# SACRED HEART COLLEGE (AUTONOMOUS)

## Department of Chemistry

## MSc Chemistry - Pharmaceutical

**Course Plan**

**Academic Year 2018-19**

**Semester One**

## PROGRAMME OUTCOMES

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|---|---|
| **PO 1** | The students are capable of exercising their critical thinking in creating new knowledge leading to innovation, entrepreneurship and employability. |
| **PO 2** | The students are able to effectively communicate the knowledge of their study and research in their respective disciplines to their employers and to the society at large. |
| **PO 3** | The students are able to make choices based on the values upheld by the college, and have the readiness and know-how to preserve environment and work towards sustainable growth and development. |
| **PO 4** | The students possess an ethical view of life, and have a broader (global) perspective transcending the provincial outlook. |
| **PO 5** | The students possess a passion for exploring new knowledge independently for the development of the nation and the world and are able to engage in a lifelong learning process. |

## PROGRAMME SPECIFIC OUTCOMES

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| ***Knowledge and Understanding*** | |
| **PSO1** | Demonstrate an in-depth knowledge and understanding of the principles of Inorganic, Organic, Physical and Theoretical Chemistry. |
| **PSO2** | Demonstrate an awareness of the relevance of chemistry in a wider multi-disciplinary context. |
| ***Intellectual Abilities*** | |
| **PSO3** | Apply their understanding in Chemistry to design solutions to unfamiliar problems in Chemistry and those involving other related disciplines. |
| **PSO4** | Use their knowledge and understanding to conceptualize appropriate models and representations. |
| ***Practical Skills*** | |
| **PSO5** | Design and conduct analytical, modelling and experimental investigations in Inorganic, Organic, Physical and Theoretical Chemistry. |
| ***Professional Skills*** | |
| **PSO6** | Ability to identify, design and conduct appropriate experiments, interpret data obtained, draw pertinent conclusions and communicate all these effectively. |

**COURSE STRUCTURE**

| Course Code | Title Of The Course | No. Hrs./Week | Credits | Total Hrs./Sem |
|---|---|---|---|---|
| 16P1CPHT01 | Inorganic Chemistry I | 4 | 4 | 72 |
| 16P1CPHT02 | Basic Organic Chemistry | 4 | 4 | 72 |
| 16P1CPHT03 | Physical Chemistry I | 3 | 3 | 54 |
| 16P1CPHT04 | Quantum Chemistry and Group Theory | 4 | 3 | 72 |

**COURSE 1**

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|---|---|---|---|
| **PROGRAMME** | **M.SC. APPLIED CHEMISTRY - PHARMACEUTICAL** | **SEMESTER** | **1** |
| **COURSE CODE AND TITLE** | **16P1CPHT01 AND INORGANIC CHEMISTRY I** | **CREDIT** | **4** |
| **HOURS/WEEK** | **4** | **HOURS/SEM** | **72** |
| **FACULTY NAME** | **DR. RAMAKRISHNAN S (RKS), DR. THOMMACHAN XAVIER (TX), MR. MIDHUN DOMINIC C D (MDCD) & MR. SENJU DEVASSYKUTTY (SD)** | | |

| | COURSE OUTCOME | POS / PSOS | CL |
|---|---|---|---|
| **CO1** | Explain stability of organometallic compounds and clusters, and their application as industrial catalysts. | PO 1<br>PSO 4 | A |
| **CO2** | Describe the key concepts of inorganic and organometallic chemistry including those related to synthesis, reaction chemistry, and structure and bonding. | PO 1<br>PSO 1 | U |
| **CO3** | Demonstrate a systematic understanding of the key aspects of nuclear chemistry and their analytical applications. | PO 1<br>PSO 1 | U |
| **CO4** | Recognize and explain the interaction of different metal ions with biological ligands. | PO 1<br>PSO 1 | U |

CL* Cognitive Level

**CO -PO/PSO Mapping**

| | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CO1 | 2 | | | | | | | | | 1 | | |
| CO2 | 3 | | | | | | 2 | | | | | |
| CO3 | 3 | | | | | | 1 | | | | | |
| CO4 | 2 | | | | | | 1 | | | | | |

| **UNIT 1: ORGANOMETALLIC COMPOUNDS-SYNTHESIS, STRUCTURE AND BONDING (18H)** | | | | |
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| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 1. | Introduction to organometallic compounds. Hapto nomenclature of organometallic compounds and 16 and 18 electron rule | Conventional Lecture using Chalk and Board and ICT -PPT | Q & A Session | CO1 |
| 2. | Organometallic compounds with linear pi donor ligands-olefins - synthesis, structure and bonding. | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 3. | Organometallic compounds with linear pi donor ligands- acetylenes, synthesis, structure and bonding. | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 4. | Organometallic compounds with linear pi donor ligands-dienes synthesis, structure and bonding. | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 5. | Organometallic compounds with linear pi donor ligands-allyl complexes-synthesis, structure and bonding | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 6. | Complexes with cyclic pi donors-metallocenes and structure and bonding. | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 7. | Complexes with cyclic pi donors cyclic arene complexes structure and bonding. | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 8. | Metal carbene and alkylidenes, carbine and alkylidynes complexes, Fisher- type and Schrock- type complexes. | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 9. | Revision | Chalk and Board | | CO1 |
| 10. | Metal Carbonyls: CO- as a π acid ligand, synergism, Molecular electronic structure and18-electron rule | Conventional Lecture using Chalk and Board | | CO1 |
| 11. | Binary Carbonyl complexes-Mononuclear and Binuclear | Conventional Lecture using Chalk and Board | | CO1 |

