

Sacred Heart College (Autonomous)

Department of Chemistry

MSc Chemistry

Course Plan

Academic Year 2014 – 15

Semester 1

COURSE PLAN			
ACADEMIC YEAR 2014-15			
PROGRAMME	:	<i>M.Sc. Chemistry</i>	LECTURE HOURS : 72
SEMESTER	:	<i>1</i>	CREDITS : 4
SUBJECT TITLE	:	ORGANOMETALLICS AND NUCLEAR CHEMISTRY	SUBJECT CODE : P1CHET01
COURSE TEACHERS	:	<i>Dr. Joseph John (JJ), Dr. Thommachan Xavuer (TX), Mr. Midhun Dominic C D (MD) & Mr. Senju Devassykutty</i>	
Course Objectives	:	<ol style="list-style-type: none"> <i>1. Ability to understand the basics of organometallic compounds, their synthesis, structure and bonding</i> <i>2. To understand the reactions and catalysis by organometallic compounds</i> <i>3. To know about the synthesis of organometallic polymers</i> <i>4. To understand the importance of inorganic chemicals in the field of biochemistry</i> <i>5. Explore the field of nuclear chemistry</i> 	

Teacher I – JJ Unit 5 : Bioinorganic Compounds (18 Hours)			
No. of Session	Session Topic and Discussion Theme	Method of Teaching	Remarks/Student Assignments
1	Essential and trace elements in biological systems	Conventional Lecture Chalk & Board	Assignment on Different types of molecules that are transported across membranes
2	Structure and functions of biological membranes	Lecture With power point presentation	
3	Mechanism of ion transport across membranes,		
4	Sodium pump, ionophores,		
5	Valinomycin and crown ether complexes of Na ⁺ and K ⁺		
6	ATP and ADP. Photosynthesis-chlorophyll a, PS I and PS II.		
7	Role of calcium in muscle contraction blood clotting mechanism and biological calcification		
First Internal Test			
8	Oxygen carriers and oxygen transport proteins-haemoglobins, Myoglobins and haemocyanin	Lecture With Powerpoint presentation	Assignment on Redoxmetalloenzymes
9	Haemerythrins and haemevanadins, cooperativity in haemoglobin		
10	Iron storage and transport in biological systems-ferritin and transferrin.		
11	Redox metalloenzymes-cytochromes,		
12	Peroxidases and superoxide dismutase and catalases.		
13	Nonredox metalloenzymes-CarboxypeptidaseA-structure and functions		
14	Nitrogen Fixation-nitrogenase, vitamin B ₁₂ and the vitamin B ₁₂ coenzymes.		

Second Internal Test			
15	Introduction to Metals in medicine	Lecture with ICT	Assignment Related to Toxic effect of metals
16	Therapeutic applications of <i>cis</i> -platin, radio-isotopes and MRI agents.		
17	Toxic effects of metals (Cd, Hg, Cr and Pb).		
18	Revision		
Reference Text Books			
<ol style="list-style-type: none"> 1. G. Wulfborg, Inorganic Chemistry, Ind. Edition, Viva, 2014. 2. Shiver & Atkins, Inorganic Chemistry, 4th Edn. Oxford University Press, 2006. 3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Cengage Learning 2nd Edn., 2014. 4. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006. 5. F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999. 6. G.L. Miessler, D. A. Tarr, Inorganic Chemistry 3rd Ed., Pearson Education, 2007. 7. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007. 8. I. Bertini, H. B Gray, S. J Lippard, J. S Valentine, Bioinorganic Chemistry. 9. R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1984. 			

