Department of Chemistry

B.Sc.,

M.Sc.,

M.Sc., (SPL)

M.Phil

B.Sc., Chemistry

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

B.Sc., CHEMISTRY COURSE STRECUTRE

SEMESTER – I

Course	Subject Code	Name of the Paper	Hrs./ week	Credit/ course	Total No. of hrs. allotted	Marks		
						CA	SE	Total
Part I Tamil	P 111	Ikkala Ilakkiyam	6	3	90	25	75	100
Part II English	P 211	English Through Prose	6	3	90	25	75	100
Core	MC 11	Organic Chemistry-I	4	4	60	25	75	100
Allied	AC 11(P)	Ancillary Physics-I	4	4	60	25	75	100
Allied	ACL 11(P)	Ancillary Physics Practical	2	-	30	-	-	-
Core Lab	MCL 11	Inorganic Qualitative Analysis	4	2	60	40	60	100
Value Education	VE 1	Value Education -I	2	2	30	15	35	50
Environmental Studies	ES 1	Environmental Science	2	2	30	15	35	50
Total			30	20				

SEMESTER – II

Course	Subject Code	Name of the Paper	Hrs./ week	Credit/ course	Total No. of hrs. allotted	Marks		
						CA	SE	Total
Part I Tamil	P 121	Bhakthi Illakiyamum Sitrillakiyam	6	3	90	25	75	100
Part II English	P 221	English Through Drama	6	]'3	90	25	75	100
Core	MC 21	Inorganic and Physical Chemistry	6	6	90	25	75	100
Allied	AC 21(P)	Ancillary Physics-II	4	4	60	25	75	100
Allied	ACL 21(P)	Ancillary Physics Practical	2	2	30	40	60	100
Core Lab	MCL 21	Organic Qualitative Analysis	4	2	60	40	60	100
Skill Based Elective 1	SBE 1	Polymer Chemistry	2	2	30	15	35	50
Total			30	22				

SEMESTER – III

Course	Subject Code	Name of the Paper	Hrs./ week	Credit/ course	Total No. of hrs. allotted	Marks		
						CA	SE	Total
Part I Tamil	P 131	Kappiya Illakiyam	6	3	90	25	75	100
Part II English	P 231	English Through Poetry	6	3	90	25	75	100
Core	MC 31	Inorganic Chemistry-I	3	3	45	25	75	100
Core	MC 32	Organic and Physical Chemistry	3	3	45	25	75	100
Allied	AC 31(M)/ AC 31(Z)	Ancillary Maths / Zoology-I	6/4	4	90/60	25	75	100
Allied	ACL 31(Z)	Ancillary Zoology Practical-I	2	-	30	-	-	-
Core Lab	MCL 31	Volumetric Analysis	2	1	30	40	60	100
Value Education II	VE 2	Value Education -II	2	2	30	15	35	50
Non Major Elective II	NME 1	Modern Cosmetics	2	2	30	15	35	50
Total			30	21				

SEMESTER – IV

Course	Subject Code	Name of the Paper	Hrs./ week	Credit/ course	Total No. of hrs. allotted	Marks		
						CA	SE	Total
Part I Tamil	P 141	Pandai Illakiyam	6	3	90	25	75	100
Part II English	P 241	English Through Fiction	6	3	90	25	75	100
Core	MC 41	Physical Chemistry-I	3	3	45	25	75	100
Core Elective I	EMC 41	Organic Chemistry-II	3	3	45	25	75	100
Allied	AC 41(M)/ AC 41(Z)	Ancillary Maths / Zoology-II	6/4	4	90/60	25	75	100
Allied	ACL 41(Z)	Ancillary Zoology Practical-I	2	2	30	40	60	100
Core Lab	MCL 41	Organic Estimations	2	1	30	40	60	100
Skill Based Elective II	SBE 2	Green Chemistry	2	2	30	15	35	50
Non Major Elective II	NME 2	Consumer Products (Lab)	2	2	30	15	35	50
Total			30	23				

SEMESTER – V

Course	Subject Code	Name of the Paper	Hrs./ week	Credit/ course	Total No. of hrs. allotted	Marks		
						CA	SE	Total
Core	MC 51	Inorganic Chemistry-II	6	6	90	25	75	100
Core	MC 52	Organic Chemistry-III	6	6	90	25	75	100
Core	MC 53	Physical Chemistry-II	6	6	90	25	75	100
Core Elective II	EMC 51	Co-ordination Chemistry	5	3	75	25	75	100
Core Lab	MCL 51	Inorganic Gravimetric Estimations & Organic Preparations	5	5	75	40	60	100
Value Education III	VE 3	Value Education III	2	2	30	15	35	50
Self Study Paper		Dairy Chemistry		Extra 5		15	35	50
Total			30	28 + Extra 5				

*** Carries Extra 5 credits that do not form part mandatory credits (140) required for completion of the course.**

SEMESTER – VI

Course	Subject Code	Name of the Paper	Hrs./ week	Credit/course	Total No. of hrs. allotted	Marks		
						CA	SE	Total
Core	MC 61	Analytical Methods & Computer Applications in Chemistry	6	6	90	25	75	100
Core	MC 62	Organic Chemistry-IV	6	6	90	25	75	100
Core	MC 63	Physical Chemistry-III	6	6	90	25	75	100
Core Elective III	EMC 61	Group Theory and Spectroscopy	5	3	75	25	75	100
Core Lab	MCL 61	Experiments in Physical Chemistry	5	2	75	40	60	100
Skill Based Elective III	SBE 3	Water Analysis	2	2	30	40	60	100
Part V				1				
Total			30	26				
Total Credits for Semesters I to VI				140				

A) CONSOLIDATION OF CONTACT HOURS AND CREDITS: UG

Semester	Contact Hrs/ Week	Credits
I	30 hrs.	20
II	30 hrs.	22
III	30 hrs.	21
IV	30 hrs.	23
V	30 hrs.	28
VI	30 hrs.	25
Part – V	--	1
Total	180 hrs	140

B) Curriculum Credits: Part wise

Part I	**Tamil**	**4x3 = 12 Credits**
Part II	**English**	**4x3 = 12 Credits**
Part III	**Core**	**= 68 Credits (6+8+7+4+23+20)**
	Allied	**5x4 = 20 Credits**
	Core Electives	**3x3 = 09 Credits**
Part IV	**Value Education**	**3x2 = 06 Credits**
	Environmental studies	**1x2 = 02 Credits**
	Skill Based Electives	**3x2 = 06 Credits**
	Non – Major Electives	**2x2 = 04 Credits**
Part V		**1x1 = 01 Credits**
	Total	**140 Credits**

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DEPARTMENT OF CHEMISTRY
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Course : B.Sc **Code No : MC-11**
Semester : I **No of Hrs allotted: 4**
Paper : Core1 **No of Credits : 4**
Title of the Paper: Organic chemistry -I

COURSE OBJECTIVES (60 hrs)

This course will emphasize basic concepts and nomenclature of organic compounds.
It deals with reaction mechanism of Aliphatic and substitution reactions and elimination reactions.
To understand the conformational analysis.

UNIT-I INTRODUCTION 12 Hrs

Different methods of purification of organic substances - distillation under reduced pressure - steam distillation - Soxhlet method – Crystallization – Sublimation -Fractional distillation. Chromatography - adsorption chromatography (column) - partition chromatography (paper) - Thin layer chromatography (TLC) - vapour phase chromatography (VPC) - Determination of molecular weight - Classification and nomenclature of organic compounds - IUPAC systems.

UNIT-II FUNDAMENTAL CONCEPTS 12 Hrs.

Types of reagents: Electrophilic and Nucleophilic reagents –Definition and examples.
Isomerism: Definition, types of isomerism- structural isomerism – chain, position, functional – metamerism – tautomerism – explanation with examples - stereo isomerism – Geometrical or cis trans isomerism – Geometrical isomerism isomerism in alkenes with examples.

UNIT-III REACTION MECHANISM 12Hrs

Factors which influence a reaction – inductive effect, mesomeric effect - Hyper conjugation- Steric effects – Homolytic and heterolytic fission.
Reaction intermediates: Carbonium ions, carbanions, carbon free radicals and carbenes – Nomenclature, structure and stability.
Types of organic reactions and mechanisms - Mechanism of aliphatic nucleophilic substitution (SN_1, SN_2 and SNi) and elimination reactions (E_1 and E_2).

UNIT-IV 12 Hrs

Cycloalkanes
Definition, nomenclature, symbols of cycloalkanes, General methods of preparations and reactions
Stability Baeyer's strain theory and its limitations, Sache-Mohr theory.
Conformations of cyclohexane and its mono and disubstituted derivatives.

UNIT-V ALIPHATIC UNSATURATED HYDROCARBONS 12 Hrs

Alkenes - mechanism of addition –Markonikov and anti-Markonikov mechanism of addition to conjugated dienes - addition on alkynes- acidity of acetylene.

ALKYL HALIDES

Mono, di and tri halogen derivatives - preparation, properties and reactions - chloroform, iodoform, carbon tetrachloride and freons - vinyl chloride and allyl halides.

Reference books:

1. I.L.Finar, Organic chemistry Vol 1, 6th edition, Pearson Edition, 2005, Singapore.
2. R.T. Morrision and R.N. Boyd, Organic chemistry, 6th edition, Prentice Hall Private Limited, 1997, New Delhi.
3. P.L. Soni, Text Book of Organic Chemistry, Sultan Chand, 2005, New Delhi.
4. K.S. Tewari, N.K. Vishil and S.N. Mehotra. A text book of Organic Chemistry, 1st edition, Vikas Publishing House Pvt Ltd, 2001, New Delhi.
5. B.S. Bahl and Arun Bahl, Advanced Organic Chemistry, 1st edition, S. Chand and Company Ltd, 1998, New Delhi.
6. Peter Sykes, a Guide book to Mechanism in Organic Chemistry 6th Edition, Longmans Scientific and Technical, 2002, Essex.

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DEPARTMENT OF CHEMISTRY
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Course : B.Sc **Code No : MCL-11**

Semester : I **No of Hrs allotted: 4**

Paper : Core Lab **No of Credits : 2**

Title of the Paper : Inorganic Qualitative Analysis-I **(60 Hrs)**

Course Objectives:

To make the students analyze simple salts containing one acid and one basic radicals

Analysis of simple salts containing one anion and one cation.

Acid radicals:

Simple: Nitrate, Sulphate, Bromide, Iodide and Carbonate

Interfering: Phosphate, Oxalate, Borate, Chromate and fluoride

Basic Radicals:

Lead, Copper, Cadmium, Iron, Nickel, Zinc, Calcium, Barium, Strantium, Magnesium, Ammonium.

Total Marks = 100 (Internal 40 + External 60)

Internal Marks Distribution:

Acid radical	= 15
Basic radical	= 15
Procedure	= 05
Record	= 05
Total	= 40

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Course : B.Sc Chemistry **Code No : MC 21**
Semester : II **No of Hrs allotted : 6**
Paper : Core 2 **No of Credits : 6**
Title of the Paper: Inorganic and Physical Chemistry

Course Objectives **90 Hours**

In this course, the students are exposed to know the different types of bonding. Preparation, properties and applications of hydrides and interhalogen compounds are discussed. Properties of matter in gaseous and liquid state are also dealt with.

Unit – I: Chemical Bonding (18 hours)

Chemical bond - definition, types of chemical bonds.
Ionic or electrovalent bond - Definition, Illustration of the formation of ionic bond (Examples: NaCl, MgO, CaF_2, Al_2O_3 only), Condition for the formation of ionic compounds, Born Haber cycle,
Covalent bond: Definition, types of covalent bond (single, double and triple), Illustration of the formation of covalent bond (Example: HF, H_2O, NH_3, O_2, N_2 only), factors favouring the formation of covalent compounds.
Coordinate bond: Definition, Illustration of the formation of coordinate bond (Example: H_2O_2, SO_2, CO, NH_4^+, Al_2Cl_6 only), comparision between ionic, covalent and coordinate bond.
Hydrogen bond: Definition, properties, types and significance of hydrogen bonding.

Unit - II : Hybridization and Shape of Covalent Molecules (18hours)

Hybridization –concept-VB theory-sp,sp^2,sp^3 sp^3_d, sp^3d^2.VSEPR theory-Geometry of $SnCl_2$ NH_3,H_2O. ClF_3,IF_5 . Formation of molecular orbitals from atomic orbitals.

Molecular Orbital Theory- Homonuclear (H_2, Li_2, N_2, O_2) and Heteronuclear (CO and NO) diatomic molecules.

Unit- III: Gaseous State (18 hours)
Ideal gases: Kinetic theory of ideal gases- gas laws- ideal gas equation- definition of most probable velocity, Mean velocity and RMS velocity- Collision diameter- Collision cross section- collision frequency- mean free path.
Real gases: Deviation from ideal behaviour- Derivation of Vander Waal's equation- Methods of liquefaction of gases- Joule Thomson effect- Inversion temperature.

Unit - IV: Liquid State (18 hours)
Properties of liquids- viscosity – surface tension- their determination- liquid crystals – smectic – nematic- Cholesteric phase of liquid crystals- Swarm theory of liquid crystals.

Unit - V: Dilute Solutions (18 hours)
Colligative properties, - vapour pressure lowering- Osmosis and Osmotic pressure- boiling point elevation- freezing point depression- experimental determinnation of vapour pressure lowering and osmotic pressure- Van't Hoff factor- Degree of association- Degree of dissociation.

Text Books:

1. B.R. Puri, L.R. Sharma and K.C.Kalia. Principles of Inorganic Chemistry, 28th edition, Vallabh Publication, 2002, NewDelhi.
2. R.D Madan, Modem Inorganic Chemistry, S. Chand & Company, 2nd edition, 2002, New Delhi.

References:

1. B.R Puri, L.R. Sharma, and S. Pathania, Principles of Physical Chemistry, 33rd edition, Vishal Publication, 2007, Jalandhar.

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Course	**: B.Sc Chemistry**	**Code No**	**: MCL-21**
Semester	**:II**	**No of Hrs allotted**	**: 4**
		No. of credit	**: 2**

Title of the Paper: ORGANIC QUALITATIVE ANALYSIS (60 hours}

Analysis of

1. Aromatic Organic Compounds like mono and dicarboxylic acids.
2. Aromatic primary and secondary amines.
3. Aromatic amides
4. Aromatic aldehyde and ketones.
5. Phenols and naphthols.
6. Chloro and nitro aromatic compounds.
7. Aliphatic diamides.

Total marks =100marks (Internal= 40, External= 60)

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Course : B.Sc **Code No : SBE1**
Semester : II **No of Hrs allotted: 2**
Paper : Skill Based Electives -I **No of Credits : 2**
Title of the Paper: Polymer Chemistry

Total Hours: 30 Hrs

Course Objectives:

To give better understanding about the basic concept of polymers and the chemistry of commercial polymers.

UNIT-I

INTRODUCTION TO POLYMERS **15 hrs**

Introduction - polymers- monomers and polymers-degree of polymerization- definition- Classification of polymers- Homo, Hetero and copolymers- Block – Graft polymers- functionality – tacticity- Addition, co-polymerisation and Condensation polymers - Thermosetting & Thermoplastics.

UNIT-II

CHEMISTRY OF COMMERCIAL POLYMERS **15 hrs**

General methods of preparation, properties and uses of the following polymers: Polyethylene (LDPE & HDPE), PVC, Polystyrene, PAN, Teflon, Polyurethanes, phenol-folmaldehydes- composites- ABS.

Text Book:

1. V.R.Gowariker, N.V. Viswanathan and J.Sreedhar, Polymer Science, Wiley Eastern Ltd., 2000, New Delhi.

Reference Book:

1. B.K.Sharma, Polymer Chemistry, Goel publishing House, 2002, Meerut.

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DEPARTMENT OF CHEMISTRY
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Course : B. Sc **Code No : MC-31**
Semester : III **No of Hrs allotted : 3**
Paper : Core Paper 3 **No of Credits : 3**

Title of the Paper : INORGANIC CHEMISTRY-I

Course Objectives 45 Hours

It deals with error analysis and the concept of acids and bases. The group metals (I, II, III, IV and V) and their compounds are discussed. Emphasize is made in the general study of lanthanides and actinides.

UNIT I Alkali and Alkaline earth metals (9 hrs)

First group metals- extraction of Lithium-general group discussion-comparison of Li with other members of the family. Group II metals- group discussion-extraction of beryllium-comparison of Be with other members of the family-diagonal relationship between Beryllium and Aluminium- **important compounds –BeO, $BeCl_2$, CaC_2,$CaCl_2$**.

UNIT II p-block, d-block and f-block elements (9 hrs)

Comparative account of group III A elements – Boron – Borazole, Borohydrides, preparation properties and structure of diboranes.

General characteristics of group IV A elements – carbon – percarbonates – carbides, silicon, silicones and their applications – silicon in semi conductors – silicates – zeolites and ultramarines.

General introduction of transition metals. Metallurgy of titanium, molybdenum and tungsten.

General study of lanthanides and actinides. Uranium and thorium – metallurgy and their compounds.

UNIT III Group- V elements (9 hrs)

V group elements – general group discussion – preparation, properties, and structure of hydrazoic acid,hydroxyl amine – compounds of As, Sb and Bi – As_2O_3, Scheele's green, tartaremetic, sodium bismuthate.

UNIT IV Acids and Bases : (9 hrs)

Arrehenius concept, proton transfer theory – concept of Lowry and Bronsted – Luxflood concept – the solvent system concept – Lewis concept – relative strength of acids and bases – effect of solvent – leveling effect – effect of polarity and dielectric constant – effect of substituents – factors influencing relative strengths of acids and bases.

UNIT V Analytical Chemistry I (Error analysis) (9 hrs)

Error analysis – terms and definitions – absolute and relative errors – precision and accuracy – classification of errors – sources and minimization of errors – significant figures and computation – mean and standard deviation – method of least squares – student T test and Q test.

References

1. B.R.Pury, L.R.Sharma and K.C.Kalia, Principles of Inorganic Chemistry, 28th edition, Vallabha Publication, 2002, New Delhi.
2. B.K.Sharma, Instrumental methods of chemical analysis, 5th edition, Goel publication, 1996, Meerut.
3. D.A.Skoog, F.James Hollar and T.A.Niemans, Principles of industrial analysis, 5th edition, Thomson Books Cole, 2004, Singapore.

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DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc Chemistry **Paper Code : MC 32**
Semester : III **No of Hrs allotted : 3**
Paper : Core Paper 4 **No. of Credits : 3**
Title of the Paper: ORGANIC AND PHYSICAL CHEMISTRY

COURSE OBJECTIVES (45 Hours)

To study the preparation, properties and uses of organometallic compounds, alcohols, ethers, aldehydes & ketones. Composition of nucleus, properties of radioactive rays, natural radioactivity and its consequences are also discussed.

UNIT-I (9 **hrs)**

ORGANOMETALLIC COMPOUNDS: Organo magnesium compounds - preparation, reactions and synthetic uses of Grignard reagents. Metal alkyl: alkyl lead (TEL- tetra ethyl lead) - their preparation, reactions and synthetic uses.

ALCOHOLS

Classification (1°, 2° and 3°) – nomenclature - preparation, properties, reactions and uses of allyl alcohol, glycol and glycerol.

UNIT-II (9 hrs)

ETHERS: Nomenclature - General methods of preparation - Properties - Estimation of number of alkoxy groups.

THIO ALCOHOLS AND THIOETHERS:

Nomenclature - General methods of preparation – properties - sulphonol and mustard gas.

UNIT-III (**9 hrs)**

ALDEHYDES AND KETONES

Nomenclature - general methods of preparation – properties - Mechanism of addition and condensation reactions of aldehyde and ketones - Differences between aldehyde and ketone- Chemistry of acrolein and crotonaldehyde.

UNIT-IV (9 hrs)

NUCLEAR CHEMISTRY

Composition of the nucleus - Nuclear forces - Mass defect -'Binding energy – Binding energy per nucleon (Problems related to this) Nuclear stability and Binding energy.

NATURAL RADIOACTIVITY

Types of radioactive rays - Detection and measurement of radioactivity - GM counter method and Wilson cloud chamber method , Fajan's - Russell - Soddy group displacement law – illustration, Laws of radioactive disintegration - derivation of radioactive disintegration constant, average life and half-life period (Problems related to this).

UNIT-V (9 hrs)

MOLECULAR PROPERTIES AND STRUCTURE

Electrical properties of molecules - polarization of a molecule in an electric field - Derivation of Clausius - Mosotti equation — Derivation of Debye equation - Dipole moments and molecular structure - Magnetic properties of molecules - Magnetic permeability - Magnetic susceptibility - Measurement of magnetic susceptibility – Diamagnetism - Paramagnetism - Ferro magnetism and Anti-Ferromagnetism.

References:

1. I.L.Finar, Organic chemistry Vol 1, 6th edition, Pearson Edition, 2005, Singapore.
2. R.T. Morrision and R.N. Boyd, Organic chemistry, 6th edition, Prentice Hall Private Limited 1997, New Delhi.
3. P.L. Soni, Text Book of Organic Chemistry, Sultan Chand, 2005, New Delhi.
4. K.S.Tewari, N.K.Vishil and S.N.Mehotra. A text book of Organic Chemistry, 1st edition, Vikas Publishing House Pvt Ltd, 2001, New Delhi.
5. B.S.Bahl and Arun Bahl, Advanced Organic Chemistry, 1st edition, S. Chand and Company Ltd, 1998, New Delhi.
6. B.R. Puri, L.R.Sharma, R.D. Madan and S. Pathania, Principles of Physical Chemistry, 33rd edition, Vishal Publication, 2007, Jalandhar.

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DEPARTMENT OF CHEMISTRY

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Course : B.Sc Chemistry Code No :MCL-31
Semester : III No of Hrs allotted: 2
Paper : Core Practical 1 No of Credits : 1
Title of the Paper: VOLUMETRIC ANALYSIS
(Iodometry , Permanganometry And Organic Preparations)
(30 Hours)

A. ACIDIMETRY - ALKALIMETRY

1. Na_2CO_3 (Std)-HCl - Na_2CO_3
2. Na_2CO_3 (Std)-HCl - NaOH
3. HCl- Na_2CO_3 (Std)-HCl
4. NaOH-Oxalic acid - (Std)-NaOH

B. PERMANGANIMETRY

1. Fe^{2+}- $KMnO_4$-FAS
2. $KMnO_4$- Fe^{2+}- $KMnO_4$
3. Oxalic acid - $KMnO_4$-Oxalic acid
4. $KMnO_4$-Oxalic acid - $KMnO_4$

C. DICHROMETRY

1. Fe^{2+}-$K_2Cr_20_7$-FAS
2. $K_2Cr_20_7$ - Fe^{2+}- $K_2Cr_20_7$

D. IODOMETRY

1. $K_2Cr_20_7$-Thio- $K_2Cr_20_7$
2. $KMnO_4$-Thio- $K_2Cr_20_7$
3. $CuSO_4$-Thio- $K_2Cr_20_7$
4. $CuSO_4$-Thio- $KMnO_4$

ORGANIC PREPARATIONS

Preparation of the following Organic Compounds:

1. Benzoic acid from Methyl benzoate
2. Salicylic acid from Methy or ethyl salicylate
3. Osazone from Glucose
4. Benzoic acid from Benzaldehyde

(Any two estimations from each of the above mentioned volumetric estimations and also any two preparations)

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Course : B.Sc	**Code No : NME1**
Semester : III	**No of Hrs allotted: 2**
Paper : Non Major Elective - I	**No. of Credits : 2**
Title of the Paper: Modern Cosmetics	**Total Hours : 30 Hrs**

Unit I MODERN COSMETICS –I (15 Hrs)

Deodorants and antiperspirants-Distinction between astringents and deodorants, formulation of antiperspirant lotions and creams and sticks, deodorant powders. Dental Preparations: Tooth pastes- ingredients, their characteristics and functions – Mouth washes. Lip sticks: Classification of ingredients and formulation. Man's Toiletries: Hair lotions and tonics, hair creams greasy and non greasy shaving creams, after shave preparations.

Unit II MODERN COSMETICS – II (15 Hrs)

Hair care preparations: Hair structure, permanent hair waving, cold waving, special additive in cold wave preparations, shampoo different types and formulations, hair conditioners and setting lotions.Hair colourants: Hair lighteners and bleaches, Temporary colourant, Semi-permanent colourants, permanent colourants – vegetable dyes, Oxidation dyes and modifiers.

Reference:

1. Poucher, W.A. Perfumes, Cosmetics and soaps, Vol. III, Modern Cosmetics.
2. Simons, J.V. Chemistry and the beauty business.

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DEPARTMENT OF CHEMISTRY

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Course : B.Sc Chemistry **Code No : MC41**
Semester : IV **No of Hrs allotted: 3**
Paper : Core Paper 5 **No of Credits: 3**
Title of the Paper: PHYSICAL CHEMISTRY-I

COURSE OBJECTIVE: **45 Hours**

In this course the students are expected to learn the three laws of the thermodynamics and their application, Chemical equilibrium will also be explained.

UNIT-I THERMODYNAMICS (9hrs)

Importance of thermodynamics- limitations of thermodynamics-concepts of a system and surrounding-state variable- Extensive and Intensive properties- State function and their differential(exact and Inexact)-Different types of processes- Isothermal, Adiabatic, Isobaric, Isochoric,Reversible,Irreversible and cyclic.

FIRST LAW OF THERMODYNAMICS

Statement, Mathematical expression-enthalpy and energy of a system-Heat capacity at constant P & V-Correlation between C_p and C_v-Workdone in reversible isothermal compression-Maximum work- Workdone in Irreversible isothermal expansion and adiabatic expansion.

UNIT-II THERMOCHEMISTRY (9hrs)

Enthalpy of combustion- Bomb calorimeter-Bond energies-Flame and Explosion temperatures-Enthalpy of neutralization- Enthalpy of formation- Standard enthalpy of formation-Enthalpy of solution- Hess's law of heat of summation and its application- Kirchoff"s equation.

UNIT-III SECOND LAW OF THERMODYNAMICS (9hrs)

Need for second law- Different forms of second law- Carnot cycle and entropy a state function- Entropy changes in Reversible and Irreversible processes –Clausius inequality-Calculation of entropy change of an ideal gas with change in P,V &T-Entropy of mixing- Physical significance of entropy- work function and free energy- variation of free energy change with temperature and pressure- Maxwell's relationships- The Gibbs-Helmholtz equation- Clapeyron equation- Clausius Clapeyron equation- Application of clapeyron clausius equation- Van't Hoff isotherm-Van't Hoff Isochore-Osmotic pressure- Relationship between osmotic pressue and relative lowering of vapour pressure.

UNIT-IV THIRD LAW AND ZEROETH LAW OF THERMODYNAMICS (9hrs)

Nernst heat theorem-Statement of third law of thermodynamics- Determination of Absolute entropy of solid, liquids & gases- Experimental verification of third law- Entropy changes in chemical reaction- Residual entropy- Exceptions to third law-Definition of zeroth law of thermodynamics.

UNIT-V CHEMICAL EQUILIBRIUM (9hrs)

The law of mass action- Thermodynamic treatment of law of mass action - Relationship between Kp and Kc- Application of Law of mass action to Homogeneous system- PCl_5 and N_2O_4-Heterogeneous system-Calcium carbonate and Copper Sulphate- LeChatlier Braun principle-LeChatlier principle and Physical equilibria.

REFERENCES:

1. B.R. Puri, L.R. Sharma and Madan S.Pathania, Elements of Physical chemistry, 30th edition, Vishal publication, 2007, Jalandhar-Delhi.
2. B.S.Bahl, G.D. Tuli and Arun Bahl,Essential of Physical chemistry,S.Chand publications, Reprint 2004, Ram nagar, New Delhi.
3. D. Van Samuel Glasstone, Thermodynamics- Nostrand company, Inc., 5th edition, Eastern Wiley Publication,2002, London.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc Chemistry **Code No : EMC- 41**
Semester : IV **No of Hrs allotted : 3**
Paper : Major Elective **No of Credits : 3**
Title of the Paper: ORGANIC CHEMISTRY -II (Choice- A)

COURSE OBJECTIVE:

- To understand the chemistry of aliphatic carboxylic acid and their derivatives and substituted acids.
- To study the preparation and properties of aliphatic nitrogen compounds.
- To have an in-depth study of stereoisomerism such as Geometrical isomerism and Optical isomerism.

(45 Hrs)

UNIT –I

CARBOXYLIC ACID AND THER DERIVATIVES (9 Hrs)

Nomenclature – saturated monocarboxylic acid – Resonance structure of the carboxyl group – relative strength of carboxylic acids (effect od substituent effect). Acid derivatives: acid chlorides, anhydrides, amides and esters.

Unsaturated monocarboxylic acids: acrylic, crotonic and oleic acids.

Substituted acids: Halogeno acids – preparation, properties and reactions – hydroxyl acids- alpha and beta hydroxyl acids – preparation and reactions – action of heat – chemistry of lactic and tartaric acids.

UNIT –II

ALDEHYDIC AND KETONIC ACIDS (9 Hrs)

Preparation and properties of glyoxalic acids, pyruvic and laevulic acid – Preparation and synthetic importance of acetoacetic ester.

Dicarboxylic acids: Preparation and properties of Oxalic acid, malonic acid, succinic acid, glutaric acids – reactive methylene group.

Unsaturated dicarboxylic acid: Prpearation and properties of fumaric and maleic acid

UNIT –III

ALIPHARTIC NITOGEN COMPOUNDS (12 Hrs)

Preparation properties and reaction of alkylnitrites and nitroalkanes – alkyl cyanides isocyanides. Distinction between nitroethane and ethylnitrite; ethylcyanide and ethylisocyanides.

Aliphatic amines: Classification – Nomenclature - General methods of preparation, Properties and reaction - separation of mixture of amines Basicity of amines - distinction between primary, secondary and tertiary amine.

Aliphatic diazo compounds: Preparation and properties of diazomethane.

UNIT-IV

GEOMETRICAL ISOMERISM (9 Hrs)

Introduction - Determination of configuration of geometrical isomers – Physical methods- Chemical methods- E and Z system of nomenclature- geometrical isomerism of Oximes – Backmann rearrangement – Tautomerism- Definition- differences between tautomerism and resonance.

Conformational isomerism – Conformational isomerism of ethane and n-butane - Newmann, sawhorse, Fischer and flying wedge projection formulae.

UNIT-V

OPTICAL ISOMERISM (9 Hrs)

Optical activity-elements of symmetry – concept of chirality – optical isomerism exhibited by compounds containing one and two asymmetric carbon atoms – enantiomers and diasteromers – methods of resolution. Walden inversion and Assymetric synthesis (partial and absolute) – enantiotopic and diastereotopic ligands and faces. Relative and absolute configuration – Relative and absolute configuration - D, L nomenclature - R, S notations.

Difference between conformation and configuration

References:

1. I.L.Finar, Organic chemistry Vol I, 6th edition, Pearson Edition, 2005, Singapore.
2. R.T. Morrision, and R.N. Boyd, Organic chemistry, 6th edition, Prentice Hall Private Limited, 1997, New Delhi.
3. P.L. Soni, Text Book of Organic Chemistry, Sultan Chand, 2005, New Delhi.
4. K.S.Tewari, N.K.Vishil and S.N.Mehotra. A text book of Organic Chemistry, 1st edition, Vikas Publishing House Pvt Ltd, 2001, New Delhi.
5. B.S. Bahl and Arun Bahl, Advanced Organic Chemistry, 1st edition, S.Chand and Company Ltd, 1998, New Delhi.
6. P.S. Kalsi, Stereo chemistry, Conformation and Mechanism, 4th edition, New Age International Publishers, 2005, New Delhi.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc Chemistry **Code No : MCL-41**

Semester : IV **No of Hrs allotted: 2**

Paper : Core Practical **No of Credits: 1**

Title of the Paper: ORGANIC ESTIMATIONS **30Hrs**

ORGANIC ESTIMATIONS

1. Estimation of Phenol
2. Estimation of Aniline
3. Estimation of Glycine
4. Estimation of Ascorbic acid (Vitamin C)
5. Estimation of Saponification value of an Oil
6. Determination of Iodine value

Total Marks = 100 Marks (Internal = 40, External = 60)

Internal marks distribution:

Estimation = 30

Record = 10

Total = 40

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DEPARTMENT OF CHEMISTRY
(From 2014-17 batch onwards)

Course	**: B. Sc**	**Code No**	**: SBE-2**
Semester	**: IV**	**No of Hrs allotted**	**: 2**
Paper	**: Skill based elective**	**No of Credits**	**: 2**
Title of the Paper	**: Green Chemistry**	**Total Hours**	**: 30 Hrs**

INTRODUCTION TO GREEN CHEMISTRY

Unit – I (15 hrs)

Requirements- Basic principles- Solid state and solvent free organic reactions (using supported reagents)- Microwave radiation- Characteristics of microwave heating- Fundamental theory- Difference between microwave heating and conventional heating.

Unit – II (15 hrs)

Microwave reaction in organic solvent, in dry media- Pericyclic reaction- Vilsmeir Haack reaction- Friedlander condensation- Ortho Ester Claisen Rearrangement- Claisen-Schmidt condensation- Michael addition- Reformatsky reaction.

Text Books:

1. V. K. Ahluwalia and Renu Aggarwal- Organic Synthesis- 2001, Narosa Publishers, New Delhi.

Reference books:

1. K. R. Desai- Green Chemistry- 2005, Himalaya Publishing House, Mumbai.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-17 batch onwards)

Course : B.Sc	**Code No : NME2**
Semester : IV	**No of Hrs allotted : 2**
Paper : Non Major Elective-2	**No. of Credits : 2**
Title of the Paper: Consumer Products (Lab)	**Total Hours : 30 Hrs**

Course Objective:

In this course, students will be given training in the laboratory preparation of the following consumer products.

(i) Soap oil
(ii) Detergent powder
(iii) Cleaning powder
(iv) Phenoyl
(v) Shampoo
(vi) Tooth powder
(vii) Face powder
(viii) Candle
(ix) Chalk
(x) Pain balm

Reference:

Mohan Malhotra, Latest Cottage Industries, 20th Edition Edn, Vishal publishers, 1980, Meerut.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-17 batch onwards)

Course : B.Sc Chemistry Code No : MC-51
Semester : V No of Hrs allotted : 6
Paper : Core Paper 6 No of Credits : 6
Title of the Paper: INORGANIC CHEMISTRY –II

Total : 90 Hours

COURSE OBJECTIVE:

- To study the solid state elaborately.
- It deals with bioinorganic chemistry and transition metal catalysts.
- It discusses the study of VI group elements.
- Gives and idea about sources and control of air and water pollution.

UNIT-I:

SOLID STATE – I (18 hrs)

Types of solids – Amorphous – crystalline – Seven Crystal systems – Unit cell & Space lattice, Symmetry elements – Simple cubic – bcc – fcc lattices –Miller indices – Bragg equation – Packing of atoms and ions – packing arrangements ccp and hcp – radius ratio – co ordination number 3, 4 and 6 – packing efficiency – simple cubic, bcc and fcc. Structures of Cesium chloride, Zinc blende, Wurtzite, Diamond and Graphite.

UNIT – II:

SOLID STATE: II (18 hrs)

Crystal defects, schottky and frenkel defects – colour centres – point defects – plane defects – edge dislocation – non-stoichiometric defects – Semiconductors – **Types of crystals Molecular , Covalent, Metallic and Ionic crystals**-Free electron theory and band theory of solids – P-N junction – Transistors – super conductors.-**High temperature and low temperature super conductors, Organic super conductors**

UNIT – III: (18 hrs)

ORGANO METALLIC COMPOUNDS

Definition-Types- Alkene complexes—Zeise's Salt-Structural Features of Zeise's Salt-Iron-Butadiene Complex-Nomenclature of organometallic compounds, 16- and 18-electron rule.