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| | carbonyls. Preparation, properties, structure, bonding in metal carbonyls | | | |
| 12. | Bridging modes of CO, Polynuclear metal carbonyls with and without bridging, oxygen bonded metal carbonyls | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 13. | Ligands similar to CO- Cyanide, nitrosyls, dinitrogen, Hydrogen and dihydrogen complexes | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 14. | Carbonyl clusters-LNCCS and HNCCS | Conventional Lecture using Chalk and Board | | CO1 |
| 15. | Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons. | Conventional Lecture using Chalk and Board and ICT -PPT | | CO1 |
| 16. | Wade-Mingos rules, cluster valence electrons. | Conventional Lecture using Chalk and Board | | CO1 |
| 17. | Wade-Mingos rules, cluster valence electrons. | Conventional Lecture using Chalk and Board | | CO1 |
| 18. | Revision | Chalk and Board | quiz | CO1 |
| **UNIT 2: REACTIONS AND CATALYSIS OF ORGANOMETALLIC COMPOUNDS (18H)** | | | | |
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 19. | Substitution reactions-nucleophilic ligand substitution | Conventional Lecture | Q & A Session | CO2 |
| 20. | Nucleophilic and electrophilic attack on coordinated ligands. Carbonylate anions as nucleophiles. | Conventional Lecture | | CO2 |
| 21. | Addition and elimination reactions-1,2 additions to double bonds | Conventional Lecture | | CO2 |
| 22. | Carbonylation and decarbonylation | Conventional Lecture | | CO2 |
| 23. | Oxidative addition and reductive elimination, | Conventional Lecture | | CO2 |
| 24. | Insertion (migration) and elimination reactions. | Conventional Lecture | | CO2 |
| 25. | Rearrangement reactions | Conventional Lecture | | CO2 |
| 26. | Redistribution reactions, fluxional isomerism. | Conventional Lecture | | CO2 |
| 27. | Revision | Conventional Lecture | Quiz | CO2 |

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| 28. | Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops | Conventional Lecture | | CO2 |
| 29. | Reactions of carbon monoxide and hydrogen-the water gas shift reaction | Conventional Lecture | | CO2 |
| 30. | Reactions of carbon monoxide and hydrogen-the Fischer-Tropsch reaction(synthesis of gasoline). | Conventional Lecture | | CO2 |
| 31. | Hydroformylation of olefins using cobalt or rhodium catalyst. Synthesis of diethyhexylphthalate. | Conventional Lecture | | CO2 |
| 32. | Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts. | Conventional Lecture | | CO2 |
| 33. | Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using Co2(CO)8 catalyst in adipic ester synthesis | Conventional Lecture | | CO2 |
| 34. | Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop"). | Conventional Lecture | | CO2 |
| 35. | Palladium catalysed oxidation of ethylene-the Wacker process. | Conventional Lecture | | CO2 |
| 36. | Revision | Conventional Lecture | Quiz | CO2 |
| **UNIT 3 : NUCLEAR CHEMISTRY (18H)** | | | | |
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 37. | Introduction to Nuclear Chemistry | Conventional Lecture | Q & A Session | CO3 |
| 38. | Radioactive decay. Alpha decay-Alpha ray spectrum, Beta decay-Types of beta decay, β+, β-, β-ray spectrum | Conventional Lecture | | CO3 |
| 39. | Neutrino antineutrino and Positron emission, Dirac theory, pair production, positron-electron annihilation | Conventional Lecture | | CO3 |
| 40. | Electron capture, double β decay. Gamma decay- de-excitation of excited molecules, change of Energy, spin, parity during photon emission | Conventional Lecture | | CO3 |

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| 41. | Nuclear isomerism and isomeric transition, internal conversion, auger electrons and auger effect | Conventional Lecture | | CO3 |
| 42. | Nuclear reactions. Q-Value and reaction threshold, reaction cross section-definition, and units | Conventional Lecture | | CO3 |
| 43. | Cross section and reaction rate, neutron capture cross section, variation of neutron cross section with energy( 1/V law) | Conventional Lecture | | CO3 |
| 44. | Photonuclear, Thermonuclear and Fusion reactions, Magnetic confinement, internal confinement. | Conventional Lecture | | CO3 |
| 45. | Nuclear fission - Fission fragment and mass distribution, fission yield, fission energy, fission cross section and threshold, fission neutrons, prompt and delayed neutrons, fission by high energy neutrons. | Conventional Lecture | | CO3 |
| 46. | Nuclear Reactors. Fissile and fissionable nuclei, fast and thermal neutrons | Conventional Lecture | | CO3 |
| 47. | Terms and symbols used in reactor technology- average no. of fission neutrons, fast fission factor, fast neutrons loss factor | Conventional Lecture | | CO3 |
| 48. | Terms and symbols used in reactor technology- Resonance capture, thermal neutrons loss factor, thermal utilization factor, relative fission cross section, reproduction factor, critical size of reactor. Breeder reactor, fast breeder test reactor. | Conventional Lecture | | CO3 |
| 49. | Terms and symbols used in reactor technology- Reproduction factor, critical size of reactor. Breeder reactor, fast breeder test reactor. | Conventional Lecture | | CO3 |
| 50. | Reactor Safety precaution, Management of radioactive waste- Low level Waste, Intermediate level Waste, High level Waste. | Conventional Lecture | | CO3 |
| 51. | Principles of counting techniques- G.M. counter, proportional, ionization and scintillation counters. | Conventional Lecture | | CO3 |
| 52. | Applications of radioisotopes. Physico-chemical study-Solubility of sparingly soluble salts | Conventional Lecture | Q & A Session | CO3 |