Teacher II – TX		Module Taken : Unit 4: Organometallic Polymers (Total – 9 Hrs)	
No. of Session	Session Topic and Discussion Theme	Method of Teaching	Remarks/Student Assignments
1	Introduction to Organometallic polymers	Conventional Lecture Using Chalk and Board	Assignment for Preparing Applications of organometallic polymers
2	Polymers with organometallic moieties as pendant groups		
3	Polymers with organometallic moieties in the main chain		
4	Condensation polymers based on ferrocene and on rigid rod polyynes		
5	Polymers prepared by ring opening polymerization.		
6	Organometallic Dendrimers		
First Internal Test			
Teacher II – TX		Module Taken : Unit 6: Nuclear Chemistry (Total – 9 Hrs)	
7	Introduction to Nuclear Chemistry	Lecture With Chalk and board	Assignments based on Different types of nuclear reactions
8	Fission products and fission yield. Neutron capture cross section and critical size.		
9	Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations.		
10	Positron annihilation and autoradiography. Principles of counting technique such as G.M. counter		
11	Principles of counting technique such as Proportional, ionization and scintillation counters. Cloud chamber		
12	Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium		
13	Synthesis of transuranic elements such as Mendeleevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.		

Second Internal Test			
14	Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants	Lecture with ICT	Seminar Based on Applications of radioactivity
15	Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry		
16	Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology		
17	Radiation safety precaution, nuclear waste disposal. Radiation chemistry of water and aqueous solutions.		
18	Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.		
Reference Text Books			
1. G. Friedlander, J.W. Kennedy, E.S. Macias, and J.M. Miller, Nuclear and Radiochemistry, John Wiley and Sons, 2nd Ed. 1981. 2. H.J. Arnikar, Essentials of Nuclear Chemistry, New Age International, 4th Edn., 2011. 3. B.R Puri, L.R. Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Milestone, 2011. 4. S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.			

Teacher III– MD Module Taken : Unit 1: Organometallic Compounds-Synthesis, Structure and Bonding (18 Hours)			
No. of Session	Session Topic and Discussion Theme	Method of Teaching	Remarks/Student Assignmets
1	Introduction to organometallic compounds	Conventional Lecture	Seminar Assignment to Students on the applications of organometallic compounds
2	Organometallic compounds with linear pi donor ligands-olefins - synthesis, structure and bonding.	Conventional lecture using Chalk and Board and ICT-PPT	
3	Organometallic compounds with linear pi donor ligands- acetylenes, synthesis, structure and bonding.		
4	Organometallic compounds with linear pi donor ligands- dienes synthesis, structure and bonding.		
5	Organometallic compounds with linear pi donor ligands- allyl complexes-synthesis, structure and bonding		
6	Complexes with cyclic pi donors- metallocenes and structure and bonding.		
7	Complexes with cyclic pi donors cyclic arene complexes structure and bonding.		
8	Carbene and carbyne complexes		
9	Revision		
First Internal Test			
10	Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls	Conventional Lecture using Chalk and Board and ICT -PPT	Assignment to Students on the applications of metal carbonyls
11	Preparation, properties, structure and bonding of metal nitrosyls		

12	Preparation, properties, structure and bonding of metal cyanides		
13	Preparation, properties, structure and bonding of simple dinitrogen complexes		
14	Polynuclear metal carbonyls with and without bridging.		
Second Internal Test			
15	Carbonyl clusters-LNCCS and HNCCS	Conventional Lecture using Chalk and Board and ICT -PPT	
16	Isoelectronic and isolobal analogy, Wade-Mingos rule, cluster valence electrons.		
17	Wade-Mingos rules, cluster valence electrons.		
18	Revision		
<ol style="list-style-type: none"> 1. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers, 1993. 2. F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999. 3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977. 4. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988. 5. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007. 6. B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010. 			

Teacher IV – SD		Module Taken : Unit 2: Reactions of Organometallic Compounds (9 Hrs)	
No. of Session	Session Topic and Discussion Theme	Method of Teaching	Remarks/Student Assignments
1	Substitution reactions-nucleophilic ligand substitution	Conventional Lecture	Preparation of Lecture Notes
2	Nucleophilic and electrophilic attack on coordinated ligands		
3	Addition and elimination reactions-1,2 additions to double bonds		
4	Carbonylation and decarbonylation		
5	Oxidative addition and reductive elimination,		
6	Insertion (migration) and elimination reactions.		
7	Rearrangement reactions		
8	Redistribution reactions, fluxional isomerism.		
9	Revision		
First Internal Test			
Reference Text Books			
<ol style="list-style-type: none"> 1. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers, 1993. 2. F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999. 3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977. 4. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988. 5. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007. 6. B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010. 			