Wilkinson catalyst (hydrogenation of olefins) – Zeigler-natta catalyst (propylene polymerization) – organo palladium catalyst – Wacker's process (oxidation of olefins) – Mechanism of these processes.

UNIT – IV: GROUP –VI ELEMENTS- SULPHUR COMPOUNDS (18 hrs)

General characteristics of group VI A elements, preparation, properties and structure of oxides and oxyacids of Sulphur. Halides of Sulphur, Thionic acids – permono and perdi sulphuric acid. Biologically important sulphur compounds – sulphur bridged Molybdenum V dimeric complexes.

UNIT – V: ENVIRONMENTAL CHEMISTRY: (18 hrs)

Air pollution – Air pollutants – Carbon monoxide – Carbon dioxide – Acid rain – Hydrogen sulphide – depletion of Ozone layer – Fluorocarbons and their effects on ozone layer – particulates – Toxic effects of particulates – smog, photochemical smog – Green House effect-monitoring and control of air pollutants. Water pollution – Biological oxygen demand – Chemical Oxygen demand – Purification of water – De-ionisation of water.

References:

1. B.R. Puri, L.R. Sharma, K.C. Kalia, Principles of Inorganic Chemistry, 28th edition, Vallabh Publication, 2004, New Delhi.
2. R.D. Madan, Advanced Inorganic Chemistry, 2nd edition.S. Chand & Company, 2005, New Delhi,
3. N. B. Hannay, Solid State Chemistry, Prentic- Hall of India Pvt Ltd, 1976, New Delhi.
4. B**.** Anthony, R. West, Solid State Chemistry and its applications West, John Wiley & Sons,1989, Singapore.
5. F.A. Albert Cotton, Advanced Inorganic Chemistry, Geofferey Wilkinson, Carlos, Murillo, Manfred Bochmann, John Wiley & Sons, Inc. 1998, New York.
6. J. E. Huheey, Ellen A. Keiter, Richard L. Keiter, Inorganic Chemistry, 4th edition, Pearson Education Pvt Ltd, Harper Collins College Publishers, 2004, Singapore.
7. A.K. De, Environmental Chemistry, 2nd edition, Wiley Easter Ltd, 1989, New Delhi.

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DEPARTMENT OF CHEMISTRY
(From 2014-17 batch onwards)

Course : B.Sc Chemistry **Code No :MC-52**
Semester : V **No of Hrs allotted : 6**
Paper : Core Paper 7 **No of Credits : 6**

Title of the Paper: ORGANIC CHEMISTRY – III **90 Hrs**

COURSE OBJECTIVE:

Senior undergraduate students will switch over their studies from aliphatic compounds to aromatic compounds. They will have an insight into the mechanism of aromatic substitution and will be exposed to structure and reaction of polynuclear hydrocarbons and their derivatives.

UNIT-I **18 hrs**

AROMATIC COMPOUNDS AND AROMATIC SUBSTITUTION

Introduction – Aromaticity and Huckel's rule – non benzenoid aromatics - Isolation of aromatic compounds from coaltar. Structure of benzene-resonance- aromatic Electrophilic substitution – Mechanism of nitration, sulphonation and Friedel-craft reaction, Directing effects of substituents – electronic interpretation - Aromatic nucleophilic substitution – Benzyne mechanism.

UNIT – II **18 hrs**

AROMATIC ALDEHYDES AND KETONES

ALDEHYDES

General methods of preparation, and properties of aromatic aldehydes – benzaldehyde – Mechanism of benzoin condensation – perkin reaction, claisen reaction, Knovenagel reaction and cannizaro reaction.

Unsaturated aldehyde – cinnamaldehyde

KETONES

Preparation and properties of acetophenone, benzophenone – Houben Hoesech synthesis.

REARRANGEMENT

Mechanism of the following rearrangements: Pinacol – Pinacolone, Hoffmann, Benzilic acid, Claisen, and Fries rearrangement

UNIT – III **18 Hrs**

AROMATIC SULPHONIC ACIDS

Methods of sulphonation – preparation and reaction of benzene sulphonic acid, sulphanilic acid – saccharin, and chloramine – T.

Aromatic hydroxy compounds

General methods of preparation and reaction of phenol – acid strength of phenol – General methods of preparation and reaction of phenolic ether (anisole).

Aromatic acids

Monocarboxylic acids – general methods of preparation, properties and reactions - benzoic acid – anthranilic acid – salicylic acid – cinnamic acid –
Dicarboxylic acid: phthalic acid and terephthalic acid.

UNIT – IV **18 Hrs**

AROMATIC COMPOUNDS CONTAINING NITROGEN

Aromatic Nitro Compounds

Nitro benzene – reduction products of nitrobenzene – T.N.T – picric acid - difference between nitro toluenes and phenylnitromethane.

Aromatic amino compounds

Aniline – Preparation and reactions - basicity of aromatic amines – effect of substituents – phenylene diamine – Toludines – benzyl amine.

Diazonium compounds

Diazotization – mechanism – benzene diazoniumchloride – structure and reactions - synthetic applications – Mechanism of diazo coupling reaction.

UNIT – V **18 Hrs**

POLY NUCLEAR HYDROCARBONES AND THEIR DERIVATIVES

(a) Naphthalene – structure, synthesis and reactions – orientation to electrophilic substitution - derivatives –napthols and naphthaquinones.

(b) Anthracene – structure, synthesis and reactions – anthraquinone - alizarin.

(c) Phenanthrene – structure, synthesis and reactions – phenanthraquinone.

Reference:

- I.L.Finar, Organic chemistry Vol 1, 6th edition, Pearson Edition, 2005, Singapore.
- P.L. Soni, Text Book of Organic chemistry, Sultans chand, 1991, New Delhi,
- K.S. Tewari, N.K. Vishil, S.N. Mehotra – A text book of org. chem – 1st edition, Vikas Publishing House Pvt Ltd., 2001, New Delhi.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc Chemistry Code No : MC-53
Semester : V No of Hrs allotted : 6
Paper : Core Paper 8 No of Credits : 6
Title of the Paper: PHYSICAL CHEMISTRY – II

Total Hours: 90

Course Objectives

Since the nanotechnology is gaining momentum, the students are introduced to Nanoscience. Non – conventional energy sources like solar energy conversion is also introduced. This course will deal with the applications of thermodynamics to dilute solutions and phase rule. The chemical kinetics, introductory quantum theory and applications of quantum theory to simple systems like particles in one dimension, three dimension and simple harmonic oscillator will be explained.

UNIT – I NANO TECHNOLOGY (18 hrs)

Definition of nanoscience- top down and bottom up approach – Sol-gel mehod- electron microscopes – transmission electron microscope (TEM) – application of nano materials – insulation materials – machine tools – phosphors – batteries, solar energy – high power magnets – motor vehicles and aircraft – medical implants.

UNIT-II PHASE RULE (18 hrs)

Statement and thermodynamic derivations – Application of phase rule – one component system (Water and Sulphur only) – Two component systems – simple eutectic (Lead – Silver only) – Compound formation – congruent melting point (Zn – Mg only) – Incongruent melting point (Na – K only)

Henry's law and Raoult's law – Two component liquid systems – completely miscible – completely immiscible – theory of fractional distillation and steam distillation.

UNIT – III CHEMICAL KINETICS (18 hrs)

Rate constant, order and molecularity – I order, II order(concentration same and different) and Zero order reactions – derivations of equations for rate constants — Half life period - zero, I, II order reactions – methods of determining order of the reaction – Arrhenius equation (ARRT) – significance of energy of activation – collision theory and its limitations.

UNIT – IV INTRODUCTION TO QUANTUM THEORY (18 hrs)

Experimental foundation of quantum theory– black body radiation and planck's theory(no derivation required) – Photoelectric effect and Einstein's theory – Hydrogen atomic spectrum and Bohr's theory of the atom model – Derivation of Ritz combination principle – Compton effect – Dualistic nature of matter – de Broglie's wave equation – uncertainty principle - spin of electron – Hund's rule – Pauli exclusion principle.

UNIT – V QUANTUM CHEMISTRY (18 hrs)

Postulates of quantum mechanics – Derivation of Schrödinger wave equation –wave function and its significance – probability of finding electrons - operators – differential and integral operators only – Application of Schrödinger wave equation - particle in one dimensional box – particle in 3D box.

References:

- M. Wilson, K.K. Geolf Smith, M. Simmons, B. Raguse Nanotechnology, overseas press, 2005, New Delhi.
- B.R. Puri, L.R Sharma, Madan S. Pathania, Principles of physical chemistry, 33rd edition, Vishal Publication, 2007, Jalandhar.
- K.J. Laidler, Chemical kinetics, 2nd edition – TaTa Mc Graw – Hill, 2005, U.K.
- A.K. Chandra, Introductory quantum chemistry,4th edition TaTa McGraw – Hill publishing company limited, 1994, U.K.
- Dr. K.S. Krishnan Marg, National Institute of Science Communication and Information Resources, 1996, New Delhi – 110012.

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DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Class: B.Sc Chemistry **Code : EMC-51**

Paper: Major Elective **Credits : 3**

Semester: V **No. of Hours : 5**

Title of the paper: COORDINATION CHEMISTRY

Course Objectives **75 hours**

It is a special paper on Coordination Chemistry. It deals with the basic concepts, theories, mechanism and application of Coordination chemistry. An emphasize is given on carbonyl compounds

UNIT – I (15 hrs)

Introduction to the transition elements – electronic configuration – variable valency – double salts and coordination compounds – coordination number and geometries, nomenclature – physical methods in the study of complexes – Werner's theory – stability of complexes – determination of stability constants – jobs method – stepwise stability constant – overall stability constant – factors affecting stability of coordination compounds – charge of central metal ion – size of central metal ion – chelate ring size – steric effects. Isomerism in coordination compounds.

UNIT – II (15 hrs)

Theories – Valence bond theory - application to octahedral and square planar complexes – crystal field theory – magnetic properties of metal complexes – factors influencing the magnitude of crystal field splitting – colour of transition metal complexes Jahn Teller distortion – Electronic spectra – Orgel diagram – d^1 and d^9 systems – MO theory applied to sigma bonding only.

UNIT – III (15 hrs)

Reactions of metal complexes. Labile and Inert complexes VBT, Taube's explanation of lability and inertness – ligand substitution reactions applied to Octahedral complexes S_N1, S_N2 reactions. Electron transfer reactions, inner sphere and outer sphere mechanism.

UNIT – IV (15 hrs)

Complexes of Pi acceptor ligands – metal carbonyls – EAN rule – classification preparation – properties – uses of metal carbonyls – bonding in metal carbonyls – IR spectra of metal complexes in cis – trans isomerism – determination of bond order of CO – differentiating terminal and bridging CO – structures of some common binary metal carbonyls – carbonyls of Ni, Fe, Co.

UNIT – V (15 hrs)

Application of coordination compounds- metal complexes in analytical chemistry – Inorganic qualitative analysis – complexometric titrations – complexes in colourimetry, gravimetry - metal complexes in therapy – metal complexes in industries –**Metal Complexes in Biological system.**

References:

J.E. Huheey, Ellen A.Keiter, Richard L.Keiter, Inorganic Chemistry, IV Edn., Pearson Education (Singapore) Pvt. Ltd., New Delhi. 2004.

1. Concise Inorganic Chemistry, J.D.Lee.
2. Selected topics in Inorganic Chemistry, Wahid U. Malik, G.D. Tuli, R.D. Madan, 7^{th} edition, S. Chand & Company Ltd, 2003, New Delhi.
3. Concise coordination chemistry – R. Gopalan, V. Ramalingam, Vikas publishing House, PVT LTD, 2001, New Delhi.

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DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc Chemistry Code No :MCL- 51
Semester : V No of Hrs allotted: 5
Paper : Core Practical 3 No of Credits :5
Title of the Paper: INORGANIC GRAVIMETRIC ESTIMATIONS AND ORGANIC PREPARATIONS 75Hrs

GRAVIMETRIC ESTIMATIONS:

1. Estimation of Lead as Lead chromate
2. Estimation of Barium as Barium chromate
3. Estimation of Nickel as Nickel-DMG complex
4. Calcium as Calcium Oxalate monohydrate
5. Magnesium as Magnesium Oxinate

ORGANIC PREPARATIONS

Preparation of the following Organic Compounds:

5. Benzoic acid from Methyl benzoate
6. Salicylic acid from Methyl or ethyl salicylate
7. Osazone from Glucose
8. Benzoic acid from Benzaldehyde

Total Marks = 100 (Internal = 40, External = 60)

Mark distribution:

Inorganic estimation	= 20
Preparation	= 10
Record	= 10
Total	40

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-17 batch onwards)

Course: BSc., **Code. No:**
Semester: V **No of hours allotted:**
Paper: Self Study **No of Credits: 5 (Extra)**
Title of the Paper: Dairy Chemistry

Course Objectives:

This paper deals with the composition of milk, processing of milk and milk products. The students will understand about the various constituents of milk and how to process the milk.

UNIT-I COMPOSITION OF MILK

Milk-definition-general composition of milk-constituents of milk-lipids, proteins, carbohydrates, vitamins and minerals-physical properties of milk-colour-odour-acidity-specific gravity-viscosity and conductivity - factors affecting the composition of milk-adulterants, preservative and neutralizer-example and their detection-estimation of fat, acidity and total solids in milk.

UNIT-II PROCESSING OF MILK

Microbiology milk-destruction of micro-organisms in milk-physico-chemical changes taking place in milk due to processing-boiling pasteurization-types of pasterurization-Bottle, batch and HTST (High Temperature Short Time)-Vacuum pasterurization-Ultra High Temperature Pasteurization.

UNIT – III MAJOR MILK PRODUCTS - I

Cream-composition-Chemistry of creaming process-gravitational and centrifugal methods of separating cream-estimation of fat in cream.

Butter –composition-theory of churning-desibutter-salted butter-estimation of acidity and moisture content in butter.

UNIT – IV

MAJOR MILK PRODUCTS – II

Ghee-major constituents-common adulterants added to ghee and their detection- rancidity-definition-prevention-antioxidants and synergists-natural and synthetic.

UNIT – V MAJOR MILK PRODUCTS - III

Special milk-definition-merits-reconstituted milk-definition-flow diagram of manufacturers-homogenized milk-flavoured milk-vitaminised milk-tonned milk-imitation milk-vegetable toned milk-humanized milk-condensed milk-definition, composition and nutritive value.

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DEPARTMENT OF CHEMISTRY
(From 2014-17 batch onwards)

Course : B.Sc., **Code No : MC 61**
Semester : VI **No of Hrs allotted : 6**
Paper : Core 9 **No of Credits : 6**
Title of the Paper: Analytical Methods and Computer Applications in Chemistry

Course Objectives: **90 Hours**

It gives a thorough understanding on the basic concepts of analytical Chemistry. It deals with the techniques like UV- visible spectrophotometry; TGA, DTA, Chromatography and cyclic voltametry.

It deals with Inorganic polymers

An introduction to computer and 'C' programming is given. Students gain hand on experience in writing c programming for their physical chemistry practical's.

UNIT I ANALYTICAL CHEMISTRY -I (18 Hrs)

Redox titrations , redox potentials, theory of redox indicators- principles involved in iodometric and iodimetric titrations- Complexometric titrations involving EDTA - indicators for Complexometric titrations –Principle, instrumentation and working of Cyclic voltametry.

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UNIT II ANALYTICAL CHMISTRY – II (18 Hrs)

i. Colorimetric and Spectrophotometric analysis-Beer's - Lambert's law and problems involving concentrations using Beer's-Lambert's law, working of double beam UV-visible spectrophotometer-determination of Nickel (II) and iron(III):

ii. Chromatography- Classification of chromatographic methods -Thin Layer-paper, column and gas. Chromatography-Theory of chromatography- R_f value applications of these methods in organic and inorganic chemistry.

iii. Thermal Analysis:- Principles, instrumentation and applications of TGA and DTA.

UNIT III: INORGANIC POLYMERS (18 hrs)

Inorganic polymers-General properties- Glass transition temperature-phosphorous based polymers-chain polymers- Maddrell's salts- kuroll's salts-phosphorous based network polymers-Sulphur based polymers-Boron based polymers.

UNIT-IV INTRODUCTION TO COMPUTERS (18 hrs)

Importance of Computers-history and development-hardware and software-structure of a computer - operating systems - DOS and UNIX – **Low level and High level languages-Interpreter and compiler**-Types of Computers - various input and output devices.

UNIT-V PROGRAMMING IN `C' LANGUAGE: (18 hrs)

a) Advantages - types-style of the language - **Structure of C-program**- keywords -variables – constants-**data types**-operators-arithmetic expressions--input and output functions- Running of C program -control-statements-Looping statements- arrays.. .

b) APPLICATION OF C PROGRAM IN CHEMISTRY

FORMULA TRANSLATIONS:

Calculation of

i). RMS and average velocities of O_2.
ii). Mean activity coefficient of an electrolyte.
iii). Calculation of pH of the given solution
iv). Use of braces in if-else ladder to obtain the lines of Lyman series
v) Applying C-programming to simple physical chemistry practicals like Rast method and Ester hydrolysis.
vi). Calculation of Normality, Molarity and molality of the given solution.
vii). Conversion of Celsius to Kelvin temperature and vice versa.

Text Books:

1. B.R. Puri, L.R. Sharma, K. C. Kalia, Principles of Inorganic Chemistry, 28th edition, Vallabh publication, 2004, New Delhi.
2. B.K.Sharma, Instrumental Methods of chemical analysis, 5th edition, Goel publication, 2000, New Delhi.
3. Chatwal Anand, Spectroscopy, Himalaya publishing house, 1994, New Delhi.
4. Skoog & West., Principles of instrumental analysis, 5th edition, Thomson Brooks Cole, 2004, Singapore.

Reference Books:

1. E.Balaguruswamy, Programming in ANSI C, 3rd edition, Tata McGraw-Hill publishing Company Ltd., 2005, New Delhi.
2. Yaswant Kanitkar, Let us C, BPB Publications, 1998, New Delhi.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc Chemistry Code No : MC-62
Semester : VI No of Hrs allotted : 6
Paper : Core Paper -10 No of Credits : 6
Title of the Paper: ORGANIC CHEMISTRY – IV

Total Hours: 90

COURSE OBJECTIVE

To study about the structure and synthesis of natural products like carbohydrates, alkaloids, terpenoids and proteins. Students are also highlighted on the spectral techniques in the identification of compounds.

UNIT – I **18 hrs**

CARBHOYDRATES

Introduction and classification — glucose – mutarotation – Killiani-Fischer synthesis – Ruff degradation - structure of glucose – Fructose: Structure of fructose - methods of interconversion between aldose and ketose – Disaccharides – sucrose – structure elucidation – Polysachharides - starch and cellulose (classification and structure only).

UNIT – II **18 hrs**

HETROCYCLIC COMPOUNDS AND DYES

Introduction to heterocyclic compounds, Nomenclature – chemistry of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole.

Introduction to dyes – colour and constitution - Classification based on structure and application – preparation and applications of the following dyes – methyl orange, congo red, malachite green, flourescein, phenolphthalene and indigo.

UNIT –III

CHEMISTRY OF NATURAL PRODUCTS **18 hrs**

Alkaloids

Introduction - general characteristics - classification – Hofmann Exhaustive methylation - structure and synthesis of the following alkaloids – piperine, nicotine, and atropine.

Terpenoids

Introduction and classification - isoprene rule – gem dialkyl rule - structure, synthesis and stereochemistry of the following terpenoids – citral, menthol and camphor.

UNIT – IV

PHOTOCHEMISTRY **18 hrs**

Difference between photochemical and thermal reaction – Jablonski diagram - introduction to photochemical reaction - photo elimination - photo reductions - photo oxidations - Cis -trans isomerisation – rearrangements – Cyclisation – woodward – Hofmann rules for cyclo additions.

UNIT – V

ORGANIC SPECTROSCOPY **18 hrs**

Introduction – laws of light absorption – UV-Visible spectroscopy - Types of electronic transitions- chromophore – auxochrome – bathochromic shift – hypsochromic shift – hyperchromic shift – applications of UV spectroscopy.

IR spectroscopy – Molecular vibrations – number of fundamental vibrations – factors affecting vibrational frequency – hydrogen bonding – applications of IR spectroscopy.

NMR spectroscopy – Introduction – relaxation process – number of signals - chemical shift – shielding and deshielding – splitting of signals – spin - spin coupling – coupling constants – Applications of NMR spectroscopy.

Reference books

- I.L.Finar, Organic chemistry Vol 1, 6th edition, Pearson Edition 2005, Singapore.
- K.S.Tewari, N.K.Vishil and S.N.Mehotra. A text book of Organic Chemistry, 1st edition, Vikas Publishing House Pvt Ltd, 2001, New Delhi.
- Y.R. Sharma, O.P. Vig, Elementary organic absorption spectroscopy – 1st edition, Goel Pulishers, 1997, Meerut.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc Chemistry **Code No : MC-63**
Semester : VI **No of Hrs allotted: 6**
Paper : Core Paper 11 **No of Credits : 6**
Title of the Paper: PHYSICAL CHEMISTRY – III

Course Objectives **Total Hours: 90**

After undergoing this course, the students are expected to know the theories of ionic conductance, EMF measurements and its applications to chemistry. In photochemistry unit, the students are explained about the various photochemical processes and their kinetics. The students will be taught about the classification and the determination of molecular masses of macromolecules. In colloid and surface chemistry, the preparation and properties of colloids are to be taught. Also the enzyme catalysis will be dealt with.

UNIT – I ELECTRO CHEMISTRY – I (18 hrs)

Electrical conductance in solution – Ohm's law and Faraday's law – specific, equivalent and molar conductance – variation of conductance with dilution – Oswald's dilution law– Kohlrausch's law and its application – ionic mobilities – transport numbers and their determination–Conductometric titrations (Strong acid and strong base, weak acid and weak base) – ionic equilibria – ionic product of water – Ionisation constant of weak acids and bases – pH, pOH and pKa – buffer solutions – Henderson equation – common ion effect.

UNIT – II ELECTROCHEMISTRY – II (18 hrs)

Electrochemical cells – Galvanic cells and Emf – electrode reaction and electrode potential – thermodynamics of cells -concentration cells– measurement of Emf (Poggendrof's method) and it's applications – representation of electrodes and cells – sign conventions – Nernst's equation - standard electrode potential – Electrochemical ells – dry cell – Ni-Cd, – lead storage battery-potentiometric titration. Fuel cells - Hydrogen – Oxygen fuel cells and solar cell

UNIT – III PHOTOCHEMISTRY (18 hrs)

Absorption of potochemical reactions – Hydrogen – bromine reaction, Hydrogen chlorine reaction, dimerisation of anthracene. Absorption of radiation – Laws of photochemistry – quantum efficiency – thermal and photochemical reactions – Jablonski diagram – fluorescence and phosphorescence – photosensitization – chemluminescence – bioluminescence.

UNIT – IV (18 hrs)

POLYMER CHEMISTRY

Classification of polymers – Functionality – Tacticity– addition, co-polymerisation and condensation polymerization – Thermoplastic resin and thermosetting resin – mechanism of cationic and anionic polymerization – number average and weight average molecular weights – Moulding of polymers – injection, compression.

UNIT – V (18 hrs)

COLLOIDS AND SURFACE CHEMISTRY

Introduction – colloids – zeta potential – coagulation – Hardy Schulze law – Hofmeister series protective effects – gold number – gels – Thixotrophy, synerisis and imbibtion – Donnan membrane equilibrium – colloidal electrolytes and detergents.

Physical adsorption, chemical adsorption and occlusion – Freundlich and Langmuir's adsorption isotherms.

Catalysis – Homogenous and heterogeneous catalysis – enzyme catalysis -Michaelis Menton Mechanism .

Reference

- B.R. Puri, L.R. Sharma and Madan S. Pathania, Principles of Physical chemistry, 33rd edition, Vishal Publication, 2007, Jalandhar.
- Glasstone – von nonstrand, Introduction to electro chemistry, Von Nonstrand Co. Inc., 2002, Toronto.
- Rahatgi Mukherjee, Fundamentals of Photochemistry, Willey Eastern Ltd., 1994, New York.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc., **Code No :EMC 61**
Semester :VI **No of Hrs allotted:5**
Paper : Major Elective **No of Credits:3**
Title of the Paper: Group Theory and Spectroscopy

Course Objective: **75 Hrs**

This is a special paper in Physical Chemistry.This paper is introduced to give an advanced knowledge for UG students in group theory,molecular spectroscopy,Raman spectroscopy and resonance spectroscopy.

UNIT-I 15 hrs

GROUP THEORY-I

Definition of a mathematical group-Characteristics-Abelian group and cyclicgroup-Group multiplication table-subgroup-similarity transformation and class of group.Symmetry operations and symmetry elements –Point group –Assignment of Point group –Symmetry elements and symmetry operations in various molecules-Symmetry operations forming mathematical group.Matrix operators for Symmetry operations –Representation of a group –Reducible and Irreducible representation.

UNIT-II 15 hrs

GROUP THEORY-II

The great orthogonality theorem –rules for writing (properties of) irreducible representations – Projection operator –Direct product representation –Character table –$C_{2V,}$ C_{3V} and C_{2h} point group character table derivation- Application of group theory-Determination of Hybridation in BF_3 and CH_4 –Normal mode analysis –Selection rule of IR and Raman activity of normal modes of H_2O, $N_{2,}$ F_2, NH_3-Allowed and Forbidden transition in HCHO.

UNIT-III 15 hrs

MOLECULAR SPECTROSCOPY

Electromegnetic Spectrum –different regions in electromagnetic spectrum-Molecular spectra-Types of molecular spectra.

Microwave spectra –Classification of molecules –Rotational spectra of diatomic molecules –Rigid rotator-Selection rules-Relative intensities of spectral lines –effect of isotopic substitution –Application of microwave spectroscopy – Determination of bond distances in diatomic molecules.

Electronic spectra –electronic spectra of diatomic molecules – Franck Cotton principle – vibronic transitions and vibrational progression – group frequencies and factors affecting band position and intensities.

UNIT-IV 15 hrs

INFRA-RED AND RAMAN SPECTROSCOPY

Infra-red: Vibrational spectra of diatomic molecule –Force constants from IR spectra-Rotation-vibration spectra of diatomic molecules-IR spectrometer-Application of vibrational spectra-Simultaneous rotation and vibration in molecules-Diatomic vibrating rotator-diatomic molecule as a harmonic oscillator and a rigid rotator-Diatomic molecule as anharmonic oscillator and a non-rigid rotator-Analysis of IR spectra on the basis of modes of vibrations,of polyatomic molecules CO_2, H_2O- Finger print region and Characteristic frequencies – Fermi resonance.

Raman spectra: Introduction – Difference between IR and Raman spectra – Pure rotational Raman spectra – polarization of light –Raman effect –Application of Raman effects to chemistry-structure determination from Raman and IR spectroscopy –Mutual exclusion principle-Instrumentation-advantages and limitations of Raman spectroscopy.

UNIT-V 15 hrs

RESONANCE SPECTROSCOPY

NMR: Introduction –Nuclear spin and magnetic moment-origin of NMRspectra- theory of NMR spectroscopy-precession of particles in a field –saturation –relaxation spin-spin process in NMR-Basic instrumentation –types of environmental effects –chemical shifts-splitting –shielding and deshielding of magnetic nuclei- factors affecting chemical shifts – NMR spectrum of CH_3CHO –the coupling constant J- factors influencing the coupling constsnt J.

ESR:ESR introduction –factors affecting the gvalue- difference between ESR and NMR-basic instrumentation-Hyperfine interactions –Applications of ESR – Limitations of ESR.

Text Books:

1. Puri & Sharma, Physical chemistry,33rd edition,Vishal Puplications,2003,NewDelhi.
2.K.V.Raman,Group theory,1st edition,Tata McGraw Hill Publishing Limited,1990, NewDelhi.
3. C. M. Banwell, Fundamentals of Molecular spectroscopy, 4 th edition, TMH company limited, 2005.
4.V.Ramakrishnan & M.S.Gopinathan,Group theory,1st edition, Vishal Puplications,1988,NewDelhi.

Reference Books:

1. Gurudeep R.Chatwal & K.Anand, Spectroscopy, 5th edition, Himalaya Puplications, 2002, NewDelhi.
2. Russel S.Drago, Physical method in Inorganic Chemistry, Affilation East-West Press Pvt Limited, NewDelhi.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc Chemistry Code No : MCL-61
Semester : VI No of Hrs allotted: 5
Paper : Core Practical 4 No of Credits : 2
Title of the Paper: EXPERIMENTS IN PHYSICAL CHEMISTRY 75Hrs

1. Potentiometric Titrations
2. Conductometric Titrations
3. Molecular weight determination by Rast Micro Method
4. Simple Eutectic system
5. Compound formation
6. Ester hydrolysis using acid HCl or H_2SO_4
7. CST of Phenol

Total Marks = 100 (Internal 40 + External 60)

Distribution:

Record	= 10 Marks
Practical	= 30 Marks
Total	40

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DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc., **Code : SBE 3**

Semester : VI **No. of hours allotted: 2**

Paper : Skill Based Elective **No. of credits: 2**

Title of the paper: WATER ANALYSIS **Total Hours: 30Hrs**

1. Estimation of temporary and permanent hardness.
2. Estimation of calcium and magnesium hardness.
3. Estimation of chloride by Mohr's method.
4. Estimation of sulphate.
5. Spectro photometric estimation of fluoride.
6. Estimation of dissolved oxygen (DO).
7. Estimation of TDS.
8. Determination of Biological Oxygen Demand (BOD).
9. Determination of Chemical Oxygen Demand (COD).
10. Flame photometric estimation of sodium.

Total Marks = 100 (Internal = 40, External = 60)

Distribution:

Short Procedure = 20 Record = 10 Experiment = 30

Total = 60

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Allied Papers

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-17 batch onwards)

Course : B.Sc., **Code : AC11**
Semester : I, III &V **No. of hours allotted: 4**
Paper : ANCILLARY CHEMISTRY - I **No. of credits : 4**

Title of the paper: GENERAL CHEMISTRY - I **Total Hours: 60Hrs**

V Sem : III B.Sc., Mathematics
III Sem : II B.Sc., Physics & II B.Sc., Botany
I Sem : I B.Sc., IMB

UNIT-1 STRUCTURE OF ATOM 12 Hrs

Rutherford model of the atom- defects of Rutherford model - Discovery of neutron, Bohr model of an atom- merits and demerits- Sommerfield modification- - de Broglie's concept of durality - quantum numbers- shapes of s, p, d atomic orbitals. Arrangement of electrons in atoms- Hund's rule – Pauli exclusion principle- Heisenberg's uncertainty principle.

UNIT-II BONDING 12 Hrs

VB theory: Postulates of VB theory- application to the formation hydrogen. Overlap of atomic orbitals- s-s, s-p and p-p overlap- principles of hybridization-brief outline of hybridization sp^3, sp^2 and *sp* with one example for each

UNIT-III HYDROGEN 12 Hrs

Isotopes of hydrogen- separation of the isotopes- properties and uses of heavy hydrogen- position of hydrogen in the Periodic table- ortho and para hydrogen- separation, difference in structure and properties- Hydrogen Peroxide and Ozone: Manufacture, properties, structure and uses.

UNIT- IV CARBOHYDRATES 12 Hrs

Classification- preparation and properties and uses of sucrose- muta rotation- conversion of aldopentose to aldohexone and vice versa. Conversion of glucose to fructose vice versa.

UNIT- V WATER 12 Hrs

Introduction – Definition- Units of Hardness- Scales and Sludge – Sterilization and flocculation. Hardness of water – Treatment of water: Ion –exchange method and reverse Osmosis – Estimation of hardness by EDTA method

Reference:

1. Fundamentals of chemistry- R.Gopalan, S.Sundaram, Sultan Chand & sons, 1998.
2. Principles of Inorganic Chemistry, B.R. Puri, L. Sharma, K.C. Kalia-Shoban, Lal Nagin Chand & co 1995.
3. Allied chemistry-R.Gopalan, S.Sundaram, Sulthan Chand & Son 1993. LTD.
4. Principles of Inorganic Chemistry, B.R. Puri, L. Sharma, K.C. Kalia-Shoban, Lal Nagin Chand & co 1998.
5. Text book of Organic Chemistry, P.L.Soni, S.Chand & Company, New Delhi, 1998.

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DEPARTMENT OF CHEMISTRY
(From 2014-17 batch onwards)

Course : B.Sc., **Code : AC21**
Semester : II, IV & VI **No. of hours allotted: 4**
Paper : ANCILLARY CHEMISTRY - II **No. of credits : 4**

Title of the paper: GENERAL CHEMISTRY - II **Total Hours: 60Hrs**

VI Sem : III B.Sc., Mathematics
IV Sem : II B.Sc., Physics & II B.Sc., Botany
II Sem : I B.Sc., IMB

UNIT – I NUCLEAR CHEMISTRY 12 Hrs

Introduction – mass defect- binding energy, neutron- proton ratio, packing fraction. *Natural Radioactivity*: Comparison of properties of alpha, beta and gamma rays- detection and measurement of radioactivity- GM counter-Fajans- Russelll- Soddy group displacement law- illustration- half life period- Nuclear fission – Nuclear Fusion. Uses of radioactive isotopes as tracers.

UNIT- II ELECTROCHEMISTRY 12 Hrs

Arrehenius theory of electrolysis- strong electrolytes- weak electrolytes- Oswald's dilution law and its significance. *Conductance*: Specific, equivalent and molar conductance- measurements, Kohlraush's Law and applications- conductometric titrations. *pH*: Definition simple calculation of pH from molarity of acids - common ion effects and its applications - Buffer solution – definition- theory of buffer action and applications.

UNIT- III CATALYSIS 12Hrs

Definition- different types of catalysts – homogenous and heterogeneous catalysis- acid-base catalysis- enzyme catalysis-mechanism. Mechanism of heterogeneous catalytic reactions - auto catalysis- catalytic poisoning- promoters.

UNIT- IV PREPARATION AND USE OF IMPORTANT COMPOUNDS 12 Hrs

BHC, DDT, TNT, Bakelite, picric acid , saccharin, Nylon 66, PVC, *Fuels*: LPG, water gas, producer gas, preparation, properties (composition) and uses. *Fertilizers*: Preparation and uses of urea, super phosphate, triple super phosphate and potassium nitrate.

UNIT- V AMINOACIDS 12 Hrs

Amino acids: Definition- general methods of preparation, properties and uses- Glycine, and alanine. *Proteins*: Definitions- Classification and general properties – colour reactions and the relation of amino acids to proteins. *Vitamins*: Definition- classification, sources and role of vitamins or deficiency symptoms - A, B complex, C, D and K (structure and synthesis not expected).

References:

1. Fundamentals of chemistry- R.Gopalan, S.Sundaram, Sultan Chand & sons, 1998.
2. Principles of Inorganic Chemistry, B.R. Puri, L. Sharma, K.C. Kalia-Shoban, Lal Nagin Chand & co 1995.
3. Allied chemistry-R.Gopalan, S.Sundaram, Sulthan Chand & Son 1993. LTD.
4. Principles of Inorganic Chemistry, B.R. Puri, L. Sharma, K.C. Kalia-Shoban, Lal Nagin Chand & co 1998.
5. Text book of Organic Chemistry, P.L.Soni, S.Chand & Company, New Delhi, 1998.

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DEPARTMENT OF CHEMISTRY

(From 2014-17 batch onwards)

Course : B.Sc., **Code No : ACL1**
Semester : IV & VI **No of Hrs allotted : 30**
Paper : ANCILLARY CHEMISTRY PRACTICALS **No of Credits : 2**
Title of the Paper: Inorganic Chemistry Practical

V & VI Sem : III B.Sc., Mathematics
III & IV Sem : II B.Sc., Physics & II B.Sc., Botany
I & II Sem : I B.Sc., IMB

(Common to B Sc Maths, Physics, Botany and IMB)

Course Objectives:

The students will get exposed to titrations alkalimetrically, permanganometrically, dichrometrically andiodometrically.

