SACRED HEART COLLEGE (AUTONOMOUS)

Department of Chemistry

MSc Chemistry

Course Plan

Academic Year 2017 - 18

Semester One

COURSE STRUCTURE

Course Code	Title Of The Course	No. Hrs./Week	Credits	Total Hrs./Sem
16P1CHET01	Inorganic Chemistry I	4	4	72
16P1CHET02	Basic Organic Chemistry	4	4	72
16P1CHET03	Physical Chemistry I	3	3	54
16P1CHET04	Quantum Chemistry and Group Theory	4	3	72

COURSE 1

PROGRAMME	**M.SC. CHEMISTRY**	**SEMESTER**	**1**
COURSE CODE AND TITLE	**16P1CHET01 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 OBJECTIVE
To explain stability of organometallic compounds and clusters, and their application as industrial catalysts.
To know the key concepts of inorganic and organometallic chemistry including those related to synthesis, reaction chemistry, and structure and bonding.
To understand the key aspects of nuclear chemistry and their analytical applications.
To explain the interaction of different metal ions with biological ligands.

UNIT 1: ORGANOMETALLIC COMPOUNDS-SYNTHESIS, STRUCTURE AND BONDING (18H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
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	
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.	Conventional Lecture using Chalk and Board and ICT -PPT		
4.	Organometallic compounds with linear pi donor ligands-dienes synthesis, structure and bonding.	Conventional Lecture using Chalk and Board and ICT -PPT		
5.	Organometallic compounds with linear pi donor ligands-allyl complexes-synthesis, structure and bonding	Conventional Lecture using Chalk and Board and ICT -PPT		
6.	Complexes with cyclic pi donors-metallocenes and structure and bonding.	Conventional Lecture using Chalk and Board and ICT -PPT		
7.	Complexes with cyclic pi donors cyclic arene complexes structure and bonding.	Conventional Lecture using Chalk and Board and ICT -PPT		
8.	Metal carbene and alkylidenes, carbine and alkylidynes complexes, Fisher- type and Schrock- type complexes.	Conventional Lecture using Chalk and Board and ICT -PPT		
9.	Revision	Chalk and Board		
10.	Metal Carbonyls: CO- as a π acid ligand, synergism, Molecular electronic structure and18-electron rule	Conventional Lecture using Chalk and Board		
11.	Binary Carbonyl complexes-Mononuclear and Binuclear carbonyls. Preparation, properties, structure, bonding in metal carbonyls	Conventional Lecture using Chalk and Board		
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		
13.	Ligands similar to CO- Cyanide, nitrosyls, dinitrogen, Hydrogen and dihydrogen complexes	Conventional Lecture using Chalk and Board and ICT -PPT		

14.	Carbonyl clusters-LNCCS and HNCCS	Conventional Lecture using Chalk and Board		
15.	Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons.	Conventional Lecture using Chalk and Board and ICT -PPT		
16.	Wade-Mingos rules, cluster valence electrons.	Conventional Lecture using Chalk and Board		
17.	Wade-Mingos rules, cluster valence electrons.	Conventional Lecture using Chalk and Board		
18.	Revision	Chalk and Board	quiz	
UNIT 2: REACTIONS AND CATALYSIS OF ORGANOMETALLIC COMPOUNDS (18H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
19.	Substitution reactions-nucleophilic ligand substitution	Conventional Lecture	Q & A Session	
20.	Nucleophilic and electrophilic attack on coordinated ligands. Carbonylate anions as nucleophiles.	Conventional Lecture		
21.	Addition and elimination reactions-1,2 additions to double bonds	Conventional Lecture		
22.	Carbonylation and decarbonylation	Conventional Lecture		
23.	Oxidative addition and reductive elimination,	Conventional Lecture		
24.	Insertion (migration) and elimination reactions.	Conventional Lecture		
25.	Rearrangement reactions	Conventional Lecture		
26.	Redistribution reactions, fluxional isomerism.	Conventional Lecture		
27.	Revision	Conventional Lecture	Quiz	
28.	Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops	Conventional Lecture		
29.	Reactions of carbon monoxide and hydrogen-the water gas shift reaction	Conventional Lecture		