Teacher IV – SD		Module Taken : Unit 3: Catalysis by Organometallic Compounds (9 Hrs)	
10	Introduction to catalysis by organometallic compounds	Conventional Lecture	Preparation of Notes on application of catalysis
11	Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.		
12	Reactions of carbon monoxide and hydrogen-the water gas shift reaction		
13	Reactions of carbon monoxide and hydrogen-the Fischer-Tropsch reaction(synthesis of gasoline).		
14	Hydroformylation of olefins using cobalt or rhodium catalyst.		
Second Internal Test			
15	Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts.	Conventional Lecture	Preparation of Notes on application of catalysis
16	Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $\text{Co}_2(\text{CO})_8$ catalyst in adipic ester synthesis.		
17	Olefin metathesis-synthesis gas based reactions, photodehydrogenation catalyst (“Platinum Pop”).		
18	Palladium catalysed oxidation of ethylene-the Wacker process.		
Reference Text Books			
<ol style="list-style-type: none"> 1. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers, 1993. 2. F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999. 3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977. 4. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988. 5. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007. 6. B.D. Gupta, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010. 			

COURSE PLAN**ACADEMIC YEAR 2014-15**

PROGRAMME	:	<i>M.Sc. Chemistry</i>	LECTURE HOURS	:	72
SEMESTER	:	<i>1</i>	CREDITS	:	4
SUBJECT TITLE	:	<i>Structural and Molecular Organic Chemistry</i>	SUBJECT CODE	:	<i>P1CHET02</i>
COURSE TEACHERS	:	<i>Dr. Joseph .T. Moolayil, Dr. V.S Sebastian, Dr. Franklin John, Dr. June Cyriac</i>			
COURSE OUTCOMES (COs)	:				
Instructional Hours	:	<i>Four Hours per Week</i>			

	No. of Session	Session Topic and Discussion Theme	Value additions	COs
JTM				
Unit 5: Conformational Analysis (18Hrs)	1.	Stereoisomerism: Definition based on symmetry and energy criteria	Assignment No: 1	
	2.	Configuration and conformational stereoisomers.		
	3.	Conformational descriptors		
	4.	Factors affecting conformational stability of molecules.		
	5.	Potential energy diagrams		
	6.	Conformational analysis of acyclic systems: substituted ethanes,		
	7.	Aldehydes,		
	8.	Ketones and olefins.		
	9.	Conformational analysis of cyclic systems -		
	10.	Cyclohexane and its derivatives. Cyclohexanone.		
	11.	Continued		
	12.	Conformational analysis of Fused and bridged bicyclic systems		
	13.	Decalins, adamantane		
	14.	Hexamethylene diamine and congressane,		
	15.	Conformation and reactivity of elimination -dehalogenation, Dehydrohalogenation,		
	16.	Dehydration, semipinacolic deamination and pyrolytic elimination-		
	17.	Saytzeff and Hofmann eliminations, substitution and oxidation of 2 ^o alcohols		
	18.	Chemical consequence of conformational equilibrium - Curtin-Hammett principle.		
	1.	D. Nasipuri, <i>Stereochemistry of Organic Compounds: Principles and Applications</i> , Third Edition, New Age Publications, New Delhi, 2010.		
	2.	E. L. Eliel and S. H. Wilen, <i>Stereochemistry of Organic Compounds</i> , John Wiley & Sons, New York, 1994.		

VSS				
Unit 4: Stereochemistry of Organic Compounds (18 Hours)	19.	Introduction to molecular symmetry and chirality – examples from common objects to molecules		
	20.	Axis, plane, centre, alternating axis of symmetry.		
	21.	Centre of chirality – molecules with C, N, S based chiral centres		
	22.	Absolute configuration - enantiomers		
	23.	Racemic modifications - R and S nomenclature using Cahn-Ingold-Prelog rules	Assignment No:2	
	24.	Continued		
	25.	Molecules with a chiral centre and C _n		
	26.	Molecules with more than one center of chirality		
	27.	Definition of diastereoisomers constitutionally symmetrical and unsymmetrical chiral molecules		
	28.	Erythro, threo nomenclature.		
	29.	Axial, planar and helical chirality – examples		
	30.	Stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls,		
	31.	Ansa and cyclophanic compounds, spirans, exo-cyclic alkylidenecycloalkenes. Identification of enantiotopic, homotopic, diastereotopic hydrogens		
	32.	Prochirality, Topicity and prostereoisomerism – topicity of ligands and faces, and their nomenclature.		
	33.	NMR distinction of enantiotopic/diastereotopic ligands. Stereospecific, stereoselective and asymmetric synthesis.		
	34.	Stereoisomerism-configuration and conformational stereoisomers		
	35.	Geometrical isomerism: E-Z notation, Methods of determination of geometrical isomers		
	36.	Interconversion of geometrical isomers		