I ACIDIMETRY - ALKALIMETRY

1 Na_2CO_3 (Std)-HCl - Na_2CO_3
2 Na_2CO_3 (Std)-HCl - NaOH
3 HCL- Na_2CO_3 (Std)-HCl
4 NaOH-Oxalic acid - (Std)-NaOH

II PERMANGANIMETRY

1 Fe^{2+}- $KMnO_4$-FAS
2 $KMnO_4$- Fe^{2+}- $KMnO_4$
3 Oxalic acid - $KMnO_4$-Oxalic acid
4 $KMnO_4$-Oxalic acid - $KMnO_4$

III DICHROMETRY

1 Fe^{2+}-$K_2Cr_20_7$-FAS
2 $K_2Cr_20_7$ - Fe^{2+}- $K_2Cr_20_7$

IV IODOMETRY

1 $K_2Cr_2O_7$-Thio- $K_2Cr_2O_7$
2 $KMnO_4$-Thio- $K_2Cr_2O_7$
3 $CuSO_4$-Thio- $K_2Cr_2O_7$
4 $CuSO_4$-Thio- $KMnO_4$

(Any two estimations from each of the above mentioned volumetric estimations to be given for Regular Class practical and for the Summative Practical Examination)

Total Marks: 100 (Internal=40, External=60)

M.Sc., Chemistry

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DEPARTMENT OF CHEMISTRY

COURSE STRUCTURE (w.e.f 2014 – 2016 Batch Onwards)

I – Semester

Course	Code	Subject	Contact Hrs.	Credits	Max. Marks (CA)	Max. Marks (SE)	Total
Core 1	1PC1	Organic Chemistry – I	5	5	25	75	100
Core -2	1PC2	Inorganic Chemistry – I	5	5	25	75	100
Core - 3	1PC3	Physical Chemistry – I	5	5	25	75	100
Lab	2PCL1	Organic Chemistry Practicals	5*	-	-	-	-
Lab	2PCL2	Inorganic Chemistry Practicals	5*	-	-	-	-
Lab	2PCL3	Physical Chemistry Practicals	5*	-	-	-	-
		Total	**30**	**15**	**75**	**225**	**300**

II – Semester

Course	Code	Subject	Contact Hrs.	Credits	Max. Marks (CA)	Max. Marks (SE)	Total
Core 4	2PC1	Organic Chemistry – II	4	4	25	75	100
Core 5	2PC2	Inorganic Chemistry – II	4	4	25	75	100
Core - 6	2PC3	Physical Chemistry – II	4	4	25	75	100
Elective - 1	2PC4(E1)	C-Programming Fundamentals & Applications in Chemistry (Elective 1) (OR) Medicinal Chemistry (Elective 2)	5	5	25	75	100
Lab	2PCL1	Organic Chemistry Practicals	5	5	40	60	100
Lab	2PCL2	Inorganic Chemistry Practicals	4	4	40	60	100
Lab	2PCL3	Physical Chemistry Practicals	4	4	40	60	100
		Total	**30**	**30**	**220**	**480**	**700**

III – Semester

Course	Code	Subject	Contact Hrs.	Credits	Max. Marks (CA)	Max. Marks (SE)	Total
Core 7	3PC1	Organic Chemistry – III	5	5	25	75	100
Core 8	3PC2	Inorganic Chemistry – III	5	5	25	75	100
Core - 9	3PC3	Physical Chemistry – III	5 (3+2)	4 (3+1)	25	75	100
Elective - 2	3PC4(E2)	Computer Applications in Chemistry (Elective 1) (OR) Advanced Organic Synthesis (Elective 2)	5	5	25	75	100
Lab	4PCL1	Organic Chemistry Practicals	5*	-	-	-	-
Lab	4PCL (E3)	Inorganic Chemistry Practicals (Elective 1) (OR) Analytical Chemistry Practicals (Elective 2)	5*	-	-	-	-
		Total	**30**	**19**	**100**	**300**	**400**

IV Semester

Course	Code	Subject	Contact Hrs.	Credits	Max. Marks (CA)	Max. Marks (SE)	Total
Core 10	4PC1	Organic Chemistry – IV	4	4	25	75	100
Core 11	4PC2	Inorganic Chemistry – IV	4	4	25	75	100
Core - 12	4PC3	Physical Chemistry – IV	4	4	25	75	100
Lab	4PCL1	Organic Chemistry Practicals	5	5	40	60	100
Elective - 3	4PCL (E3)	Inorganic Chemistry Practicals (Elective 1) (OR) Analytical Chemistry Practicals (Elective 2)	5	5	40	60	100
PJ	PJ	Project	8	4	40	60	100
		Total	**30**	**26**	**195**	**405**	**600**

* Credits will be given at the end of II / IV Semester

A. <u>Consolidation of contact hours and credits: PG</u>

Semester	Contact Hrs/week	Credits
I	30	15
II	30	30
III	30	19
IV	30	26
Total	**120**	**90**

B) <u>Curriculum Credits</u>

Core	--- 75Credits
Elective	---15 Credits

Total	90 Credits

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 1PC1**
Semester	**: I**	**No. of Hrs allotted**	**: 5**
Paper	**: Core -I**	**No. of Credits**	**: 5**
Title of the Paper	**: Organic Chemistry –I**		

Course Objective:

This paper aims at enriching the students' knowledge about bonding and reaction mechanism in organic molecules.

UNIT-I Delocalized chemical bonding, Aromaticity and Reaction intermediate (15 hrs)

Electron displacement – Steric effect – Tautomerism

Concept of aromaticity – Benzenoid and non-benzenoid compounds – Huckel's rule - Non aromatic and anti aromaticity - Alternant and non alternant hydrocarbons - aromaticity of cyclopentadienyl anion and Tropylium cation – Azulenes and annulenes.

Synthesis , structure, stability, reactivity and reactions of carbocations, carbanions, free radicals (reactions include Pinacol coupling, McMurray reactions, acyloin reaction, selective radical bromination). Carbenes: Stability - Structure – Generation – Types – Reactions. Nitrenes: Generation and reactions.

UNIT - II Reaction mechanism-I (15 hrs)

Guidelines for proposing reasonable mechanism – Energetics and energy profile diagrams – transition state – Intermediate – Hammond's postulate – principle of microscopic reversibility - kinetic and thermodynamic controls – kinetic and non-kinetic methods of determining organic reaction mechanism – primary and secondary kinetic isotope effects – Effect of structure on reactivity: Resonance and field effects – Quantitative treatments – Hammett and Taft equation.

UNIT - III Reaction mechanism-II (15 Hrs)

Substitution Reactions:

Aliphatic Nucleophilic Substitution Reactions - Mechanism – S_N1 and S_N2, mixed S_N1& S_N2, S_Ni, SET, Neighboring group participation by σ and π bonds – Reactivity at an allylic, aliphatic trigonal and vinylic carbon – Effect of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity - Ambident nuleophiles.

Aromatic Nucleophilic Substitution Reactions – Unimolecular, Bimolecular and Benzyne mechanism – Effect of substrate, leaving group and attacking nucleophile.

Electrophilic substitution reactions:

Aliphatic: Bimolecular mechanism SE2 and SE1 – Aromatic: Arenium ion mechanism – Orientation and reactivity: Ortho and Para ratio, partial rate factor

UNIT-IV Reaction Mechanism III (15 hrs)

Elimination reactions

E_1, E_2 and E_1CB mechanism- Competition between substitution and elimination – orientation of double bonds (Bredt's rule and Hofmann and saytzeff rules) – Effect of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity – Mechanism and orientation in pyrolytic eliminations - Cope and Chugaev reaction (cis-elimination)

UNIT-V Reaction Mechanism IV (15 hrs)

Addition to carbon – carbon multiple bonds:

Electrophilic, Nucleophilic & free radical addition – Mechanism, Orientation and reactivity and reactions - addition to conjugated systems- addition to α,β-unsaturated carbonyl and nitrile systems- Michael addition – addition of Grignard reagents-Diels Alder reaction- Enamine reaction - Mechanism of Reformatsky reaction- Darzen reaction- Mannich reaction - Wittig reaction - Stobbe and Dieckman condensation.

Text books:

1. Jerry March, Advanced Organic Chemistry, Reaction mechanism and structure, John Wiley and sons, 4th Edition, New york, 1992.
2. R.O.C Norman, Principles of organic synthesis, 3rd Edition Nelson Thorines, Hong kang 2001.
3. P.J.Garrat, Aromaticity, Mc Graw Hill, 1991
4. F.A.Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and B, Plenum Press, 3rd Edition 1990).
5. G.M. Badger, Aromatic character and Aromaticity, Cambridge, USA, 2001.

Reference Books:

1. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, 2007.
2. E.S. Gould, Mechanism and structure in Organic Chemistry, Holtoo INC, 1960.
3. G. Solomon, Organic Chemistry, John Wiley and sons INC, 5th Edition, 1992.
4. R.K. Mackie and D.M. Smith, Guide Book to Organic synthesis,Longman, UK,1993.
5. Peter sykes, A Guidebook to Mechanism in Organic Chemistry, Longman, 6th Edition, 2003.

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DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 1PC2**
Semester	**: I**	**No. of Hrs allotted**	**: 5**
Paper	**: Core -2**	**No. of Credits**	**: 5**
Title of the Paper	**: Inorganic Chemistry-I**		

Course Objectives: **75 Hours**

- ✓ This paper deals with the concepts of bonding and electronic structure of Atom.
- ✓ It deals with the study of acid base systems and non aqueous solvents.
- ✓ It gives a thorough understanding on nuclear Chemistry.

UNIT – I: ELECTRONIC STRUCTURE OF ATOM 15 Hrs

Introduction to quantum Chemistry –Postulates of quantum mechanics-Operators – Wave equation –Orthogonality and normalisation -hydrogen like atoms-radial wave function-symmetry orbitals -significance of quantum numbers-shapes of atomic orbitals - poly electronic atoms –Pauli's exclusion principle- Aufbau principle -L.S Coupling scheme- Russel- Saunders method- Term Symbols -Hunds rule –eletronic configuration.. **Ionisation potential, Ionic radii and covalent radii, Electron affinity, Electro negativity- their trend in the periodic table.**

UNIT – II: NATURE OF THE CHEMICAL BOND 15Hrs

Ionic bond – Lattice energy and its determination by Born-Haber cycle and Born Lande Equation – Hardness, electrical conductivity and solubility of ionic compounds – ionic radii. Goldschmidths radius ratio-packing of atoms and ions in solids. **Calculation of ionic radius –Pauling's method and Linde's method. Effective nuclear charge-Slater's rule.**

Covalent bond – qualitative treatment of valence bond theory – Heitler-London theory – Pauling theory and Molecular orbital theory LCAO theory – Hybridisation and resonance.

UNIT – III: BONDING APPLICATION 15 Hrs

Application of VB and MO theories to the structure of homonuclear (H_2, B_2, C_2, N_2) and heteronuclear (CO,NO,HCl,HF) diatomic and selective polyatomic molecules (CO_3^{2-}, NO_2, BeH_2, CO_2), comparison of VB and MO theories. Bond properties, bond order, bond energy, bond length and bond polarity. Partial ionic character of covalent bonds-**Fajan's Rule** -VSEPR theory and its applications to H_2O, NH_3, , IF_5 IF_7, ClO_4^- ions. **VSEPR applied to Xenon compounds like Xenon halides and xenon oxides**

UNIT – IV : ACID-BASE SYSTEMS AND NON-AQUEOUS SOLVENTS. 15Hrs

A generalized acid base concepts – steric effects and solvation effects – Measures of Acid-Base strength –**Factors affecting the strength of acids and bases- Common ion effect and Henderson's equation-** - Hard and Soft acids and bases – symbiosis – theoretical basis of hardness and softness. Classification of solvents – properties of ionizing solvents. Typical reactions in non–aqueous solvents- liquid HF, Hydrogen cyanide, Sulphuric acid and acetic acid.

UNIT – V : NUCLEAR CHEMISTRY 15Hrs

Radioactive decay and equilibrium- Different types of nuclear reaction – spallation – fission and fusion. Theories of fission. Fissile and Fertile isotopes.

Nuclear fusion – stellar energy

Nuclear forces: Liquid drop model, shell model

Calculation of Q-values – Cross section.

Detectors: Scintillation counter , Gas Ionisation chamber. Proportional Counter, Cerenkov Counter

Accelerators: Cyclotron, Synchrocyclotron, Betatron.

Applications: Activation analysis, Isotopic dilution technique-radiometric titration.

Nuclear reactors: Types (Thermo nuclear and breeder reactors) feed materials production. Reprocessing of nuclear materials waste disposal. Atomic power projects in India. **Hazardous of radioactive materials and Safety measures.**

TEXT BOOKS:

1. **P.J.Durrant and B.Durrant**, Introduction to advanced inorganic chemistry, Longman Group Ltd, London,1970.
2. **A.K.Chandra,** Introductory Quantum Chemistry, Tata McGraw Hill, New Delhi, 3rd Edn., 1988.
3. **J.D. Lee**, Concise Inorganic Chemistry, Blackwell Science Ltd., V Edn., London. 2002.
4. **S. Glasstone**, Source Book of Atomic Energy, Van Nostrand, III Edn,East West Press (P) Ltd., New Delhi.1967
5. **G. Friedlander, J.S. Kennedy and M.M. Millodr**, Nuclear and radiochemistry, John Wiley & Sons ,New York..1984.
6. **M. Clyde Day, Jr & Joel Selbin**, Theoretical Inorganic Chemistry, Chapman & Hall Ltd., London, 5th Reprint, 1967.

REFERENCE BOOKS :

1. **J.E. Huheey, Ellen A.Keiter, Richard L.Keiter,** Inorganic Chemistry, IV Edn., Pearson Education (Singapore) Pvt. Ltd., New Delhi. 2004.
2. **H.J. Arnikar**, IV Edn., Essentials of Nuclear Chemistry, vNew Age international (P) Ltd., New Delhi. 2005.
3. **R.D. Madan,** Modern Inorganic Chemistry, S. Chand & Company Ltd., New Delhi, 2004.
4. **Wahid U. Malik, G.D. Tuli and R. D. Madan**, Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi. 2006.
5. **Gary L. Miessler and Donald A. Tarr**, Inorganic Chemistry, Pearson Education, Inc., 3rd Edn., New Delhi. 2004.
6. **William W. Porterfield**, Inorganic Chemistry, II Edn., Elsevier,New Delhi,2005.
7. **A.G. Sharpe**, Inorganic Chemistry, III Edn., Addition – Wesley Longman, UK, 2004.
8. **D. F. Shriver and P.W. Atkins**, Inorganic Chemistry, Oxford University Press, London.1999.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry**	**Code No**	**: 1PC3**
Semester	**: I**	**No. of Hrs allotted**	**: 5**
Paper	**: Core Paper - 3**	**No. of Credits**	**: 5**
Title of the Paper	**: PHYSICAL CHEMISTRY-I**		**75Hrs**

Course Objective:

To understand the concepts of gaseous and liquid states, their thermodynamic properties, basic principles of quantum mechanics & its applications to simple systems & application of thermodynamics to biological reactions.

UNIT-I - PROPERTIES OF GASES AND LIQUIDS (15 HRS)

Equations of states - Molecular speeds- Maxwell distribution of molecular velocities - one, two and three dimensions-Energy distribution-Maxwell – Boltzmann distribution law- Principle of equipartition of energy and heat capacity- Rotation, vibrations and translational degree of freedom- Molecular collisions- Mean free path- Transport properties- thermal conductivity- Viscosity of gases- momentum transfer and diffusion.

Liquid state- theory of liquids- Internal pressure- liquid crystals- Nematic (p-methoxycinnamic acid), cholesteric (cholestryl benzoate), smectic (ethyl-p-azoxybenzoate)- theory and its application in Liquid Crystals Display.

UNIT-II- THERMODYNAMICS – EQUILIBRIUM AND NON-EQUILIBRIUM (15 HRS)

A general review of enthalpy, entropy and free energy concepts – Nernst heat theorem-Genesis of third law and its limitations- Derivation of third law and their application to real gases-calculation of $(\delta H/dP)_T$, $(\delta E/dV)_T$ and $\mu_j.T$ for gases- Thermodynamics of system of variable composition- partial molar quantities and their determination- Chemical potential- relationship between partial molal quantities.

Gibbs Duhem equation- Duhem Margules equation- thermodynamic properties of real gases- Fugacity concept- Determination of Fugacity of real gases- Activity and Activity coefficient- Electrolytes and Non-Electrolytes- Equilibrium thermodynamics- Gibbs phase rule and its application to three component systems- Extent of reaction- quantitative treatment of Le Chatlier principle- Reaction potential- Basic concepts of Non-equilibrium thermodynamics-Principle of Microscopic reversibility-Onsager's reciprocal relationship.

UNIT –III - QUANTUM CHEMISTRY-I (15 HRS)

Black Body radiation- de Broglies wave particle duality- Experimental verification of matter waves- Compton effect- Heisenberg's Uncertainity principle- The Schrodinger equation and the postulates of quantum mechanics- operators –linear and non-linear operators- commutative and non-commutative operators- Hermitian operators- Eigen function, Eigen values and degeneracy-Orthogonality and Normalization of wave functions- Derivation of Schrodinger's wave equation.

UNIT- IV- QUANTUM CHEMISTRY-II (15 HRS)

Application of quantum mechanics to simple system-Application of SWE to free particle moving in one dimension- particle moving in a one dimension box - particle moving in 3D cubical and rectangular box- Quantum Mechanical tunneling - particle in a ring- rigid rotor- Simple Harmonic oscillator - hydrogen atom- angular momentum spin momentum- ladder operator.

UNIT-V - PHYSICO-CHEMICAL PRINCIPLES AND BIOLOGICAL REACTIONS

(15 HRS)

Studies on biochemical equilibria- buffer system of intracellular fluids- H_2CO_3/HCO_3^- - $HPO_4^{2-}/H_2PO_4^-$ -Application of Henderson- Hassel bach equation- Ion channels – membrane and Static potentials – Role of Na^+ / K^+ ions in neural communications.– allosterism and oxygen – Saturation curves for Hb and Mb- Hill equation.

Medicinal chemistry- QSAR-partition coefficient, p and concentration, c of drugs – use of hydrophobicity constant Π- Πc and ρ- Hamett substituent constants σ and ρ, steric factor: Es- Hansch equation-Craig plot- Topliss scheme.

Text Books:

1. S. Glasstone, A text book of Physical Chemistry, McMillan India Ltd., 1999.
2. R. A. Alberty and F. Daniels, Physical Chemistry, John Wiley & Sons, New York 1978.
3. G. W. Castellan, Physical chemistry, 3rd edition, Wesley Publishing Company, UK, 1986. (Unit –I)
4. S. Glasstone, Thermodynamics for Chemists, Eastern Wiley publications, 2002. (Unit –II)
5. P.Atkins, Physical Chemistry, Oxford University Press, VII Edition, 2002.
6. K. Chandra- Introductory Quantum Chemistry-3rd edition, Tata Mcgraw Hill Publishing company, New Delhi, 1988.
7. H. W. Hanna, Quantum Mechanics in Chemistry- Benjamin- Cummiza, London Publishing company, 1983.
8. P. W. Atkins, Molecular Quantum Mechanics, Oxford University Press, II Edition, UK, 1986. (Unit –III)
9. H. W. Hanna, Quantum Mechanics in Chemistry- Benjamin- Cummiza London Publishing company, UK, 1983.
10. A.K. Chandra-Introductory quantum chemistry-3rd edition Tata McGrow- Hill Publishing Co Ltd., New Delhi, 1988.
11. P. W. Atkins, Molecular Quantum Mechanics, Oxford University Press, II Edition, Oxford, 1986. (Unit –IV)
12. J. Gareth Morris- A. Biologists physical chemistry, Edward Arnold , UK, 1974.
13. G. M. Barrow- physical chemistry for the life sciences ,McGraw Hill Kogakusha Ltd., New York, 1994. (Unit –V)

Reference Books:

1. S. Glasstone, A text book of Physical Chemistry, McMillan India Ltd., Alasca, 1999.
2. Walter J. Moore, Physical Chemistry, 6th edition, Orient Longman, New York, 2006. (Unit –I)
3. M. Klotz and R. M. Rosenberg-Chemical thermodynamics, 4th edition, Benjamin, New York, 1996.
4. S. Glasstone - Thermodynamics for Chemists, 5th edition, Eastern Wiley publications,2002.
5. J. Rajaram and J. C. Kuriakose, Thermodynamics, 3rd edition, S. N. Chand, New Delhi, 1999. (Unit –II)
6. Levine, Quantum Chemistry, 6th edition, Prentice-Hall, New Delhi, 2006
7. D. A. Mcquarrie, Quantum Chemistry,Viva Books Pvt. Ltd., New Delhi, 2003. (Unit –III)
8. Levine , Quantum Chemistry, 5th edition, Prentice-Hall, UK, 2003.
9. D. A. Mcquarrie, Quantum Chemistry,Viva Books Pvt. Ltd., New Delhi, 2003.
10. P.Atkins, Physical Chemistry, Oxford University Press, VII Edition, 2002. (Unit –IV)
11. Raymond Chang – Physical Chemistry with application to biochemical system Mc Millan Publishing Company. Inc., New Delhi, 2002.
12. Graham L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, New York, 1995 (Unit – V)

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 2PC1**
Semester	**: II**	**No. of Hrs allotted**	**: 60**
Paper	**: Core - 4**	**No. of Credits**	**: 4**
Title of the Paper	**: Organic Chemistry - II**		

Course Objective: **(60 Hrs)**

This paper aims at enriching the students' knowledge about organic spectroscopy and stereochemistry

Unit-I UV and IR Spectrsocopy **(12 Hrs)**

Ultraviolet spectroscopy – basic principle – instrumentation – the absorption laws, types of electronic transitions – Effect of solvent and hydrogen bonding on λ_{max} values - Woodward rules to calculate λ_{max} values of conjugated dienes, conjugated polyenes, and carbonyl compounds

Infrared spectroscopy – basic principle – Molecular Vibrations – instrumentation – characteristic IR absorption of different functional groups – factors influencing the vibrational frequencies

Unit-II ^{1}H NMR and ^{13}C NMR spectroscopy **(12 Hrs)**

^{1}H NMR spectroscopy: Basic principles – number of signals – chemical shift factors influencing chemical shift – spin-spin coupling – coupling constant and factors influencing coupling constant. Simplification of complex spectra – shift reagents, deuterium substitution and spin decoupling. **Advanced NMR Spectroscopy -** Introduction to 2D-NMR - Classification of 2D experiments – 2D resolved spectroscopy – HOMO and HETERO – 2D – J resolved spectra. Correlation Spectroscopy (COSY) – HOMO – COSY, HETERO – COSY, 2D – INADEQUATE and NOESY.

^{13}C NMR spectroscopy: Basic principle – comparison with ^{1}H NMR – noise decoupling – off resonance decoupling – factors affecting the C-13 chemical shifts.

UNIT-III: Mass Spectroscopy, ORD and CD **(12 hrs)**

Basic instrumentation of Mass spectrometer - types of ions – molecular, isotopic, metastable and fragmentation ions – Tests for molecular ion peak – General fragmentation modes- Retro Diels - Alder reactions – Mc Lafferty rearrangement – Fragmentation pattern of simple organic molecules. Application – Accurate Molecular weight, Molecular formula (Nitrogen rule) – Determination of structures of organic molecules. Introduction to ESI, MALDI and FAB mass spectrometer.

Optical rotatory dispersion (ORD) and Circular Dichroism (CD): Circularly polarized light – Circular birefringence and CD – plain curves and their applications – Cotton effects curves – structural applications – axial haloketone rule, octant rule and their applications.

Solving problems based on UV, IR, NMR and Mass data.

UNIT IV - Organic Stereochemistry **(12 hrs)**

Optical isomerism

Symmetry elements – the concept of chirality – chirality about a center – specification by Cahn-Ingold-Prelog notations – compounds with more than one chiral center – erythro, threo and meso nomenclature – concept of prochirality – homotopic, enantiotopic and diastereotopic ligands and faces – Asymmetric synthesis – Cram's rule and Prelog's rule. Optical activity in allenes and spiranes – StereoChemistry of nitrogen compounds.

Geometrical isomerism

E and Z notation – Determination of configuration of geometrical isomers by simple techniques like hydroxylation, hydroboration and methods based on physical properties – Stereoisomerism in cyclic compounds – 3, 4 and 5 membered ring systems.

UNIT V -Conformational Analysis (12 hrs)

Configuration and conformation – definition – conformational free energy – atropisomers – conformational analysis of cyclohexane system – stability and isomerism in mono and disubstituted cyclohexanes – conformation and reactivity of cyclohexane derivatives – conformational analysis of fused ring system – decalins, and perhydrophenanthrene.

Text Books:

1. D. Nasipuri, Stereochemistry of Organic compounds 2nd edition, New Age International, New Delhi 2004.
2. William Kemp, Organic Spectroscopy, 4th Edition, ELBS, UK, 1994.
3. R.M. Silverstein, G.C. Bassler and T.C. Morrill, Spectrometric Identification of organic compounds, 6th Edition, John Wiley, New York, 2005.

Reference Books:

1. E.L. Eliel and S.H.Wiley, Stereochemistry of carbon compounds. John Wiley & Son, Inc 2003.
2. V.M.Potapov, Stereochemistry, MIR Publisher, Moscow, 1999.
3. H.Kagan, Organic Stereochemistry, Edward Arnold, London, 2001.
4. E.L. Eliel, N.L. Allinger, S.J. Angyal and G.A. Morrison, Conformational Analysis, Interscience, New York, 2004.
5. P. Wetirli Marchand, Interpretation of ^{13}C NMR Spectra, VCH Weinheim, UK, 1987.
6. Atta-ur Rahman, Nuclear Magnetic Resonance, Springer Verlog, New York, 1990.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 2PC2**
Semester	**:II**	**No. of Hrs allotted**	**: 4**
Paper	**: Core - 5**	**No. of Credits**	**: 4**
Title of the Paper	**:Inorganic Chemistry-II**		

Course Objectives: 60 Hours

- To study the solid state elaborately.
- It deals with polymeric inorganic compounds.
- It gives a thorough understanding on analytical Chemistry.
- It deals with the techniques like Colorimetry, Fluorimetry, AAS, TGA, DTA, Chromatography and cyclic voltammetry.

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UNIT I SUPRAMOLECULAR CHEMISTRY (12 Hrs)

Definition, Nature of supramolecular interactions- Non - Covalent interactions, Host - guest interaction, Molecular recognition, Types of recognition, Self- assembly. General properties of Supra molecular complexes- Molecular Library- **Transition metal mediated supramolecules-** Directional bond approach- Molecular triangles (Pd and Pt)- Molecular squares (Pd, Pt and Re)- Molecular rectangles-(Pd, Pt, Cu and Re) Molecular Cages (Pd, Pt and Re).

UNIT II SOLID-STATE CHEMISTRY (12 Hrs)

Packing of atoms and ions- close packing arrangements-HCP,CCP and BCC lattice. Radius ratio rules- Limiting radius ratio. Structure of typical lattices such as calcite, cesium chloride, Nickel arsenide, Fluorite, Antifluorite, Cadmium iodide, Perovskite, Spinels (normal and inverse**). Bragg's equation- problems involving Bragg's equation. Crystal structure determination- X-ray diffraction study, Electron and Neutron diffractions.**

Crystal defects- point – Schotky and Frenkel defect - line and plane defects- colour centers- non- stoichiometric Compounds- effect of imperfections and non- stoichiometry on physical properties-types of solids-electronic structure of solids- free electron and band theories.

Electrical conductivity and superconductivity – High temperature superconductivity-types of Semi-conductors-thermoelectric power and Hall effect- PN junction- transistors- optical properties- photovoltaic effect- semiconductors in solar energy conversion.

UNIT-III CAGES AND METAL CLUSTERS- POLYMERIC INORGANIC COMPOUNDS (12 Hrs)

Electron deficient compounds: Borane and carboranes- Synthesis, structure and bonding (VBT and MO approach)-bonding –topological treatment-wades rule –styx numbers. **P-N HETEROCYCLICS**- Phosphonitrilic compounds: Synthesis, Structure and bonding.

S-N HETEROCYCLICS:

Synthesis, structure and bonding in Binary sulphur nitrils, S-N cations and anions, cyclic S-N compounds, S-N halogen compounds.

METAL CLUSTERS

Synthesis, structure and bonding in Poly anions and isopoly anions of phosphorous,vanadium, chromium,Nolybdenum and tugston. Hetero poly anions of molybdenum and tungsten.

UNIT-IV ANALYTICAL CHEMISTRY-1 (12 Hrs)

Principles and practice of complexometric estimations/- Spectro analytical methods:- Principles and applications of colorimetry and spectro photometry, fluorimetry, nephelometry and turbidimetry-emission and atomic absorption spectroscopy (AAS) and atomic fluorescence spectroscopy.

UNIT-V ANALYTICAL CHEMISTRY-II (12 Hrs)

Instrumentation and applications of Cyclic Voltametry, Thermogravimetry, Differential thermal analysis and differential scanning colorimetry, Chromatography: GC, HPLC and Ion Exchange Chromatographic techniques.

Text book:

1. **D.A.Skoog and D.M.West,** Fundamentals of Analytical Chemistry, Holler Saunders college publishing,USA.VI Edn., 1998.
2. **F.A. Cotton and G. Wilkinson**, Advanced Inorganic Chemistry, Wiley-Interscience publications, John Wiley & Sons, V Edn.,New Delhi, 1988.
3. **Purcell K.F. and Kotz J.C., Saunders**, Inorganic Chemistry, Philadelphia, 1977.
4. **H.G.Heal**, The Inorganic Heterocyclic Chemistry of Sulphur, Nitrogen and Phosphorus, Academic press, New York , 1980.
5. **J.D.Woolings**, Non Metal Rings, Cages and Clusters, John Wiley and sons, New York, 1989**.**
6. **H.V. Keer**, Principles of the Solid State, Wiley Eastern Ltd., 1993.
7. **Walter E. Harris and Byron Kratochvil**, An Introduction to Chemical Analysis, Saunders Golden Sunburst Series, Philadelphia,1982.
8. **Galen W. Ewing**, Instrumental Methods of Chemical Analysis, Mc Graw Hill International Editions, V Edn., New Delhi, 1987.
9. **B.K. Sharma**, Instrumental Methods of Chemical Analysis, GOEL Publishing House, 12th Reprint., New Delhi, 1993.

REFERENCE BOOKS:

1. **A.I.Vogel,** Textbook of Quantitative Chemical Analysis, ELBS Longman Singapore Publisher Pte Ltd., Singapore.V Edn., 2002.
2. **J.E.Huheey**, Ellen A.Keiter,Richard L.Keiter, Inorganic Chemistry, Pearson Education (Singapore) Pte.Ltd., IV Edn., Delhi, 2004.
3. **I. Azaroff** , Introduction to Solids, Tata McGraw hill, New Delhi, 2004.
4. **Wahid U. Malik, G.D. Tuli and R. D. Madan**, Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi, 2006.
5. **William W. Porterfield**, Inorganic Chemistry, II Edn.,Elsevier,New Delhi, 2005.
6. **A.G. Sharpe**, Inorganic Chemistry, III Edn., Addition – Wesley Longman, UK 2004.
7. **K. Chakrabarthy**, Solid State Chemistry, New Age International Publishers, (P) Ltd., 2005.
8. **Bradley J. Holliday & Chad A. Mirkin**, Strategies for the Construction of Supramolecular Compounds through Coordination Chemistry- Reviews , Angew. Chem. Int. Ltd., Ed., 2001, 40, 2022-2043., ~CHEMIE@WILEY-VCH

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry**	**Code No**	**: 2PC3**
Semester	**: II**	**No. of Hrs allotted**	**: 4**
Paper	**: Core Paper - 6**	**No. of Credits**	**: 4**
Title of the Paper	**: PHYSICAL CHEMISTRY-II**		**60 Hrs**

Course Objective:

To understand the various concepts involved in electrochemistry and to have a detailed study on statistical thermodynamics. This course will also focus on the various approximation methods involved in quantum mechanics.

UNIT-I **(12 Hrs)**

ELECTROCHEMISTRY-I

Theory of strong electrolytes -Interionic attraction theory- Debye – Huckel theory of strong electrolytes - Debye-Huckel model of ionic atmosphere–Debye–Huckel Onsager equation-derivation, verification and modifications- Debye – Falkenhagen effect and Wien effect - Electrical double layers – formation – Structure of electrified interfaces – Stern model.

Debye Huckel limiting law- extension- Huckel Bronsted equation - Determination of activity coefficients using Bronsted equation – Applications of conductivity measurements – Nernst equation and its significance – Reversible and irreversible cells - Electrodes – SHE – Calomel – Glass electrode – Platinum electrode – Glassy carbon electrode – ion selective electrode and measurement of pH.

Text Books:

1. J. O. M. Bokris and A. K. N. Reddy, Modern Electrochemistry, Vol I, Plenum Press, New York, 1978.
2. Dr. Crow, Principles and Applications of Electrochemistry, Chapman Hall, UK, 1988.
3. R. Venkataraman, K. Rengarajan and P. S. Raghavan Electrochemistry, First edition, 2007
4. J. O. M. Bokris and A. K. N. Reddy, Modern Electrochemistry Vol II Plenum Press, New Delhi, 1978.

Reference Books:

1. L. Antropov, Theoretical electrochemistry, MIR Publications, New Delhi, 1999.
2. S. Glasstone, An Introduction to Electrochemistry, Von Nostrand Co. Inc., Toronto, 2002.

UNIT-II **(12 Hrs)**

ELECTROCHEMISTRY-II

Over voltage- Theories of over voltage- applications of over voltage- electrode processes - Kinetics of electrode processes - Butler-Volmer equation- Tafel equation- corrosion- principles of electrochemical corrosion – dry and wet corrosion and its mechanism – Pilling-Bedworth rule. Types of corrosion- galvanic, aeration, stress, pitting corrosion and passivity – factor influencing corrosion – corrosion control- cathodic production - corrosion inhibitors.

Principles of Polorography - Cyclic Voltametry –quasi – reversible – irreversible voltamogram – electrochemical energy conversions-Nickel Cadmium, lead acid battery. Fuel cells – H_2 - O_2 Fuel cell – methyl alcohol fuel cell.

Text Books:

1. J. O. M. Bokris and A. K. N. Reddy, Modern Electrochemistry Vol II Plenum Press, New Delhi, 1978.
2. Dr. Crow, Principles and applications of Electrochemistry, Chapman Hall, UK, 1988.

Reference books:

1. L. Antropov, Theoretical electrochemistry, MIR Publications, New Delhi, 1999.
2. S. Glasstone, An Introduction to Electrochemistry, Von Nostrand Co Inc., Toronto, 2002.

UNIT-III **(12 Hrs)**

STATISTICAL THERMODYNAMICS-I

Need for statistical thermodynamics- Definition of state of a system- assembly- ensemble- canonical and micro canonical ensembles- phase space- microstates- probability and distribution. Boltzmann distribution law- derivation- partition functions – Translational, rotational, vibrational, and electronic partition functions. Thermodynamic properties from partition functions for energy, heat capacity, enthalpy and entropy, Helmholtz free energy, Gibbs free energy, pressure and chemical potential. Sackur-Tetrode equation- thermodynamic properties of monoatomic gases.

Text Books:

1. S. Glasstone- Thermodynamics for Chemists, Eastern Wiley Publication, 2002.
2. Lee, Sears and Tercotte, Statistical Thermodynamics- Addision Wesley Publishing Co., London – I Edition, 1973.