30.	Reactions of carbon monoxide and hydrogen-the Fischer-Tropsch reaction(synthesis of gasoline).	Conventional Lecture		
31.	Hydroformylation of olefins using cobalt or rhodium catalyst. Synthesis of diethyhexylphthalate.	Conventional Lecture		
32.	Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts.	Conventional Lecture		
33.	Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $(CO)_8$ catalyst in adipic ester synthesis	Conventional Lecture		
34.	Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop").	Conventional Lecture		
35.	Palladium catalysed oxidation of ethylene-the Wacker process.	Conventional Lecture		
36.	Revision	Conventional Lecture	Quiz	
UNIT 3 : NUCLEAR CHEMISTRY (18H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
37.	Introduction to Nuclear Chemistry	Conventional Lecture	Q & A Session	
38.	Radioactive decay. Alpha decay-Alpha ray spectrum, Beta decay-Types of beta decay, β+, β-, β-ray spectrum	Conventional Lecture		
39.	Neutrino antineutrino and Positron emission, Dirac theory, pair production, positron-electron annihilation	Conventional Lecture		
40.	Electron capture, double β decay. Gamma decay- de-excitation of excited molecules, change of Energy, spin, parity during photon emission	Conventional Lecture		
41.	Nuclear isomerism and isomeric transition, internal conversion, auger electrons and auger effect	Conventional Lecture		
42.	Nuclear reactions. Q-Value and reaction threshold, reaction cross section-definition, and units	Conventional Lecture		
43.	Cross section and reaction rate, neutron capture cross section,	Conventional Lecture		

	variation of neutron cross section with energy(1/V law)			
44.	Photonuclear, Thermonuclear and Fusion reactions, Magnetic confinement, internal confinement.	Conventional Lecture		
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		
46.	Nuclear Reactors. Fissile and fissionable nuclei, fast and thermal neutrons	Conventional Lecture		
47.	Terms and symbols used in reactor technology- average no. of fission neutrons, fast fission factor, fast neutrons loss factor	Conventional Lecture		
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		
49.	Terms and symbols used in reactor technology- Reproduction factor, critical size of reactor. Breeder reactor, fast breeder test reactor.	Conventional Lecture		
50.	Reactor Safety precaution, Management of radioactive waste- Low level Waste, Intermediate level Waste, High level Waste.	Conventional Lecture		
51.	Principles of counting techniques- G.M. counter, proportional, ionization and scintillation counters.	Conventional Lecture		
52.	Applications of radioisotopes. Physico-chemical study-Solubility of sparingly soluble salts	Conventional Lecture	Q & A Session	
53.	Applications of radioisotopes. Analytical applications-Isotope dilution analysis, radiometric titrations, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.	Conventional Lecture		
54.	Applications of radio isotopes medicine-Thyroiditis, Tumour	Conventional Lecture		

	identification, Determination of volume of blood in patient			
UNIT 4 : BIOINORGANIC CHEMISTRY (18H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
55.	Biochemistry of Iron Oxygen Carriers-Structure and functions of haemoglobin and myoglobin	Conventional Lecture Chalk & Board		
56.	Oxygen transport mechanism of Hemoglobin, cooperativity in haemoglobin.	Lecture With power point presentation		
57.	Bohr effect and phosphate effect. Hemerythrin Structure and function.	Lecture With power point presentation		
58.	Redox Metalloenzymes-Cytochromes, Classification, Structure and function .	Lecture With power point presentation		
59.	Role in Oxidative Phosphorylation of ADP to ATP. Iron Sulphur Proteins-Rubredoxin, Ferredoxin	Conventional Lecture		
60.	Nitrogenase, Structure and function, Nitrogen Fixation. Peroxidases and catalases	Conventional Lecture		
61.	Cytochrome P450- Structure and functions. Storage and transport of iron in biological systems-Ferritin, transferrin and Siderophores	Conventional Lecture		
62.	Biochemistry of Zn and Copper. Structure and functions of carboxypeptidase and carbonic anhydrase	Conventional Lecture		
63.	Superoxide dismutase. Structure and functions of various Copper proteins and enzymes.	Conventional Lecture		
64.	Blue copper proteins (Type-1) - Electron transfer agents - Plastocyanin, Stellacyanin and Azurin.	Conventional Lecture		
65.	Blue copper Enzymes (Type II) - Ascorbateoxidase, Laccase and ceruloplsmin.	Conventional Lecture		
66.	Non Blue copper enzyme (Type III) - Cytochrome oxidase, Amine oxidases, Structure and functions of Hemocyanin.	Conventional Lecture		
67.	Vitamin B_{12}- Structure and biological importance	Conventional Lecture		

68.	Chlorophyll-Photosynthesis, PS I & PS II.	Conventional Lecture		
69.	Therapeutic applications of cis-platin, Mechanism of action, MRI agents	Conventional Lecture		
70.	Mechanism of muscle contraction, blood clotting mechanism.	Conventional Lecture		
71.	Essential and trace elements in biological systems, Toxic effects of metals (Cd, Hg, Cr and Pb)	Conventional Lecture	Q & A Session	
72.	Mechanism of ion transport across membranes, Sodium Potassium pump.	Conventional Lecture		

INDIVIDUAL ASSIGNMENTS/SEMINAR – DETAILS & GUIDELINES

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc.)**
1	18/08/17	Assignment on Redox metalloenzymes, blue copper proteins
2	22/08/17	Application of metal carbonyls and organometallic compounds

GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc.)**
1	02/08/17	Application of: Radioactivity Fission & fusion

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.
- F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999.
- 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.
- H.J. Arnikar, Essentials of Nuclear Chemistry, New Age International,4th Edn., 2011.