<i>Text Books</i>	<ol style="list-style-type: none"><li data-bbox="331 231 2076 263">3. D. Nasipuri, <i>Stereochemistry of Organic Compounds: Principles and Applications</i>, Third Edition, New Age Publications, New Delhi, 2010.<li data-bbox="331 279 2076 311">4. E. L. Eliel and S. H. Wilen, <i>Stereochemistry of Organic Compounds</i>, John Wiley & Sons, New York, 1994.
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FJ				
Unit 1: Basic Concepts in Organic Chemistry (18 Hours)	37.	Review of basic concepts in organic chemistry	Assignment No.3	
	38.	Bonding, hybridization, MO picture.		
	39.	Continued and electron displacement effects-inductive effect		
	40.	Electrometric effect, resonance effect, hyperconjugation, steric effect. Steric inhibition of resonance.		
	41.	Bonding weaker than covalent bonding- H-bonding, π - π interactions.	Group Discussion	
	42.	Other non-covalent interactions		
	43.	Concept of aromaticity: delocalization of electrons –Huckel’s rule		
	44.	Craig rule- criteria for aromaticity -examples of neutral and charged aromatic systems,		
	45.	Annulenes		
	46.	Tropolone, Azulene. NMR as a tool for aromaticity		
	47.	Anti- and homo-aromatic systems–Alternate and non-alternate hydrocarbons,		
	48.	Fullerenes, Carbon nanotubes and Graphene.		
	49.	Mechanism of electrophilic aromatic substitution		
	50.	Continued		
	51.	Mechanism of nucleophilic aromatic substitution		
	52.	Arenium ion intermediates		

	53.	Mechanism of SN1, SNAr,		
	54.	SRN1 and Benzyne mechanisms.		
	5.	D. Hellwinkel, Systematic nomenclature of organic chemistry, Springer international edition		
	6.	R. Bruckner, <i>Advanced Organic Chemistry: Reaction Mechanisms</i> , Academic Press, 2002.		
	7.	F. A. Carey and R. A. Sundberg, <i>Advanced Organic Chemistry, Part A: Structure and Mechanisms</i> , Fifth Edition, Springer, New York, 2007.		
	8.	J. Clayden, N. Greeves, S. Warren, P. Wothers, <i>Organic Chemistry</i> , Oxford University Press, New York, 2004		

JUC				
Unit 2: Physical Organic Chemistry and Photochemistry (18 Hours)	55.	Introduction to carbon acids		
	56.	HSAB principle and its application		
	57.	Catalysis by acids and bases		
	58.	Nucleophiles with examples from acetal, cyanohydrin		
	59.	Ester formation and hydrolysis reactions – A_{AC}^2 mechanisms		
	60.	A_{AC}^1 mechanism.		
	61.	A_{AL}^1 , B_{AC}^2 mechanisms.		
	62.	B_{AL}^1 mechanism.		
	63.	Jablonski diagram, triplet and singlet states. Photoreactions of carbonyl compounds: Norrish reactions of acyclic ketons		
	64.	Cyclic ketones.		
	65.	Paterno-Buchi reaction.		
	66.	Barton reaction and photo reduction of ketones.		
	67.	Di- π -methane reaction		
	68.	Photochemistry of Nitro and Azo groups. Photochemistry of vision		