Reference Books:

1. M. C. Gupta – Statistical Thermodynamics – Wiley Eastern limited, New Delhi- 1993.
2. J. C. Kuriakose and J. Rajaram – Thermodynamics III edition, Shoban lal Nagin Chand, New Delhi, 1999.

UNIT-IV **(12 Hrs)**

STATISTICAL THERMODYNAMICS-II

Quantum statistics-Fermi-Dirac and Bose-Einstein Statistics derivations-Application of Fermi-Dirac statistics to electron gas in metal – average energy of electron in metals. Application of Bose-Einstein statistics to photon gas – Planck's radiation formula-Derivation of Rayleigh-Jeans law-Stefan Boltzman equation.

Population inversion-negative absolute temperature -heat capacity of diatomic gases- Einstein's theory and Debye's theory of heat capacities of solids- third law of thermodynamics and statistical entropy - hydrogen ortho and para nuclear states. ***Reference Books***

No: 1 and 2 given in Unit-III

UNIT –V **(12 Hrs)**

Approximation methods, application of SWE to many electron systems.

Necessity for approximation methods- Variation methods for the Hydrogen atom – Perturbation (first order) method to Helium atom - Slater determinant wave function- secular determinant – Hartree – Fock self consistent field method to Helium atom – HMO bielectron theory of Ethylene and Butadiene.

Text Books:

1. A. K. Chandra- Introductory Quantum Chemistry-3rd edition Tata McGraw-Hill Publishing Co, New Delhi, 1988.
2. D.A.Mc Quarie , Quantum Mechanics, Oxford University press, Oxford, 1983.
3. R.K. Prasad, Quantum mechanics,

Reference Books:

1. Levine , Quantum Chemistry, 6th Edition, Prentice-Hall, New Delhi, 2006.
2. H.W. Hanna, Quantum Mechanics in Chemistry-Benjamin –Cummiza London Publishing Company, New Delhi, 1993.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 2PC4 (E1)**
Semester	**: II**	**No. of Hrs allotted**	**: 5**
Paper	**: MAJOR ELECTIVE**	**No. of Credits**	**: 5**
Title of the Paper	**: C-PROGRAMMING: FUNDAMENTALS AND APPLICATIONS INCHEMISTRY (Optional 1)**		

OBJECTIVE: **75 Hours**

- To have an Overview of C-Programme.
- To comprehend the basic ideas of Operators, Data input and Output.
- To know about Decision Making , Arrays, and Functions
- And to understand Applications of C in Chemistry

UNIT-I Introduction and overview of C (15 HRS)

Introduction – Importance of C-structure of C-programs- Simple programs-style of the language.

Characters–Keywords, Variables and parameters-Data types-Constants-Declaration of and assignments of values to variables.

Operators-Arithmetic, Relational, Logical, assignment, Increment and Decrement, Conditional and bitwise operators-Special operators.

Expressions- Arithmetic - Evaluation of expression- Procedure of arithmetic operators-Library functions.

UNIT-II Data input and Output (T: 7 HRS + P: 8 HRS)

Character input- The getchar function – Character output- The putchar function – Entering input data- the Scanf function-Writing output data- The printf function- Formatted input and output data-the gets and puts functions-preparing and running a complete program.

Decision making and branching

Decision making with IF statement –simple IF statement-the IF…ELSE statement-Nesting of IF…Else statements – The ELSE IF ladder –The Switch statement – The ?: operator – the GOTO statement.

UNIT-III (T: 8 HRS + P: 7 HRS)

Decision making and Looping:

The WHILE statement – The DO statement-The FOR statement – Jumps in loops.

Arrays:

One dimensional array –Two dimensional arrays –Initializing two dimensional arrays-Multidimensional arrays.

User defined functions

Need for user–defined functions – A multifunction program – The form of C functions - Return values and their types- Calling a function –Category of function- No arguments and no return values –Nesting functions- Recursions- The scope and life time of variables in function.

UNIT-IV Applications of C in Chemistry-I (T: 6 HRS + P: 9 HRS)

Explanation of the formulae, equations and programs to solve the following problems in chemistry:

1. Calculation of Molecular weight of Organic Compounds.
2. Calculation of pH.
3. Determination on First Order rate constant for the given reaction
4. Evaluation of lattice energy using

i). Born- Haber Cycle
ii). Born –Lande equation

5. Computing ionic radii- Lande's method and Paulings method
6. Calculation of Normality, Molarity and Molality of a given solution
7. Converting Kelvin to Celsius temperature and vice versa.
8. Determination of enthalpy of a given solution
9. Evaluation of Cell constant
10. Calculation of energy of Hydrogen atom spectral lines.

UNIT-V: Applications of C in Chemistry-II (T: 6 HRS + P: 9 HRS)

Explanation of the formulae, equations and programs to solve the following problems in chemistry:

Organic Chemistry:

1. Use of Recursive functions to calculate the number of π Resonance structures for an organic conjugated system using
   res - str = n! / ((n/2)! * ((n/2) + 1)!)
2. Empirical formula of Hydrocarbons and other Organic compounds.

Inorganic Chemistry:

1. Array manipulation to balance the chemical equations.
2. Half life and average life periods of radioactive nuclei.
3. Binding energy of nucleus.
4. Program to get output as First ten elements of Periodic Table with their Name, Symbol, Atomic number and Atomic Weight.

Physical chemistry:

1. Calculation of RMS, average and MPV of gases.
2. Solving Quadratic equation to evaluate the Equilibrium constant for the reaction
   $H_2 + I_2 \quad 2HI$
3. Illustrate use of Loop to calculate the NMR frequency for a nucleus with Spin ½
4. Mean activity coefficient of an Electrolyte (KCl)

TEXT BOOK

1. **E. Balagurusamy**, Programming in ANSI C, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 3rd Edn., 10th Reprint, 2005.

REFERENCES:

1. **Brian W. Kernighan & Dennis M. Ritchie**, The C Programming Language, Prentice Hall of India Private Limited, New Delhi, 2nd Edn., 2001.
2. **Byron S. Gottfried**, Programming with C, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 2nd Edn., 2001.
3. **R. Rajaram**, C Programming Made Easy, Scitech Publications, Chennai, 1999.
4. **Yeshavant Kanitkar**, Let Us C, BPB Publications, New Delhi, 3rd Edn.,1999.
5. **Yeshavant Kanitkar**, C - Projects, BPB Publications, New Delhi, 1998.
6. **K. V. Raman** , Computers in Chemistry, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 3rd Edn., 1993.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course : M.Sc., Code No : 2PC4(E1)
Semester : II No. of Hrs allotted : 5
Paper : MAJOR ELECTIVES No.of.credits :5
Title of the Paper : MEDICINAL CHEMISTRY (Optional 2)

Course Objective : 75 Hours

To introduce the concept of pharmacokinetics, pharmacodynamics drug discovery by design, QSAR, combinatorial chemistry and synthesis of drugs

Unit – I :: Introduction to Drug Design: 15 hrs

a) ADME Properties

The pharmacokinetics phase-Adsorption-Distribution, Metabolism-Elimination-Bioavailability of drug. pharmacokinetics models, Intravascular and Extravascular administration. The use of pharmacokinetics in Drug dsign**.**

b) Pharmacodynamics - Stereoelectronic structure.

Unit II Drug Discovery by Design 15 hrs

a) Streochemistry and Drug Design

Structurally rigid Groups –procaine, Acetylcholine. Conformation-Syn and Anti Acetylcholine, Phenyl ethanoate methiodides. Configuration-Variations in the biological activities of stereoisomers

b) Strutural –Activity –Relationship (SAR)

Changing the size and shape.Changing th degree of unsaturation. Introduction or removal of ring system. Introduction of new substituents-methyl group, Halogens, hydroxyl groups, Basic groups, carboxylic and sulphonic acid groups. Changing the excisting substituents of lead-isosteres,bioisoteres.

Unit III a)Quantitative-structural Activity-Relationship (QSAR) 15 hrs

Partition parameters-partition coefficients(p), Lipophilic subtituents constants (π) Electronic parameters-The Hammett constants-Steric parameters-The Taft Steric parameters (Es), Molar refractivity (MR), Hansch analysis-craig plots, The toplss decision tree. Compute –aided drug design- Modelling Drug-Receptor Interaction.

b) Combinatorial Chemistry

Basic concepts-The design of combinatorial syntheses. The general technique used in combinatorial synthesis i) Solid support mthod-parrllel synthesis –Furka's mix and splt techniques-sequential chemical tagging methods-Still;s binary code Tag systemcomputerised tagging. ii) Combinaterial synthesis in solution iii) Screening and deconvolution

Unit – IV

a) Antineoplastic Agents: 15 hrs

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer

b) Psychoactive drugs – The chemotherapy of Mind:

Introduction, neutotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, neurochemistry of mental diseases

c) Cardiovascular Drugs and Local Antiinfective Drugs:

Introduction, Cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output.

Unit V Synthesis of Drugs 15 hrs

a) Synthesis of Antineoplastic agents

Mechlorethamine, Cyclophosphamide uracil, mustards and 6-mercaptopurine

b) Synthesis of cardiovascular drugs

Amyl-nitrate, sorbitrate, , Verapamil.

c) Synthesis of Phychoactive drugs

Synthesis of Diazepam, Chlorazepam, oxazepam, Alprazolam, Phenyltocin or Diphenylhydantoin, Barbitol, Phenobarbital.

Text Books:

1.Gringuage, Introduction to Medical Chemistry, Wiley – VCH, 2004.
2.Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed., Robert F.Dorge, 2003.
3. S.S.Pandeya and J.R.Dimmock, An Introduction to Drug Design, New Age International, 2006.
4. Burger's Medicinal Chemistry and Drug Discovery,Vol-1 (Chapter-9 and Ch-14) Ed., M.E. Wolff, John Wiley, 2005.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill, 2006.
6. R.B.Silverman, The Organic Chemistry of Drug Design and Drug Action, Academic Press, 2006.

Reference Books:

1 D. Lednicer, Strategies for Organic Drug Synthesis and Design, John Wiley.
2 Gareth Thomas, Medicinal Chemistry, An introduction, John wiley& sons,Ltd., 2004.
3 M.L Gangwal Medicinal chemistry Lectures on Drug design and Synthetic Drugs, Student publishing House, 2007.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 2PCL1**
Semester	**: I & II**	**No. of Hrs allotted**	**: 5**
Paper	**: CORE PRACTICAL -1**	**No. of Credits**	**: 5**
Title of the Paper	**: Organic Chemistry Practicals**		

Course Objective: 75 **hrs**

To develop the practical skills in analyzing a mixture of two organic substances and also in preparation of organic compounds.

ANALYSIS

Analysis of Organic mixtures : Two component Systems
(Maximum of SIX Mixtures)

Spectral identification of those organic compounds by the provided UV, IR, NMR and Mass data.

Marks **Internal - 40**
External - 60

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 2PCL2**
Semester	**: I / II**	**No. of Hrs allotted**	**: 4**
Paper	**: Core Practical - II**	**No. of Credits**	**: 4**
Title of the Paper	**: Inorganic Chemistry Practicals**		

Course objective: **60 hrs**

To impart skills in both qualitative and quantitative inorganic analysis

I. COMPLEXOMETRIC TITRATIONS WITH EDTA

1. Estimation of ZINC
2. Estimation of MAGNESIUM
3. Estimation of COPPER
4. Estimation of NICKEL
   a) By Direct Method
   b) By Indirect Method

II. SEMI MICRO ANALYSIS

Semi micro analysis of samples containing two Familiar Cations and two Less Familiar Cations. – Maximum of Five samples.

Marks

Internal- 40 **(Estimation=15, Analysis=15, Record=5, Viva=5)**
External- 60

Distribution of marks for External Exam

Estimations	- 25 Marks	Analysis (20)
Analysis	- 20 Marks	Two Familiar Cations : 5+5 = 10
Record	- 10 Marks	Two Less Familiar
Viva	- 05 Marks	Cations : 5+5 = 10
Total	60 marks	

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry**	**Code No**	**: 2PCL3**
Semester	**: I / II**	**No. of Hrs allotted**	**: 4**
Paper	**: Core Practicals 3**	**No. of Credits**	**: 4**

Title of the Paper : PHYSICAL CHEMISTRY PRACTICALS

Course objective: 60 hrs

To develop practical skills in various Conductometric, Potentiometric titrations, Phase diagram, Kinetics and calculation of enthalpy of solutions by Rast's micro method.

I. THERMOCHEMISTRY-enthalpy of solution by solubility method-unknown concentration.

II. ADSORPTION-adsorption of oxalic acid\acetic acid on activated charcoal-freundlich adsorption isotherm-determination of unknown concentration.

III. CHEMICAL KINETICS-

Kinetics of acid hydrolysis of an ester

Evaluation of Arrhenius parameters E_a & A (for practice only)

IV. CONDUCTIVITY EXPERIMENTS

1. Determination of cell constant-verification of Ostwald's dilution law-determination of dissociation constant of weak acid.
2. Solubility product of sparingly soluble salt.

3. Conductometric titration

a) HCl Vs NaOH Vs HCl

b) AcOH Vs NaOH Vs AcOH

c) HCl Vs NaOH Vs Mixture of acids

4. Displacement of titration

(a) NH_4Cl-NaOH, NH_4Cl

(b) NaOAC, HCl-NaOAC

(c) Quinhydrone electrode

(1) Determination of pH

(2) Dissociation constant of weak acid by e.m.f. method.

V. EMF EXPERIMENTS

A) Redox titrations:

1) KI-$KMnO_4$-KI

2)FAS-Ce^{4+}-FAS

B) Precipitation titrations;

1) KCl Vs $AgNO_3$- K_{sp} of AgCl

2)KCl Vs $AgNO_3$ Vs KCl + KI (mixture of halides)

VI. Determination of Molecular weight by Rast method

VII. Phase Diagram – Simple and Compound

VIII. Transition Temperature

IX. Critical Solution Temperature

X. Determination of Coefficient of Viscosity

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Cours : M.Sc., **Paper Code : 3PC1**
Semester : III **No. of hours allotted : 5**
Paper : Core **No. of credits : 5**
Title of the paper: Organic chemistry - III

Course objective: **(75 Hours)**

This paper gives a detailed information about the following topics:
(i) Usage of various reagents in organic synthesis (ii) Advanced synthetic routes for an ideal organic synthesis. (iii) Interaction of organic molecules at thermal and photochemical condition. (iv) Reactions involving molecular rearrangements.

Unit-I Reagents in Organic Synthesis **(15 Hrs)**

Use of the following reagents in organic syntheses and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate – lithium diisopropylamide (LDA) — trimethyl silyliodide – tri-*n*-butyl tin hydride – Jones reagent – pyridinium chloro chromate – SeO_2 – peracids – DMSO – $Pb(OAc)_4$ – HIO_4 – Prevost and Woodward hydroxylation – Etard's reagent – Waker's reagent – RuO_4 – $Hg(OAc)_2$ – Oppenauer oxidation – DDQ – $LiAlH_4$, $NaBH_4$, Lawesson's reagent – Crown ethers – Thallium nitrate – Phase transfer catalysts – Birch reduction.

UNIT-II Advanced Organic Synthesis I **(15 hrs)**

Disconnection Approach: Importance of organic synthesis- requirement of an ideal synthesis- Planning synthesis – Synthons and types – synthetic equivalents – latent functionality – Reactions involving functional group interconversions – Reterosynthetic analysis – concept of umpolung – two group C-X disconnections and synthetic strategies 1,2-, 1,3-, 1,4-, 1,5- and 1,6-difunctionalised disconnection.

UNIT-III Advanced Organic Synthesis II **(15 hrs)**

Steroselective and stereospecific reactions - Chemoselectivity – Stereoselectivity- Regioselectivity
Asymmetric synthesis: Definition of enantiomeric, disatereomeric excess – analytical methods to determine ee and de – strategy and classification of methods of asymmetric synthesis – chiral substrates – Chiral auxiliaries – chiral reagents – chiral catalysts.
Chiral catalysts and chiral reagents: BINAP-ruthenium (II) Mc Murray's reagent – Mc Murray's reagent – $Ti(Oi\text{-}Pr)_4$ Mc Murray's reagent – OsO_4 and $K_2Os_2(OH)_4$ Mc Murray's reagent – Sharpless asymmetric epoxidation Mc Murray's reagent – Heck reactions – Suzuki Coupling – Sonogashira coupling – Mc Murray's reagent.

UNIT-IV Photochemistry and Pericyclic reactions **(15 hrs)**

General principles – orbital symmetry considerations related to photochemical reactions, thermal versus photochemical reactions – principles of energy transfer – photochemical reactions of ketones – Norrish type I and type II reactions – Paterno Buchi reaction – Dienone photochemistry – photo reduction, photochemical oxidation, Barton reaction – photochemistry of alkenes and dienes.

Pericyclic reactions

Application of symmetry to orbital interactions – selection rules (Woodward and Hoffmann rules) – Concept of con and dis rotation – Electrocyclisation, cycloaddition and sigmatropic rearrangements – cheletropic reactions – Diels-Alder Reactions: Endoselectivity and regioselectivity – Explanation of these reaction in terms of correlation diagrams approach, FMO approach and Dewar – Zimmermann approach – (PMO) Huckel-Mobius concepts.

UNIT-V Molecular rearrangements (15 hrs)

Classification – Nucleophilic, electrophilic, and radical – Mechanism of Favorski, Benzil-Benzilic acid, Bayer-Villiger, Wagner-Meerwin rearrangement, Carbanionic rearrangements, Stevan's rearrangement, Sommelet-Hauser, Cope, aza and Wesly-Moses rearrangement, Fries Rearrangement.

Acid catalyzed rearrangement – Arndt-Eistert synthesis – carbon to nitrogen migration – Hofmann rearrangement, Curtius rearrangement, Lossen rearrangement, Schmidt and Beckmann rearrangement.

Text book:

1. Jerry March, Advanced Organic Chemistry, Reaction mechanism and structure, John Wiley and sons, 4th Edition, New york, 1992.
2. S. Warren, Organic synthesis - The disconnection approach, John Wiley & Sons, UK, 2004**.**
3. Cary and Sundberg, Advanced Organic Chemistry, Part B, Reactions and Synthesis, Plenum Press, 3rd Edition, 1990.
4. R. K. Mackei and D. M. Smith, Guide Book to Organic synthesis, ELBS, 1982.
5. I.L. Finar, Organic Chemistry, Vol. II, V Edition, ELBS, New York, 2005.
6. W. Caruthers, Some modern methods of organic synthesis, Cambridge university.
7. C.H. Depuy and O.L. Chapman, Molecular reactions and Photo Chemistry, Eastern and Economic Edition, Tata MacGraw Hill, 1975.

Reference Books:

1. Graham Solomons, Organic Chemistry, John Wiley and Sons INC, 5th Edition, 1992.
2. Michael B. Smith, Organic Synthesis, McGraw Hill, International Edition, 1994.
3. Clayden, Greeve, Warren and Wothers, Organic Chemistry, OXFORD University Press, 2007.
4. A.J. Bellamy, An introduction to conservation of orbital symmetry, Longman group Limited, 1974.
5. H. O. House, Modern synthetic reactions, Cambridge University press, 3rd Edition, 1972.
6. W. Carruthers and I. Coldham, Modern methods of organic synthesis, Cambridge University Press, 4th Edition, 2004.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 3PC2**
Semester	**: III**	**No. of Hrs allotted**	**: 5**
Paper	**: Core**	**No. of Credits**	**: 5**
Title of the Paper	**: Inorganic Chemistry-III**		

Course Objectives: **75 hrs**

- This paper deals with coordination Chemistry , lanthanides and actinides.
- It deals with the basic concept, theories , mechanism and spectra of coordination compounds..
- An emphasize is given on Separation techniques of lanthanides and synthesis of actinides.
- To introduce the basics and the advanced technology to study about the synthesis, properties, characterization and the applications of nano materials.

UNIT I COORDINATION CHEMISTRY-1 15 Hrs

Nomenclature of coordination complexes-Stereochemistry of coordination compounds: Geometrical isomerism- optical isomerism of complexes having C.N.4,6-stability constants of complexes-stepwise and overall stability constant- their determination-Jobs' continuous variation method-Chelate effect

CFT. LFT and MO theories- Influence of ligands on crystal field splitting- Octahedral and Tetrahedral splitting of "d" orbitals, CFSE. Spectrochemical series- Nephelauxetic effect– John Teller effect-site preferences. Spectral properties of complexes- Magnetic properties- Para, Dia, ferro magnetism and antiferro magnetism- **Determination of magnetic properties – Gouy's method.**

UNIT-II COORDINATION CHEMISTRY-III (INORGANIC REACTION MECHANISMS) 15 Hrs

Substitution reactions- lability-inertness- square planar substitution reactions- Factors affecting reactivity of square planar complexes- Trans effect- Theories of Trans effect- Stereo chemistry of substitution in octahedral complexes.(SN1,SN2,SNiCB)- Reactions of coordinated ligands- Acid hydrolysis- anation reactions and base hydrolysis.

Mechanism of electron transfer reactions- Outer sphere, inner sphere electron transfer reactions.- Marcus Theory and its applications.

Synthesis of coordination compounds using electron transfer and substitution reaction.

UNIT- III CHEMISTRY OF NANOSCIENCE AND TECHNOLOGY 15 Hrs

Introduction- Types of nano materials-Nanoparticles, nanotubes-Carbon nanotubes: SWCNT and MWCNT,nanowires,nanoribbons,nanorods, nano composites.

Preparation methods-Chemical vapour deposition, Sol-Gel method, Electrodeposition method, Ball milling method, Chemical reduction method, spin coating technique, Solvothernal synthesis, Colloidal method, Co-precipitation method,Flame spray synthesis(Arc Plasma)-Peparation of metal oxide nanoparticles

Properties of nanoparticles- Optical, mechanical, magnetic,electrical, thermal properties.

Characterisation Techniques like SEM,TEM,AFM, XRD, UV-DRS, B.E.T analysis , DLS, PL -Applications of Nanoparticles.

UNIT – IV PHYSICAL METHODS IN INGORGANIC CHEMISTRY-I 15 Hrs

Electronic spectra : selection rules – polarization – splitting of spectral terms – Orgel and Tanabe-Sugano diagram. – Effect of distortion and spin orbit coupling. Evaluation of 10 Dq and beta for octahedral Ni and tetrahedral Co complexes.

IR and Raman spectra : symmetry of normal vibrations – fundamental vibrations – selection rules – applications of IR and Raman. selection rules to structure determination – IR spectral studies of carbonyl compounds.

Nuclear magnetic resonance : Application of chemical shift and spin coupling to structure determination using multiple NMR (H,P,F) chemical exchange, dynamic processes in inorganic and organometallic compounds-kinetics of rearrangement reaction and metal chelates.- Fluxional NMR of metal carbonyls and allyl complexes – paramagnetic NMR and contact and pseudo contact shifts.

NQR- Basic theory, principles and applications.

UNIT-V LANTHANIDES AND ACTINIDES 15 Hrs

a) Lanthanides:-

Occurrence- Separation techniques (Fractional crystallisation, precipitation, ion-exchange, solvent-extraction and thermal decomposition- Selective reduction and oxidation)- Electronic configuration- Oxidation states, Lanthanide contraction- Spectral and Magnetic properties- Lanthanides as shift reagents in NMR- uses of lanthanides and their compounds- position in the periodic table.

b) Actinides:-

Synthesis of elements- Extraction of Th and U and Pu- electronic configuration and oxidation states, spectral and magnetic properties- position in the periodic table.

TEXT BOOKS:

1. **F.A. Cotton and G. Wilkinson**, Advanced Inorganic Chemistry, Wiley-Interscience publications, John Wiley & Sons, V Edn.New York. 1988.
2. **R.S. Drago, Van Nostrand and Reinhold**, Physical methods in Chemistry, 1976.
3. **Purcell K.F. Kotz J.C. Holt Saunders**, Inorganic Chemistry, Philedelphia, 1977.
4. **Gurdeep R. Chatwal & M. S. Yadav**, Coordination Chemistry, Himalaya Publishing House, I Edn.,1993.
5. **Nakamoto, Kazuo**, Infrared and Raman Spectra of Inorganic and coordination compounds, IV edition, John Wiley and Sons,New Yark,1986.
6. **Figgis, B.N.,** Introduction to Ligand Fields, Interscience, Wiley Eartern Ltd., I Edn., New Delhi.1964.
7. **Raymond Chang**- Basic principles of Spectroscopy, Mc Graw Hill,New Delhi. 1971
8. **B.P.Straughan and S. Walker**- Spectroscopy Vol.3, Chapman and Hall 1976.
9. **D. Banerjea** , Coordination Chemistry , Tata McGraw- Hill Publishing Co. Ltd., 1993.

REFERENCES:

1. **Douglas and McDaniel**, A Concise of Inorganic Chemistry , - Oxford and IBH Publishing company (P)Ltd., New Delhi. 2002.
2. **E. Huheey** , Ellen A.Keiter,Richard L.Keiter, Inorganic Chemistry, IV Edn., Pearson Education (Singapore) Pte.Ltd., Delhi, 2004.
3. **Wahid U. Malik, G.D. Tuli and R. D. Madan**, Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi, 2006
4. **William W. Porterfield** , Inorganic Chemistry, Elsevier,II Edn., New Delhi. 2005.
5. **A.G. Sharpe**, Inorganic Chemistry, Addition – Wesley Longman,UK III Edn., 2004.
6. **Gary L. Miessler and Donald A. Tarr**, Inorganic Chemistry, Pearson Education, Inc., 3rd Edn.,New Delhi. 2004.
7. **D.N. Sathyanarayana**, Electronic Absorption Spectroscopy and Related Techniques, Universities Press(India) Limited, 2001.
8. **Mick Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons and Burkhard Raguse:** Nano technology-Basic Science and Emerging Technologies, Overseas Press India Pvt. Ltd. New Delhi-First Edition-2005.
9. **Mark Ratner and Daniel Ratnar**, Nanotechnology-A Gentle Introduction to the Next Big Idea, Pearson Education Inc., US and UK, 2003

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry**	**Code No**	**: 3PC3**
Semester	**: III**	**No. of Hrs allotted**	**: 5**
Paper	**: Core - 9**	**No. of Credits**	**: 4**
Title of the Paper	**: PHYSICAL CHEMISTRY-III**		
			75 Hrs

Course objective:

To understand the symmetry of molecules through the study of group theory and to have an advanced knowledge about the principle and application of various spectral techniques.

UNIT – I **15 Hrs**

Mathematical group – definition – four cardinal properties – cyclic group – commutative property and abelian group – group multiplication table, sub group – similarity transformation and class of group – symmetry of molecules – symmetry elements – symmetry operations – relationship between symmetry operations of a molecule and a mathematical group – point group of a molecule and its deduction – matrix representation of a symmetry operations : **E, C_n, σ_v, i, S_n** – character of a symmetry operation – representation of a group – matrix representation – character representation – similarity transformation – block factorization

Reducible and irreducible representations – the great orthogonality theorem – results of great orthogonality theorem – construction of character table for **C_{2v}, D_{3h}, T_d** – projection operators – direct product representation.

UNIT – II **Applications of group theory** **15 Hrs**

Prediction of symmetries of atomic orbitals, linear vectors, rotation vectors – symmetries of tensor like properties (α & g) – Application to predict the selection rules for IR / Raman activity of normal modes of H_2O and NH_3 – selection rules to predict allowed and forbidden transition in UV-Visible electronic transition for example formaldehyde and behaviour of hamiltonian operator – Prediction of orbitals and hybridization for the molecules BF_3 and CH_4 – HMO energy calculation for ethylene and butadiene.

TEXT BOOKS: **(UNIT I & II)**

1. F.A. cotton – chemical applications of group theory – 3rd edition – wiley eastern Ltd., UK – 1971.
2. V.Ramakrishnan and M.S.gopinathan – group theory in chemistry, vishal publication – Newdelhi, 1988.
3. Veera Reddy, K. symmetry and spectroscopy of molecules, New age International (p) Ltd., 1998.

REFERENCE BOOKS: **(UNIT I & II)**

1. K.V. Raman - Group theory and its applications of chemistry, TMH publishing company Ltd., New Delhi, 1990.

UNIT – III **SPECTROSCOPY - I** **15 Hrs**

Absorbtion and emission of emr – LASER — Interaction of emr with matter – Einstein coefficients. Microwave, IR and Raman spectroscopy of diatomic molecules – determination of molecular paramaters – vibrational spectra of polyatomic molecules – IR and Raman active modes – overtone and combination bands – Fermi resonance – group frequencies and coupling interaction.

REFERENCE BOOKS:

1. G.M. Barrow, Introduction to molecular spectroscopy, McGraw-Hill, Newyork.
2. G.M.Banwell, Fundamentals of molecular spectroscopy, IV Edn., TMH company Ltd.
3. R.Chang, Basic principles of spectroscopy, McGraw-Hill, 1971.
4. K.Veera Reddy, Symmetry and spectroscopy of molecular, New Age International (p) Ltd. 1998.
5. B.P.Straughan and S.Walker, spectroscopy – Vol.-2, Chapman and Hall, 1976.

UNIT – IV SPECTROSCOPY - II 15 Hrs

Electronic spectra of diatomic molecules – molecular quantum numbers – dissociation energy calculations – Birge – sponer extrapolation technique, pre-dissociation spectra – charge transfer spectra – Fortrat diagram – electronic spectra of molecules – absorbance – oscillator strength.

Photoelectron spectroscopy – basic principles, spectrum, X-ray PES, (ESCA) – vibrational structure – koopman's theorem – PES of argon, oxygen and nitrogen.

REFRENCE BOOKS:

1 to 3 as given in **UNIT III**

B.P.Straughan and S.Walker, Spectroscopy Vol.3, Chapman and Hall, 1976.

UNIT – V SPECTROSCOPY - III 15 Hrs

ESR spectroscopy – principle, g-factor, experimental method, spectrum, fine and hyperfine structures and applications (H-atom, CH_3 radical, *p*-1,4 benzosemiquinone radical anion, naphthalene anion, Tempol)

NQR spectroscopy – quadrupole movement, coupling constant, quadrupole transition-electric field gradient and molecular structure ($_7N^{14}$, $_5B^{11}$, $_{17}Cl^{36}$)

Mossbauer spectroscopy – recoilless emission and resonance absorbtion, experimental method, isomeric shift and electric quadrupole splitting in Fe^{57}.

REFERENCE BOOKS:

1. R.Chang, Basic principles of spectroscopy, McGraw-Hill, 1971.
2. R.S.Drago, Physical methods in chemistry, Saunder college publishing, 1999.
3. B.P.Straughan and S.Walker, spectroscopy Vol.I, Chapman and hall, 1976.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course : M.Sc., **Code No : 3PC4 (E2)**
Semester : III **No. of Hrs allotted : 5**
MAJOR ELECTIVES **No. of Credits : 5**
Title of the Paper : COMPUTER APPLICATIONS IN CHEMISTRY(Optional 1)

Course objectives: **75 hours**

To understand the concepts in internet and E-mail.
To have an understanding on HTML and JAVA APPLET and also to emphazise on their applications in chemistry.
To understand Chemistry related software and their applications

UNIT-I: INTERNET AND E-MAIL **T: 10 + P: 5 Hrs**

INTERNET: Introduction- History- Importance of the Internet- Internet Access- Dial-Up connection, Direct connection and equipments –- Internet protocol(TCP/IP,FTP HTTP, TELNET and WAP)-Internet addressing – Domain Name-Mail address-Uniform Resource Locator(URL)-Web Browsing- Searching the Web- Search Engines(Yahoo, Google)- Intranet

Searching and utilizing Popular websites in Chemistry. On line literature survey- accessing of e-journals. Preparing articles for e-publications. Online structure drawing- Collection of spectral data using databases.

ELECTRONIC MAIL: Introduction-Working of E-Mail - Word processor for E-Mail- Mailing Basics – Composing and sending of an E-Mail- Address Book – Signature- File Attachments-Customizing your Mail program –Advantages and Disadvantages of E-Mail - Tips for effective E-Mail use- Smile keys.

UNIT- II: HTML **T: 8 + P: 7 Hrs**

HTML - Need- Structure of HTML Document- HTML Tags- Horizontal line Tags-Background and Text color Tags- Font Tags- MARQUEES Tags- Adding pictures - Ordered and Unordered Lists- Creating Links- Construction of Periodic Table with required data for first ten elements- Frames – Developing and hosting of Web Pages for a given molecule / chemical.

JAVA APPLETS: - Simple and Java applets with graphics- Applications of applet to draw 2D and 3D view of molecules.

UNIT-III: APPLICATIONS OF DESK TOP SOFTWARE IN CHEMISTRY-I
T: 8 + P: 7 Hrs

Chemical drawing programs:- Chem- Draw and Chem 3D

Introduction- Tool Pallets- Construction of the molecule using Chem Draw- Tools-Manipulating a molecule-Model display- Display type- Structure displays- Molecular Surface display- NMR simulation and interpretation- Naming IUPAC- Structure from Name and Name from Structure-Computational Concepts: - Computational methods: - Potential energy surface, geometry Optimizations property (calculations)-Molecular Mechanics Theory in brief - Animations- Difference between Chemdraw and Chem 3D.

UNIT-IV: APPLICATIONS OF *SHELX PROGRAM* IN CHEMISTRY-II

T: 5 + P: 10 Hrs

1. Basics of Crystals- Symmetry and operations- Seven Crystal systems- Bravais lattices- X-Ray Diffractometers- Unit cell parameters- X-ray data- Deduction of Space group- - Structure solution and refinement using SHELX- Structure building using PLATON- H-Bonding.

ORIGIN software- Importing of ASCII file- plotting-manipulation of plots-multiple plots-Linear regression, Multi-regression.

UNIT-V: APPLICATIONS OF *RASMOL* and *MATLAB* IN CHEMISTRY-III

T: 8 + P: 7 Hrs

RASMOL: -

Introduction- User commands– Identification of disulfide-bridges and visualization of :- hydrophobic and polar residues, the distribution of polar and non polar amino acids, side chain of carboxylate and amine , the different structural motives like α-helix, β-sheet and β - turn, the amino acids bound to Zn, active site of carboxypeptidase A, the environment of the active center.

MATLAB: -

Introduction-advantages- getting started- windows for workspace, command interpretation, command history and current history- Addition- Use of sine and Cosine of angles(pi)- variable 'ans'- order of operations- significant decimals- Representation of matrix- getting transpose of a matrix- display of images- saving images-solving linear equations(case m=n only).

Text Books:

1. . **Alexis Leon and Mathews Leon**. Fundamentals of Information Technology Leon TECH World, UBS Publishers & Distributors Ltd., 1999.
2. **E. Balagurusmy**, Programming with Java- A Primer, , Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2nd Edn., 15th Reprint-2003
3. **C. Xavier**, World wide web design with HTML, , Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2nd Reprint 2000.

REFERENCE BOOKS:

1. **Margaret Levine Young**, Internet- Complete Reference, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2001.
2. **Barbara Kassev**, Using the Internet, EE edition, New Delhi, IV Edition, 1998.
3. **Alexis Leon and Mathews Leon**, Internet for Everyone, Leon TECH World, UBS Publishers & Distributors Ltd., 2000.
4.. **John Zukowski**, Mastering Java 2, BPB Publications, New Delhi, 2000.
5 **Patrick Naughten**, The Java Hand Book, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 11th Reprint 2002.
6. **Herbert Schildt**, Java 2- The Complete Reference, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 4th Edn., 2001.
7. **Holzner, John Zukowski**, Java 2 Complete: Steven BPB Publications, New Delhi, 1st Indian Edn., 1999.
8. **Harley Hahn**, The Internet Complete Reference, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2nd Edn., 2001.
9 Chem Draw & Chem 3D –Manual
10. Shelx, Rasmol and MATLAB- Manuals.