- B.R Puri,L.R. Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Milestone,2011.
- 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

PROGRAMME	**M.SC. CHEMISTRY**	**SEMESTER**	**1**
COURSE CODE AND TITLE	**16P1CHET02 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 OBJECTIVE
To explain the basic concepts of organic chemistry.
To know the principles of physical organic chemistry.
To have an idea about the reactivity and stability of organic molecules based on structure, including conformation and stereochemistry.
To recognize the importance of organic photochemical reactions.

UNIT 1: BASIC CONCEPTS IN ORGANIC CHEMISTRY (12H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
1.	IUPAC nomenclature of polycyclic, heterocyclic	Conventional Lecture	Q & A Session	
2.	Benzenoid, non-benzenoid and spiro compounds.	Conventional Lecture		
3.	Review of basic concepts in organic chemistry: Electron displacement effects-inductive effect	Conventional Lecture		
4.	Electrometric effect, resonance effect, hyperconjugation, steric effect. Steric inhibition of resonance.	Conventional Lecture		

5.	Bonding weaker than covalent bonding- H-bonding, π- π interactions.	Conventional Lecture		
6.	Other non-covalent interactions	Conventional Lecture		
7.	Concept of aromaticity: delocalization of electrons –Huckel's rule	Conventional Lecture	Q & A Session	
8.	Craig rule- criteria for aromaticity - examples of neutral and charged aromatic systems,	Conventional Lecture		
9.	Annulenes [10], [14], [18], [22]	Conventional Lecture		
10.	Tropolone, Azulene. NMR as a tool for aromaticity	Conventional Lecture		
11.	Anti- and homo-aromatic systems– Alternate and non-alternate hydrocarbons	Conventional Lecture		
12.	Fullerenes, Carbon nanotubes and Graphene.	Conventional Lecture	Quiz	
Teacher II – JUC : Unit 2: Physical Organic Chemistry (11h)				
13.	Energy profiles. Hammond postulate	Conventional Lecture		
14.	Kinetic versus thermodynamic control of product formation	Conventional Lecture		
15.	Captodative effect –- kinetic isotope effects with examples	Conventional Lecture		
16.	Continued	Conventional Lecture		
17.	Stereochemical studies-use of isotopes, Hammet equation	Conventional Lecture	Q & A Session	
18.	Taft equation, cross-over experiments, Hammond postulates.	Conventional Lecture		
19.	Salt and Solvent effect.	Conventional Lecture		
20.	Intermediates *vs*. Transition state, linear free energy relationship.	Conventional Lecture		
21.	Introduction to carbon acids - pK_a of weak acids	Conventional Lecture		
22.	Kinetic and thermodynamic acidity.	Conventional Lecture		
23.	Introduction to organic bases- pK_b of weak bases.	Conventional Lecture	Q & A Session	
Teacher III – FJ : Unit 3 : Review of basic reaction mechanisms (8h)				
24.	Mechanism of SN1, SNAr	Conventional Lecture		
25.	SRN1 and Benzyne mechanisms.	Conventional Lecture		

26.	Catalysis by acids and bases	Conventional Lecture		
27.	Nucleophiles with examples from acetal, cyanohydrin	Conventional Lecture	Q & A Session	
28.	Ester formation and hydrolysis reactions –A_{AC}^2 mechanisms	Conventional Lecture		
29.	A_{AC}^1 mechanism.	Conventional Lecture		
30.	A_{AL}^1, B_{AC}^2 mechanisms.	Conventional Lecture		
31.	B_{AL}^1 mechanism.	Conventional Lecture	Quiz	
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	
33.	Axis, plane, centre, alternating axis of symmetry.	Conventional Lecture		
34.	Centre of chirality – molecules with C, N, S based chiral centres	Conventional Lecture		
35.	Absolute configuration - enantiomers	Conventional Lecture		
36.	Racemic modifications - R and S nomenclature using Cahn-Ingold-Prelog rules	Conventional Lecture		
37.	Continued	Conventional Lecture		
38.	Molecules with a chiral centre and Cn	Conventional Lecture		
39.	Molecules with more than one center of chirality	Conventional Lecture		
40.	Definition of diastereoisomers constitutionally symmetrical and unsymmetrical chiral molecules	Conventional Lecture		
41.	Erythro, threo nomenclature.	Conventional Lecture	Q & A Session	
42.	Axial, planar and helical chirality – examples	Conventional Lecture		
43.	Stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls	Conventional Lecture		
44.	Ansa and cyclophanic compounds, spirans, exo-cyclic alkylidenecycloalkenes. Identification of enantiotopic, homotopic, diastereotopic hydrogens	Conventional Lecture		