	69.	Energy profiles. Hammond postulate		
	70.	Kinetic versus thermodynamic control of product formation		
	71.	Kinetic isotope effects with examples -		
	72.	Stereochemical studies-use of isotopes Hammett equation, Taft equation, cross-over experiments, Hammond postulates.		
	9.	J.Clayden, N.Greeves, S.Warren, P.Wothers, <i>Organic Chemistry</i> , Oxford University Press, New York, 2004.		
	10.	Aditi Sangal, <i>Krishna's Advanced Organic Chemistry</i> ; Volume 1 – Krishna Prakashn Media(P) Ltd.		
	11.	T. H. Lowry and K. S. Richardson, <i>Mechanism and Theory in Organic Chemistry</i> , Second Edition, Harper & Row, New York, 1981.		
	12.	N. S. Isaacs, <i>Physical Organic Chemistry</i> , ELBS, Longman, UK, 1987.		
	13.	Jack Hine, <i>Physical Organic Chemistry</i> , McGraw-Hill; 2nd Edition, 1962.		
	14.	Anslyn, E. V.; Dougherty, D. A. <i>Modern Physical Organic Chemistry</i> , University Science Books, 2006		
	15.	N. J. Turro, V. Ramamurthy and J. C. Scaiano, <i>Principles of Molecular Photochemistry: An Introduction</i> , University Science books 2009.		
	16.	N.J Turro, <i>Modern Molecular Photochemistry</i> , Benjamin Cummings Publishing Company, Menlo Park, 1978.		
	17.	K.K.R.Mukherjee, <i>Fundamentals of Photochemistry</i> , New Age Publications, New Delhi, 1978.		

DEPARTMENT OF CHEMISTRY, SACRED HEART COLLEGE (AUTONOMOUS), THEVARA

COURSE PLAN : ACADEMIC YEAR 2014 - 2015

PROGRAMME	: <i>M.Sc. Chemistry</i>	SEMESTER	: <i>1</i>
LECTURE HOURS	: <i>54</i>	CREDITS	: <i>3</i>
SUBJECT TITLE	: <i>Classical and Statistical Thermodynamics</i>	SUBJECT CODE	: <i>P1CHET04</i>
COURSE TEACHERS	: Dr. K. B. Jose (KBJ), Dr. Jinu George (JG), Dr. Ignatious Abraham (IGA)		
Instructional Hours	: <i>Tuesday : Period 1 (9:30 to 10:30 am) - KBJ</i> <i>Wednesday : Period 1 (9:30 to 10:30 am) - JG</i> <i>Thursday : Period 5 (2:30 to 3:30 pm) - IGA</i>		

IGNATIUS ABRAHAM

Unit I : CLASSICAL THERMODYNAMICS

Sessions	Session Topic and Discussion Theme	Value additions
1	Entropy, dependence of entropy on variables of a system (S,T and V; S,T and P).	Numerical Problems
2	Thermodynamic equations of state. Irreversible processes - Clausius inequality	
3	Free energy, Maxwell relations and significance, temperature dependence of free energy	Numerical Problems
4	Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.	
5	Partial molar quantities, chemical potential and Gibbs-Duhem equations. Determination of partial molar volume and enthalpy.	Power Point Presentation

6	Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas. Variation of fugacity with temperature and pressure.	
7	Activity, dependence of activity on temperature and pressure.	Assignment
8	Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law.	
9	Excess thermodynamic functions-free energy, enthalpy, entropy and volume. Determination of excess enthalpy and volume.	
1st Internal Examination		
10	Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- vant Hoff reaction isochore and isotherm.	Numerical Problems
11	Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.	
12	Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance	Power Point Presentation
13	Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations.	
14	The Onsager reciprocal relations - principle of microscopic reversibility.	
15	Electrokinetic phenomena. Thermoelectric phenomena	
2nd Internal Examination		
Unit II : Statistical Thermodynamics		
16	Need for quantum statistics, Bose-Einstein statistics: Bose-Einstein distribution, example of particles,	