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| 53. | Applications of radioisotopes. Analytical applications-Isotope dilution analysis, radiometric titrations, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry. | Conventional Lecture | | CO3 |
| 54. | Applications of radio isotopes medicine-Thyroiditis, Tumour identification, Determination of volume of blood in patient | Conventional Lecture | | CO3 |
| **UNIT 4 : BIOINORGANIC CHEMISTRY (18H)** | | | | |
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 55. | Biochemistry of Iron Oxygen Carriers- Structure and functions of haemoglobin and myoglobin | Conventional Lecture Chalk & Board | | CO4 |
| 56. | Oxygen transport mechanism of Hemoglobin, cooperativity in haemoglobin. | Lecture With power point presentation | | CO4 |
| 57. | Bohr effect and phosphate effect. Hemerythrin Structure and function. | Lecture With power point presentation | | CO4 |
| 58. | Redox Metalloenzymes-Cytochromes, Classification, Structure and function . | Lecture With power point presentation | | CO4 |
| 59. | Role in Oxidative Phosphorylation of ADP to ATP. Iron Sulphur Proteins-Rubredoxin, Ferredoxin | Conventional Lecture | | CO4 |
| 60. | Nitrogenase, Structure and function, Nitrogen Fixation. Peroxidases and catalases | Conventional Lecture | | CO4 |
| 61. | Cytochrome P450- Structure and functions. Storage and transport of iron in biological systems-Ferritin, transferrin and Siderophores | Conventional Lecture | | CO4 |
| 62. | Biochemistry of Zn and Copper. Structure and functions of carboxypeptidase and carbonic anhydrase | Conventional Lecture | | CO4 |
| 63. | Superoxide dismutase. Structure and functions of various Copper proteins and enzymes. | Conventional Lecture | | CO4 |
| 64. | Blue copper proteins (Type-1) - Electron transfer agents - Plastocyanin, Stellacyanin and Azurin. | Conventional Lecture | | CO4 |

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| 65. | Blue copper Enzymes (Type II) - Ascorbateoxidase, Laccase and ceruloplsmin. | Conventional Lecture | | CO4 |
| 66. | Non Blue copper enzyme (Type III) - Cytochrome oxidase, Amine oxidases, Structure and functions of Hemocyanin. | Conventional Lecture | | CO4 |
| 67. | Vitamin $B_{12}$- Structure and biological importance | Conventional Lecture | | CO4 |
| 68. | Chlorophyll-Photosynthesis, PS I & PS II. | Conventional Lecture | | CO4 |
| 69. | Therapeutic applications of cis-platin, Mechanism of action, MRI agents | Conventional Lecture | | CO4 |
| 70. | Mechanism of muscle contraction, blood clotting mechanism. | Conventional Lecture | | CO4 |
| 71. | Essential and trace elements in biological systems, Toxic effects of metals (Cd, Hg, Cr and Pb) | Conventional Lecture | Q & A Session | CO4 |
| 72. | Mechanism of ion transport across membranes, Sodium Potassium pump. | Conventional Lecture | | CO4 |

**INDIVIDUAL ASSIGNMENTS/SEMINAR – DETAILS & GUIDELINES**

| | **Date of completion** | **Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc.)** | **Course Outcome** |
|---|---|---|---|
| 1 | 18/08/18 | Assignment on Redox metalloenzymes, blue copper proteins | CO4 |
| 2 | 22/08/18 | Application of metal carbonyls and organometallic compounds | CO2 |

**GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES**

| | **Date of completion** | **Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc.)** | **Course Outcome** |
|---|---|---|---|
| 1 | 02/08/18 | Application of: Radioactivity Fission & fusion | CO3 |

**REFERENCES**


- G. Wulfberg, Inorganic Chemistry, Ind. Edition, Viva, 2014.
- Shiver & Atkins, Inorganic Chemistry, 4th Edn. Oxford University Press, 2006.
- K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Cengage Learning 2nd Edn., 2014.
- J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and

Reactivity, 4th Edn., Pearson Education India, 2006.
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- G.L. Miessler, D. A. Tarr, Inorganic Chemistry 3rd Ed., Pearson Education, 2007.
- B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
- I. Bertini,H. B Gray, S. J Lippard, J. S Valentine, Bioinorganic Chemistry.
- G. Friedlander,J.W.Kennedy,E.S.Macias,and J.M. Miller, Nuclear and Radiochemistry, John Wiley and Sons, 2nd Ed.1981.
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- S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.
- J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers, 1993.
- F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999.
- K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
- P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988.
- B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
- B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

**COURSE 2**

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| **PROGRAMME** | **M.SC. APPLIED CHEMISTRY - PHARMACEUTICAL** | **SEMESTER** | **1** |
| **COURSE CODE AND TITLE** | **16P1CPHT02 AND BASIC ORGANIC CHEMISTRY** | **CREDIT** | **4** |
| **HOURS/WEEK** | **4** | **HOURS/SEM** | **72** |
| **FACULTY NAME** | **DR. JOSEPH .T. MOOLAYIL (JTM), DR. V.S SEBASTIAN(VSS), DR. FRANKLIN JOHN (FJ) , DR. JUNE CYRIAC (JUC)** | | |

| | COURSE OUTCOME | POS / PSOS | CL |
|---|---|---|---|
| **CO1** | Explain the basic concepts of organic chemistry. | PO 1<br>PSO 1 | R |
| **CO2** | Illustrate the principles of physical organic chemistry. | PO 1<br>PSO 1 | U |
| **CO3** | Demonstrate the reactivity and stability of organic molecules based on structure, including conformation and stereochemistry. | PO 1<br>PSO 3 | U |
| **CO4** | Recognize the importance of organic photochemical reactions. | PO 1<br>PSO 4 | U |

