# Sacred Heart College (Autonomous)

## Department of Chemistry

## MSc Chemistry

## Course Plan

## Academic Year 2015 – 16

## Semester 1

| COURSE PLAN | | | | | |
|---|---|---|---|---|---|
| **ACADEMIC YEAR 2015 - 16** | | | | | |
| **PROGRAMME** | **:** | *M.Sc. Chemistry* | **LECTURE HOURS** | **:** | *72* |
| **SEMESTER** | **:** | *1* | **CREDITS** | **:** | *4* |
| **SUBJECT TITLE** | **:** | **ORGANOMETALLICS AND NUCLEAR CHEMISTRY** | **SUBJECT CODE** | **:** | **P1CHET01** |
| **COURSE TEACHERS** | **:** | ***Dr. Joseph John (JJ), Dr. Thommachan Xavuer (TX), Mr. Midhun Dominic C D (MD) & Mr. Senju Devassykutty*** | | | |
| **Course Objectives** | **:** | *1. Ability to understand the basics of organometallic compounds, their synthesis, structure and bonding*<br>*2. To understand the reactions and catalysis by organometallic compounds*<br>*3. To know about the synthesis of organometallic polymers*<br>*4. To understand the importance of inorganic chemicals in the field of biochemistry*<br>*5. Explore the field of nuclear chemistry* | | | |

| **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 | | |
| 3 | Mechanism of ion transport across membranes, | Lecture With power point presentation | |
| 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. | Conventional Lecture | |
| 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 *cis*-platin, radio-isotopes and MRI agents. | | |
| 17 | Toxic effects of metals (Cd, Hg, Cr and Pb). | | |
| 18 | Revision | | |

**Reference Text Books**


1. G. Wulfberg, 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 Mendelevium, 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 Wiiley and Sons, 2nd Ed.1981.<br>2. H.J. Arnikar, Essentials of Nuclear Chemistry, New Age International,4th Edn., 2011.<br>3. B.R Puri,L.R. Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Milestone,2011.<br>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 rules, cluster valence electrons. | | |
| 17 | Wade-Mingos rules, cluster valence electrons. | | |
| 18 | Revision | | |


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**


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 $Co_2(CO)_8$ catalyst in adipic ester synthesis. | | |
| **17** | Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop"). | | |
| **18** | Palladium catalysed oxidation of ethylene-the Wacker process. | | |

**Reference Text Books**


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.

| COURSE PLAN | | | | | |
|---|---|---|---|---|---|
| **ACADEMIC YEAR 2015 - 16** | | | | | |
| **PROGRAMME** | **:** | *M.Sc. Chemistry* | **LECTURE HOURS** | **:** | *72* |
| **SEMESTER** | **:** | *1* | **CREDITS** | **:** | *4* |
| **SUBJECT TITLE** | **:** | *Structural and Molecular Organic Chemistry* | **SUBJECT CODE** | **:** | *P1CHET02* |
| **COURSE TEACHERS** | **:** | *Dr. Joseph .T. Moolayil, Dr. V.S Sebastian, Dr. Franklin John, Dr. June Cyriac* | | | |
| **COURSE OUTCOMES (COs)** | **:** | | | | |
| **Instructional Hours** | **:** | *Four Hours per Week* | | | |

| | 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 oxidationof $2^0$ alcohols | | |
| | 18. | Chemical consequence of conformational equilibrium - Curtin-Hammett principle. | | |
| | 1. D. Nasipuri,*Stereochemistry of Organic Compounds: Principles and Applications*, Third Edition, New Age Publications, New Delhi, 2010.<br>2. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, 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 Cn | | |
| | 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 assymetric synthesis. | | |
| | 34. | Stereoisomerism-configuration and conformational stereoisomers | | |
| | 35. | Geometrical isomerism: E-Z notation, Methods of determination of geometrical isomers | | |
| | 36. | Interconversion of geometrical isomers | | |

| | |
|---|---|
| ***Text Books*** | 3. D. Nasipuri,*Stereochemistry of Organic Compounds: Principles and Applications*, Third Edition, New Age Publications, New Delhi, 2010.<br>4. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994. |

| | | | | |
|---|---|---|---|---|
| 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. | Continnued | | |
| | 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<br>6. R. Bruckner, *Advanced Organic Chemistry*: Reaction Mechanisms, Academic Press, 2002.<br>7. F. A. Carey and R. A. Sundberg, *Advanced Organic Chemistry*, Part A: Structure and Mechanisms, Fifth Edition, Springer, New York, 2007.<br>8. J.Clayden, N.Greeves, S.Warren, P.Wothers, *Organic Chemistry*, 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.<br>Photoreactions of carbonyl compounds: Norrish reactions of acyclic ketons | | |
| | 64. | Cyclic ketones. | | |
| | 65. | Patterno-Buchi reaction. | | |
| | 66. | Barton reaction and photo reduction of ketones. | | |
| | 67. | Di-π-methane reaction | | |
| | 68. | Photochemistry of Nitro and Azo groups.<br>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 Hammet equation, Taft equation, cross-over experiments, Hammond postulates. | | |