REFERENCES in the NET

1.http://SCS 99.unige. Che/eng/toc.html
2.http://hackberry.chem.niu.edu: to/o/webpage.html
3.http://java.Sun.Com/applet/applets/chemical Models/index.html
4.http://ccl.osc.edu/chemistry.html
5. http://www.umass.eud/microbio/rasmol/
6. http://www. Mdli.com/cgi/dynamic/welcome.html/ (for CHIME similar to Rasmol)

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 3PC4(E2)**
Semester	**:III**	**No. of Hrs allotted**	**: 5**
Paper	**: MAJOR ELECTIVES**	**No. of Credits**	**: 5**
Title of the Paper	**: ADVANCED ORGANIC SYNTHESIS (Optional 2)**		

75hrs

Course Objective:

To impart knowledge in Stereoselective and retrosynthetic analysis
To understand about the guest-host interaction.
To gain scientific and technical knowledge in Green chemistry and biotransformation

UNIT-I REETEROSYNTHETIC ANALYSIS (15 Hrs)

Synthetic Strategy of the following target molecules: longifolene-juvabione-jasmone- 5-hexenoic acid-trans-9-methyl I-decalone- bicyclo (4,1,0) heptan-2 one- α-onocerin-isonootketone.

UNIT-II BIOGENESIS OF ALKALOIDS,TERPENOIDS & FLAVONES: **(15 Hrs)**

Alkaloids(pyridine,phenanthrene and indole type)-nicotine-gramine-harmine-morphine-codine- terpenoids of classes with examples Lanosterol & Cholesterol from squalene-coumarins-carbohydrates-fructose-6-phosphate-xylose-5-phosphate-ribulose-5-phosphate-sucrose-amylose and amylopectin-flavones-proteins

Terpenoids: Geranyl diphosphate-Geraniol-Farnesol–Camphor-limonene-citronellol-caryophyllene(Corey methods) – santonin

UNIT-III BIOSYNTHESIS OF FATTY ACIDS (15 Hrs)

Introduction-acetate pathway-acetyl co-enzyme-A-biosynthesis of fatty acids-malonyl co-A-malonyl ACP-Acyl ACP-Acetoacetyl Co-A- biosynthesis of unsaturated fatty acids Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives 3)Mevalonic acid pathway : Biosynthesis of mevalonic acid.

UNIT-IV: DYES (15 Hrs)

Introduction, various methods of dyeing, classification of dyes, nitroso dyes,Azodyes,-Fast green, Methyl Orange, Methyl Red, Fast Red, tripheylmethane dyes-Malachite green, Rosaniline, Aniline blue, Crystal violet, Xanethene dyes-Fluorescein,Rhodamine B, Anthroquinone dyes – Alizarin –Preparation and uses.

UNIT – V : BIOTRANSFORMATION (15 Hrs)

Advantages and disadvantages of Biocatalysts – Biocatalytic application. Hydrolytic reaction, reduction, oxidation, peroxidation – addition and elimination Reaction. Formation of C-C bond-glycosyl transfer reactions - Immobilisation – adsorbtion – ion binding entrapment into gels, into membranes – compartments – Micells and vesicles – modified and artificial enzymes – semisynthetic enzymes – catalytic antibodies.

Text Books:

1. R.K. Mackie, D.M. Smith and R.A.Aitken, Guide book to Organic synthesis, Longman group, UK, 2n edition, 1990.
2. S.Warren, Organic synthesis, The disconnection approach, John Wiley & Son, 1997.
3. C.Daniel Gutsche, Calixarent, Royal Society of Chemistry, Cambridge, 1989.

References:

1. Organnic Synthesis-Robert E.Ireland-Prantice Hall of India Pvt Ltd,NewDelhi.
2. Advanced Organic Chemistry-Reaction & Synthesis-Francis A.Corey & Richard J.Sundberg-V Edition-Springer.
3. Organic Chemistry-Francis A.Corey & Robert M.Giuliano-Tata McGraw-Hill Edition
4.Organic Chemistry-Natural Products Volume II-Dr.O.P.Agarwal-Goel Publishing House.
5. Chemistry of Carbocyclic Compounds-Azhuwalia
6. Pharmaceutical,Medicinal and Natural Product Chemistry-P.S.Kalsi & Sangeetha Jagtap-Narosa Publishing House
7. Organic Chemistry-Jonathan Clayden,Nick Greeves and Stuart Warren-Second Editiion-Oxford University Press
8. Synthetic Dyes-Gurudeep Chatwal
9.Biotransformation in Organic Chemistry-Kurt Faber-A Textbook-V Edition-Springer

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 4PC1**
Semester	**: IV**	**No. of Hrs allotted**	**: 4**
Paper	**: Core - 10**	**No. of Credits**	**: 4**
Title of the Paper	**: Organic Chemistry - IV**		

Course objective: **60 hrs**

To kindle the synthetic aptitude among students on the hetrocycles, Green Chemistry and biologically important compounds and to have a detailed discussion on the natural products.

Unit - I CHEMISTRY OF HETEROCYCLIC COMPOUNDS (12 hrs)

Heterocyclics – Nomenclature – Compounds containing two hetero atoms: Synthesis and reactivity of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, quinoline and isoquinoline. diazines: the chemistry of pyridazine, pyrimidine and pyrazine – Comparison of basicity of diazines Chemistry of anthrocyanins and flavonoids

Unit - II CHEMISTRY OF TERPENOIDS AND ALKALOIDS (12 hrs)

Chemistry of terpenoids: General methods of determining structure of terpenoids – α-pinene, α-cadinene, Zingiberene, Abietic acid and Heliangine.

Chemistry of alkaloids: Alkaloids and Drugs: General methods of determining structure of alkaloids – Structure elucidation of (i) Morphine (ii) Reserpine (iii) Lysergic acid.

Unit- III CHEMISTRY OF STEROIDS AND VITAMINS (12 hrs)

Chemistry of steroids : Introduction – Structural elucidation of Cholesterol – Androsterone and Testosterone (male sex hormones) – Oesterone, progesterone (Female sex hormone).

Classification of Vitamins: Nomenclature of Vitamins – Biological functions of vitamins (Synthesis not included): Vitamin A (Retinol), Vitamin-B (Thiamine), Vitamin B6 (Pyridoxine), Vitamin B12, Vitamin B2 (Riboflavin), Vitamin C, Vitamins K, D and E

Unit IV CHEMISTRY OF PEPTIDES AND NUCLEIC ACID (12 hrs)

(a) Polypeptides – Classification - the peptide linkage - Structure of amino acids – 1^0, 2^0, 3^0 and quaternary structure) – Solid phase peptide synthesis (Merifield) – use of protecting groups and reagents – Structural elucidation of glutathione, thyroxin and oxytocin.

(b) Nucleosides, Nucleotides and Nucleic acids – structure and synthesis of nucleosides and nucleotides – Elementary treatment on the structure of DNA and RNA

Unit – V GREEN CHEMISTRY, CARBODYDRATES AND ANTIBIOTICS (12 hrs)

Green Chemistry: Importance and principles of Green chemistry - Solid state and Solvent free organic reactions – Solid supported reagents – Microwave assisted reactions - Sonochemical approach - Reactions in ionic liquids – supercritical CO_2 medium – aqueous medium - enzymatic and electrochemical methods.

Carbohydrates: Polysaccharides: Startch and cellulose

Antibiotics: Strucural features of following antibiotics (synthesis need not to be discussed)

β-lactam anitibiotics: Penicillin – Chloramphenicol – Griseofulvin

Text Books:

1. I.L. Finar, Organic Chemistry, Vol. II, V Edition, ELBS, UK, 2005.
2. S.F. Dyke, Chemistry of Vitamins, Interscience, Toronto, 1965.
3. O.P. Agarwal, Chemistry of Natural products, Vol. I and II, Himalaya Publishing House, New Delhi, 2002.
4. V.K. Ahluwalia, M. Kidwai " New trends in Green Chemistry" Second Edition, Anamaya publishers, New Delhi, 2006.
5. Gurdeep Chatwal, Organic Chemistry of natural products, Vol. I, Himalaya Publishing House 1997.
6. Morrison and Boyd, Organic Chemistry, Prentice-Hall of India private limited, New Delhi, 6th Edition.

Reference Books

1. Hermann Dugus, Bioorganic Chemistry, Springer International, III Edition, New Delhi, 2004.
2. D.L. Nelson and M.M. Cox, Lehningers' Principal of Biochemistry, W.H. Freeman and Company, New York, 5th Edition, 2008.
3. L.F Fieser and M. Fieser, Steroids, Reinhold Press, Atlanta, 1991.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 4PC2**
Semester	**: IV**	**No. of Hrs allotted**	**: 4**
Paper	**: Core Paper - 11**	**No. of Credits**	**: 4**
Title of the Paper	**: Inorganic Chemistry-IV**		

Course Objectives: **60 hours**

- This paper deals with Organo metallic chemistry and transition metal catalysts.
- It discusses the study of bioinorganic chemistry.
- It gives an idea about inorganic photochemistry.
- It deals with PES, EPR, Mossbauer spectroscopic studies of complexes.

UNIT –I ORGANOMETALLIC CHEMISTRY –I 12 Hrs

Stability of organo metallic compounds- β hydrogen elimination- the sixteen and eighteen electron rule. Synthesis – structure and bonding in metal carbonyls ,- use of IR in the structural elucidation of carbonyl compounds– metal nitrosyls – dinitrogen complexes. π donors. Synthesis structure bonding and reactivity of carbenes, carbines, metallocenes and other aromatic cyclopolyenes – Ferrocene – bonding and structure – sigma, pi and hapto nomenclature. Arene complexes – olefin – acetylene and pi allyl complexes.

UNIT – II ORGANOMETALLIC CHEMISTRY –II 12 Hrs

Catalysis involving organometallic compounds – properties of metals and ligands in homogeneous catalysis – oxidative addition and reductive elimination – hydrogen abstraction – hydrogenation of olefins – Wilkinson's catalyst – hydroformylation – oxidation of olefins – Wacker process – propylene polymerization - Ziegler natta catalyst -cyclo oligomerisation of acetylene , **butadiene-** Reppe's catalyst . **Mansanto's acetic acid synthesis-Fischer-Troppe's synthesis of Synthetic gasoline.**

UNIT –III BIO-INORGANIC CHEMISTRY 12 Hrs

Essential and trace elements in biological systems – metalloporphyrins – the porphyrine ring system – chlorophyll – photosynthetic electron transfer - Electron transport sequence – biological electron transfer – electron transfer agents – cytochromes – Hemoglobin – myoglobins – and synthetic oxygen carriers – nitrogen fixation – in vivo and in vitro – copper proteins-**Metal complexes in medicine.**

UNIT-IV PHYSICAL METHODES IN INORGANIC CHEMISTRY-II 12Hrs

Photoelectron spectroscopy: Fine structure in PES. Chemical shift in Auger spectroscopy -principle and applications.

Electron paramagnetic resonance spectroscopy: Applications of hyperfine splitting and g factor to structural elucidation- Zero field splitting-Krammer's Degeneracy- EPR spectra of Cu (II) and Mn (II) in various site symmetry- covalency of metal-ligand bonding by EPR- study of dynamic processes in solids- Study of phase transition by Mn (II) – John Teller distortions in Cu (II) complexes.

Mossbauer spectroscopy: Basic principles- Doppler effect- Isomer shift- Electron nuclear hyperfine interactions- Quadrupole and magnetic interactions in the study of structure and bonding in Iron and Tin complexes and in Biological systems.

UNIT –V INORGANIC PHOTOCHEMISTRY 12 Hrs

Excited states of coordination complexes – properties of excited states charge transfer and energy transfer – photochemical pathways.

Photoredox reactions of Co(III) and Cr(III) complexes – photosubstitution reactions – photoaquation, photoanation and photorearrangements - Role of TiO_2 in solar energy conversion – Photoredox chemistry of Ruthenium bipyridyl and Ruthenium(II) poly pyridyl compounds-**Chemiluminescence reactions.**

TEXT BOOKS: -

1. **F.A. Cotton and G. Wilkinson** , Advanced Inorganic Chemistry, Wiley-Interscience publications, John Wiley & Sons, V Edn. New York, 1988.
2 **R.S.Drago**, Van Nostrand and Reinhold , Physical Methods in Chemistry 1976.
3. **Purcell K.F. and Kotz J.C., Holt Saunders**, Inorganic chemistry, Philadelphia, 1977
4.**Arthur W. Adamson & Paul D. Fleischauer**, Concepts of Inorganic Photochemistry, John Wiley & Sons. In.,New York, 1975.
5. **Nakamoto, Kazuo, Paul J. McCarthy**,Spectroscopy and Structure of Metal Chelate Compounds, IV edition, John Wiley and Sons. Inc. , New York. 1986.
6. **Wahid U. Malik, G.D. Tuli and R. D. Madan**,Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi, 2006
7. **Raymond Chang**, Basic principles of Spectroscopy - Spectroscopy, Mc Graw Hill, New Delhi, 1971.
8. **B.P.Straughan and S. Walker** , Spectroscopy. - Vol.3, Chapman and Hall ,New York,1976.
9.. **T.C.Gibbs,** Principles of Mossbauer Spectroscopy, Chapman and Hall, New York,1978.

REFERENCE BOOKS: -

1. **J.E.Huheey, Ellen A.Keiter,Richard L.Keiter** , Inorganicchemistry, IV Edn., pearson Education (Singapore) Pte.Ltd., Delhi, 2004.
2. K. Hussain Reddy, Bioinorganic Chemistry, New Age International (P) Ltd., Delhi, 2005.
3. **F. Albert Cotton, Geoffrey Wilkinson, Paul L.Gans**, Basic Inorganic Chemistry, John Wiley & Sons. Inc., III Edn.,New York, 2004.
4. **William W. Porterfield**, Inorganic Chemistry, II Edn., Elsevier,New Delhi, 2005.
5. **A.G. Sharpe**, Inorganic Chemistry, III Edn.,Addition – Weskey Longman,UK 2004.
6. **Gary L. Miessler and Donald A. Tarr,** Inorganic Chemistry, Pearson Education, Inc., 3rd Edn., New Delhi, 2004.
7. **Wahid U. Malik, G.D. Tuli and R. D. Madan**,Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi, 2006

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry**	**Code No**	**: 4PC3**
Semester	**: IV**	**No. of Hrs allotted**	**: 4**
Paper	**: Core Paper - 12**	**No. of Credits**	**: 4**
Title of the Paper	**: PHYSICAL CHEMISTRY-IV**		**60 Hrs**

Course Objectives:

To impart knowledge on the various theories of reaction rates; to understand the concepts of catalysis as well as fast, chain and explosive reactions. To explain the concepts of photochemistry, surface chemistry and polymer chemistry.

UNIT-I **(12 hrs)**

CHEMICAL KINETICS-I

Simple Collision theory- modification - Absolute reaction rate theory (ARRT) - Statistical and thermodynamics formulation - Comparison of ARRT with collision theory- Significance of entropy of activation- Relation between ΔH and Ea- Transmission co-efficient – ARRT of termolecular reactions – Unimolecular reactions - Lindemann, Hinshelwood, RRKM and Slater treatments. –Solution kinetics – ARRT of reaction in solution – Influence of ionic strength on the rates of ionic reactions (salt effects).

Reference Books:

1. K.J. Laidler, Chemical Kinetics, II Edition, Tata McGraw Hill, UK, 2005.
2. A.A. Frost and R.G. Pearson, Kinetics and Mechanism, New York, 1990.
3. F.Wilkinson, Chemical Kinetics and Reaction Mechanism, Var Nostrard Reinhold Co., New York, 2000.

UNIT-II **(12 hrs)**

CHEMICAL KINETICS-II

Fast reactions-flow and relaxation techniques, Temperature Jump and pressure jump method - complex reactions – opposing, consecutive and parallel reactions. Chain reaction – kinetics and general characteristic – H_2 – Br_2 reaction, Rice – Herzfeld mechanism for decomposition of acetaldehyde & ethane – Branched chain reaction – study of H_2 – O_2 Explosive reaction- Homogeneous catalysis – acid, base catalysis.

Reference Books:

1. K.J. Laidler, Chemical Kinetics, Tata McGraw Hill, UK, 2005.
2. A.A. Frost and R.G. Pearson, Kinetics and Mechanism, New York, 1990.
3. F.Wilkinson, Chemical Kinetics and Reaction Mechanism, Var Nostrard Reinhold Co., New York, 2000.

UNIT-III **(12 hrs)**

PHOTOCHEMISTRY

Physical properties of the electronically excited molecules-radiationless transitions-Internal conversion and intersystem crossing-Stern-Volmer equation and its application-radiative transition – fluorescence, phosphorescence and other deactivation processes. Effect of temperature on emission process- photosensitization and Chemiluminescence. - Experimental techniques in photochemistry, Chemical actinometers.

Photochemical Kinetics of H_2-X_2 reactions – Photolysis of acetaldehyde Photodimerisation of anthracene-Photoequation of $(Cr(NH_3)_5NCS)^{2+}$ and photo isomerisation of Cis-bis glycinato Pt(II). Applications of photochemistry – Solar energy conversion and storage -photo synthesis.

Reference Books:

1. Fundamentals of Photochemistry, K.K. Rohatgi-Mukherjee, Wiley Eastern Ltd., Revised edition, New York, 1999.

UNIT-IV **(12 hrs)**

SURFACE CHEMISTRY

Physisorption and Chemisorption- adsorption isotherms-Langmuirs, Freundlich and B.E.T equations- surface area determination –Gibbs adsorption isotherm. Heterogeneous catalysis- and their kinetics. Chemical reactions on solid surfaces. Mechanism & Kinetics of unimolecular and bimolecular surface reactions-Langmuir –Hinshelwood, Langmuir –Ridel mechanism. ARRT of surface reactions-Basic concepts of Micelles and Reverse Micelles.

Text Books:

1. S.Glasstone – Textbook of Physical chemistry – III Edition McMillan, Alasca, 1974.
2. F.Daniels and R.A. Alberty – Physical Chemistry – John willey and sons , UK, 1974.
3. W.J. Moore – Physical Chemistry – V Edition – Orient Longman , UK, 1972.

Reference Books:

1. A.M. Adamson – Physical Chemistry of Surfaces – V.Edition John Willey, UK, 2002.
2. K.S. Laider – Chemical kinetics – III Edition – TMH, New York, 2005.

UNIT-V **(12 hrs)**

POLYMER CHEMISTRY

Introduction of Polymers -Classification-Tacticity - Polymerisation - Addition, Co-polymerisation and Condensation polymerisation – Kinetics of polymerization-Free radical Chain polymerization-Cationic- anionic polymerization- Molecular weight determination – Osmotic pressure methods- Light Scattering method-Ultra Centrifuge and Viscosity methods.

Classification of Plastics-Thermosetting & Thermoplastic resins-Adhesives-Compounding of Plastic - Fabrication - Compression moulding, Injection moulding, Extrusion moulding and Blow moulding.

Industrially important polymers – Preparation, Properties and uses of (LDPE & HDPE), PS, polyester, acrylo polymer, Teflon, Phenolic resins, amino resins and epoxy resins, Polyvinyl acetate-composites of Resins-ABS-Conducting Polymers-Polyacetylene, Polyaniline, Inorganic polymer-Silicone and Biopolymers-cellulose.

Reference Books:

1. H.R. Allcock and W. Lampe – Contemporary polymer chemistry – Prentice Hall UK, 1991.
2. Young, Polymer Chemistry II, Chapman Hall, 2002.
3. Arora Singh, Polymer Chemistry, Anmol Publications Pvt. Ltd., 2001.

Text Books

1. F.W. Billmeyer Jr., A text book of Polymer Chemistry – III edition, John Willey and Sons, UK, 1984.
2. V. Gowarikar, et al., Polymer Science, Willey Eastern Limited, New York, 1986.
3. F. Rodriguez, Principles of polymer chemistry, Tata McGraw- Hill Publishing Co. Ltd., New Delhi, 1987.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 4PCL1**
Semester	**: III & IV**	**No. of Hrs allotted**	**: 5**
Paper	**: Major Elective**	**No. of Credits**	**: 5**
Title of the Paper	**: Organic Chemistry Practicals**		

COURSE OBJECTIVE **75 hrs**

To include the spirit of organic synthesis in senior chemistry students, to train them in the quantitative estimation of organic compounds, glucose, methyl ketones, etc. and some extraction methods and TLC analysis,

DOUBLE STAGE PREPARATION

1. p-Nitroaniline
2. p-Bromoaniline
3. 1,3,5-Tribromobenzene
4. Benzanilide
5. m-Nitrobenzoic acid
6. p-Iodonitrobenzene (III stage)
7. 2,5-dihydroxy acetophenone

(any five preparations only)

ESTIMATION

1. Estimation of glucose – Lane and Eynon method
2. Estimation of ethyl methyl ketone
3. Separation of amino acids by thin layer chromatography (including hydrolysis of aspartame present in the sugar-free tablet)
4. Extraction of Caffeine from Tea leave using Soxhlet apparatus
5. Extraction of lemongrass oil by steam distillation
6. Isolation of curcumin from turmeric powder by column chromatography

MARKS

Internal 40 External 60

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 4PCL(E3)**
Semester	**:IV**	**No. of Hrs allotted**	**: 5**
Paper	**: Major Electives**	**No. of Credits**	**: 5**
Title of the Paper	**: Inorganic Chemistry Practicals (Optional-1)**		

Course objective: 75 hrs

This course mainly emphazise on developing practical skills on quantitative inorganic estimations and also in spectrometric determination of metal ions and also to focus on the preparation of inorganiccomplexes.

	ESTIMATIONS: By VOLUMETRIC METHOD		**By GRAVIMETRIC METHOD**
1.	Estimation of COPPER	and	NICKEL
2.	Estimation of CALCIUM	and	MAGNESIUM
3.	Estimation of BARIUM	and	ZINC
4.	Estimation of IRON	and	NICKEL
5.	Estimation of COPPER	and	SILVER
6.	Estimation of COPPER	and	ZINC
7.	Estimation of COPPER	and	NICKEL

II PREPARATIONS (Any FIVE Estimations only)

1. Tetramminecopper(II) sulphate
2. Potassium cupricsulphate
3. Potassium trioxalatoaluminate(III)
4. Sodium nitroprusside
5. Trithioureacopper(II) sulphate
6. Pentathioureadicuprous nitrate
7. Hexathioureaplumbus nitrate
8. Nitropentamminecobalt(III)
9. DithiocyanatotetrapyridineIron(III)
10. Potassium troxalatoferrate III

(Any Five Preparations only)

Marks

Internal- 40 (Estimation= 20, Preparation= 10, Record=5, Viva=5)
External- 60 (Estimation=30, Preparation=10, Record=10, Viva= 10)

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: 4PCL(E3)**
Semester	**:IV**	**No. of Hrs allotted**	**: 5**
Paper	**: Core practical**	**No. of Credits**	**: 5**
Title of the Paper	**: Analytical Chemistry Practicals (Optional-2)**		

Course objective: 75 hrs

This course mainly emphazise on developing practical skills on analytical chemistry in the analysis of soil, water, fertilizer, oil etc.

I SOIL ANALYSIS

Collection of soil sample – soil pH, EC – Nutrient analysis – soil N_2, P

II WATER ANALYSIS

Determination of pH, EC, COD, BOD

III FERTILIZER ANALYSIS

Analysis of Urea, Super phosphate, DAP, Determination of micro nutrient analysis using Atomic absorption spectroscopy, Flame Photometry. Determination of Zn, Ca, S.

IV ANALYSIS OF OIL

Determination of I_2 value – saponification value- acid value

V RAW MATERIAL TESTING

Analysis of cement – milk and milk products

VI INSTRUMENTAL ANALYSIS

FTIR: Recording and interpretation of FTIR spectra of organic and inorganic samples.

UV-Visible : Determination of unknown concentration of Ni^{2+}, Cu^{2+} and Fe^{2+}

VII ELECTROCHEMICAL ANALYSIS

CV and impedence measurements of ferrocyanide / ferricyanide and other redoc systems, heme solution and cells / batteries

VIII MODELLING AND SHELX

(i) Sructure drawing, visualization and energy minimization of simple molecules using Chem Draw, Rasmol, Kinemages and Alchemy 2000

(ii) Structure solution of simple inorganic and organic molecules using SHELX.

Reference Books

1. S.M.Khopkar, Analytical chemistry, New Age International, 2002
2. A.I.Vogel, A text book of Quantitative Inorganic Analysis, Longman, 1961
3. D.G.Peters, J.M.Hayes and G.M.Hejije- A Brief Introduction to modern chemical analysis, WB Saunders, 1976.

Marks: **Internal** : 40 **External : 60**

Analysis	**= 45**
Record	**= 10**
Viva voce	**= 05**
Total	**= 60**

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,**	**Code No**	**: SPJ 8**
Semester	**: IV**	**No. of Hrs allotted**	**: 8**
Paper	**: Core Project**	**No. of Credits**	**: 4**
Title of the Paper	**: PROJECT**		

Course Objective: **120 hours**

The objective is to impart to the students, the skills on developing new materials through new synthetic routes and characterization of these using different techniques including their applications. The students thus learn research methodologies along with literature survey and creativity.

Marks

External Examiner : Viva : 20

External Examiner Evaluation of Project : 40

Internal Examiner Evaluation of Project : 40

(only) ----------

100

M.Sc., Chemistry Special (SF)

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY (SPL)
COURSE STRUCTURE – (w.e.f 2014 – 2016 Batch Onwards)
I – Semester

Course	Code	Subject	Contact Hrs.	Credits	Max. Marks (CA)	Max. Marks (SE)	Total
Core -1	S1PC1	Organic Chemistry – I	4	4	25	75	100
Core 2	S1PC2	Inorganic Chemistry – I	4	4	25	75	100
Core -3	S1PC3	Physical Chemistry – I	4	4	25	75	100
Core -4	S1PCL4	Separation techniques and quantitative analysis.	4	4	40	60	40
Lab	S2PCL1	Organic Chemistry Practicals	5*	-	-	-	-
Lab	S2PCL2	Inorganic Chemistry Practicals	5*	-	-	-	-
Lab	S2PCL3	Physical Chemistry Practicals	4*	-	-	-	-
		Total	**30**	**16**	**115**	**285**	**340**

II – Semester

Course	Code	Subject	Contact Hrs.	Credits	Max. Marks (CA)	Max. Marks (SE)	Total
Core 5	S2PC1	Organic Chemistry – II	4	4	25	75	100
Core –6	S2PC2	Inorganic Chemistry – II	4	4	25	75	100
Core -7	S2PC3	Physical Chemistry – II	4	4	25	75	100
Elective 1	S2PC4 (E1)	C-Programming Fundamentals & Applications in Chemistry (Elective 1) (OR) Medicinal Chemistry	4	5	25	75	100
Lab	S2PCL1	Organic Chemistry Practicals	5	4	40	60	100
Lab	S2PCL2	Inorganic Chemistry Practicals	4	4	40	60	100
Lab	S2PCL3	Physical Chemistry Practicals	5	4	40	60	100
		Total	**30**	**29**	**220**	**480**	**700**

III – Semester

Course	Code	Subject	Contact Hrs.	Credits	Max. Marks (CA)	Max. Marks (SE)	Total
Core -8	S3PC1	Organic Chemistry – III	5	4	25	75	100
Core - 9	S3PC2	Inorganic Chemistry – III	5	4	25	75	100
Core -10	S3PC3	Physical Chemistry – III	5	4	25	75	100
Elective 2	S3PC4 (E2)	Computer Applications in Chemistry (Elective) (OR) Advanced Organic Synthesis (Elective)	5	5	25	75	100
Lab	S4PCL1	Organic Chemistry Practicals	5*	-	-	-	-
Lab	S4PCL (E2)	Inorganic Chemistry Practicals (Elective) (OR)Analytical Chemistry (Elective)	5*	-	-	-	-
		Total	**30**	**17**	**100**	**300**	**400**

IV Semester

Course	Code	Subject	Contact Hrs.	Credits	Max. Marks (CA)	Max. Marks (SE)	Total
Core -11	S4PC1	Organic Chemistry – IV	4	4	25	75	100
Core - 12	S4PC2	Inorganic Chemistry – IV	4	4	25	75	100
Core -13	S4PC3	Physical Chemistry – IV	4	4	25	75	100
Lab	S4PCL1	Organic Chemistry Practicals	5	4	40	60	100
Elective – 3	S4PCL(E3)	Inorganic Chemistry Practicals (Elective 1) (OR) Analytical Chemistry (Elective 2)	5	5	40	60	100
Lab	S4PCL3	Synthesis and spectral analysis	5	4	40	75	40
SPJ	SPJ	Project	3	3	40	60	100
		Total	**30**	**28**	**235**	**480**	**640**

* Credits will be given at the end of II / IV Semester

(A) <u>Consolidation of Contact Hours and Credits: PG</u>

Semester	Contact Hrs. / Week	Credits
I	30	16
II	30	29
III	30	17
IV	30	28
Total	**120**	**90**

B) <u>Curriculum Credits</u>

Core	--- 75Credits
Elective	---15 Credits

Total	90 Credits

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course : M.Sc., Chemistry (Spl) **Code No : S1PC1**
Semester : I **No. of Hrs allotted : 4Hr/week**
Paper : Core **No. of Credits : 4**
Title of the Paper : Organic Chemistry- I

Course Objective: **Total Hours: 60**

This paper aims at enriching the students' knowledge about bonding and reaction mechanism in organic molecules.

UNIT-I Delocalized chemical bonding, Aromaticity and Reaction intermediate (12 hrs)

Electron displacement – Steric effect – Tautomerism

Concept of aromaticity – Benzenoid and non-benzenoid compounds – Huckel's rule - Non aromatic and anti aromaticity - Alternant and non alternant hydrocarbons - aromaticity of cyclopentadienyl anion and Tropylium cation – Azulenes and annulenes.

Synthesis , structure, stability, reactivity and reactions of carbocations, carbanions, free radicals (reactions include Pinacol coupling, McMurray reactions, acyloin reaction, selective radical bromination). Carbenes: Stability - Structure – Generation – Types – Reactions. Nitrenes: Generation and reactions.

UNIT - II Reaction mechanism-I (12 hrs)

Guidelines for proposing reasonable mechanism – Energetics and energy profile diagrams – transition state – Intermediate – Hammond's postulate – principle of microscopic reversibility - kinetic and thermodynamic controls – kinetic and non-kinetic methods of determining organic reaction mechanism – primary and secondary kinetic isotope effects – Effect of structure on reactivity: Resonance and field effects – Quantitative treatments – Hammett and Taft equation.

UNIT - III Reaction mechanism-II (12 Hrs)

Substitution Reactions:

Aliphatic Nucleophilic Substitution Reactions - Mechanism – S_N1 and S_N2, mixed S_N1& S_N2, S_Ni, SET, Neighboring group participation by σ and π bonds – Reactivity at an allylic, aliphatic trigonal and vinylic carbon – Effect of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity - Ambident nuleophiles.

Aromatic Nucleophilic Substitution Reactions – Unimolecular, Bimolecular and Benzyne mechanism – Effect of substrate, leaving group and attacking nucleophile.

Electrophilic substitution reactions:

Aliphatic: Bimolecular mechanism SE2 and SE1 – Aromatic: Arenium ion mechanism – Orientation and reactivity: Ortho and Para ratio, partial rate factor

UNIT-IV Reaction Mechanism III (12 hrs)

Elimination reactions : E_1, E_2 and E_1CB mechanism- Competition between substitution and elimination – orientation of double bonds (Bredt's rule and Hofmann and saytzeff rules) – Effect of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity – Mechanism and orientation in pyrolytic eliminations - Cope and Chugaev reaction (cis-elimination)

UNIT-V Reaction Mechanism IV (12 hrs)

Addition to carbon – carbon multiple bonds:

Electrophilic, Nucleophilic & free radical addition – Mechanism, Orientation and reactivity reactions - addition to conjugated systems- addition to α,β-unsaturated carbonyl and nitrile systems- Michael addition – addition of Grignard reagents-Diels Alder reaction- Enamine reaction - Mechanism of Reformatsky reaction- Darzen reaction- Mannich reaction - Wittig reaction - Stobbe and Dieckman condensation.

Text books:

1. Jerry March, Advanced Organic Chemistry, Reaction mechanism and structure, John Wiley and sons, 4th Edition, New york, 1992.
2. R.O.C Norman, Principles of organic synthesis, 3rd Edition Nelson Thorines, Hong kang 2001.
3. P.J.Garrat, Aromaticity, Mc Graw Hill, 1991
4. F.A.Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and B, Plenum Press, 3rd Edition 1990).
5. G.M. Badger, Aromatic character and Aromaticity, Cambridge, USA, 2001.

Reference Books:

1. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, 2007.
2. E.S. Gould, Mechanism and structure in Organic Chemistry, Holtoo INC, 1960.
3. G. Solomon, Organic Chemistry, John Wiley and sons INC, 5th Edition, 1992.
4. R.K. Mackie and D.M. Smith, Guide Book to Organic synthesis,Longman, UK,1993.
5. Peter sykes, A Guidebook to Mechanism in Organic Chemistry, Longman, 6th Edition, 2003.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S1PC2**
Semester	**: I**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core**	**No. of Credits**	**: 4**
Title of the Paper	**: Inorganic Chemistry-I**		

Course Objectives: **60 Hours**

- ✓ This paper deals with the concepts of bonding and electronic structure of Atom.
- ✓ It deals with the study of acid base systems and non aqueous solvents.
- ✓ It gives a thorough understanding on nuclear Chemistry.

UNIT – I: ELECTRONIC STRUCTURE OF ATOM 12 Hrs

Introduction to quantum Chemistry –Postulates of quantum mechanics-Operators – Wave equation –Orthogonality and normalisation -hydrogen like atoms-radial wave function-symmetry orbitals -significance of quantum numbers-shapes of atomic orbitals - poly electronic atoms –Pauli's exclusion principle- Aufbau principle -L.S Coupling scheme- Russel- Saunders method- Term Symbols -Hunds rule –eletronic configuration.. **Ionisation potential, Ionic radii and covalent radii, Electron affinity, Electro negativity- their trend in the periodic table.**

UNIT – II: NATURE OF THE CHEMICAL BOND 12 Hrs

Ionic bond – Lattice energy and its determination by Born-Haber cycle and Born Lande Equation – Hardness, electrical conductivity and solubility of ionic compounds – ionic radii. Goldschmidths radius ratio-packing of atoms and ions in solids. **Calculation of ionic radius –Pauling's method and Linde's method. Effective nuclear charge-Slater's rule.**

Covalent bond – qualitative treatment of valence bond theory – Heitler-London theory – Pauling theory and Molecular orbital theory LCAO theory – Hybridisation and resonance.

UNIT – III: BONDING APPLICATION 12 Hrs

Application of VB and MO theories to the structure of homonuclear (H_2, B_2, C_2, N_2) and heteronuclear (CO,NO,HCl,HF) diatomic and selective polyatomic molecules (CO_3^{2-}, NO_2, BeH_2, CO_2), comparison of VB and MO theories. Bond properties, bond order, bond energy, bond length and bond polarity. Partial ionic character of covalent bonds-**Fajan's Rule** -VSEPR theory and its applications to H_2O, NH_3, IF_5, IF_7, ClO_4 **VSEPR applied to Xenon compounds like Xenon halides and xenon oxides**

UNIT – IV : ACID-BASE SYSTEMS AND NON-AQUEOUS SOLVENTS. 12 Hrs

A generalized acid base concepts – steric effects and solvation effects – Measures of Acid-Base strength –**Factors affecting the strength of acids and bases- Common ion effect and Henderson's equation-** - Hard and Soft acids and bases – symbiosis – theoretical basis of hardness and softness. Classification of solvents – properties of ionizing solvents. Typical reactions in non–aqueous solvents- liquid HF, Hydrogen cyanide, Sulphuric acid and acetic acid.