CL* Cognitive Level

**CO -PO/PSO Mapping**

| | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CO1 | 2 | | | | | | 2 | | | | | |
| CO2 | 3 | | | | | | 2 | | | | | |
| CO3 | 3 | | | | | | | | 2 | | | |
| CO4 | | | | | | | | | | 1 | | |

| **UNIT 1: BASIC CONCEPTS IN ORGANIC CHEMISTRY (12H)** | | | | |
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| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 1. | IUPAC nomenclature of polycyclic, heterocyclic | Conventional Lecture | Q & A Session | CO 1 |
| 2. | Benzenoid, non-benzenoid and spiro compounds. | Conventional Lecture | | CO 1 |
| 3. | Review of basic concepts in organic chemistry: Electron displacement effects-inductive effect | Conventional Lecture | | CO 1 |
| 4. | Electrometric effect, resonance effect, hyperconjugation, steric effect. Steric inhibition of resonance. | Conventional Lecture | | CO 1 |
| 5. | Bonding weaker than covalent bonding-H-bonding, π- π interactions. | Conventional Lecture | | CO 1 |
| 6. | Other non-covalent interactions | Conventional Lecture | | CO 1 |
| 7. | Concept of aromaticity: delocalization of electrons –Huckel's rule | Conventional Lecture | Q & A Session | CO 1 |
| 8. | Craig rule- criteria for aromaticity - examples of neutral and charged aromatic systems, | Conventional Lecture | | CO 1 |
| 9. | Annulenes [10], [14], [18], [22] | Conventional Lecture | | CO 1 |
| 10. | Tropolone, Azulene. NMR as a tool for aromaticity | Conventional Lecture | | CO 1 |
| 11. | Anti- and homo-aromatic systems– Alternate and non-alternate hydrocarbons | Conventional Lecture | | CO 1 |
| 12. | Fullerenes, Carbon nanotubes and Graphene. | Conventional Lecture | Quiz | CO 1 |
| **Teacher II – JUC : Unit 2: Physical Organic Chemistry (11h)** | | | | |
| 13. | Energy profiles. Hammond postulate | Conventional Lecture | | CO 2 |

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| 14. | Kinetic versus thermodynamic control of product formation | Conventional Lecture | | CO 2 |
| 15. | Captodative effect –- kinetic isotope effects with examples | Conventional Lecture | | CO 2 |
| 16. | Continued | Conventional Lecture | | CO 2 |
| 17. | Stereochemical studies-use of isotopes, Hammet equation | Conventional Lecture | Q & A Session | CO 1 |
| 18. | Taft equation, cross-over experiments, Hammond postulates. | Conventional Lecture | | CO 2 |
| 19. | Salt and Solvent effect. | Conventional Lecture | | CO 2 |
| 20. | Intermediates *vs*. Transition state, linear free energy relationship. | Conventional Lecture | | CO 2 |
| 21. | Introduction to carbon acids - $pK_a$ of weak acids | Conventional Lecture | | CO 2 |
| 22. | Kinetic and thermodynamic acidity. | Conventional Lecture | | CO 2 |
| 23. | Introduction to organic bases- $pK_b$ of weak bases. | Conventional Lecture | Q & A Session | CO 1 |
| **Teacher III – FJ : Unit 3 : Review of basic reaction mechanisms (8h)** | | | | |
| 24. | Mechanism of SN1, SNAr | Conventional Lecture | | CO 3 |
| 25. | SRN1 and Benzyne mechanisms. | Conventional Lecture | | CO 3 |
| 26. | Catalysis by acids and bases | Conventional Lecture | | CO 3 |
| 27. | Nucleophiles with examples from acetal, cyanohydrin | Conventional Lecture | Q & A Session | CO 1 |
| 28. | Ester formation and hydrolysis reactions –$A_{AC}^2$ mechanisms | Conventional Lecture | | CO 3 |
| 29. | $A_{AC}^1$ mechanism. | Conventional Lecture | | CO 3 |
| 30. | $A_{AL}^1$, $B_{AC}^2$ mechanisms. | Conventional Lecture | | CO 3 |
| 31. | $B_{AL}^1$ mechanism. | Conventional Lecture | Quiz | CO 3 |
| **Teacher IV – VSS : Unit 4: Stereochemistry of Organic Compounds (15h)** | | | | |
| 32. | Introduction to molecular symmetry and chirality – examples from common objects to molecules | Conventional Lecture | Q & A Session | CO 1 |
| 33. | Axis, plane, centre, alternating axis of symmetry. | Conventional Lecture | | CO 3 |
| 34. | Centre of chirality – molecules with C, N, S based chiral centres | Conventional Lecture | | CO 3 |
| 35. | Absolute configuration - enantiomers | Conventional Lecture | | CO 3 |