9. J.Clayden, N.Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.
10. Aditi Sangal, *Krishna's Advanced Organic Chemistry*; Volume 1 – Krishna Prakashn Media(P) Ltd.
11. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, Second Edition, Harper & Row, New York, 1981.
12. N. S. Isaacs, *Physical Organic Chemistry*, ELBS, Longman, UK, 1987.
13. Jack Hine,*Physical Organic Chemistry*, McGraw-Hill; 2nd Edition,1962.
14. *Anslyn, E. V.; Dougherty, D. A. Modern Physical Organic Chemistry, University Science Books, 2006*
15. N. J. Turro, V. Ramamurthy and J. C. Scaiano, *Principles of Molecular Photochemistry: An Introduction*, University Science books 2009.
16. N.J Turro, *Modern Molecular Photochemistry*, Benjamin Cummings Publishing Company, Menlopark, 1978.
17. K.K.R.Mukherjee, *Fundamentals of Photochemistry*, New Age Publications, New Delhi, 1978.

| DEPARTMENT OF CHEMISTRY, SACRED HEART COLLEGE (AUTONOMOUS), THEVARA | | | | | |
|---|---|---|---|---|---|
| **COURSE PLAN : ACADEMIC YEAR 2015 - 2016** | | | | | |
| **PROGRAMME** | **:** | *M.Sc. Chemistry* | **SEMESTER** | **:** | *1* |
| **LECTURE HOURS** | **:** | *54* | **CREDITS** | **:** | *3* |
| **SUBJECT TITLE** | **:** | *Classical and Statistical Thermodynamics* | **SUBJECT CODE** | **:** | *CH1C04* |
| **COURSE TEACHERS** | **:** | Dr. K. B. Jose (KBJ), Dr. Jinu George (JG), Dr. Ignatious Abraham (IGA) | | | |
| **Instructional Hours** | **:** | *Tuesday : Period 1 (9:30 to 10:30 am) - KBJ*<br>*Wednesday : Period 1 (9:30 to 10:30 am) - JG*<br>*Thursday : Period 5 (2:30 to 3:30 pm) - IGA* | | | |

| IGNATIOUS 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:**


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, Physiacl 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 2015 - 16** | | | | | |
| **PROGRAMME** | **:** | *M.Sc. Chemistry* | **LECTURE HOURS** | **:** | *72 hours* |
| **SEMESTER** | **:** | *1* | **CREDITS** | **:** | *3* |
| **SUBJECT TITLE** | **:** | *Quantum Chemistry and Group Theory* | **SUBJECT CODE** | **:** | *16P1CHET04* |
| **COURSE TEACHERS** | **:** | *Dr. Jorphin Joseph(JRJ), Dr. Abi T.G. (ATG)* | **INSTRUCTIONAL HOURS/WEEK** | : | *4 hours* |
| **COURSE OBJECTIVES** | **:** | To make the student<br>01 - Learn the basic principles and concepts of quantum mechanics like operators, observables, probabilities, amplitudes, average values etc.<br>02 - Understand how to solve the Schrodinger equation for model systems and relate these to different atomic/molecular phenomena.<br>03 - Recognize symmetry elements in a molecule, state the point group a molecule belongs to and understand degenerate and non-degenerate representations<br>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 (Lx, Ly, Lz and L2)-commutation relations between these operators. | Lecture method | |
| | 22 | Spherical harmonics as eigen functions of angular momentum operators Lz 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** | • I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.<br>• P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 4th Edition, Oxford University Press, 2005<br>• Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983<br>• J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993<br>• A.K. Chandra, *Introduction to Quantum Chemistry*, 4th Edition, Tata McGraw-Hill, 1994<br>• R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006<br>• Jack Simons, *An Introduction to Theoretical Chemistry*, 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 orthogonalmatrices, character of a matrix | Lecture method | |
| | **First Internal Examination** | | | |
| | 10 | block diagonalisation, matrix representation ofsymmetry 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 OrthogonalityTheorem (GOT) | Power Point Presentation | |
| | 15 | Properties of irreducible representations. | Power Point Presentation | |
| | 16 | Construction ofirreducible representation using GOT | Power Point Presentation | |
| | 17 | construction of character tables for C2v,C2h, C3, C3v and C4v | 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 polyatomicmolecules-selection rules for vibrational absorption.. | Power Point Presentation | |
| | 23 | Determination of thesymmetry of normal modes of $H_2O$, $C_2H_4$, | Power Point Presentation | |
| | 24 | Trans $N_2F_2$,$CHCl_3$and $NH_3$ using Cartesiancoordinates 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)$H_2O$ (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** | • F.A. Cotton, *Chemical applications of Group Theory*, 3rd Edition, John Wiley &Sons Inc., 2003<br>• H. H. Jaffe and M. Orchin, *Symmetry in Chemistry*, John Wiley &Sons Inc., 1965.<br>A. Salahuddin Kunju & G. Krishnan, *Group Theory & its Applications in Chemistry*, PHI Learning Pvt. Ltd. 2010.<br>• Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.<br>• S.F.A. Kettle, Symmetry and Structure: Readable Group Theory for Chemists, 3rd Edn.**,**Wiley, 2007<br>• K.Veera Reddy, *Symmetry & Spectroscopy of Molecules 2nd Edn.*, New Age International 2009 | | | |