mass equation, nuclear models, the liquid drop model, the shell model, the Fermi gas model & collective nuclear model, nuclear spin, parity & magnetic moments of odd mass numbers nuclei.

Unit 2 **20 hours**

Nuclear reaction

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

Nuclear fission

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and Asymmetric fission, decay chains and delayed neutrons.

Unit 3 **20 hours**

Reactor Theory

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

Nuclear Resources in India

Uranium and Thorium resources in India and their extractions, Heavy water manufacturing in India.

Unit 4 **16 hours**

Elements of Radiation Chemistry

Radiation Chemistry, Interaction of radiation with matter, Passage of neutrons through matter, Interaction of gamma radiation with matter, Units for measuring radiation absorption, Radiolysis of water, Free radicals in water radiolysis, Radiolysis of some aqueous solutions

ESSENTIAL BOOKS:

1. Friedlander, Kennedy and Miller, Nuclear and Radio Chemistry: John Wiley
2. B.G. Harvey, Nuclear Chemistry
3. Hassinsky: Translated by D.G. Tuck, Nuclear Chemistry and its application: Addison Wiley

4. B.G. Harvey, Introduction to Nuclear Physics and Chemistry
5. Maeclefort: Nuclear Chemistry: D.Van Nostrand
6. An N.Nesmeyannoy: Radiochemistry: Mir
7. Jacobs et al: Basic Principles of nuclear Science and Reactors, V.Nost & EWAP
8. N. Jay: Nuclear Power Today Tomorrow: ELBS
9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
10. Essentials of Nuclear Chemistry, H.J. Arnikar, John Wiley
11. Nuclear and Radiation Chemistry: B.K. Sharma, Krishna Publication
12. A Introduction to Nuclear Physics: R. Babber and Puri

Course Title: Medicinal Chemistry-II
Paper Code: MCL.610
Total Hours: 72

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 **18 Hours**

Steroids: Introduction, nomenclature, stereochemistry of cholesterol, stigmasterol, ergosterol, diosgenin, solasodine, bile acids, biosynthesis of testosterone, β-estradiol and aldosterone form cholesterol, Estrogens, SAR among estrogens, progestational agents, synthesis of progesterone from diosgenin and stigmasterol, ethisterone from dehydroepiandrosterone, oral contraceptives, SAR of progestins, **Androgens and Anabolic Agents:** Synthesis of testosterone from diosgenin, methyltestosterone from dehydroepiandrosterone, methandienone from methy1 testosterone, stanozolol from testosterone. **Aderenocorticoids:** Glucocorticoids and their SAR, mineralocorticoids, modifications in structure of hydrocortisone.

Unit 2 **18 Hours**

Opioid analgesics: Morphine and related drugs, synthetic modifications of morphine, codeine and thebaine, synthetic analgesics, endogenous opioid peptides, opioid antagonists, **CNS stimulants:** natural and synthetic, Methylxanthines and modified Methylxanthines, Psychopharmacological agents, Antipsychotics, Phenothiazines, **Antidepressants:** Tricyclic antidepressants, MAO inhibitors, atypical antidepressants, **Antianxiety drugs:** Meprobamate and related drugs, Benzodiazepines, Hallucinogens Hallucinogenic agents related to indoles, phenethylamines and Cannabinoids.

Unit 3 **18 Hours**

Diuretics carbonic anhydrase inhibitors: Thiazides and related drugs, High-ceiling diuretics. Aldosterone, antagonists, other potassium sparing diuretics, Osmotic diuretics, **Cardiovascular Agents:** cardiac glycosides, SAR, mechanism of action, toxic effects. Antihypertensive agents; introduction, ganglion blocking agents, antiadrenergic agents, drugs acting directly on smooth muscles, drugs acting on CNS. **Antianginals and vasodilators:** introduction, mechanism of smooth muscle vasodilation, esters of nitrous and nitric acid, side-effects. Antiarrhythmic and antifibrillytic drugs classification of antiarrhythmic drugs, mechanism of action, side effects.

Unit 4 **18 Hours**

Sulphonamides: Introduction and classification, antimicrobial spectrum, DHFR inhibitors, toxicity and side effects, reduction. **Antibiotics:** Classification, cycloserine, chloramphenicol, penicillins, cephalosporins, aminoglycosides, tetracyclines, polypeptides. **Antimycobacterial agents:** Introduction, uses in therapeutics. **Antimalarials:** quinoline and analogues, 8-amino quinolines, 9-amino acridines, 4-amino quinolines, diamino pyrimidine, and biguanides and recently introduced compounds. **Antiamoebic agents:** quinoline derivatives, metal free substances, diloxanide furoate, etc. **Anthelmintic drugs** in cestode infections in trematode infections and for intestinal nematode infections, antifilarial agents, **Antiviral agents:** Introduction to DNA, RNA and retroviruses, viral application, amantidine hydrochloride, interferones, acyclovir, idoxuridine, trifluorothymidine and vidarabine etc.

Suggested Readings:

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., 7th edition, Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, 6th edition, Philadelphia.
3. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd Edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3rd edition, New York.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4th edition. UK.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, 4th edition, UK.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier), 3rd edition.
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery*, John Wiley and Sons, New York.

Course Title: Project
Paper Code: MCD.600

L	T	P	Credits	Marks
-	-	-	20	500