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| 36. | Racemic modifications - R and S nomenclature using Cahn-Ingold-Prelog rules | Conventional Lecture | | CO 3 |
| 37. | Continued | Conventional Lecture | | CO 3 |
| 38. | Molecules with a chiral centre and Cn | Conventional Lecture | | CO 3 |
| 39. | Molecules with more than one center of chirality | Conventional Lecture | | CO 3 |
| 40. | Definition of diastereoisomers constitutionally symmetrical and unsymmetrical chiral molecules | Conventional Lecture | | CO 3 |
| 41. | Erythro, threo nomenclature. | Conventional Lecture | Q & A Session | CO 1 |
| 42. | Axial, planar and helical chirality – examples | Conventional Lecture | | CO 3 |
| 43. | Stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls | Conventional Lecture | | CO 3 |
| 44. | Ansa and cyclophanic compounds, spirans, exo-cyclic alkylidenecycloalkenes. Identification of enantiotopic, homotopic, diastereotopic hydrogens | Conventional Lecture | | CO 3 |
| 45. | Prochirality, Topicity and prostereoisomerism – topicity of ligands and faces, and their nomenclature. | Conventional Lecture | Quiz | CO 3 |
| 46. | NMR distinction of enantiotopic/diastereotopic ligands. Stereospecific, stereoselective and assymetric synthesis. | Conventional Lecture | | CO 3 |
| **Teacher V – JTM : Unit 5: Conformational Analysis (20h)** | | | | |
| 47. | Stereoisomerism: Definition based on symmetry and energy criteria | Conventional Lecture | Q & A Session | CO 1 |
| 48. | Configuration and conformational stereoisomers. | Conventional Lecture | | CO 3 |
| 49. | Conformational descriptors | Conventional Lecture | | CO 3 |
| 50. | Factors affecting conformational stability of molecules. | Conventional Lecture | | CO 3 |
| 51. | Potential energy diagrams | Conventional Lecture | | CO 3 |
| 52. | Conformational analysis of acyclic systems: substituted ethanes | Conventional Lecture | | CO 3 |
| 53. | Aldehydes | Conventional Lecture | Q & A Session | CO 1 |

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| 54. | Ketones and olefins. | Conventional Lecture | | CO 3 |
| 55. | Conformational analysis of cyclic systems | Conventional Lecture | | CO 3 |
| 56. | Cyclohexane and its derivatives. Cyclohexanone. | Conventional Lecture | | CO 3 |
| 57. | Continued | Conventional Lecture | | CO 3 |
| 58. | Conformational analysis of Fused and bridged bicyclic systems | Conventional Lecture | Quiz | CO 3 |
| 59. | Decalins, adamantane | Conventional Lecture | | CO 3 |
| 60. | Hexamethylene diamine and congressane | Conventional Lecture | | CO 3 |
| 61. | Conformation of sugars-glucose, sucrose and lactose | Conventional Lecture | | CO 3 |
| 62. | Conformation and reactivity of elimination -dehalogenation | Conventional Lecture | | CO 3 |
| 63. | Dehydrohalogenation | Conventional Lecture | | CO 3 |
| 64. | Dehydration, semipinacolic deamination and pyrolytic elimination | Conventional Lecture | | CO 3 |
| 65. | Saytzeff and Hofmann eliminations, substitution and oxidation of $2^0$ alcohols. | Conventional Lecture | | CO 3 |
| 66. | Chemical consequence of conformational equilibrium - Curtin-Hammett principle. | Conventional Lecture | | CO 3 |
| **Teacher VI – JUC : Unit 6: Organic Photochemistry (6h)** | | | | |
| 67. | Jablonski diagram, triplet and singlet states.<br>Photoreactions of carbonyl compounds: Norrish reactions of acyclic ketones | Conventional Lecture | Q & A Session | CO 1 |
| 68. | Cyclic ketones. | Conventional Lecture | | CO 4 |
| 69. | Patterno-Buchi reaction. | Conventional Lecture | | CO 4 |
| 70. | Barton reaction and photo reduction of ketones. | Conventional Lecture | Quiz | CO 4 |
| 71. | Di-π-methane reaction | Conventional Lecture | | CO 4 |
| 72. | Photochemistry of Nitro and Azo groups.<br>Photochemistry of vision | Conventional Lecture | | CO 4 |

**INDIVIDUAL ASSIGNMENTS/SEMINAR – DETAILS & GUIDELINES**

| | Date of completion | Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc) | Course Outcome |
|---|---|---|---|
| 1 | 11/8/18 | IUPAC nomenclature of polycyclic, heterocyclic | CO 1 |
| 2 | 20/8/18 | Racemic modifications - R and S nomenclature using Cahn-Ingold-Prelog rules | CO 3 |

**GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES**

| | Date of completion | Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc) | Course Outcome |
|---|---|---|---|
| 1 | 02/8/18 | Non-covalent interactions | CO 1 |

**REFERENCES**


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- E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994
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**COURSE 3**

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| **PROGRAMME** | **M.SC. APPLIED CHEMISTRY - PHARMACEUTICAL** | **SEMESTER** | **1** |
| **COURSE CODE AND TITLE** | **16P1CPHT03 AND PHYSICAL CHEMISTRY – I** | **CREDIT** | **3** |
| **HOURS/WEEK** | **3** | **HOURS/SEM** | **54** |
| **FACULTY NAME** | **DR. K. B. JOSE (KBJ), DR. JINU GEORGE (JG), DR. IGNATIOUS ABRAHAM (IGA)** | | |

| | **COURSE OUTCOME** | **POS / PSOS** | **CL** |
|---|---|---|---|
| **CO1** | Application of mathematical tools to calculate thermodynamic and kinetic properties. | PO 1<br>PSO 3 | A |
| **CO2** | Explain the relationship between microscopic properties of molecules with macroscopic thermodynamic observables. | PO 1<br>PSO 2 | U |
| **CO3** | Explain the kinetic behaviour of gases and their transport properties. | PO 1<br>PSO 4 | U |