UNIT – V : NUCLEAR CHEMISTRY 12 Hrs

Radioactive decay and equilibrium- Different types of nuclear reaction – spallation – fission and fusion. Theories of fission. Fissile and Fertile isotopes.

Nuclear fusion – stellar energy

Nuclear forces: Liquid drop model, shell model

Calculation of Q-values – Cross section.

Detectors: Scintillation counter , Gas Ionisation chamber. Proportional Counter, Cerenkov Counter

Accelerators: Cyclotron, Synchrocyclotron, Betatron.

Applications: Activation analysis, Isotopic dilution technique-radiometric titration.

Nuclear reactors: Types (Thermo nuclear and breeder reactors) feed materials production. Reprocessing of nuclear materials waste disposal. Atomic power projects in India. **Hazardous of radioactive materials and Safety measures.**

TEXT BOOKS:

1. **P.J.Durrant and B.Durrant**, Introduction to advanced inorganic chemistry, Longman Group Ltd, London,1970.
2. **A.K.Chandra,** Introductory Quantum Chemistry, Tata McGraw Hill, New Delhi, 3rd Edn., 1988.
3. **J.D. Lee**, Concise Inorganic Chemistry, Blackwell Science Ltd., V Edn., London. 2002.
4. **S. Glasstone**, Source Book of Atomic Energy, Van Nostrand, III Edn,East West Press (P) Ltd., New Delhi.1967
5. **G. Friedlander, J.S. Kennedy and M.M. Millodr**, Nuclear and radiochemistry, John Wiley & Sons ,New York..1984.
6. **M. Clyde Day, Jr & Joel Selbin**, Theoretical Inorganic Chemistry, Chapman & Hall Ltd., London, 5th Reprint, 1967.

REFERENCE BOOKS :

1. **J.E. Huheey, Ellen A.Keiter, Richard L.Keiter,** Inorganic Chemistry, IV Edn., Pearson Education (Singapore) Pvt. Ltd., New Delhi. 2004.
2. **H.J. Arnikar**, IV Edn., Essentials of Nuclear Chemistry, vNew Age international (P) Ltd., New Delhi. 2005.
3. **R.D. Madan,** Modern Inorganic Chemistry, S. Chand & Company Ltd., New Delhi, 2004.
4. **Wahid U. Malik, G.D. Tuli and R. D. Madan**, Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi. 2006.
5. **Gary L. Miessler and Donald A. Tarr**, Inorganic Chemistry, Pearson Education, Inc., 3rd Edn., New Delhi. 2004.
6. **William W. Porterfield**, Inorganic Chemistry, II Edn., Elsevier,New Delhi,2005.
7. **A.G. Sharpe**, Inorganic Chemistry, III Edn., Addition – Wesley Longman, UK, 2004.
8. **D. F. Shriver and P.W. Atkins**, Inorganic Chemistry, Oxford University Press, London.1999.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry (Spl)**	**Code No**	**: S1PC3**
Semester	**: I**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core Paper - 3**	**No. of Credits**	**: 4**
Title of the Paper	**: PHYSICAL CHEMISTRY-I**		**60 Hrs**

Course Objective:

To understand the concepts of gaseous and liquid states, their thermodynamic properties, basic principles of quantum mechanics & its applications to simple systems & application of thermodynamics to biological reactions.

UNIT-I

PROPERTIES OF GASES AND LIQUIDS (12 Hr)

Equations of states - Molecular speeds- Maxwell distribution of molecular velocities - one, two and three dimensions-Energy distribution-Maxwell – Boltzmann distribution law- Principle of equipartition of energy and heat capacity- Rotation, vibrations and translational degree of freedom- Molecular collisions- Mean free path- Transport properties- thermal conductivity- Viscosity of gases- momentum transfer and diffusion.

Liquid state- theory of liquids- Internal pressure- liquid crystals- Nematic (p-methoxycinnamic acid), cholesteric (cholestryl benzoate), smectic (ethyl-p-azoxybenzoate)- theory and its application in Liquid Crystals Display.

Text Books:

1. S. Glasstone, A text book of Physical Chemistry, McMillan India Ltd., 1999.
2. R. A. Alberty and F. Daniels, Physical Chemistry, John Wiley & Sons, New York 1978.
3. G. W. Castellan, Physical chemistry, 3rd edition, Wesley Publishing Company, UK, 1986.

Reference Books:

1. S. Glasstone, A text book of Physical Chemistry, McMillan India Ltd., Alasca, 1999.
2. Walter J. Moore, Physical Chemistry, 6th edition, Orient Longman, New York, 2006.

UNIT-II

THERMODYNAMICS – EQUILIBRIUM AND NON-EQUILIBRIUM (12 Hr)

A general review of enthalpy, entropy and free energy concepts – Nernst heat theorem- Genesis of third law and its limitations- Derivation of third law and their application to real gases- calculation of $(\delta H/dP)_T$, $(\delta E/dV)_T$ and $\mu_j.T$ for gases- Thermodynamics of system of variable composition- partial molar quantities and their determination- Chemical potential- relationship between partial molal quantities.

Gibbs Duhem equation- Duhem Margules equation- thermodynamic properties of real gases- Fugacity concept- Determination of Fugacity of real gases- Activity and Activity coefficient- Electrolytes and Non-Electrolytes- Equilibrium thermodynamics- Gibbs phase rule and its application to three component systems- Extent of reaction- quantitative treatment of Le Chatlier principle- Reaction potential- Basic concepts of Non-equilibrium thermodynamics- Principle of Microscopic reversibility-Onsager's reciprocal relationship.

Text Books:

1. S. Glasstone, Thermodynamics for Chemists, Eastern Wiley publications, 2002.

Reference Books:

1. M. Klotz and R. M. Rosenberg-Chemical thermodynamics, 4th edition, Benjamin, New York, 1996.
2. S. Glasstone - Thermodynamics for Chemists, 5th edition, Eastern Wiley publications, 2002.
3. J. Rajaram and J. C. Kuriakose, Thermodynamics, 3rd edition, S. N. Chand, New Delhi, 1999.

UNIT –III

QUANTUM CHEMISTRY-I (12 Hr)

Black body radiation- de Broglies wave particle duality- Experimental verification of matter waves- Compton effect- Heisenberg's Uncertainity principle- The Schrodinger equation and the postulates of quantum mechanics- operators –linear and non-linear operators- commutative and non-commutative operators- Hermitian operators- Eigen function, Eigen values and degeneracy- Orthogonality and Normalization of wave functions- Derivation of Schrodinger's wave equation.

Text Books:

1. P.Atkins, Physical Chemistry, Oxford University Press, VII Edition, 2002.
2. A. K. Chandra- Introductory Quantum Chemistry-3rd edition, Tata Mcgraw Hill Publishing company, New Delhi, 1988.
3. H. W. Hanna, Quantum Mechanics in Chemistry- Benjamin- Cummiza, London Publishing company, 1983.
4. P. W. Atkins, Molecular Quantum Mechanics, Oxford University Press, II Edition, UK, 1986.

Reference Books:

1. Levine, Quantum Chemistry, 6th edition, Prentice-Hall, New Delhi, 2006.
2. D. A. Mcquarrie, Quantum Chemistry,Viva Books Pvt. Ltd., New Delhi, 2003.

UNIT- IV

QUANTUM CHEMISTRY-II (12 Hr)

Application of quantum mechanics to simple system- Application of SWE to free particle moving in one dimension- particle moving in a one dimension box - particle moving in 3D cubical and rectangular box- Quantum Mechanical tunneling - particle in a ring- rigid rotor- Simple Harmonic oscillator - hydrogen atom- angular momentum spin momentum- ladder operator.

Text Books:

1. H. W. Hanna, Quantum Mechanics in Chemistry- Benjamin- Cummiza London Publishing company, UK, 1983.
2. A.K. Chandra-Introductory quantum chemistry-3rd edition Tata McGrow- Hill Publishing Co Ltd., New Delhi, 1988.
3. P. W. Atkins, Molecular Quantum Mechanics, Oxford University Press, II Edition, Oxford, 1986.

Reference Books:

1. Levine , Quantum Chemistry, 5th edition, Prentice-Hall, UK, 2003.
2. . D. A. Mcquarrie, Quantum Chemistry,Viva Books Pvt. Ltd., New Delhi, 2003.
3. P.Atkins, Physical Chemistry, Oxford University Press, VII Edition, 2002.

UNIT-V (12 Hr)

PHYSICO-CHEMICAL PRINCIPLES AND BIOLOGICAL REACTIONS

Studies on biochemical equilibria- buffer system of intracellular fluids- H_2CO_3/HCO_3^- - $HPO_4^{2-}/H_2PO_4^-$ -Application of Henderson- Hassel bach equation- Ion channels – membrane and Static potentials – Role of Na^+ / K^+ ions in neural communications.– allosterism and oxygen – Saturation curves for Hb and Mb- Hill equation.

Medicinal chemistry- QSAR-partition coefficient, p and concentration, c of drugs – use of hydrophobicity constant Π- Πc and ρ- Hamett substituent constants σ and ρ, steric factor: Es- Hansch equation-Craig plot- Topliss scheme.

Text Books:

1. J. Gareth Morris- A. Biologists physical chemistry, Edward Arnold , UK, 1974.
2. G. M. Barrow- physical chemistry for the life sciences ,McGraw Hill Kogakusha Ltd., New York, 1994.

Reference book:

1. Raymond Chang – Physical Chemistry with application to biochemical system Mc Millan Publishing Company. Inc., New Delhi, 2002.
2. Graham L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, New York, 1995.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry(Spl)**	**Code No**	**: S1PCL4**
Semester	**: I**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core Practical**	**No. of Credits**	**: 4**
Title of the Paper	**: Separation Technique and Quantitative Analysis**		

Course objective: 60 hrs

To impart the knowledge of separation technique and make the student to get known about the extraction of product from the natural source.

I.SEPARATION TECHNIQUE

(i) Chromatographic Separation of Carbohydrates.

(ii) Separation of amino acids by TLC.

(iii) Separation of amino acids by paper chromatography

(iv) Separation of organic compounds by Column chromatography

II. EXTRACTION

(i) Isolation of lactose from milk.

(ii) Isolation of Citric acid from lemon

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III. ESTIMATIONS

(i) Iodine value on an Oil using Hanus method.

(ii) Saponification value of an oil.

(iii) Estimation of Ascorbic acid.

(iv) Reichert-Meissel value of an oil.

INTERNAL : 40 Marks

Assessment = 25
Record = 10
Viva = 5

40

EXTERNAL : 60 Marks

Extraction/Estimation = 30
Separation = 15
Viva = 5
Record = 10

60

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S2PC1**
Semester	**: II**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core - 5**	**No. of Credits**	**: 4**
Title of the Paper	**: Organic chemistry -II**		

Course Objective: **Total:60 Hr**

This paper aims at enriching the students' knowledge about organic spectroscopy and stereochemistry

Unit-I UV and IR Spectrsocopy (12 Hr)

Ultraviolet spectroscopy – basic principle – instrumentation – the absorption laws, types of electronic transitions – Effect of solvent and hydrogen bonding on λ_{max} values - Woodward rules to calculate λ_{max} values of conjugated dienes, conjugated polyenes, and carbonyl compounds

Infrared spectroscopy – basic principle – Molecular Vibrations – instrumentation – characteristic IR absorption of different functional groups – factors influencing the vibrational frequencies

Unit-II ^{1}H NMR and ^{13}C NMR spectroscopy (12 Hr)

^{1}H NMR spectroscopy: Basic principles – number of signals – chemical shift factors influencing chemical shift – spin-spin coupling – coupling constant and factors influencing coupling constant. Simplification of complex spectra – shift reagents, deuterium substitution and spin decoupling. **Advanced NMR Spectroscopy -** Introduction to 2D-NMR - Classification of 2D experiments – 2D resolved spectroscopy – HOMO and HETERO – 2D – J resolved spectra. Correlation Spectroscopy (COSY) – HOMO – COSY, HETERO – COSY, 2D – INADEQUATE and NOESY.

^{13}C NMR spectroscopy: Basic principle – comparison with ^{1}H NMR – noise decoupling – off resonance decoupling – factors affecting the C-13 chemical shifts.

UNIT-III: Mass Spectroscopy, ORD and CD (12 Hr)

Basic instrumentation of Mass spectrometer - types of ions – molecular, isotopic, metastable and fragmentation ions – Tests for molecular ion peak – General fragmentation modes- Retro Diels - Alder reactions – Mc Lafferty rearrangement – Fragmentation pattern of simple organic molecules. Application – Accurate Molecular weight, Molecular formula (Nitrogen rule) – Determination of structures of organic molecules. Introduction to ESI, MALDI and FAB mass spectrometer.

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD): Circularly polarized light – Circular birefringence and CD – plain curves and their applications – Cotton effects curves – structural applications – axial haloketone rule, octant rule and their applications.

Solving problems based on UV, IR, NMR and Mass data.

UNIT IV - Organic Stereochemistry (12 Hr)

Optical isomerism

Symmetry elements – the concept of chirality – chirality about a center – specification by Cahn-Ingold-Prelog notations – compounds with more than one chiral center – erythro, threo and meso nomenclature – concept of prochirality – homotopic, enantiotopic and diastereotopic ligands and faces – Asymmetric synthesis – Cram's rule and Prelog's rule. Optical activity in allenes and spiranes – StereoChemistry of nitrogen compounds.

Geometrical isomerism

E and Z notation – Determination of configuration of geometrical isomers by simple techniques like hydroxylation, hydroboration and methods based on physical properties – Stereoisomerism in cyclic compounds – 3, 4 and 5 membered ring systems.

UNIT V -Conformational Analysis (12 Hr)

Configuration and conformation – definition – conformational free energy – atropisomers – conformational analysis of cyclohexane system – stability and isomerism in mono and disubstituted cyclohexanes – conformation and reactivity of cyclohexane derivatives – conformational analysis of fused ring system – decalins, and perhydrophenanthrene.

Text Books:

1. D. Nasipuri, Stereochemistry of Organic compounds 2nd edition, New Age International, New Delhi 2004.
2. William Kemp, Organic Spectroscopy, 4th Edition, ELBS, UK, 1994.
3. R.M. Silverstein, G.C. Bassler and T.C. Morrill, Spectrometric Identification of organic compounds, 6th Edition, John Wiley, New York, 2005.

Reference Books:

1. E.L. Eliel and S.H.Wiley, Stereochemistry of carbon compounds. John Wiley & Son, Inc 2003.
2. V.M.Potapov, Stereochemistry, MIR Publisher, Moscow, 1999.
3. H.Kagan, Organic Stereochemistry, Edward Arnold, London, 2001.
4. E.L. Eliel, N.L. Allinger, S.J. Angyal and G.A. Morrison, Conformational Analysis, Interscience, New York, 2004.
5. P. Wetirli Marchand, Interpretation of ^{13}C NMR Spectra, VCH Weinheim, UK, 1987.
6. Atta-ur Rahman, Nuclear Magnetic Resonance, Springer Verlog, New York, 1990.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S2PC2**
Semester	**: II**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core - 6**	**No. of Credits**	**: 4**
Title of the Paper	**: Inorganic Chemistry-II**		

Course Objectives: Total: 60 Hours

- To study the solid state elaborately.
- It deals with polymeric inorganic compounds.
- It gives a thorough understanding on analytical Chemistry.
- It deals with the techniques like Colorimetry, Fluorimetry, AAS, TGA, DTA, Chromatography and cyclic voltammetry.

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UNIT I SUPRAMOLECULAR CHEMISTRY (12 Hr)

Definition, Nature of supramolecular interactions- Non - Covalent interactions, Host - guest interaction, Molecular recognition, Types of recognition, Self- assembly. General properties of Supra molecular complexes- Molecular Library- **Transition metal mediated supramolecules-** Directional bond approach- Molecular triangles (Pd and Pt)- Molecular squares (Pd, Pt and Re)- Molecular rectangles-(Pd, Pt, Cu and Re) Molecular Cages (Pd, Pt and Re).

UNIT II SOLID-STATE CHEMISTRY (12 Hr)

Packing of atoms and ions- close packing arrangements-HCP,CCP and BCC lattice. Radius ratio rules- Limiting radius ratio. Structure of typical lattices such as calcite, cesium chloride, Nickel arsenide, Fluorite, Antifluorite, Cadmium iodide, Perovskite, Spinels (normal and inverse**). Bragg's equation- problems involving Bragg's equation. Crystal structure determination- X-ray diffraction study, Electron and Neutron diffractions.**

Crystal defects- point – Schotky and Frenkel defect - line and plane defects- colour centers- non-stoichiometric Compounds- effect of imperfections and non- stoichiometry on physical properties-types of solids-electronic structure of solids- free electron and band theories.

Electrical conductivity and superconductivity – High temperature superconductivity-types of Semi-conductors-thermoelectric power and Hall effect- PN junction- transistors- optical properties- photovoltaic effect- semiconductors in solar energy conversion.

UNIT-III CAGES AND METAL CLUSTERS- POLYMERIC INORGANIC COMPOUNDS (12 Hr)

Electron deficient compounds: Borane and carboranes- Synthesis, structure and bonding (VBT and MO approach)-bonding –topological treatment-wades rule –styx numbers. **P-N HETEROCYCLICS**- Phosphonitrilic compounds: Synthesis, Structure and bonding.

S-N HETEROCYCLICS:

Synthesis, structure and bonding in Binary sulphur nitrils, S-N cations and anions, cyclic S-N compounds, S-N halogen compounds.

METAL CLUSTERS

Synthesis, structure and bonding in Poly anions of vanadium, chromium, Molybdenum and tungston. Hetero poly anions of molybdenum and tungsten.

UNIT-IV ANALYTICAL CHEMISTRY-1 (12 Hr)

Principles and practice of complexometric estimations - Spectro analytical methods:- Principles and applications of colorimetry and spectro photometry, fluorimetry, nephelometry and turbidimetry-emission and atomic absorption spectroscopy (AAS) and atomic fluorescence spectroscopy.

UNIT-V ANALYTICAL CHEMISTRY-II (12 Hr)

Instrumentation and applications of Cyclic Voltametry, Thermogravimetry, Differential thermal analysis and differential scanning colorimetry, Chromatography: GC, HPLC and Ion Exchange Chromatographic techniques.

Text book:

1. **D.A.Skoog and D.M.West,** Fundamentals of Analytical Chemistry, Holler Saunders college publishing,USA.VI Edn., 1998.
2.. **F.A. Cotton and G. Wilkinson**, Advanced Inorganic Chemistry, Wiley-Interscience publications, John Wiley & Sons, V Edn.,New Delhi, 1988.
3. **Purcell K.F. and Kotz J.C., Saunders**, Inorganic Chemistry, Philadelphia, 1977.
4 . **H.G.Heal**, The Inorganic Heterocyclic Chemistry of Sulphur, Nitrogen and Phosphorus, Academic press, New York , 1980.
5. **J.D.Woolings**, Non Metal Rings, Cages and Clusters, John Wiley and sons, New York, 1989**.**
6. **H.V. Keer**, Principles of the Solid State, Wiley Eastern Ltd., 1993.
7. **Walter E. Harris and Byron Kratochvil**, An Introduction to Chemical Analysis, Saunders Golden Sunburst Series, Philadelphia,1982.
8. **Galen W. Ewing**, Instrumental Methods of Chemical Analysis, Mc Graw Hill International Editions, V Edn., New Delhi, 1987.
9. B.K. Sharma, Instrumental Methods of Chemical Analysis, GOEL Publishing House, 12th Reprint., New Delhi, 1993.

REFERENCE BOOKS:

1. **A.I.Vogel,** Textbook of Quantitative Chemical Analysis, ELBS Longman Singapore Publisher Pte Ltd., Singapore.V Edn., 2002.
2. **J.E.Huheey**, Ellen A.Keiter,Richard L.Keiter, Inorganic Chemistry, Pearson Education (Singapore) Pte.Ltd., IV Edn., Delhi, 2004.
3. **I. Azaroff** , Introduction to Solids, Tata McGraw hill, New Delhi, 2004.
4. **Wahid U. Malik, G.D. Tuli and R. D. Madan**, Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi, 2006.
5. **William W. Porterfield**, Inorganic Chemistry, II Edn.,Elsevier,New Delhi, 2005.
6. **A.G. Sharpe**, Inorganic Chemistry, III Edn., Addition – Wesley Longman, UK 2004.
7. **K. Chakrabarthy**, Solid State Chemistry, New Age International Publishers, (P) Ltd., 2005.
8. **Bradley J. Holliday & Chad A. Mirkin**, Strategies for the Construction of Supramolecular Compounds through Coordination Chemistry- Reviews , Angew. Chem. Int. Ltd., Ed., 2001, 40, 2022-2043., ~CHEMIE@WILEY-VCH

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry(Spl)**	**Code No**	**: S2PC3**
Semester	**: II**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core Paper - 7**	**No. of Credits**	**: 4**
Title of the Paper	**: PHYSICAL CHEMISTRY-II**		

Course Objective: **Total:60 Hr**

To understand the various concepts involved in electrochemistry and to have a detailed study on statistical thermodynamics. This course will also focus on the various approximation methods involved in quantum mechanics.

UNIT-I **(12 Hr)**

ELECTROCHEMISTRY-I

Theory of strong electrolytes -Interionic attraction theory- Debye – Huckel theory of strong electrolytes - Debye-Huckel model of ionic atmosphere–Debye–Huckel Onsager equation-derivation, verification and modifications- Debye – Falkenhagen effect and Wien effect - Electrical double layers – formation – Structure of electrified interfaces – Stern model.

Debye Huckel limiting law- extension- Huckel Bronsted equation - Determination of activity coefficients using Bronsted equation – Applications of conductivity measurements – Nernst equation and its significance – Reversible and irreversible cells - Electrodes – SHE – Calomel – Glass electrode – Platinum electrode – Glassy carbon electrode – ion selective electrode and measurement of pH.

Text Books:

1. J. O. M. Bokris and A. K. N. Reddy, Modern Electrochemistry, Vol I, Plenum Press, New York, 1978.
2. Dr. Crow, Principles and Applications of Electrochemistry, Chapman Hall, UK, 1988.
3. R. Venkataraman, K. Rengarajan and P. S. Raghavan Electrochemistry, First edition, 2007
4. J. O. M. Bokris and A. K. N. Reddy, Modern Electrochemistry Vol II Plenum Press, New Delhi, 1978.

Reference Books:

1. L. Antropov, Theoretical electrochemistry, MIR Publications, New Delhi, 1999.
2. S. Glasstone, An Introduction to Electrochemistry, Von Nostrand Co. Inc., Toronto, 2002.

UNIT-II **(12 Hr)**

ELECTROCHEMISTRY-II

Over voltage- Theories of over voltage- applications of over voltage- electrode processes - Kinetics of electrode processes - Butler-Volmer equation- Tafel equation- corrosion- principles of electrochemical corrosion – dry and wet corrosion and its mechanism – Pilling-Bedworth rule. Types of corrosion- galvanic, aeration, stress, pitting corrosion and passivity – factor influencing corrosion – corrosion control- cathodic production - corrosion inhibitors.

Principles of Polorography - Cyclic Voltametry –quasi – reversible – irreversible voltamogram – electrochemical energy conversions-Nickel Cadmium, lead acid battery. Fuel cells – H_2 - O_2 Fuel cell – methyl alcohol fuel cell.

Text Books:

1. J. O. M. Bokris and A. K. N. Reddy, Modern Electrochemistry Vol II Plenum Press, New Delhi, 1978.
2. Dr. Crow, Principles and applications of Electrochemistry, Chapman Hall, UK, 1988.

Reference books:

1. L. Antropov, Theoretical electrochemistry, MIR Publications, New Delhi, 1999.
2. S. Glasstone, An Introduction to Electrochemistry, Von Nostrand Co Inc., Toronto, 2002.

UNIT-III **(12 Hr)**

STATISTICAL THERMODYNAMICS-I

Need for statistical thermodynamics- Definition of state of a system- assembly- ensemble- canonical and micro canonical ensembles- phase space- microstates- probability and distribution. Boltzmann distribution law- derivation- partition functions – Translational, rotational, vibrational, and electronic partition functions. Thermodynamic properties from partition functions for energy, heat capacity, enthalpy and entropy, Helmholtz free energy, Gibbs free energy, pressure and chemical potential. Sackur-Tetrode equation- thermodynamic properties of monoatomic gases.

Text Books:

1. S. Glasstone- Thermodynamics for Chemists, Eastern Wiley Publication, 2002.
2. Lee, Sears and Tercotte, Statistical Thermodynamics- Addision Wesley Publishing Co., London – I Edition, 1973.

Reference Books:

1. M. C. Gupta – Statistical Thermodynamics – Wiley Eastern limited, New Delhi- 1993.
2. J. C. Kuriakose and J. Rajaram – Thermodynamics III edition, Shoban lal Nagin Chand, New Delhi, 1999.

UNIT-IV **(12 Hr)**

STATISTICAL THERMODYNAMICS-II

Quantum statistics-Fermi-Dirac and Bose-Einstein Statistics derivations-Application of Fermi-Dirac statistics to electron gas in metal – average energy of electron in metals. Application of Bose-Einstein statistics to photon gas – Planck's radiation formula-Derivation of Rayleigh-Jeans law-Stefan Boltzman equation.

Population inversion-negative absolute temperature -heat capacity of diatomic gases- Einstein's theory and Debye's theory of heat capacities of solids- third law of thermodynamics and statistical entropy - hydrogen ortho and para nuclear states. ***Reference Books***

No: 1 and 2 given in Unit-III

UNIT –V **(12 Hr)**

Approximation methods, application of SWE to many electron systems.

Necessity for approximation methods- Variation methods for the Hydrogen atom – Perturbation (first order) method to Helium atom - Slater determinant wave function- secular determinant – Hartree – Fock self consistent field method to Helium atom – HMO bielectron theory of Ethylene and Butadiene.

Text Books:

1. A. K. Chandra- Introductory Quantum Chemistry-3rd edition Tata McGraw-Hill Publishing Co, New Delhi, 1988.
2. D.A.Mc Quarie , Quantum Mechanics, Oxford University press, Oxford, 1983.
3. R.K. Prasad, Quantum mechanics,

Reference Books:

1. Levine , Quantum Chemistry, 6th Edition, Prentice-Hall, New Delhi, 2006.
2. H.W. Hanna, Quantum Mechanics in Chemistry-Benjamin –Cummiza London Publishing Company, New Delhi, 1993.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc.,Chemistry (Spl)**	**Code No**	**: S2PC4 (E1)**
Semester	**: II**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: MAJOR ELECTIVE -I**	**No. of Credits**	**: 5**
Title of the Paper	**: C-PROGRAMMING: FUNDAMENTALS AND APPLICATIONS IN CHEMISTRY (Optional 1)**		

OBJECTIVE: **Total:60 Hour**

- To have an Overview of C-Programme.
- To comprehend the basic ideas of Operators, Data input and Output.
- To know about Decision Making , Arrays, and Functions
  And to understand Applications of C in Chemistry

UNIT-I Introduction and overview of C (12 Hr)

Introduction – Importance of C-structure of C-programs- Simple programs-style of the language.

Characters–Keywords, Variables and parameters-Data types-Constants-Declaration of and assignments of values to variables.

Operators-Arithmetic, Relational, Logical, assignment, Increment and Decrement, Conditional and bitwise operators-Special operators.

Expressions- Arithmetic - Evaluation of expression- Procedure of arithmetic operators-Library functions.

UNIT-II Data input and Output (T: 6 Hr + P: 6 Hr)

Character input- The getchar function – Character output- The putchar function – Entering input data- the Scanf function-Writing output data- The printf function- Formatted input and output data-the gets and puts functions-preparing and running a complete program.

Decision making and branching

Decision making with IF statement –simple IF statement-the IF…ELSE statement-Nesting of IF…Else statements – The ELSE IF ladder –The Switch statement – The ?: operator – the GOTO statement.

UNIT-III (T: 8 Hr + P: 4 Hr)

Decision making and Looping:

The WHILE statement – The DO statement-The FOR statement – Jumps in loops.

Arrays:

One dimensional array –Two dimensional arrays –Initializing two dimensional arrays-Multidimensional arrays.

User defined functions

Need for user–defined functions – A multifunction program – The form of C functions - Return values and their types- Calling a function –Category of function- No arguments and no return values –Nesting functions- Recursions- The scope and life time of variables in function.

UNIT-IV Applications of C in Chemistry-I (T: 3 Hr + P: 9 Hr)

Explanation of the formulae, equations and programs to solve the following problems in chemistry:

1. Calculation of Molecular weight of Organic Compounds.
2. Calculation of pH.
3. Determination on First Order rate constant for the given reaction
4. Evaluation of lattice energy using
   i). Born- Haber Cycle
   ii). Born –Lande equation
5. Computing ionic radii- Lande's method and Paulings method
6. Calculation of Normality, Molarity and Molality of a given solution
7. Converting Kelvin to Celsius temperature and vice versa.
8. Determination of enthalpy of a given solution
9. Evaluation of Cell constant
10. Calculation of energy of Hydrogen atom spectral lines.

UNIT-V: Applications of C in Chemistry-II (T: 3 Hr + P: 9 Hr)

Explanation of the formulae, equations and programs to solve the following problems in chemistry:

Organic Chemistry:

3. Use of Recursive functions to calculate the number of π Resonance structures for an organic conjugated system using
   res - str = n! / ((n/2)! * ((n/2) + 1)!)
4. Empirical formula of Hydrocarbons and other Organic compounds.

Inorganic Chemistry:

1. Array manipulation to balance the chemical equations.
2. Half life and average life periods of radioactive nuclei.
3. Binding energy of nucleus.
4. Program to get output as First ten elements of Periodic Table with their Name, Symbol, Atomic number and Atomic Weight.

Physical chemistry:

1. Calculation of RMS, average and MPV of gases.
2. Solving Quadratic equation to evaluate the Equilibrium constant for the reaction
   $H_2 + I_2 \quad 2HI$
3. Illustrate use of Loop to calculate the NMR frequency for a nucleus with Spin ½
4. Mean activity coefficient of an Electrolyte (KCl)

TEXT BOOK

1. **E. Balagurusamy**, Programming in ANSI C, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 3rd Edn., 10th Reprint, 2005.

REFERENCES:

1. **Brian W. Kernighan & Dennis M. Ritchie**, The C Programming Language, Prentice Hall of India Private Limited, New Delhi, 2nd Edn., 2001.
2. **Byron S. Gottfried**, Programming with C, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 2nd Edn., 2001.
3. **R. Rajaram**, C Programming Made Easy, Scitech Publications, Chennai, 1999.
4. **Yeshavant Kanitkar**, Let Us C, BPB Publications, New Delhi, 3rd Edn.,1999.
5. **Yeshavant Kanitkar**, C - Projects, BPB Publications, New Delhi, 1998.
6. **K. V. Raman** , Computers in Chemistry, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 3rd Edn., 1993.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course : M.Sc., Chemistry (Spl) Code No : S2PC4 (E1)
Semester : II No. of Hrs allotted : 4 Hr/week
Paper : MAJOR ELECTIVES -I No.of.credits :5
Title of the Paper : MEDICINAL CHEMISTRY (Optional 2)

Course Objective : **Total: 60 Hour**

To introduce the concept of pharmacokinetics, pharmacodynamics drug discovery by design, QSAR, combinatorial chemistry and synthesis of drugs

Unit – I :: Introduction to Drug Design: **12 Hr**

a) ADME Properties

The pharmacokinetics phase-Adsorption-Distribution, Metabolism-Elimination-Bioavailability of drug. pharmacokinetics models, Intravascular and Extravascular administration. The use of pharmacokinetics in Drug dsign**.**

b) Pharmacodynamics - Stereoelectronic structure.

Unit II Drug Discovery by Design **12 Hr**

a) Streochemistry and Drug Design

Structurally rigid Groups –procaine, Acetylcholine. Conformation-Syn and Anti Acetylcholine, Phenyl ethanoate methiodides. Configuration-Variations in the biological activities of stereoisomers

b) Strutural –Activity –Relationship (SAR)

Changing the size and shape.Changing th degree of unsaturation. Introduction or removal of ring system. Introduction of new substituents-methyl group, Halogens, hydroxyl groups, Basic groups, carboxylic and sulphonic acid groups. Changing the excisting substituents of lead-isosteres,bioisoteres.

Unit III a)Quantitative-structural Activity-Relationship (QSAR) **12 Hr**

Partition parameters-partition coefficients(p), Lipophilic subtituents constants (π) Electronic parameters-The Hammett constants-Steric parameters-The Taft Steric parameters (Es), Molar refractivity (MR), Hansch analysis-craig plots, The toplss decision tree. Compute –aided drug design- Modelling Drug-Receptor Interaction.

b) Combinatorial Chemistry

Basic concepts-The design of combinatorial syntheses. The general technique used in combinatorial synthesis i) Solid support mthod-parrllel synthesis –Furka's mix and splt techniques-sequential chemical tagging methods-Still;s binary code Tag systemcomputerised tagging. ii) Combinaterial synthesis in solution iii) Screening and deconvolution

Unit – IV

a) Antineoplastic Agents: **12 Hr**

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer.

b) Psychoactive drugs – The chemotherapy of Mind:

Introduction, neutotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, neurochemistry of mental diseases

c) Cardiovascular Drugs and Local Antiinfective Drugs:

Introduction, Cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output.

Unit V Synthesis of Drugs 12 Hr

a) Synthesis of Antineoplastic agents

Mechlorethamine, Cyclophosphamide uracil, mustards and 6-mercaptopurine

b) Synthesis of cardiovascular drugs

Amyl-nitrate, sorbitrate, , Verapamil.

c) Synthesis of Phychoactive drugs

Synthesis of Diazepam, Chlorazepam, oxazepam, Alprazolam, Phenyltocin or Diphenylhydantoin, Barbitol, Phenobarbital.

Text Books:

1.Gringuage, Introduction to Medical Chemistry, Wiley – VCH, 2004.
2.Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed., Robert F.Dorge, 2003.
3. S.S.Pandeya and J.R.Dimmock, An Introduction to Drug Design, New Age International, 2006.
4. Burger's Medicinal Chemistry and Drug Discovery,Vol-1 (Chapter-9 and Ch- 14) Ed., M.E. Wolff, John Wiley, 2005.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill, 2006.
6. R.B.Silverman, The Organic Chemistry of Drug Design and Drug Action, Academic Press, 2006.

Reference Books:

1 D. Lednicer, Strategies for Organic Drug Synthesis and Design, John Wiley.
2 Gareth Thomas, Medicinal Chemistry, An introduction, John wiley& sons, Ltd., 2004.
3 M.L Gangwal Medicinal chemistry Lectures on Drug design and Synthetic Drugs, Student publishing House, 2007.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)

DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S2PCL1**
Semester	**: I & II**	**No. of Hrs allotted**	**: 5 Hr/week**
Paper	**: CORE PRACTICAL -1**	**No. of Credits**	**: 4**
Title of the Paper	**: Organic Chemistry Practicals**		

Course Objective: Total: 75 Hr

To develop the practical skills in analyzing a mixture of two organic substances and also in preparation of organic compounds.

ANALYSIS

Analysis of Organic mixtures : Two component Systems

(Maximum of SIX Mixtures)

Spectral identification of those organic compounds by the provided UV, IR, NMR and Mass data.

Marks **Internal - 40**

External - 60

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S2PCL2**
Semester	**: I / II**	**No. of Hrs allotted:**	**4 Hr/week**
Paper	**: Core Practical - II**	**No. of Credits**	**: 4**
Title of the Paper	**: Inorganic Chemistry Practicals**		

Course objective: Total: **60** Hr

To impart skills in both qualitative and quantitative inorganic analysis

I. COMPLEXOMETRIC TITRATIONS WITH EDTA

1. Estimation of ZINC
2. Estimation of MAGNESIUM
3. Estimation of COPPER
4. Estimation of NICKEL
   a) By Direct Method
   b) By Indirect Method

II. **SEMI MICRO ANALYSIS**

Semi micro analysis of samples containing two Familiar Cations and two Less Familiar Cations. – Maximum of Five samples.