17	Bose-Einstein condensation, Difference between first order and higher order phase transitions, liquid helium, super cooled liquids.	Videos showing BEC
18	Fermi-Dirac distribution, examples of particles, Application in electron gas, thermionic emission. Comparison of three statistics.	
JINU GEORGE		
Sessions	Session Topic and Discussion Theme	Value additions
Unit I : CLASSICAL THERMODYNAMICS		
1	Phase equilibrium	
2	Gibbs phase rule	Individual Assignment:
3	Three component systems - Introduction	
4	Graphical representation of three component systems.	Power Point Presentation:
5	Solid-liquid equilibria - Introduction	
Unit II : BIOENERGETICS		
6	Solid-liquid equilibria - ternary solutions with common ions	
7	Solid-liquid equilibria - Hydrate formation	
8	Solid-liquid equilibria - compound formation.	
9	Liquid-liquid equilibria - One pair of partially miscible liquids	
1st Internal Examination		
Unit IV : GASEOUS STATE		
10	Liquid-liquid equilibria - Two pairs of partially miscible liquids	
11	Liquid-liquid equilibria -Three pairs of partially miscible liquids	
12	Bioenergetics: Coupled reactions	Power Point Presentation
13	ATP and its role in bioenergetics. High energy bond.	

14	Free energy and entropy change in ATP hydrolysis.	
15	Thermodynamic aspects of metabolism	
2nd Internal Examination		
16	Thermodynamic aspects of respiration	
17	Thermodynamic aspects of glycolysis	Power Point Presentation:
18	Thermodynamic aspects of biological redox reactions.	
K B Jose		
Unit III : STATISTICAL THERMODYNAMICS		
Sessions	Session Topic and Discussion Theme	Value additions
1	Permutation, probability, apriori and thermodynamic probability.	
2	Stirlings approximation, macrostates and microstates.	Power point presentation
3	Boltzmann distribution law	Mathematical treatment
4	Partition function and its physical significance	
5	Phase space, different ensembles	
6	Canonical partition function, distinguishable and indistinguishable molecules	Mathematical treatment
7	Partition function and thermodynamic functions	
8	Separation of partition function	
9	Translational and rotational partition functions.	Mathematical treatment
1st Internal Examination		
10	Vibrational and electronic partition functions.	Assignment
11	Thermal de-Broglie wavelength. Calculation of thermodynamic functions and equilibrium constants.	
12	Statistical interpretation of work and heat	

13	Sakur-Tetrode equation	
14	Statistical formulation of third law of thermodynamics	
15	Thermodynamic probability and entropy, residual entropy	
2nd Internal Examination		
16	Heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.	
17	Heat capacity of solids- the vibrational properties of solids, Einstein's theory and its limitations,	
18	Debye theory and its limitations.	
References:		
<ol style="list-style-type: none"> 1. R.P. Rastogi, R.R. Misra, An introduction to Chemical Thermodynamics, Vikas publishing house, 2009. 2. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999. 3. M.C. Gupta, Statistical Thermodynamics, New age international, 2007. 4. M.W. Zemansky, R.H. Dittman, Heat and Thermodynamics, Tata McGraw Hill, 1981. 5. P.W. Atkins, Physical Chemistry, ELBS, 1994. 6. K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4thEdn. Houghton Mifflin, 2003. 7. L.K. Nash, Elements of Classical and Statistical Mechanics, 2ndEdn., Addison Wesley, 1972. 8. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997 9. C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002. 10. R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper's Biochemistry, Tata McGraw Hill, 1999. 11. I. Tinoco, K. Sauer, J.C. Wang, J.D. Puglisi, Physical Chemistry: Principles and Applications in Biological Science, Prentice Hall, 2002. 12. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, 1975. 13. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971 		

COURSE PLAN**ACADEMIC YEAR 2014-15**

PROGRAMME	:	<i>M.Sc. Chemistry</i>	LECTURE HOURS	:	<i>72 hours</i>
SEMESTER	:	<i>1</i>	CREDITS	:	<i>3</i>
SUBJECT TITLE	:	<i>Quantum Chemistry and Group Theory</i>	SUBJECT CODE	:	<i>P1CHET03</i>
COURSE TEACHERS	:	<i>Dr. Jorphin Joseph(JRJ), Dr. Abi T.G. (ATG)</i>	INSTRUCTIONAL HOURS/WEEK	:	<i>4 hours</i>

**COURSE
OBJECTIVES**

To make the student

- 01 - Learn the basic principles and concepts of quantum mechanics like operators, observables, probabilities, amplitudes, average values etc.
- 02 - Understand how to solve the Schrodinger equation for model systems and relate these to different atomic/molecular phenomena.
- 03 - Recognize symmetry elements in a molecule, state the point group a molecule belongs to and understand degenerate and non-degenerate representations
- 04 - Able to apply formalisms based on molecular symmetry to predict spectroscopic properties.