CL* Cognitive Level

**CO -PO/PSO Mapping**

| | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CO1 | 2 | | | | | | | | 3 | | | |
| CO2 | 3 | | | | | | | 2 | | | | |
| CO3 | 3 | | | | | | | | | 1 | | |

| **Teacher I – JG and IGA : Unit 1 : CLASSICAL THERMODYNAMICS (9h)** | | | | |
|---|---|---|---|---|
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 1. | Entropy - Free energy, Clausius Inequality, Maxwell's relations – significance. Partial molar properties – Chemical potential, Fugacity and Activity. | Chalk and board | Q & A Session | CO 1 |
| 2. | Thermodynamic functions of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law. | Chalk and board | | CO 1 |
| 3. | Excess thermodynamic functions-free energy, enthalpy, entropy and volume. Chemical affinity and thermodynamic | Chalk and board | | CO 1 |

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| | functions | | | |
| 4. | Nernst heat theorem, development of third law of thermodynamics, determination of absolute entropies using third law, entropy changes in chemical reactions. | Chalk and board | | CO 1 |
| 5. | Effect of temperature and pressure on chemical equilibrium- van't Hoff equations | Chalk and board | | CO 1 |
| 6. | Three component systems: Gibbs phase rule, graphical representation of three component systems. | Chalk and board | Quiz | CO 1 |
| 7. | Solid-liquid equilibria, ternary solutions with common ions Hydrate formation, compound formation. | Chalk and board | | CO 1 |
| 8. | Liquid-liquid equilibria-one pair of partially miscible liquids | Chalk and board | | CO 1 |
| 9. | Two pairs of partially miscible liquids, three pairs of partially miscible liquids. | Chalk and board | | CO 1 |
| **Teacher II – JG and IGA : Unit 2: Thermodynamics of Irreversible Processes & Bioenergetics (10h)** | | | | |
| 10. | Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. | Chalk and board | Q & A Session | CO 1 |
| 11. | Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations. | Chalk and board | | CO 1 |
| 12. | The Onsager reciprocal relations - principle of microscopic reversibility. | Chalk and board | | CO 1 |
| 13. | Electrokinetic phenomena. | Chalk and board | | CO 1 |
| 14. | Thermoelectric phenomena | Chalk and board | Quiz | CO 1 |
| 15. | Bioenergetics: Coupled reactions, ATP and its role in bioenergetics. | Power point presentation | | CO 1 |
| 16. | High energy bond, free energy and entropy change in ATP hydrolysis. | Power point presentation | | CO 1 |
| 17. | Thermodynamic aspects of metabolism and respiration | Power point presentation | | CO 1 |
| 18. | Thermodynamic aspects of glycolysis and biological redox reactions. | Power point presentation | | CO 1 |
| 19. | Revision | Power point presentation | Quiz | CO 1 |
| **Teacher III – KBJ : Unit 3 : STATISTICAL THERMODYNAMICS (27h)** | | | | |
| 20. | Permutation, probability, apriori and thermodynamic probability. | Chalk and board | | CO 2 |

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| 21. | Stirlings approximation, macrostates and microstates. | Chalk and board | | CO 2 |
| 22. | Boltzmann distribution law | Chalk and board | Q & A Session | CO 2 |
| 23. | Partition function and its physical significance | Chalk and board | | CO 2 |
| 24. | Phase space, different ensembles | Chalk and board | | CO 2 |
| 25. | Canonical partition function, distinguishable and indistinguishable molecules | Chalk and board | | CO 2 |
| 26. | Partition function and thermodynamic functions | Chalk and board | | CO 2 |
| 27. | Separation of partition function | Chalk and board | | CO 2 |
| 28. | Translational and rotational partition functions. | Chalk and board | | CO 2 |
| 29. | Vibrational and electronic partition functions. | Chalk and board | | CO 2 |
| 30. | Thermal de-Broglie wavelength. Calculation of thermodynamic functions and equilibrium constants. | Chalk and board | | CO 2 |
| 31. | Statistical interpretation of work and heat | Chalk and board | | CO 2 |
| 32. | Sakur-Tetrode equation | Chalk and board | | CO 2 |
| 33. | Statistical formulation of third law of thermodynamics | Chalk and board | | CO 2 |
| 34. | Thermodynamic probability and entropy, residual entropy | Chalk and board | Quiz | CO 2 |
| 35. | Heat capacity of gases - classical and quantum theories | Chalk and board | | CO 2 |
| 36. | Heat capacity of hydrogen | Chalk and board | | CO 2 |
| 37. | Heat capacity of solids- the vibrational properties of solids | Chalk and board | | CO 2 |
| 38. | Einstein’s theory and its limitations | Chalk and board | Q & A Session | CO 2 |
| 39. | Debye theory and its limitations | Chalk and board | | CO 2 |
| 40. | Bose-Einstein statistics: Bose-Einstein distribution, example of particles | Chalk and board | | CO 2 |
| 41. | Bose-Einstein condensation | Power point presentation | | CO 2 |
| 42. | Difference between first order and higher order phase transitions | Chalk and board | | CO 2 |
| 43. | liquid helium, super cooled liquids | Chalk and board | | CO 2 |

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| 44. | Fermi-Dirac distribution, examples of particles | Chalk and board | | CO 2 |
| 45. | Application in electron gas, thermionic emission | Chalk and board | | CO 2 |
| 46. | Comparison of three statistics | Chalk and board | Q & A Session | CO 2 |
| **Teacher IV – JG : Unit 4 : GASEOUS STATE (8h)** | | | | |
| 47. | Derivation of Maxwell's law of distribution of velocities | Chalk and board | | CO 3 |
| 48. | Graphical representation, experimental verification of the law. | Power point presentation | | CO 3 |
| 49. | Derivation of average, RMS and most probable velocities, most probable velocity | Chalk and board | Quiz | CO 3 |
| 50. | Collision diameter, collision frequency in a single gas and in a mixture of two gases | Power point presentation | | CO 3 |
| 51. | Mean free path | Chalk and board | | CO 3 |
| 52. | Effusion, the rate of effusion | Chalk and board | | CO 3 |
| 53. | Transport properties of gases - viscosity | Chalk and board | | CO 3 |
| 54. | Thermal conductivity and diffusion | Chalk and board | | CO 3 |