Marks

Internal- 40 (Estimation=15, Analysis=15, Record=5, Viva=5)
External- 60

Distribution of marks for External Exam

Estimations	- 25 Marks	Analysis (20)
Analysis	- 20 Marks	Two Familiar Cations : 5+5 = 10
Record	- 10 Marks	Two Less Familiar
Viva	- 05 Marks	Cations : 5+5 = 10
Total	60 marks	

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry(Spl)**	**Code No**	**: S2PCL3**
Semester	**: I / II**	**No. of Hrs allotted**	**: 5 Hr/week**
Paper	**: Core Practicals 3**	**No. of Credits**	**: 4**
Title of the Paper	**: PHYSICAL CHEMISTRY PRACTICALS**		

Course objective: **Total:75 Hr**

To develop practical skills in various Conductometric, Potentiometric titrations, Phase diagram, Kinetics and calculation of enthalpy of solutions by Rast's micro method.

I. THERMOCHEMISTRY-enthalpy of solution by solubility method-unknown concentration.

II. ADSORPTION-adsorption of oxalic acid\acetic acid on activated charcoal-freundlich adsorption isotherm-determination of unknown concentration.

III. CHEMICAL KINETICS-

Kinetics of acid hydrolysis of an ester

Evaluation of Arrhenius parameters E_a & A (for practice only)

IV. CONDUCTIVITY EXPERIMENTS

1. Determination of cell constant-verification of Ostwald's dilution law-determination of dissociation constant of weak acid.
2. Solubility product of sparingly soluble salt.

3. Conductometric titration

a) HCl Vs NaOH Vs HCl

b) AcOH Vs NaOH Vs AcOH

c) HCl Vs NaOH Vs Mixture of acids

4. Displacement of titration

(a) NH_4Cl-NaOH, NH_4Cl

(b) NaOAC, HCl-NaOAC

(c) Quinhydrone electrode

(1) Determination of pH

(2) Dissociation constant of weak acid by e.m.f. method.

V. EMF EXPERIMENTS

A) Redox titrations:

1) KI-$KMnO_4$-KI

2)FAS-Ce^{4+}-FAS

B) Precipitation titrations;

1) KCl Vs $AgNO_3$- K_{sp} of AgCl

2)KCl Vs $AgNO_3$ Vs KCl + KI (mixture of halides)

VI. Determination of Molecular weight by Rast method

VII. Phase Diagram – Simple and Compound

VIII. Transition Temperature

IX. Critical Solution Temperature

X. Determination of Coefficient of Viscosity

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Cours : M.Sc., Chemistry (Spl) **Paper Code : S3PC1**
Semester : III **No. of hours allotted : 5 Hr/week**
Paper : Core – 8 **No. of credits : 4**
Title of the paper: Organic Chemistry - III

Course objective: **Total:75 Hour**

This paper gives a detailed information about the following topics:
(i) Usage of various reagents in organic synthesis (ii) Advanced synthetic routes for an ideal organic synthesis. (iii) Interaction of organic molecules at thermal and photochemical condition. (iv) Reactions involving molecular rearrangements.

Unit-I Reagents in Organic Synthesis (15 Hr)

Use of the following reagents in organic syntheses and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate – lithium diisopropylamide (LDA) — trimethyl silyliodide – tri-*n*-butyl tin hydride – Jones reagent – pyridinium chloro chromate – SeO_2 – peracids – DMSO – $Pb(OAc)_4$ – HIO_4 – Prevost and Woodward hydroxylation – Etard's reagent – Waker's reagent – RuO_4 – $Hg(OAc)_2$ – Oppenauer oxidation – DDQ – $LiAlH_4$, $NaBH_4$, Lawesson's reagent – Crown ethers – Thallium nitrate – Phase transfer catalysts – Birch reduction.

UNIT-II Advanced Organic Synthesis I (15 Hr)

Disconnection Approach: Importance of organic synthesis- requirement of an ideal synthesis- Planning synthesis – Synthons and types – synthetic equivalents – latent functionality – Reactions involving functional group interconversions – Reterosynthetic analysis – concept of umpolung – two group C-X disconnections and synthetic strategies 1,2-, 1,3-, 1,4-, 1,5- and 1,6-difunctionalised disconnection.

UNIT-III Advanced Organic Synthesis II (15 Hr)

Steroselective and stereospecific reactions - Chemoselectivity – Stereoselectivity- Regioselectivity
Asymmetric synthesis: Definition of enantiomeric, disatereomeric excess – analytical methods to determine ee and de – strategy and classification of methods of asymmetric synthesis – chiral substrates – Chiral auxiliaries – chiral reagents – chiral catalysts.
Chiral catalysts and chiral reagents: BINAP-ruthenium (II) Mc Murray's reagent – Mc Murray's reagent – $Ti(O\textit{i}\text{-}Pr)_4$ Mc Murray's reagent – OsO_4 and $K_2Os_2(OH)_4$ Mc Murray's reagent – Sharpless asymmetric epoxidation Mc Murray's reagent – Heck reactions – Suzuki Coupling – Sonogashira coupling – Mc Murray's reagent.

UNIT-IV Photochemistry and Pericyclic reactions (15 Hr)

General principles – orbital symmetry considerations related to photochemical reactions, thermal versus photochemical reactions – principles of energy transfer – photochemical reactions of ketones – Norrish type I and type II reactions – Paterno Buchi reaction – Dienone photochemistry – photo reduction, photochemical oxidation, Barton reaction – photochemistry of alkenes and dienes.

Pericyclic reactions

Application of symmetry to orbital interactions – selection rules (Woodward and Hoffmann rules) – Concept of con and dis rotation – Electrocyclisation, cycloaddition and sigmatropic rearrangements – cheletropic reactions – Diels-Alder Reactions: Endoselectivity and regioselectivity – Explanation of these reaction in terms of correlation diagrams approach, FMO approach and Dewar – Zimmermann approach – (PMO) Huckel-Mobius concepts.

UNIT-V Molecular rearrangements (15 Hr)

Classification – Nucleophilic, electrophilic, and radical – Mechanism of Favorski, Benzil-Benzilic acid, Bayer-Villiger, Wagner-Meerwin rearrangement, Carbanionic rearrangements, Stevan's rearrangement, Sommelet-Hauser, Cope, aza and Wesly-Moses rearrangement, Fries Rearrangement.

Acid catalyzed rearrangement – Arndt-Eistert synthesis – carbon to nitrogen migration – Hofmann rearrangement, Curtius rearrangement, Lossen rearrangement, Schmidt and Beckmann rearrangement.

Text book:

1. Jerry March, Advanced Organic Chemistry, Reaction mechanism and structure, John Wiley and sons, 4th Edition, New york, 1992.
2. S. Warren, Organic synthesis - The disconnection approach, John Wiley &
3. Sons, UK, 2004.
4. Cary and Sundberg, Advanced Organic Chemistry, Part B, Reactions and Synthesis, Plenum Press, 3rd Edition, 1990.
5. R. K. Mackei and D. M. Smith, Guide Book to Organic synthesis, ELBS, 1982.
6. I.L. Finar, Organic Chemistry, Vol. II, V Edition, ELBS, New York, 2005.
7. W. Caruthers, Some modern methods of organic synthesis, Cambridge university.
8. C.H. Depuy and O.L. Chapman, Molecular reactions and Photo Chemistry, Eastern and Economic Edition, Tata MacGraw Hill, 1975.

Reference Books:

1. Graham Solomons, Organic Chemistry, John Wiley and Sons INC, 5th Edition, 1992.
2. Michael B. Smith, Organic Synthesis, McGraw Hill, International Edition, 1994.
3. Clayden, Greeve, Warren and Wothers, Organic Chemistry, OXFORD University Press, 2007.
4. A.J. Bellamy, An introduction to conservation of orbital symmetry, Longman group Limited, 1974.
5. H. O. House, Modern synthetic reactions, Cambridge University press, 3rd Edition, 1972.
6. W. Carruthers and I. Coldham, Modern methods of organic synthesis, Cambridge University Press, 4th Edition, 2004.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S3PC2**
Semester	**: III**	**No. of Hrs allotted**	**: 5 Hr/week**
Paper	**: Core - 9**	**No. of Credits**	**: 4**
Title of the Paper	**: Inorganic Chemistry-III**		

Course Objectives: **Total:75 Hour**

- This paper deals with coordination Chemistry , lanthanides and actinides.
- It deals with the basic concept, theories , mechanism and spectra of coordination compounds..
- An emphasize is given on Separation techniques of lanthanides and synthesis of actinides.
- To introduce the basics and the advanced technology to study about the synthesis, properties, characterization and the applications of nano materials.

UNIT I COORDINATION CHEMISTRY-1 15 Hrs

Nomenclature of coordination complexes-Stereochemistry of coordination compounds: Geometrical isomerism- optical isomerism of complexes having C.N.4,6-stability constants of complexes-stepwise and overall stability constant- their determination-Jobs' continuous variation method-Chelate effect

CFT. LFT and MO theories- Influence of ligands on crystal field splitting- Octahedral and Tetrahedral splitting of "d" orbitals, CFSE. Spectrochemical series- Nephelauxetic effect– John Teller effect-site preferences. Spectral properties of complexes- Magnetic properties- Para, Dia, ferro magnetism and antiferro magnetism- **Determination of magnetic properties – Gouy's method.**

UNIT-II COORDINATION CHEMISTRY-III (INORGANIC REACTION MECHANISMS) 15 Hrs

Substitution reactions- lability-inertness- square planar substitution reactions- Factors affecting reactivity of square planar complexes- Trans effect- Theories of Trans effect- Stereo chemistry of substitution in octahedral complexes.(SN1,SN2,SNiCB)- Reactions of coordinated ligands- Acid hydrolysis- anation reactions and base hydrolysis.

Mechanism of electron transfer reactions- Outer sphere, inner sphere electron transfer reactions.- Marcus Theory and its applications.

Synthesis of coordination compounds using electron transfer and substitution reaction.

UNIT- III CHEMISTRY OF NANOSCIENCE AND TECHNOLOGY 15 Hrs

Introduction- Types of nano materials-Nanoparticles, nanotubes-Carbon nanotubes: SWCNT and MWCNT,nanowires,nanoribbons,nanorods, nano composites.

Preparation methods-Chemical vapour deposition, Sol-Gel method, Electrodeposition method, Ball milling method, Chemical reduction method, spin coating technique, Solvothermal synthesis Colloidal method, Co-precipitation method,Flame spray synthesis(Arc Plasma)-Preparation of metal oxide nanoparticles

Properties of nanoparticles- Optical, mechanical, magnetic,electrical, thermal properties.

Characterisation Techniques like SEM,TEM,AFM, XRD, UV-DRS, B.E.T analysis , DLS, PL -Applications of Nanoparticles.

UNIT – IV PHYSICAL METHODS IN INGORGANIC CHEMISTRY-I 15 Hr

Electronic spectra : selection rules – polarization – splitting of spectral terms – Orgel and Tanabe-Sugano diagram. – Effect of distortion and spin orbit coupling. Evaluation of 10 Dq and beta for octahedral Ni and tetrahedral Co complexes.

IR and Raman spectra : symmetry of normal vibrations – fundamental vibrations – selection rules – applications of IR and Raman. selection rules to structure determination – IR spectral studies of carbonyl compounds.

Nuclear magnetic resonance : Application of chemical shift and spin coupling to structure determination using multiple NMR (H,P,F) chemical exchange, dynamic processes in inorganic and organometallic compounds-kinetics of rearrangement reaction and metal chelates.- Fluxional NMR of metal carbonyls and allyl complexes – paramagnetic NMR and contact and pseudo contact shifts.

NQR- Basic theory, principles and applications.

UNIT-V LANTHANIDES AND ACTINIDES 15 Hrs

a) Lanthanides:-

Occurrence- Separation techniques (Fractional crystallisation, precipitation, ion-exchange, solvent-extraction and thermal decomposition- Selective reduction and oxidation)- Electronic configuration- Oxidation states, Lanthanide contraction- Spectral and Magnetic properties- Lanthanides as shift reagents in NMR- uses of lanthanides and their compounds- position in the periodic table.

b) Actinides:-

Synthesis of elements- Extraction of Th and U and Pu- electronic configuration and oxidation states, spectral and magnetic properties- position in the periodic table.

TEXT BOOKS:

1. **F.A. Cotton and G. Wilkinson**, Advanced Inorganic Chemistry, Wiley-Interscience publications, John Wiley & Sons, V Edn.New York. 1988.
2. **R.S. Drago, Van Nostrand and Reinhold**, Physical methods in Chemistry, 1976.
3. **Purcell K.F. Kotz J.C. Holt Saunders**, Inorganic Chemistry, Philedelphia, 1977.
4. **Gurdeep R. Chatwal & M. S. Yadav**, Coordination Chemistry, Himalaya Publishing House, I Edn.,1993.
5. **Nakamoto, Kazuo**, Infrared and Raman Spectra of Inorganic and coordination compounds, IV edition, John Wiley and Sons,New Yark,1986.
6. **Figgis, B.N.,** Introduction to Ligand Fields, Interscience, Wiley Eartern Ltd., I Edn., New Delhi.1964.
7. **Raymond Chang**- Basic principles of Spectroscopy, Mc Graw Hill,New Delhi. 1971
8. **B.P.Straughan and S. Walker**- Spectroscopy Vol.3, Chapman and Hall 1976.
9. **D. Banerjea** , Coordination Chemistry , Tata McGraw- Hill Publishing Co. Ltd., 1993.

REFERENCES:

1. **Douglas and McDaniel**, A Concise of Inorganic Chemistry , - Oxford and IBH Publishing company (P)Ltd., New Delhi. 2002.
2. **E. Huheey** , Ellen A.Keiter,Richard L.Keiter, Inorganic Chemistry, IV Edn., Pearson Education (Singapore) Pte.Ltd., Delhi, 2004.
3. **Wahid U. Malik, G.D. Tuli and R. D. Madan**, Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi, 2006
4. **William W. Porterfield** , Inorganic Chemistry, Elsevier,II Edn., New Delhi.2005.
5. **A.G. Sharpe**, Inorganic Chemistry, Addition – Wesley Longman,UK III Edn., 2004.
6. **Gary L. Miessler and Donald A. Tarr**, Inorganic Chemistry, Pearson Education, Inc., 3rd Edn.,New Delhi. 2004.
7. **D.N. Sathyanarayana**, Electronic Absorption Spectroscopy and Related Techniques, Universities Press(India) Limited, 2001.
8. **Mick Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons and**
9. **Burkhard Raguse:** Nano technology-Basic Science and Emerging Technologies, Overseas Press India Pvt. Ltd. New Delhi-First Edition-2005.
10. **Mark Ratner and Daniel Ratnar**, Nanotechnology-A Gentle Introduction to the Next Big Idea, Pearson Education Inc., US and UK, 2003

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry (SPl)**	**Code No**	**: S3PC3**
Semester	**: III**	**No. of Hrs allotted**	**: 5 Hr/week**
Paper	**: Core - 10**	**No. of Credits**	**: 4**
Title of the Paper	**: PHYSICAL CHEMISTRY-III**		

Total:75 Hour

Course objective:

To understand the symmetry of molecules through the study of group theory and to have an advanced knowledge about the principle and application of various spectral techniques.

UNIT – I **`15 Hrs**

Mathematical group – definition – four cardinal properties – cyclic group – commutative property and abelian group – group multiplication table, sub group – similarity transformation and class of group – symmetry of molecules – symmetry elements – symmetry operations – relationship between symmetry operations of a molecule and a mathematical group – point group of a molecule and its deduction – matrix representation of a symmetry operations : **E, C_n, σ_v, i, S_n** – character of a symmetry operation – representation of a group – matrix representation – character representation – similarity transformation – block factorization

Reducible and irreducible representations – the great orthogonality theorem – results of great orthogonality theorem – construction of character table for **C_{2v}, D_{3h}, T_d** – projection operators – direct product representation.

UNIT – II **Applications of group theory** **15 Hrs**

Prediction of symmetries of atomic orbitals, linear vectors, rotation vectors – symmetries of tensor like properties (α & g) – Application to predict the selection rules for IR / Raman activity of normal modes of H_2O and NH_3 – selection rules to predict allowed and forbidden transition in UV-Visible electronic transition for example formaldehyde and behaviour of hamiltonian operator – Prediction of orbitals and hybridization for the molecules BF_3 and CH_4 – HMO energy calculation for ethylene and butadiene.

TEXT BOOKS: **(UNIT I & II)**

1. F.A. cotton – chemical applications of group theory – 3rd edition – wiley eastern Ltd., UK – 1971.
2. V.Ramakrishnan and M.S.gopinathan – group theory in chemistry, vishal publication – Newdelhi, 1988.
3. Veera Reddy, K. symmetry and spectroscopy of molecules, New age International (p) Ltd., 1998.

REFERENCE BOOKS: **(UNIT I & II)**

1. K.V. Raman - Group theory and its applications of chemistry, TMH publishing company Ltd., New Delhi, 1990.

UNIT – III **SPECTROSCOPY - I** **15 Hrs**

Absorbtion and emission of emr – LASER — Interaction of emr with matter – Einstein coefficients. Microwave, IR and Raman spectroscopy of diatomic molecules – determination of molecular paramaters – vibrational spectra of polyatomic molecules – IR and Raman active modes – overtone and combination bands – Fermi resonance – group frequencies and coupling interaction.

REFERENCE BOOKS:

1. G.M. Barrow, Introduction to molecular spectroscopy, McGraw-Hill, Newyork.
2. G.M.Banwell, Fundamentals of molecular spectroscopy, IV Edn., TMH company Ltd.
3. R.Chang, Basic principles of spectroscopy, McGraw-Hill, 1971.
4. K.Veera Reddy, Symmetry and spectroscopy of molecular, New Age International (p) Ltd. 1998.
5. B.P.Straughan and S.Walker, spectroscopy – Vol.-2, Chapman and Hall, 1976.

UNIT – IV SPECTROSCOPY - II 15 Hrs

Electronic spectra of diatomic molecules – molecular quantum numbers – dissociation energy calculations – Birge – sponer extrapolation technique, pre-dissociation spectra – charge transfer spectra – Fortrat diagram – electronic spectra of molecules – absorbance – oscillator strength.

Photoelectron spectroscopy – basic principles, spectrum, X-ray PES, (ESCA) – vibrational structure – koopman's theorem – PES of argon, oxygen and nitrogen.

REFRENCE BOOKS:

1 to 3 as given in **UNIT III**

B.P.Straughan and S.Walker, Spectroscopy Vol.3, Chapman and Hall, 1976.

UNIT – V SPECTROSCOPY - III 15 Hrs

ESR spectroscopy – principle, g-factor, experimental method, spectrum, fine and hyperfine structures and applications (H-atom, CH_3 radical, *p*-1,4 benzosemiquinone radical anion, naphthalene anion, Tempol)

NQR spectroscopy – quadrupole movement, coupling constant, quadrupole transition-electric field gradient and molecular structure ($_7N^{14}$, $_5B^{11}$, $_{17}Cl^{36}$)

Mossbauer spectroscopy – recoilless emission and resonance absorbtion, experimental method, isomeric shift and electric quadrupole splitting in Fe^{57}.

REFERENCE BOOKS:

1. R.Chang, Basic principles of spectroscopy, McGraw-Hill, 1971.
2. R.S.Drago, Physical methods in chemistry, Saunder college publishing, 1999.
3. B.P.Straughan and S.Walker, spectroscopy Vol.I, Chapman and hall, 1976.

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course : M.Sc., Chemistry(Spl) **Code No : S3PC4 (E2)**
Semester : III **No. of Hrs allotted : 5 Hr/week**
MAJOR ELECTIVES - 2 **No. of Credits : 5**
Title of the Paper : COMPUTER APPLICATIONS IN CHEMISTRY (Optional 1)

Course objectives: **Total:75 Hour**

To understand the concepts in internet and E-mail.
To have an understanding on HTML and JAVA APPLET and also to emphazise on their applications in chemistry.
To understand Chemistry related software and their applications

UNIT-I: INTERNET AND E-MAIL T: 10 + P: 5 Hrs

INTERNET: Introduction- History- Importance of the Internet- Internet Access- Dial-Up connection, Direct connection and equipments –- Internet protocol(TCP/IP,FTP HTTP, TELNET and WAP)-Internet addressing – Domain Name-Mail address-Uniform Resource Locator(URL)-Web Browsing- Searching the Web- Search Engines(Yahoo, Google)- Intranet

Searching and utilizing Popular websites in Chemistry. On line literature survey- accessing of e-journals. Preparing articles for e-publications. Online structure drawing- Collection of spectral data using databases.

ELECTRONIC MAIL: Introduction-Working of E-Mail - Word processor for E-Mail- Mailing Basics – Composing and sending of an E-Mail- Address Book – Signature- File Attachments-Customizing your Mail program –Advantages and Disadvantages of E-Mail - Tips for effective E-Mail use- Smile keys.

UNIT- II: HTML ***T: 8 + P: 7 Hrs***

HTML - Need- Structure of HTML Document- HTML Tags- Horizontal line Tags- Background and Text color Tags- Font Tags- MARQUEES Tags- Adding pictures - Ordered and Unordered Lists- Creating Links- Construction of Periodic Table with required data for first ten elements- Frames – Developing and hosting of Web Pages for a given molecule / chemical.

JAVA APPLETS: - Simple and Java applets with graphics- Applications of applet to draw 2D and 3D view of molecules.

UNIT-III: APPLICATIONS OF DESK TOP SOFTWARE IN CHEMISTRY-I
T: 8 + P: 7 Hrs

Chemical drawing programs:- Chem- Draw and Chem 3D

Introduction- Tool Pallets- Construction of the molecule using Chem Draw- Tools-Manipulating a molecule-Model display- Display type- Structure displays- Molecular Surface display- NMR simulation and interpretation- Naming IUPAC- Structure from Name and Name from Structure-Computational Concepts: - Computational methods: - Potential energy surface, geometry Optimizations property (calculations)-Molecular Mechanics Theory in brief - Animations- Difference between Chemdraw and Chem 3D.

UNIT-IV: APPLICATIONS OF *SHELX PROGRAM* IN CHEMISTRY-II

T: 5 + P: 10 Hrs

Basics of Crystals- Symmetry and operations- Seven Crystal systems- Bravais lattices- X-RayDiffractometers- Unit cell parameters- X-ray data- Deduction of Space group- - Structure solution and refinement using SHELX- Structure building using PLATON- H-Bonding.

ORIGIN software- Importing of ASCII file- plotting-manipulation of plots-multiple plots- Linear regression, Multi-regression.

UNIT-V: APPLICATIONS OF *RASMOL* and *MATLAB* IN CHEMISTRY-III **T: 8 + P: 7 Hrs**

RASMOL: -

Introduction- User commands– Identification of disulfide-bridges and visualization of :- hydrophobic and polar residues, the distribution of polar and non polar amino acids, side chain of carboxylate and amine , the different structural motives like α-helix, β-sheet and β - turn, the amino acids bound to Zn, active site of carboxypeptidase A, the environment of the active center.

MATLAB: -

Introduction-advantages- getting started- windows for workspace, command interpretation, command history and current history- Addition- Use of sine and Cosine of angles(pi)- variable 'ans'- order of operations- significant decimals- Representation of matrix- getting transpose of a matrix- display of images- saving images-solving linear equations(case m=n only).

Text Books:

1. . **Alexis Leon and Mathews Leon**. Fundamentals of Information Technology Leon TECH World, UBS Publishers & Distributors Ltd., 1999.
2. **E. Balagurusmy**, Programming with Java- A Primer, , Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2nd Edn., 15th Reprint-2003
3. **C. Xavier**, World wide web design with HTML, , Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2nd Reprint 2000.

REFERENCE BOOKS:

1. **Margaret Levine Young**, Internet- Complete Reference, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2001.
2. **Barbara Kassev**, Using the Internet, EE edition, New Delhi, IV Edition, 1998.
3. **Alexis Leon and Mathews Leon**, Internet for Everyone, Leon TECH World, UBS Publishers & Distributors Ltd., 2000.
4.. **John Zukowski**, Mastering Java 2, BPB Publications, New Delhi, 2000.
5 **Patrick Naughten**, The Java Hand Book, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 11th Reprint 2002.
6. **Herbert Schildt**, Java 2- The Complete Reference, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 4th Edn., 2001.
7. **Holzner, John Zukowski**, Java 2 Complete: Steven BPB Publications, New Delhi, 1st Indian Edn., 1999.
8. **Harley Hahn**, The Internet Complete Reference, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2nd Edn., 2001.
9 Chem Draw & Chem 3D –Manual
10. Shelx, Rasmol and MATLAB- Manuals.

REFERENCES in the NET

1.http://SCS 99.unige. Che/eng/toc.html
2.http://hackberry.chem.niu.edu: to/o/webpage.html
3.http://java.Sun.Com/applet/applets/chemical Models/index.html
4.http://ccl.osc.edu/chemistry.html
5. http://www.umass.eud/microbio/rasmol/
6. http://www. Mdli.com/cgi/dynamic/welcome.html/ (for CHIME similar to Rasmol)

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course : M.Sc., Chemistry(Spl) Code No : S3PC4 (E2)

Semester :III No. of Hrs allotted : 5

Paper : MAJOR ELECTIVES -2 No. of Credits : 5

Title of the Paper : ADVANCED ORGANIC SYNTHESIS (Optional 2)

Course Objective: Total:75 Hours

To impart knowledge in Stereoselective and retrosynthetic analysis

To understand about the guest-host interaction.

To gain scientific and technical knowledge in Green chemistry and biotransformation

UNIT-I REETEROSYNTHETIC ANALYSIS (15 Hr)

Synthetic Strategy of the following target molecules: longifolene-juvabione-jasmone- 5-hexenoic acid-trans-9-methyl I-decalone- bicyclo (4,1,0) heptan-2 one- α-onocerin-isonootketone.

UNIT-II BIOGENESIS OF ALKALOIDS,TERPENOIDS & FLAVONES: **(15 Hr)**

Alkaloids(pyridine,phenanthrene and indole type)-nicotine-gramine-harmine-morphine-codine-terpenoids of classes with examples Lanosterol & Cholesterol from squalene-coumarins-carbohydrates-fructose-6-phosphate-xylose-5-phosphate-ribulose-5-phosphate-sucrose-amylose and amylopectin-flavones-proteins

Terpenoids: Geranyl diphosphate-Geraniol-Farnesol–Camphor-limonene-citronellol-caryophyllene(Corey methods) – santonin

UNIT-III BIOSYNTHESIS OF FATTY ACIDS (15 Hr)

Introduction-acetate pathway-acetyl co-enzyme-A-biosynthesis of fatty acids-malonyl co-A-malonyl ACP-Acyl ACP-Acetoacetyl Co-A- biosynthesis of unsaturated fatty acids Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives 3)Mevalonic acid pathway : Biosynthesis of mevalonic acid.

UNIT-IV: DYES (15 Hr)

Introduction, various methods of dyeing, classification of dyes, nitroso dyes,Azodyes,-Fast green, Methyl Orange, Methyl Red, Fast Red, tripheylmethane dyes-Malachite green, Rosaniline, Aniline blue, Crystal violet, Xanethene dyes-Fluorescein,Rhodamine B, Anthroquinone dyes –Alizarin – Preparation and uses.

UNIT – V : BIOTRANSFORMATION (15 Hr)

Advantages and disadvantages of Biocatalysts – Biocatalytic application. Hydrolytic reaction, reduction, oxidation, peroxidation – addition and elimination Reaction. Formation of C-C bond-glycosyl transfer reactions - Immobilisation – adsorbtion – ion binding entrapment into gels, into membranes – compartments – Micells and vesicles – modified and artificial enzymes – semisynthetic enzymes – catalytic antibodies.

Text Books:

1. R.K. Mackie, D.M. Smith and R.A.Aitken, Guide book to Organic synthesis, Longman group, UK, 2n edition, 1990.
2. S.Warren, Organic synthesis, The disconnection approach, John Wiley & Son, 1997.
3. C.Daniel Gutsche, Calixarent, Royal Society of Chemistry, Cambridge, 1989.

References:

1. Organic Synthesis-Robert E.Ireland - Prantice Hall of India Pvt Ltd, NewDelhi.
2. Advanced Organic Chemistry-Reaction & Synthesis-Francis A.Corey & Richard J.Sundberg-V Edition - Springer.
3. Organic Chemistry-Francis A.Corey & Robert M.Giuliano-Tata McGraw-Hill Edition
4 Organic Chemistry-Natural Products Volume II-Dr.O.P.Agarwal-Goel Publishing House.
5. Chemistry of Carbocyclic Compounds-Azhuwalia
6. Pharmaceutical,Medicinal and Natural Product Chemistry-P.S.Kalsi & Sangeetha Jagtap-Narosa Publishing House
7. Organic Chemistry-Jonathan Clayden,Nick Greeves and Stuart Warren-Second Editiion-Oxford University Press
8. Synthetic Dyes-Gurudeep Chatwal
9. Biotransformation in Organic Chemistry-Kurt Faber-A Textbook-V Edition-Springer

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., (Spl)**	**Code No**	**: S4PC1**
Semester	**: IV**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core**	**No. of Credits**	**: 4**
Title of the Paper	**: Organic Chemistry - IV**		

Course objective: **Total:60 Hour**

To kindle the synthetic aptitude among students on the hetrocycles, Green Chemistry and biologically important compounds and to have a detailed discussion on the natural products.

Unit - I CHEMISTRY OF HETEROCYCLIC COMPOUNDS (12 Hr)

Heterocyclics – Nomenclature – Compounds containing two hetero atoms: Synthesis and reactivity of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, quinoline and isoquinoline.

diazines: the chemistry of pyridazine, pyrimidine and pyrazine – Comparison of basicity of diazines Chemistry of anthrocyanins and flavonoids

Unit - II CHEMISTRY OF TERPENOIDS AND ALKALOIDS (12 Hr)

Chemistry of terpenoids: General methods of determining structure of terpenoids – α-pinene, α-cadinene, Zingiberene, Abietic acid and Heliangine.

Chemistry of alkaloids: Alkaloids and Drugs: General methods of determining structure of alkaloids – Structure elucidation of (i) Morphine (ii) Reserpine (iii) Lysergic acid.

Unit- III CHEMISTRY OF STEROIDS AND VITAMINS (12 Hr)

Chemistry of steroids : Introduction – Structural elucidation of Cholesterol – Androsterone and Testosterone (male sex hormones) – Oesterone, progesterone (Female sex hormone).

Classification of Vitamins: Nomenclature of Vitamins – Biological functions of vitamins (Synthesis not included): Vitamin A (Retinol), Vitamin-B (Thiamine), Vitamin B6 (Pyridoxine), Vitamin B12, Vitamin B2 (Riboflavin), Vitamin C, Vitamins K, D and E

Unit IV CHEMISTRY OF PEPTIDES AND NUCLEIC ACID (12 Hr)

a) Polypeptides – Classification - the peptide linkage - Structure of amino acids – 1^0, 2^0, 3^0 and quaternary structure) – Solid phase peptide synthesis (Merifield) – use of protecting groups and reagents – Structural elucidation of glutathione, thyroxin and oxytocin.
b) Nucleosides, Nucleotides and Nucleic acids – structure and synthesis of nucleosides and nucleotides – Elementary treatment on the structure of DNA and RNA

Unit – V GREEN CHEMISTRY, CARBODYDRATES AND ANTIBIOTICS (12 Hr)

Green Chemistry: Importance and principles of Green chemistry - Solid state and Solvent free organic reactions – Solid supported reagents – Microwave assisted reactions - Sonochemical approach - Reactions in ionic liquids – supercritical CO_2 medium – aqueous medium - enzymatic and electrochemical methods.

Carbohydrates: Polysaccharides: Starch and cellulose

Antibiotics: Strucural features of following antibiotics (synthesis need not to be discussed)

β-lactam antibiotics: Penicillin – Chloramphenicol – Griseofulvin

Text Books:

1. I.L. Finar, Organic Chemistry, Vol. II, V Edition, ELBS, UK, 2005.
2. S.F. Dyke, Chemistry of Vitamins, Interscience, Toronto, 1965.
3. O.P. Agarwal, Chemistry of Natural products, Vol. I and II, Himalaya Publishing House, New Delhi, 2002.
4. V.K. Ahluwalia, M. Kidwai " New trends in Green Chemistry" Second Edition, Anamaya publishers, New Delhi, 2006.
5. Gurdeep Chatwal, Organic Chemistry of natural products, Vol. I, Himalaya Publishing House 1997.
6. Morrison and Boyd, Organic Chemistry, Prentice-Hall of India private limited, New Delhi, 6th Edition.

Reference Books

1. Hermann Dugus, Bioorganic Chemistry, Springer International, III Edition, New Delhi, 2004.
2. D.L. Nelson and M.M. Cox, Lehningers' Principal of Biochemistry, W.H. Freeman and Company, New York, 5th Edition, 2008.
3. L.F Fieser and M. Fieser, Steroids, Reinhold Press, Atlanta, 1991.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S4PC2**
Semester	**: IV**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core Paper - 12**	**No. of Credits**	**: 4**
Title of the Paper	**: Inorganic Chemistry-IV**		

Course Objectives: **Total:60 Hour**

- This paper deals with Organo metallic chemistry and transition metal catalysts.
- It discusses the study of bioinorganic chemistry.
- It gives an idea about inorganic photochemistry.
- It deals with PES, EPR, Mossbauer spectroscopic studies of complexes.

UNIT –I ORGANOMETALLIC CHEMISTRY –I 12 Hr

Stability of organo metallic compounds- β hydrogen elimination- the sixteen and eighteen electron rule. Synthesis – structure and bonding in metal carbonyls ,- use of IR in the structural elucidation of carbonyl compounds– metal nitrosyls – dinitrogen complexes. π donors. Synthesis structure bonding and reactivity of carbenes, carbines, metallocenes and other aromatic cyclopolyenes – Ferrocene – bonding and structure – sigma, pi and hapto nomenclature. Arene complexes – olefin – acetylene and pi allyl complexes.

UNIT – II ORGANOMETALLIC CHEMISTRY –II 12 Hr

Catalysis involving organometallic compounds – properties of metals and ligands in homogeneous catalysis – oxidative addition and reductive elimination – hydrogen abstraction – hydrogenation of olefins – Wilkinson's catalyst – hydroformylation – oxidation of olefins – Wacker process – propylene polymerization - Ziegler natta catalyst -cyclo oligomerisation of acetylene , **butadiene-** Reppe's catalyst . **Mansanto's acetic acid synthesis-Fischer-Troppe's synthesis of Synthetic gasoline.**

UNIT –III BIO-INORGANIC CHEMISTRY 12 Hr

Essential and trace elements in biological systems – metalloporphyrins – the porphyrine ring system – chlorophyll – photosynthetic electron transfer - Electron transport sequence – biological electron transfer – electron transfer agents – cytochromes – Hemoglobin – myoglobins – and synthetic oxygen carriers – nitrogen fixation – in vivo and in vitro – copper proteins-**Metal complexes in medicine.**

UNIT-IV PHYSICAL METHODES IN INORGANIC CHEMISTRY-II 12 Hr

Photoelectron spectroscopy: Fine structure in PES. Chemical shift in Auger spectroscopy -principle and applications.

Electron paramagnetic resonance spectroscopy: Applications of hyperfine splitting and g factor to structural elucidation- Zero field splitting-Krammer's Degeneracy- EPR spectra of Cu (II) and Mn (II) in various site symmetry- covalency of metal-ligand bonding by EPR- study of dynamic processes in solids- Study of phase transition by Mn (II) – John Teller distortions in Cu (II) complexes.