JRJ	No. of Session	Session Topic and Discussion Theme	Method of Teaching	Value Addition
Unit 1: Postulates of Quantum Mechanics (9 Hrs)	1	State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions	Lecture method	
	2	Operator postulate: operator algebra, linear and nonlinear operators, Laplacian operator,	Lecture method	
	3	Hermitian operators and their properties	Lecture method	
	4	Eigen functions and eigen values of an operator. Eigen value postulate: eigen value equation, eigen functions of commuting operators.	Lecture method	
	5	Expectation value postulate		
	6	Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.	Lecture method	Assignment No: 1
	7	commuting and non commuting operators	Lecture method	
	8	Problems based on the topics discussed	Interaction/Discussion	
	9	Problems based on the topics discussed	Interaction/Discussion	Assignment No:2
Unit 2: Application to Exactly Solvable Model Problems (18 Hrs)	10	First Internal Examination		
	11	Translational motion: free particle in one-dimension, particle in a one dimensional box with infinite potential walls	Lecture method	
	12	Particle in a one-dimensional box with finite potential walls-tunnelling	Lecture method	
	13	Particle in a three dimensional box separation of variables, degeneracy.	Lecture method	
	14	Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation	Lecture method	
	15	Wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.	Lecture method	Assignment No.3
	16	Rotational motion: co-ordinate systems, cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates	Lecture method	
	17	Particle on a ring, the phi equation and its solution, wave functions in the real form	Lecture method	Assignment No.4
	18	Non-planar rigid rotor (or particle on a sphere)- separation of variables, the phi and the theta equations	Lecture method	

	19	Legendre and associated Legendre equations, Legendre and associated Legendre polynomials.	Lecture method	
	20	Spherical harmonics (imaginary and real forms) - polar diagrams of spherical harmonics.	Lecture method	Assignment No.5
	21	Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x , L_y , L_z and L^2)-commutation relations between these operators.	Lecture method	
	22	Spherical harmonics as eigen functions of angular momentum operators L_z and L^2	Lecture method	
	23	Ladder operator method for angular momentum. Space quantization.	Lecture method	
	24	Problems based on the above topics	Interaction/Discussion	
	25	Problems based on the above topics	Interaction/Discussion	
	26	Revision	PowerPoint presentation	
	27	Revision	PowerPoint presentation	
Second Internal Examination				
Unit 3: Quantum Mechanics of Hydrogen-like Atoms (9 Hrs)	28	Potential energy of hydrogen-like systems	Lecture method	
	29	The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions	Lecture method	
	30	The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions	Lecture method	
	31	Wave functions and energies of hydrogen-like atoms. Orbitals-radial functions	PowerPoint presentation	
	32	Radial distribution functions, angular functions and their plots.	PowerPoint presentation	Assignment No.6

	33	The postulate of spin by Uhlenbeck and Goudsmith	Lecture method	
	34	discovery of spin-Stern Gerlach experiment	Lecture method	
	35	Spin orbitals-construction of spin orbitals from orbitals and spin functions.	Lecture method	
	36	Revision	PowerPoint presentation	
Text Books	<ul style="list-style-type: none"> • I.N. Levine, <i>Quantum Chemistry</i>, 6th Edition, Pearson Education Inc. • P.W. Atkins and R.S. Friedman, <i>Molecular Quantum Mechanics</i>, 4th Edition, Oxford University Press, 2005 • Donald, A. McQuarrie, <i>Quantum Chemistry</i>, University Science Books, 1983 • J.P. Lowe, <i>Quantum Chemistry</i>, 2nd Edition, Academic Press Inc., 1993 • A.K. Chandra, <i>Introduction to Quantum Chemistry</i>, 4th Edition, Tata McGraw-Hill, 1994 • R.K. Prasad, <i>Quantum Chemistry</i>, 3rd Edition, New Age International, 2006 • Jack Simons, <i>An Introduction to Theoretical Chemistry</i>, Cambridge University Press, 2003 			