**INDIVIDUAL ASSIGNMENTS/SEMINAR – DETAILS & GUIDELINES**

| | Date of completion | Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc) | Course Outcome |
|---|---|---|---|
| 1 | 22/08/18 | Solid-liquid equilibria, ternary solutions with common ions | CO 1 |

**GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES**

| | Date of completion | Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc) | Course Outcome |
|---|---|---|---|
| 1 | 11/09/18 | Different statistical models and comparison | CO 2 |

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- J. Kestin, J. R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971

**COURSE 4**

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|---|---|---|---|
| **PROGRAMME** | **M.SC. APPLIED CHEMISTRY - PHARMACEUTICAL** | **SEMESTER** | **1** |
| **COURSE CODE AND TITLE** | **16P1CPHT04 AND QUANTUM CHEMISTRY AND GROUP THEORY** | **CREDIT** | **3** |
| **HOURS/WEEK** | **4** | **HOURS/SEM** | **72** |
| **FACULTY NAME** | **DR. JORPHIN JOSEPH (JRJ), DR. ABI T.G. (ATG)** | | |

| | **COURSE OUTCOME** | **POS / PSOS** | **CL** |
|---|---|---|---|
| **CO1** | Understand the foundation and postulates of quantum mechanics. | PO1, PSO3 | U |
| **CO2** | Describe the use of simple models for predictive understanding of different molecular systems and phenomena. | PO1, PSO4 | U |
| **CO3** | Illustrate the concept of atomic orbitals by quantum mechanics. | PO1, PSO3 | U |
| **CO4** | Explain the fundamentals of group theory. | PO1, PSO1 | R |
| **CO5** | Apply the principles of group theory in chemical bonding. | PO1, PSO3 | A |

CL* Cognitive Level

**CO -PO/PSO Mapping**

| | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CO1 | 2 | | | | | | | | 3 | | | |
| CO2 | 3 | | | | | | | | | 1 | | |
| CO3 | 3 | | | | | | | | 2 | | | |
| CO4 | 3 | | | | | | 2 | | | | | |
| CO5 | 2 | | | | | | | | 2 | | | |

| **UNIT 1: POSTULATES OF QUANTUM MECHANICS (9H)** | | | | |
|---|---|---|---|---|
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 1. | State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions | Lecture method | | CO 1 |
| 2. | Operator postulate: operator algebra, linear and nonlinear operators, Laplacian operator | Lecture method | | CO 1 |
| 3. | Hermitian operators and their properties | Lecture method | | CO 1 |
| 4. | Eigen functions and eigen values of an operator. Eigen value postulate: eigen value equation, eigen functions of commuting operators. | Lecture method | | CO 1 |
| 5. | Expectation value postulate | | | CO 1 |
| 6. | Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation. | Lecture method | | CO 1 |
| 7. | Commuting and non-commuting operators | Lecture method | | CO 1 |
| 8. | Problems based on the topics discussed | Interaction/Discussion | Q & A Session | CO 1 |
| 9. | Problems based on the topics discussed | Interaction/Discussion | Q & A Session | CO 1 |
| **UNIT 2: APPLICATION TO EXACTLY SOLVABLE MODEL PROBLEMS (18H)** | | | | |
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 10. | Translational motion: free particle in one-dimension, particle in a one dimensional box with infinite potential walls | Lecture method | | CO 2 |

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| 11. | Particle in a one-dimensional box with finite potential walls-tunnelling | Lecture method | | CO 1 |
| 12. | Particle in a three dimensional box separation of variables, degeneracy. | Lecture method | | CO 1 |
| 13. | Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation | Lecture method | | CO 1 |
| 14. | Wave functions and energies-important features, Harmonic oscillator model and molecular vibrations. | Lecture method | | CO 1 |
| 15. | Rotational motion: co-ordinate systems, cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates | Lecture method | | CO 1 |
| 16. | Particle on a ring, the phi equation and its solution, wave functions in the real form | Lecture method | | CO 1 |
| 17. | Non-planar rigid rotor (or particle on a sphere)- separation of variables, the phi and the theta equations | Lecture method | | CO 1 |
| 18. | Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. | Lecture method | | CO 1 |
| 19. | Spherical harmonics (imaginary and real forms) - polar diagrams of spherical harmonics. | Lecture method | | CO 1 |
| 20. | Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (Lx, Ly, Lz and L2)-commutation relations between these operators. | Lecture method | | CO 1 |
| 21. | Spherical harmonics as eigen functions of angular momentum operators Lz and $L^2$ | Lecture method | | CO 1 |
| 22. | Ladder operator method for angular momentum. Space quantization. | Lecture method | | CO 1 |
| 23. | Problems based on the above topics | Interaction/Discussion | | CO 1 |
| 24. | Problems based on the above topics | Interaction/Discussion | | CO 1 |
| 25. | Revision | PowerPoint presentation | | CO 1 |
| 26. | Revision | PowerPoint presentation | Q & A Session | CO 1 |