Mossbauer spectroscopy: Basic principles- Doppler effect- Isomer shift- Electron nuclear hyperfine interactions- Quadrupole and magnetic interactions in the study of structure and bonding in Iron and Tin complexes and in Biological systems.

UNIT –V INORGANIC PHOTOCHEMISTRY 12 Hr

Excited states of coordination complexes – properties of excited states charge transfer and energy transfer – photochemical pathways.

Photoredox reactions of Co(III) and Cr(III) complexes – photosubstitution reactions – photoaquation, photoanation and photorearrangements - Role of TiO_2 in solar energy conversion –

Photoredox chemistry of Ruthenium bipyridyl and Ruthenium(II) poly pyridyl compounds- **Chemiluminescence reactions.**

TEXT BOOKS: -

1. **F.A. Cotton and G. Wilkinson** , Advanced Inorganic Chemistry, Wiley-Interscience publications, John Wiley & Sons, V Edn. New York, 1988.
2 **R.S.Drago**, Van Nostrand and Reinhold , Physical Methods in Chemistry 1976.
3. **Purcell K.F. and Kotz J.C., Holt Saunders**, Inorganic chemistry, Philadelphia, 1977
4.**Arthur W. Adamson & Paul D. Fleischauer**, Concepts of Inorganic Photochemistry, John Wiley & Sons. In.,New York, 1975.
5. **Nakamoto, Kazuo, Paul J. McCarthy**,Spectroscopy and Structure of Metal Chelate Compounds, IV edition, John Wiley and Sons. Inc. , New York. 1986.
6. **Wahid U. Malik, G.D. Tuli and R. D. Madan**,Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi, 2006
7. **Raymond Chang**, Basic principles of Spectroscopy - Spectroscopy, Mc Graw Hill, New Delhi, 1971.
8. **B.P.Straughan and S. Walker** , Spectroscopy. - Vol.3, Chapman and Hall ,New York,1976.
9.. **T.C.Gibbs,** Principles of Mossbauer Spectroscopy, Chapman and Hall, New York,1978.

REFERENCE BOOKS: -

1. **J.E.Huheey, Ellen A.Keiter,Richard L.Keiter** , Inorganicchemistry, IV Edn., pearson Education (Singapore) Pte.Ltd., Delhi, 2004.
2. K. Hussain Reddy, Bioinorganic Chemistry, New Age International (P) Ltd., Delhi, 2005.
3. **F. Albert Cotton, Geoffrey Wilkinson, Paul L.Gans**, Basic Inorganic Chemistry, John Wiley & Sons. Inc., III Edn.,New York, 2004.
4. **William W. Porterfield**, Inorganic Chemistry, II Edn., Elsevier,New Delhi, 2005.
5. **A.G. Sharpe**, Inorganic Chemistry, III Edn.,Addition – Weskey Longman,UK 2004.
6. **Gary L. Miessler and Donald A. Tarr,** Inorganic Chemistry, Pearson Education, Inc., 3rd Edn., New Delhi, 2004.
7. **Wahid U. Malik, G.D. Tuli and R. D. Madan**,Selected Topics in Inorganic Chemistry, S. Chand & Co.Ltd., New Delhi, 2006

THIAGARAJAR COLLEGE, MADURAI – 9.

(Re-Accredited with 'A' Grade by NAAC)
DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc Chemistry(Spl)**	**Code No**	**: S4PC3**
Semester	**: IV**	**No. of Hrs allotted**	**: 4 Hr/week**
Paper	**: Core Paper - 13**	**No. of Credits**	**: 4**
Title of the Paper	**: PHYSICAL CHEMISTRY-IV**		

Course Objectives: Total: 60Hour

To impart knowledge on the various theories of reaction rates; to understand the concepts of catalysis as well as fast, chain and explosive reactions. To explain the concepts of photochemistry, surface chemistry and polymer chemistry.

UNIT-I **(12 Hr)**

CHEMICAL KINETICS-I

Simple Collision theory- modification - Absolute reaction rate theory (ARRT) - Statistical and thermodynamics formulation - Comparison of ARRT with collision theory- Significance of entropy of activation- Relation between ΔH and Ea- Transmission co-efficient – ARRT of termolecular reactions – Unimolecular reactions - Lindemann, Hinshelwood, RRKM and Slater treatments. –Solution kinetics – ARRT of reaction in solution – Influence of ionic strength on the rates of ionic reactions (salt effects).

Reference Books:

1. K.J. Laidler, Chemical Kinetics, II Edition, Tata McGraw Hill, UK, 2005.
2. A.A. Frost and R.G. Pearson, Kinetics and Mechanism, New York, 1990.
3. F.Wilkinson, Chemical Kinetics and Reaction Mechanism, Var Nostrard Reinhold
4. Co., New York, 2000.

UNIT-II **(12 Hr)**

CHEMICAL KINETICS-II

Fast reactions-flow and relaxation techniques, Temperature Jump and pressure jump method - complex reactions – opposing, consecutive and parallel reactions. Chain reaction – kinetics and general characteristic – H_2 – Br_2 reaction, Rice – Herzfeld mechanism for decomposition of acetaldehyde & ethane – Branched chain reaction – study of H_2 – O_2 Explosive reaction- Homogeneous catalysis – acid, base catalysis.

Reference Books:

1. K.J. Laidler, Chemical Kinetics, Tata McGraw Hill, UK, 2005.
2. A.A. Frost and R.G. Pearson, Kinetics and Mechanism, New York, 1990.
3. F.Wilkinson, Chemical Kinetics and Reaction Mechanism, Var Nostrard Reinhold Co., New York, 2000.

UNIT-III **(12 Hr)**

PHOTOCHEMISTRY

Physical properties of the electronically excited molecules-radiationless transitions-Internal conversion and intersystem crossing-Stern-Volmer equation and its application-radiative transition – fluorescence, phosphorescence and other deactivation processes.

Effect of temperature on emission process- photosensitization and Chemiluminescence. - Experimental techniques in photochemistry, Chemical actinometers.

Photochemical Kinetics of H_2-X_2 reactions – Photolysis of acetaldehyde Photodimerisation of anthracene-Photoequation of $(Cr(NH_3)_5NCS)^{2+}$ and photo isomerisation of Cis-bis glycinato Pt(II). Applications of photochemistry – Solar energy conversion and storage - photo synthesis.

Reference Books:

1. Fundamentals of Photochemistry, K.K. Rohatgi-Mukherjee, Wiley Eastern Ltd., Revised edition, New York, 1999.

UNIT-IV **(12 Hr)**

SURFACE CHEMISTRY

Physisorption and Chemisorption- adsorption isotherms-Langmuirs, Freundlich and B.E.T equations- surface area determination –Gibbs adsorption isotherm. Heterogeneous catalysis- and their kinetics. Chemical reactions on solid surfaces. Mechanism & Kinetics of unimolecular and bimolecular surface reactions-Langmuir –Hinshelwood, Langmuir –Ridel mechanism. ARRT of surface reactions-Basic concepts of Micelles and Reverse Micelles.

Text Books:

1. S.Glasstone – Textbook of Physical chemistry – III Edition McMillan, Alasca, 1974.
2. F.Daniels and R.A. Alberty – Physical Chemistry – John willey and sons , UK, 1974.
3. W.J. Moore – Physical Chemistry – V Edition – Orient Longman , UK, 1972.

Reference Books:

1. A.M. Adamson – Physical Chemistry of Surfaces – V.Edition John Willey, UK, 2002.
2. K.S. Laider – Chemical kinetics – III Edition – TMH, New York, 2005.

UNIT-V **(12 Hr)**

POLYMER CHEMISTRY

Introduction of Polymers -Classification-Tacticity - Polymerisation - Addition, Co-polymerisation and Condensation polymerisation – Kinetics of polymerization-Free radical Chain polymerization-Cationic- anionic polymerization- Molecular weight determination – Osmotic pressure methods- Light Scattering method-Ultra Centrifuge and Viscosity methods.

Classification of Plastics-Thermosetting & Thermoplastic resins-Adhesives-Compounding of Plastic - Fabrication - Compression moulding, Injection moulding, Extrusion moulding and Blow moulding.

Industrially important polymers – Preparation, Properties and uses of (LDPE & HDPE), PS, polyester, acrylo polymer, Teflon, Phenolic resins, amino resins and epoxy resins, Polyvinyl acetate-composites of Resins-ABS-Conducting Polymers-Polyacetylene, Polyaniline, Inorganic polymer-Silicone and Biopolymers-cellulose.

Reference Books:

1. H.R. Allcock and W. Lampe – Contemporary polymer chemistry – Prentice Hall UK, 1991.
2. Young, Polymer Chemistry II, Chapman Hall, 2002.
3. Arora Singh, Polymer Chemistry, Anmol Publications Pvt. Ltd., 2001.

Text Books

1. F.W. Billmeyer Jr., A text book of Polymer Chemistry – III edition, John Willey and Sons, UK, 1984.
2. V. Gowarikar, et al., Polymer Science, Willey Eastern Limited, New York, 1986.
3. F. Rodriguez, Principles of polymer chemistry, Tata McGraw- Hill Publishing Co. Ltd., New Delhi, 1987.

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY

(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S4PCL 1**
Semester	**: III & IV**	**No. of Hrs allotted**	**: 5 Hr/week**
Paper	**: Major Elective**	**No. of Credits**	**: 4**
Title of the Paper	**: Organic Chemistry Practicals**		

COURSE OBJECTIVE **75 hrs**

To include the spirit of organic synthesis in senior chemistry students, to train them in the quantitative estimation of organic compounds, glucose, methyl ketones, etc. and some extraction methods and TLC analysis,

DOUBLE STAGE PREPARATION

1. p-Nitroaniline
2. p-Bromoaniline
3. 1,3,5-Tribromobenzene
4. Benzanilide
5. m-Nitrobenzoic acid
6. p-Iodonitrobenzene (III stage)
7. 2,5-dihydroxy acetophenone

   (any five preparations only)

ESTIMATION

1. Estimation of glucose – Lane and Eynon method
2. Estimation of ethyl methyl ketone
3. Separation of amino acids by thin layer chromatography (including hydrolysis of aspartame present in the sugar-free tablet)
4. Extraction of Caffeine from Tea leave using Soxhlet apparatus
5. Extraction of lemongrass oil by steam distillation
6. Isolation of curcumin from turmeric powder by column chromatography

MARKS

Internal 40 External 60

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S4PCL(E3)**
Semester	**:IV**	**No. of Hrs allotted**	**: 5 Hr/week**
Paper	**: Major Electives**	**No. of Credits**	**: 5**
Title of the Paper	**: Inorganic Chemistry Practicals (Optional-1)**		

Course objective: 75 hrs

This course mainly emphazise on developing practical skills on quantitative inorganic estimations and also in spectrometric determination of metal ions and also to focus on the preparation of inorganiccomplexes.

	ESTIMATIONS: By VOLUMETRIC METHOD			**By GRAVIMETRIC METHOD**
1.	Estimation of	COPPER	and	NICKEL
2.	Estimation of	CALCIUM	and	MAGNESIUM
3.	Estimation of	BARIUM	and	ZINC
4.	Estimation of	IRON	and	NICKEL
5.	Estimation of	COPPER	and	SILVER
6.	Estimation of	COPPER	and	ZINC
7.	Estimation of	COPPER	and	NICKEL

II PREPARATIONS (Any FIVE Estimations only)

1. Tetramminecopper(II) sulphate
2. Potassium cupricsulphate
3. Potassium trioxalatoaluminate(III)
4. Sodium nitroprusside
5. Trithioureacopper(II) sulphate
6. Pentathioureadicuprous nitrate
7. Hexathioureaplumbus nitrate
8. Nitropentamminecobalt(III)
9. DithiocyanatotetrapyridineIron(III)
10. Potassium troxalatoferrate III

(Any Five Preparations only)

Marks

Internal- 40 (Estimation= 20, Preparation= 10, Record=5, Viva=5)
External- 60 (Estimation=30, Preparation=10, Record=10, Viva= 10)

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S4PCL(E3)**
Semester	**:IV**	**No. of Hrs allotted**	**: 5 Hr/week**
Paper	**: Core practical**	**No. of Credits**	**: 5**
Title of the Paper	**: Analytical Chemistry Practicals (Optional-2)**		

Course objective: 75 hrs

This course mainly emphazise on developing practical skills on analytical chemistry in the analysis of soil, water, fertilizer, oil etc.

I SOIL ANALYSIS

Collection of soil sample – soil pH, EC – Nutrient analysis – soil N_2, P

II WATER ANALYSIS

Determination of pH, EC, COD, BOD

III FERTILIZER ANALYSIS

Analysis of Urea, Super phosphate, DAP, Determination of micro nutrient analysis using Atomic absorption spectroscopy, Flame Photometry. Determination of Zn, Ca, S.

IV ANALYSIS OF OIL

Determination of I_2 value – saponification value- acid value

V RAW MATERIAL TESTING

Analysis of cement – milk and milk products

VI INSTRUMENTAL ANALYSIS

FTIR: Recording and interpretation of FTIR spectra of organic and inorganic samples.

UV-Visible : Determination of unknown concentration of Ni^{2+}, Cu^{2+} and Fe^{2+}

VII ELECTROCHEMICAL ANALYSIS

CV and impedence measurements of ferrocyanide / ferricyanide and other redoc systems, heme solution and cells / batteries

VIII MODELLING AND SHELX

(iii) Sructure drawing, visualization and energy minimization of simple molecules using Chem Draw, Rasmol, Kinemages and Alchemy 2000

(iv) Structure solution of simple inorganic and organic molecules using SHELX.

Reference Books

1. S.M.Khopkar, Analytical chemistry, New Age International, 2002
2. A.I.Vogel, A text book of Quantitative Inorganic Analysis, Longman, 1961
3. D.G.Peters, J.M.Hayes and G.M.Hejije- A Brief Introduction to modern chemical analysis, WB Saunders, 1976.

Marks: **Internal** : 40 **External : 60**

Analysis	**= 45**
Record	**= 10**
Viva voce	**= 05**
Total	**= 60**

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: S4PCL3**
Semester	**: IV**	**No. of Hrs allotted**	**: 5 Hr/week**
Paper	**: Core Practical**	**No. of Credits**	**: 4**
Title of the Paper	**: Synthesis and Spectral Analysis**		

Course Objevtives: Total: 75 Hours

The students will be able to characterize compounds using spectrometric techniques.

I. Characterization of the following complexes by electronic and IR spectral data.
(i) Tetraammine Copper (II) sulphate
(ii) Zinc-Oxine
(iii) Nickel-DMG

II. Study the folllowing reaction using IR and UV spectra.
(i) benzophenon ---------- benzophenone oxime
(ii) acetone + benzaldehyde ---------- dibenzalacetone
(iii) salicylic acid ---------- aspirin

III. Study the Adduct formation using the spectral data.
(i) hydroquinone ---------- p-benzoquinone ---------- anthracene adduct
(ii) urea-salicylic acid

IV. Compare the spectra of the following:
(i) [Cu(NH3)4)]2+ of solution and solid-vapor process
(ii) Reaction between CuSO4 and aniline under solution and solid-vapor process

INTERNAL : 40 Marks

Assessment = 25
Record = 10
Viva = 5

40

EXTERNAL : 60 Marks

Characterization = 30
Synthesis = 15
Viva = 5
Record = 10

60

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DEPARTMENT OF CHEMISTRY
(From 2014-16 batch onwards)

Course	**: M.Sc., Chemistry (Spl)**	**Code No**	**: SPJ 8**
Semester	**: IV**	**No. of Hrs allotted**	**: 3 Hr/week**
Paper	**: Core Project**	**No. of Credits**	**: 4**
Title of the Paper	**: PROJECT**		

Course Objective: **120 Hour**

The objective is to impart to the students, the skills on developing new materials through new synthetic routes and characterization of these using different techniques including their applications. The students thus learn research methodologies along with literature survey and creativity.

Marks

External Examiner :	Viva	: 20
External Examiner	Evaluation of Project	: 40
Internal Examiner	Evaluation of Project (only)	: 40
		100

M.Phil Chemistry

THIAGARAJAR COLLEGE, MADURAI – 9.

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DEPARTMENT OF CHEMISTRY
(From 2014-15 batch onwards)

Post Graduate and Research Department of Chemistry

M. Phil., PROGRAMME IN CHEMISTRY (SF)

Objectives of the Programme:

1. To develop research aptitude.
2. To equip the students with latest concepts and techniques in chemical research.
3. To enable the students to present their research work in conferences.
4. To encourage the students to publish research papers in reputed journals.
5. To facilitate students to acquire the Ph. D degree.

M. Phil., PROGRAMME IN CHEMISTRY (SF)

SNo	Title of the Paper	Contact Hrs / Week	Total no of hrs. Allotted	Marks		Total
				Internal	External	
I	1.Research Methodology (Paper - 1)	6	90	40	60	100
	2. Course Work (Paper - 2)	6	90	40	60	100
II	1. In-depth Study (Paper - 3)	6	90	40	60	100
	2. Project (Paper - 4)	6	90	100 (Dissertation – 75; Viva - 25)	100 (Dissertation – 75; Viva - 25)	200
	Total Marks			220	280	500

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DEPARTMENT OF CHEMISTRY
(From 2014-15 batch onwards)
M. Phil., PROGRAMME IN CHEMISTRY (SF)

Paper - 1 Research Methodology

(With effect from 2014 Batch onwards)

Semester - I
Course Hours per week : 6 **1SMC1**
Total Hours per Semester: 90

Objective:

- This paper deals with the general research methods and analytical skills required to carryout chemistry research projects with the help of latest web based chemical literature using chemical databases.

Unit I - Literature Survey: 18 Hrs

Searching the chemical literature, primary sources – journals and patents, secondary sources – Beilstein, reviews, periodicals – serials - monograph and text books - dictionaries, encyclopedias, catalogues and index of tabulated data, location of data - Science Citation Index - chemistry journal index - choosing a problem - Computers in literature search using Internet websites- ACS-pubs, Royal Society, Springer link, science direct, Wiley - Interscience, search engines-Google, Yahoo, Alta Vista, etc., and Chemical Abstract Online.

Unit II - Computers in Chemistry: 18 Hrs

Desk-top chemical software: **Chemoffice:** Chemdraw, Chem 3D & Chem finder, Linear regression, Multi regression. MS Excel: Graph drawing and calculations -Origin.

Rasmol: Visualization of Protein molecules – highlighting amino acids, helices, beta sheets, non-hydrogen, hydrogen and sulphur bonds, identification of metal atoms and active sites.

SHELX : Structure solving and refinement using Shelxs and Shelxl.

Molecular modeling:

Coordinate systems - Cartesian and internal coordinate systems-wire frame, ball and stick, space filling and surface models - potential energy surfaces – force fields in molecular mechanics and potential energy calculation.

Unit III- Instrumental Methods of Chemical Analysis: 18 Hrs

Principle, instrumentation and applications of spectroscopic techniques - Flame Emission spectroscopy - Atomic absorption spectroscopy (AAS). Thermal analysis-Thermo Gravimetry (TGA), Differential Thermal Analysis (DTA) & Differential scanning calorimetry (DSC)-Scanning Electron Microscopy(SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM) and Scanning Tunneling Microscope (STM).

Principle, instrumentation and applications- HPLC, GC-MS and cyclic voltammetry-Spectrofluorimetry.

Unit IV- Laboratory techniques: 18 Hrs

Safety in chemical lab - explosion and fire hazards - hazards due to toxic chemicals - electrical safety - UV radiation - first aids for various kinds of accidents including toxic chemicals - preparation and purification of reagents - precipitation- filtration - evaporation- preparation of deionised water - choice of solvents and liquids - purification - distillation - steam and fractional distillation - solvents and reagents.

Unit V-Effective thesis writing: 18 Hrs

Thesis layout - preliminaries - title page - certificates - declaration- abstracts - preface - acknowledgements - table of contents - list of tables - figures and symbols - text of the thesis - chapter division - subdivision - heading - subheadings - pagination - margins - paragraph - format and conventions - use of tables and figures - numbering - captions - referencing- Reference Systems - paranthetical documentation-documenting book and articles-alphabetical methods-chronological order-editing works-some special list of references-cases-in text citation - documenting –appendices - use of appendix and its format - puntuation and mechanics - presenting a scientific seminar - art of writing a thesis- publication of research paper.

References:

1. Barbara Kasser, Using the internet, IV Edn., EE edition, New Delhi, 1998.
2. Jerry March, Advanced Organic Chemistry, John Wiley & Sons Ltd., IV Edn., New York, 2004.
3. G. H. Geffery, J. Basselt, J. Mendhan and R.C. Denney, Vogel's Text book of Quantitative Chemical Analysis, V Edn., Longman Scientific and Industrial, UK, 1989.
4. D.A. Skoog, D.M. West & F.J. Holler, Fundamentals of Analytical Chemistry, VII Edn., Saunders College Publishing, New York, 1996.
5. Hobart H. Willard, Lynne L. Merritt,Jr., John A. Dean, Frank A. Settle,Jr, Instrumental Methods of Analysis, VII edition, CBS publishers and distributors, New Delhi, 1986.
6. R.M. Silverstein, G.C. Bassler & T.C. Morril, Spectrometric Identification of Organic Compounds, John Wiley & Sons, V Edn., New York, 2001.
7. R.S Drago, Physical Methods in Chemistry, Saunders College Publishing, Philadelphia, 1977.
8. Andrew R. Leach, Molecular Modeling Principles and Applications, II Edn., Dorset publishers, Dorchester, 2001.
9. J. Anderson, B.H. Durston and M. Poole, Thesis and Assigment Writing, Wiley Eastern Ltd., New Delhi,1997.
10. F.Abdul Rahim - Thesis Writing - A Manual Researcher, New age International Ltd., New Delhi,1996.
11. Bradley J. Holliday & Chad A. Mirkin, Strategies for the Construction of Supramolecular Compounds through Coordination Chemistry- Reviews, Angew. Chem. Int. Ltd., Ed., 2001, 40, 2022-2043., ~CHEMIE@WILEY-VCH
12. Mick Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons & Burkhard Raguse, Nanotechnology, Ist Indian Edition, New Delhi, 2005.

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DEPARTMENT OF CHEMISTRY
(From 2014-15 batch onwards)
M. Phil., PROGRAMME IN CHEMISTRY (SF)

Paper - 2 **COURSE WORK**

Semester – I
Course Hours per Week : 6 **1SMC2**
Total Hours per Semester: 90

Objectives:

To enable the learners:

i) to know about ***Organic synthesis.***

ii) to understand the concept and applications of ***various Spectral Techniques***.

iii) to derive advanced knowledge on ***Polymer Chemistry***.

iv) to set themselves exposed to ***Nano / Green Chemistry***

v) to have an understanding of ***Bio-inorganic Chemistry***.

UNIT I: Advanced Organic synthesis: 18 Hrs

Types of (Carbon to carbon bond forming) reactions - Key intermediates - starting materials - Retro synthetic analysis- synthesis involving functional group interconversion - chemo selectivity, regioselecitivity, stereo selectivity- two group C-X disconnection and synthetic strategies 1,2-1,3-1,4-1,5-1,6 difunctionalised disconnection- use of inclusion compounds such as cyclodextrin, calixarene.

UNIT II: Nano / Green Chemistry: 18 Hrs

Nanoparticles and Carbon nanotubes (singlewalled and multiwalled carbon nanotubes) - Introduction - Methods of preparations – CVD, Laser ablation method – Uses – Metal oxide nanoparticles - Zinc Oxide, Cadmium sulphide, Titanium dioxide – Synthesis and characterization - Application of nanoparticles: Phosphors, Batteries - Information storage - Solar cells .

Need for Green Chemistry - Solvent free reactions - Microwave assisted synthesis - Role of ionic liquids in green chemistry - Cleaner technology with super critical fluids - Catalytic approach to green chemistry (use of Zeolites, clays, mesoporous materials).

UNIT III: Bio-Inorganic Chemistry: 18 Hrs

Metalloproteins: Transport and storage protein: e.g Fe-S protein, Blue-copper protein, Ferritin, Transferritin, Hemocyanin and Heme erythrin. Metalloenzymes: Hydrolases (e.g. Carboxy peptidases and amino peptidases), Oxido reductases (e.g. Superoxide dismutase), Isomerases and Synthatases – (e.g. Vit B_{12}) - Nickel containing enzymes - Structure of DNA - types of Nucleic acid interactions - Coordination, intercalation and hydrogen bonding - Interactions of metal ion with Nucleic acid, Redox Chemistry, Hydrolytic Chemistry.

UNIT IV: Polymer Chemistry: 18 Hrs

Polymer-Intoduction-Classification-Tactictity-Polymerization- Addition, Co-polymerisation and condensation – Mechanism of polymerization – Free radical mechanism, Ionic mechanism, Zeigler-Nata polymerization- Stucture-Property relationships in polymer-Classification of plastics- Thermosetting and Thermoplastic resins- Additives-Compounding of plastic-Fabrication-Compression moulding, Injection moulding, Extrusion moulding and Blow moulding- Molecular weight determination-Light scattering, viscosity, osmometry methods-Number average and Average number weight polymer.

Preparation, properties and uses of some important polymeric resins-PE (LDPE and HDPE), Phenol-formaldehyde resins, Silicon resins- composite-ABS, Cellulose-Bio-degradable plolymer.

UNIT V-Spectroscopy: 18 Hrs

NMR Spectroscopy - Proton and ^{13}C- fluxional NMR, 2-dimensional NMR - uses of Shift reagents.

ESR spectroscopy - Hyperfine splitting -factors affecting ‘g’ value - anisotropy of ‘g’ and ‘A’ tensors - Zero field splitting - Krammer’s degernacy - EPR spectra of Cu (II) Complexes. Jahn -Teller distortion in Cu(II) complexes. Evaluation of bonding parameters.

Analysis and Interpretation of Spectra of simple Aliphatic and Aromatic compounds using IR, UV, NMR, MASS, XRD techniques.

References:

1) Jerry March, Advanced Organic Chemistry, (Appendix A), IV edition, John Wiley and Sons, NewDelhi, 2000.
2) S. Warren, Organic Synthesis, The disconnection approach, John Wiley and Sons, U.K , 2004.
3) F. A. Carey and R. I. Sundburg, Advanced Organic Chemistry, plenum press, Newyork, 2000.
4) R. K. Mackie and D. M. Smith, Guide book to Organic Synthesis, Longman, Newyork, 1999.
5) V.R. Gowarikar, etal., Polymer Science I Edn., Wiley Eastern Ltd., New York,1986.
6) H. R. Allcock, Lampe, Contemporary, Polymer Chemistry, II Edn., Prentice Hall, New Jersey, 1990.
7) Fred. W. Billmeyer, JR, Text book of Polymer Science III Edition, John Wiley and Sons, NewYork.
8) James E. Huheey, Eller A. Keiter and Richard L. Keiter, Inorganic Chemistry, IV Edn., Harper Collins College Publishers, New York,1993.
9) Bertini I.G.,Bio-Inorganic Chemistry, Viva books private Limited,1998.
10) Lippard S.T., and Berg T.M., Principles of Bio-inorganic Chemistry, Panima Publishing Company, New York,1997.
11) K. Hussain Reddy, Bioinorganic Chemistry New Age Internation (p) limited, New Delhi-2003.
12) Kenneth, J. Klabunde, Nanoscale Materials in Chemistry, Wiley Interscience, New York, 2001
13) M.M. Srivastava, Green Chemistry, Rasshmi Singhi Narosa publishing House Pvt. Ltd., New Delhi, 2003.
14) K. R. Desai, Green Chemistry, Himalaya Publishing House, New Delhi, 2005
15) C.N.R Rao, A. Muller and A.K. Cheethar, The Chemistry of Nanomaterials-Synthesis, Properties and Applications Vol. 1 and 2, Wiley –VCH – Verlag GmoH & Co., Wilhelm, 2004.
16) Mick Wilson, Kamali Kannangara, Geolf Smith, Michelle Simmons, Burkhard Ragnse, Nanotechnology Overseas press, New Delhi-2005.
17) Charles P. Poole, Jr, Frank J. Owens, Introduction to NanoTechnology, John Wiley and Sons, Inc., New York , 2003.
18) R.S. Drago, Physical Methods in Chemistry, Saunders Golden Sunburst Series, W.B. Saunders Company, London, 1977.
19) Silverstein, Bassler and Morrill, Spectroscopic Identification of Organic Compounds, IV Edn., John Wiley and Sons, Inc., New York ,1991.

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DEPARTMENT OF CHEMISTRY

(From 2014-15 batch onwards)

M. Phil., PROGRAMME IN CHEMISTRY (SF)

Paper - 3 **IN - DEPTH STUDY**

Semester - II

Course Hours per Week : 6 **2SMC1**

Total Hours per Semester : 90

This paper is based on the project work proposed by the guide for each student. **The Department shall provide *10-research articles* related to the project work from reputed international and other journals every year**. The Internal Evaluation and the Summative Examination will be conducted based on the research articles provided by the Department.

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DEPARTMENT OF CHEMISTRY

(From 2014-15 batch onwards)

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Paper - 4 **PROJECT**

Semester – IISMPJ

Project work for Two Semesters Sequential Course:

- The objective of this course is to enable the student to carry out the project selected in the first semester supplemented by experimental investigations.

Progress Report:

The first progress report should be presented to the Department before the 60th working day of the second semester.

Preview of Project:

The student will present the preview of the dissertation by the 75th working day of the semester to the Department.

Submission of Project:

The student has to submit four typed copies of dissertation by the 85th working day of the second semester to the department. A copy of this dissertation will be sent to the external examiner for review.

Evaluation of Project:

The Head of the PG department will be the chairman and the convener of the research committee. Internal valuation will be done by the guide. A public viva-voce examination will be conducted by a panel of examiners consisting of an external examiner who valued the dissertation and the guide.

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DEPARTMENT OF CHEMISTRY

(From 2014 – 2015 Batch onwards)

CERTIFICATE COURSE IN INDUSTRIAL SAFETY

Course : B.Sc., **Code No :**
Semester : I & II **No. of Hrs allotted: 40**
Paper : **No. of Credits :**
Title of the Paper : Fire Prevention and Environmental Safety
Course objectives:

This paper aims at enriching the students' knowledge about fire prevention and industrial safety.

UNIT I

Physical and chemical properties of fire. Fire prevention and protection – sources of ignition – fire triangle- principles of fire extinguishing – active and passive fire protection systems – various classes of fire – A, B, C, D, E – types of fire extinguishers – fire stoppers – hydrant pipes – hoses – monitors – fire watchers.

UNIT II

Industrial fire protecting systems – sprinkler-hydrants-stand pipes – special fire suppression system like deluge and emulsifier – selection criteria of the above installations – reliability – maintenance - evaluation standards – alarm and detection systems. Other suppression systems – CO_2 systems – foam system – dry chemical powder (DCP) system-Fire safety in buildings-Fire load-Fire resistant materials and fire testing.

UNIT III

Water pollutants-health hazards-sampling and analysis of water-water treatment – different industrial effluents and their treatment and disposal – advanced waste water treatment – effluent quality standards and laws – chemical industries, tannery, textile effluents-common treatment.

UNIT IV

Hazardous waste management in India-waste identification, characterization and classification-technological options for collection, treatment and disposal of hazardous waste-selection charts for treatment of different hazardous wastes-methods of collection and disposal of solid wastes-health hazards-toxic and radioactive wastes-incineration and vitrification – hazards due to bio-process-dilution-standards and restrictions – recycling and reuse.

UNIT V

Pollution control in process industries like cement, paper, petroleum-petroleum products – textile-tanneries-thermal power plants – dying and pigment industries – eco-friendly energy.

Text Book:

1. R.S. Gupta, "A Hand book of fire Technology", Orient Longman.

Reference Book:

1. N.K. Uberor, Environmental Management, Second Edition, Excel Books, New Delhi-2007

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DEPARTMENT OF CHEMISTRY

(From 2014 – 2015 Batch onwards)

Course : PG Diploma **Code No :**
Semester : I & II **No. of Hrs allotted: 30**
Paper : Core **No. of Credits :**
Title of the Paper : Molecular Modeling & Spectroscopy

Course objectives:

This paper aims at enriching the students' knowledge about Spectroscopy, QSAR studies and molecular modeling.

Unit I FTIR spectroscopy 6 Hours

FTIR- Basic Principle - Selection Rules - Instrumentation. Applications- Interpretation of FT-IR spectra of organic and Inorganic samples.

Unit II UV-Visible spectroscopy 6 Hours

Basic Principle- Selection Rules-Instrumentation, splitting of spectral terms- Orgel diagram, Evaluation of 10Dq . Evaluation onof 10Dq and β values, Determination of unknown concentration of Ni^{2+}, Cu^{2+} and Fe^{2+}.

Unit III Fluorescence spectroscopy 6 Hours

Basic theory, principle, instrumentation and applications. Study of selected fluorescence molecule.

Unit IV QSAR Studies 6 Hours

QSAR- Partition coefficient, hydrophobicity constant, Hammet substituent constant, Taft steric factor, Hansch equation, Craig plot, Topliss scheme, QSAR studies of comparing, identifying suitable organic lead compounds as drug using softwarelike Alchemy/Hyper Chem.

Unit V Molecular modeling and Docking Studies 6 Hours

Structure drawing, visualization and energy minimization of simple molecule using Chem Office, Rasmol. Docking of organic molecule, drugs in relevant enzyme or protein using Hex software.

Text Books:

1. C.M.Banwel, Introduction of molecular spectroscopy IV Edi., TMH Company Ltd., 2005.
2. B.P.Straughan and S.Walkar,Spectroscopy, vol.I II and III ,chapman and Hill. U.K., 1976.
3. R.S.Drago, Physical methods in chemistry, saunders collge publishing, New delhi_1999.
4. Nakamato, Kazuo, Paul J.Macartry, spectroscopy and structure of metal chealte Compounds,IV Edision, John Wiley and sons, Inc., New York 1986.
5. .B.K.Sharma, Instrumental method of chemical Analysis, GOEL publishing house, 12th Reprint, New Delhi, 1993.
6. William Kemp .Organic spectroscopy , 4th Edition, ELBS , U,K.,1994.
7. Y.R.sharma, Elementry organic Absorption spectroscopy, S. Chand & Co., New Delhi 1991.

Reference Books:

1. .R.M.Silverstein , G.C.Bassler and T.C. Morrill, spectrometric Identification of Organic Compounds 6th Edition, John Wiley , New York ,2005.
2. M.I. Gangwal Medical chemistry Lectures on Drug Design and Synthetic Drugs, Student publishing house, 2007.
3. Chem office, Rasmol, Hex- Hand book prepred in the Department.

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DEPARTMENT OF CHEMISTRY

(From 2014 – 2015 Batch onwards)

Course : PG Diploma **Code No :**
Semester : I & II **No. of Hrs allotted: 30**
Paper : Core **No. of Credits :**
Title of the Paper : Spectroscopic Analysis & Software Utility

Course objectives:

This paper aims at enriching the students' knowledge to analyze and interpret simple organic and inorganic compounds spectroscopically and utilize softwares available in chemistry.

1. FT-IR spectroscopy 6 Hours

FT-IR spectral recording of organic and Inorganic samples and their interpretation

2. UV-Visible spectroscopy 6 Hours

Determination of unknown concentration of Ni^{2+}, Cu^{2+} and Fe^{2+} complexes

3. Fluorescence spectroscopy 6 Hours

Spectral Recording and Study of selected fluorescence molecule and their interpretation

4. QSAR Studies 6 Hours

Drawing of some organic molecules using Chem office. File conversion using Open BABEl. QSAR Studies using Alchemy/Hyper Chem softwares.

5. Molecular modeling and Docking Studies 6 Hours

Structure drawing, visualization and energy minimization of simple molecule using Chem Office, Rasmol. Docking of organic molecule, drugs in relevant enzyme or protein using Hex software.