ATG	No. of Sessions	Session Topic and Discussion Theme		Value addition	
	1	Symmetry elements, symmetry operations	PowerPoint presentation		
	2	Symmetry elements, symmetry operations	PowerPoint presentation		
	3	Point groups and their symbols	PowerPoint presentation		
	4	Subgroups, classes, abelian and cyclic groups	PowerPoint presentation		
Unit 4 : Group Theory and Molecular Symmetry (18 hours)	5	Group multiplication tables	PowerPoint presentation	Assignment No: 1	
	7	Classes in a group and similarity transformation	PowerPoint presentation		
	8	Matrices: addition and multiplication of matrices	Lecture method		
	9	Inverse and orthogonal matrices, character of a matrix	Lecture method		
	First Internal Examination				
	10	block diagonalisation, matrix representation of symmetry operations	PowerPoint presentation		
	11	representation of groups by matrices,	Power Point Presentation		
	12	construction of representation using vectors and atomic orbitals as basis	Power Point Presentation		
	13	construction of representation using vectors and atomic orbitals as basis	Power Point Presentation		
	14	Statement of Great Orthogonality Theorem (GOT)	Power Point Presentation		
	15	Properties of irreducible representations.	Power Point Presentation		
	16	Construction of irreducible representation using GOT	Power Point Presentation		
	17	construction of character tables for C_{2v} , C_{2h} , C_3 , C_{3v} and C_{4v}	Power Point Presentation	Assignment No: 2	
	18	Direct product of representations	Power Point Presentation		
Unit 5: Application of group theory in Spectroscopy and	19	Applications in vibrational spectra	PowerPoint presentation		
	20	transition moment integral	Power Point Presentation		
	21	vanishing of integrals	Power Point Presentation		
	22	Symmetry aspects of molecular vibrations, vibrations of polyatomic molecules- selection rules for vibrational absorption..	Power Point Presentation		
	23	Determination of the symmetry of normal modes of H_2O , C_2H_4 ,	Power Point Presentation		
	24	Trans N_2F_2 , $CHCl_3$ and NH_3 using Cartesian coordinates and internal coordinates	PowerPoint presentation		
	25	Complementary character of IR and Raman spectra-determination of the IR and Raman active vibrational modes.	Power Point Presentation	Assignment No: 3	

	26	Application in electronic spectra: selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.	PowerPoint presentation	
	27	Applications in chemical bonding	Power Point Presentation	
		Second Internal Examination		
	28			
	29	Applications in chemical bonding	PowerPoint presentation	
	30	construction of hybrid orbitals with (1)H ₂ O (2), NH ₃	Power Point Presentation	
	31	(3) BF ₃ (4) CH ₄	Power Point Presentation	Assignment No: 4
	32	PCl ₅	Power Point Presentation	
	33	Transformation properties of atomic orbitals	Power Point Presentation	
	34	Symmetry adapted linear combinations (SALC).	Power Point Presentation	
	35	Revision	Power Point Presentation	
	36	MO diagram for water and ammonia	Power Point Presentation	Assignment No: 5
Text Books	<ul style="list-style-type: none"> • F.A. Cotton, <i>Chemical applications of Group Theory</i>, 3rd Edition, John Wiley & Sons Inc., 2003 • H. H. Jaffe and M. Orchin, <i>Symmetry in Chemistry</i>, John Wiley & Sons Inc., 1965. • A. Salahuddin Kunju & G. Krishnan, <i>Group Theory & its Applications in Chemistry</i>, PHI Learning Pvt. Ltd. 2010. • Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, <i>A Simple Approach to Group Theory in Chemistry</i>, Universities Press, 2008. • S.F.A. Kettle, <i>Symmetry and Structure: Readable Group Theory for Chemists</i>, 3rd Edn., Wiley, 2007 • K. Veera Reddy, <i>Symmetry & Spectroscopy of Molecules 2nd Edn.</i>, New Age International 2009 			