| UNIT 3: QUANTUM MECHANICS OF HYDROGEN-LIKE ATOMS (9H) | | | | |
|---|---|---|---|---|
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 27. | Potential energy of hydrogen-like systems | Lecture method | | CO 2 |
| 28. | The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions | Lecture method | | CO 2 |
| 29. | The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions | Lecture method | | CO 2 |
| 30. | Wave functions and energies of hydrogen-like atoms. Orbitals-radial functions | PowerPoint presentation | | CO 3 |
| 31. | Radial distribution functions, angular functions and their plots. | PowerPoint presentation | | CO 3 |
| 32. | The postulate of spin by Uhlenbeck and Goudsmith | Lecture method | | CO 2 |
| 33. | Discovery of spin-Stern Gerlach experiment | Lecture method | | CO 3 |
| 34. | Spin orbitals-construction of spin orbitals from orbitals and spin functions. | Lecture method | | CO 3 |
| 35. | Revision | PowerPoint presentation | Quiz | CO 2 & CO 3 |
| **UNIT 4 : GROUP THEORY AND MOLECULAR SYMMETRY (18H)** | | | | |
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 36. | Symmetry elements, symmetry operations | PowerPoint presentation | Q & A Session | CO 4 |
| 37. | Symmetry elements, symmetry operations | PowerPoint presentation | | CO 4 |
| 38. | Point groups and their symbols | PowerPoint presentation | | CO 4 |
| 39. | Subgroups, classes, abelian and cyclic groups | PowerPoint presentation | | CO 4 |
| 40. | Group multiplication tables | PowerPoint presentation | | CO 4 |
| 41. | Classes in a group and similarity transformation | PowerPoint presentation | | CO 4 |
| 42. | Matrices: addition and multiplication of matrices | Lecture method | | CO 4 |
| 43. | Inverse and orthogonalmatrices, character of a matrix | Lecture method | | CO 4 |
| 44. | Block diagonalisation, matrix representation of symmetry operations | PowerPoint presentation | | CO 4 |

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| 45. | Representation of groups by matrices, | Power Point Presentation | | CO 4 |
| 46. | Construction of representation using vectors and atomic orbitals as basis | Power Point Presentation | | CO 4 |
| 47. | Construction of representation using vectors and atomic orbitals as basis | Power Point Presentation | | CO 4 |
| 48. | Statement of Great OrthogonalityTheorem (GOT) | Power Point Presentation | | CO 4 |
| 49. | Properties of irreducible representations. | Power Point Presentation | | CO 4 |
| 50. | Construction of irreducible representation using GOT | Power Point Presentation | | CO 4 |
| 51. | Construction of character tables for C2v, C2h, C3, C3v and C4v | Power Point Presentation | | CO 4 |
| 52. | Direct product of representations | Power Point Presentation | | CO 4 |
| 53. | Revision | Power Point Presentation | Quiz | CO 4 |
| **UNIT 5: APPLICATION OF GROUP THEORY IN SPECTROSCOPY AND CHEMICAL BONDING (18H)** | | | | |
| **SESSION** | **TOPIC** | **LEARNING RESOURCES** | **VALUE ADDITIONS** | **COURSE OUTCOME** |
| 54. | Applications in vibrational spectra | PowerPoint presentation | | CO 5 |
| 55. | Transition moment integral | Power Point Presentation | | CO 5 |
| 56. | Vanishing of integrals | Power Point Presentation | | CO 5 |
| 57. | Symmetry aspects of molecular vibrations, | Power Point Presentation | Q & A Session | CO 5 |
| 58. | Vibrations of polyatomicmolecules-selection rules for vibrational absorption. | Power Point Presentation | | CO 5 |
| 59. | Determination of thesymmetry of normal modes of $H_2O$, $C_2H_4$, | Power Point Presentation | | CO 5 |
| 60. | Trans $N_2F_2$,$CHCl_3$and $NH_3$ using Cartesian coordinates and internal coordinates | PowerPoint presentation | | CO 5 |
| 61. | Complementary character of IR and Raman spectra-determination of the IR and Raman active vibrational modes. | Power Point Presentation | | CO 5 |
| 62. | Applications in chemical bonding | PowerPoint presentation | | CO 5 |
| 63. | Applications in chemical bonding | PowerPoint presentation | | CO 5 |
| 64. | Construction of hybrid orbitals with (1)$H_2O$ (2), $NH_3$ | Power Point Presentation | | CO 5 |
| 65. | (3) $BF_3$ (4) $CH_4$ | Power Point Presentation | | CO 5 |

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| 66. | $PCl_5$ | Power Point Presentation | | CO 5 |
| 67. | Transformation properties of atomic orbitals | Power Point Presentation | | CO 5 |
| 68. | Symmetry adapted linear combinations (SALC). | Power Point Presentation | Q & A Session | CO 5 |
| 69. | Revision | Power Point Presentation | | CO 5 |
| 70. | MO diagram for water and ammonia | Power Point Presentation | | CO 5 |
| 71. | Revision | Power Point Presentation | | CO 5 |
| 72. | Revision | Power Point Presentation | Quiz | CO 5 |

**INDIVIDUAL ASSIGNMENTS/SEMINAR – DETAILS & GUIDELINES**

| | **Date of completion** | **Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)** | **Course Outcome** |
|---|---|---|---|
| 1. | 29/07/18 | Wave functions and energies-important features, Harmonic oscillator model and molecular vibrations. | CO 2 |
| 2. | 16/08/18 | construction of character tables for C2v,C2h, C3, C3v and C4v | CO 4 |

**GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES**

| | **Date of completion** | **Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)** | **Course Outcome** |
|---|---|---|---|
| 1. | 03/09/18 | Radial distribution functions, angular functions and their plots. | CO 2 |

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