45.	Prochirality, Topicity and prostereoisomerism – topicity of ligands and faces, and their nomenclature.	Conventional Lecture	Quiz	
46.	NMR distinction of enantiotopic/diastereotopic ligands. Stereospecific, stereoselective and assymetric synthesis.	Conventional Lecture		
Teacher V – JTM : Unit 5: Conformational Analysis (20h)				
47.	Stereoisomerism: Definition based on symmetry and energy criteria	Conventional Lecture	Q & A Session	
48.	Configuration and conformational stereoisomers.	Conventional Lecture		
49.	Conformational descriptors	Conventional Lecture		
50.	Factors affecting conformational stability of molecules.	Conventional Lecture		
51.	Potential energy diagrams	Conventional Lecture		
52.	Conformational analysis of acyclic systems: substituted ethanes	Conventional Lecture		
53.	Aldehydes	Conventional Lecture	Q & A Session	
54.	Ketones and olefins.	Conventional Lecture		
55.	Conformational analysis of cyclic systems	Conventional Lecture		
56.	Cyclohexane and its derivatives. Cyclohexanone.	Conventional Lecture		
57.	Continued	Conventional Lecture		
58.	Conformational analysis of Fused and bridged bicyclic systems	Conventional Lecture	Quiz	
59.	Decalins, adamantane	Conventional Lecture		
60.	Hexamethylene diamine and congressane	Conventional Lecture		
61.	Conformation of sugars-glucose, sucrose and lactose	Conventional Lecture		
62.	Conformation and reactivity of elimination -dehalogenation	Conventional Lecture		
63.	Dehydrohalogenation	Conventional Lecture		
64.	Dehydration, semipinacolic deamination and pyrolytic elimination	Conventional Lecture		
65.	Saytzeff and Hofmann eliminations, substitution and oxidation of 2^0 alcohols.	Conventional Lecture		

66.	Chemical consequence of conformational equilibrium - Curtin-Hammett principle.	Conventional Lecture		
Teacher VI – JUC : Unit 6: Organic Photochemistry (6h)				
67.	Jablonski diagram, triplet and singlet states. Photoreactions of carbonyl compounds: Norrish reactions of acyclic ketones	Conventional Lecture	Q & A Session	
68.	Cyclic ketones.	Conventional Lecture		
69.	Patterno-Buchi reaction.	Conventional Lecture		
70.	Barton reaction and photo reduction of ketones.	Conventional Lecture	Quiz	
71.	Di-π-methane reaction	Conventional Lecture		
72.	Photochemistry of Nitro and Azo groups. Photochemistry of vision	Conventional Lecture		

INDIVIDUAL ASSIGNMENTS/SEMINAR – DETAILS & GUIDELINES

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	11/8/17	IUPAC nomenclature of polycyclic, heterocyclic
2	20/8/17	Racemic modifications - R and S nomenclature using Cahn-Ingold-Prelog rules

GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	02/8/17	Non-covalent interactions

REFERENCES

- D. Nasipuri,Stereochemistry of Organic Compounds: Principles and Applications, Third Edition, New Age Publications, New Delhi, 2010
- E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994
- D. Hellwinkel, Systematic nomenclature of organic chemistry, Springer international edition
- J.Clayden, N.Greeves, S.Warren, P.Wothers, Organic Chemistry, Oxford University Press, New York, 2004
- F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Fifth Edition, Springer, New York, 2007.
- R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002

- Aditi Sangal, Krishna's Advanced Organic Chemistry; Volume 1 – Krishna Prakashn Media(P) Ltd.
- K.K.R.Mukherjee, Fundamentals of Photochemistry, New Age Publications, New Delhi, 1978
- N. J. Turro, V. Ramamurthy and J. C. Scaiano, Principles of Molecular Photochemistry: An Introduction, University Science books 2009.
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- Jack Hine,Physical Organic Chemistry, McGraw-Hill; 2nd Edition,1962.
- Anslyn, E. V.; Dougherty, D. A. Modern Physical Organic Chemistry, University Science Books, 2006

COURSE 3

PROGRAMME	**M.SC. CHEMISTRY**	**SEMESTER**	**1**
COURSE CODE AND TITLE	**16P1CHET03 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 OBJECTIVE
To know mathematical tools to calculate thermodynamic and kinetic properties.
To explain the relationship between microscopic properties of molecules with macroscopic thermodynamic observables.
To explain the kinetic behaviour of gases and their transport properties.

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

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		
5.	Effect of temperature and pressure on chemical equilibrium- van't Hoff equations	Chalk and board		
6.	Three component systems: Gibbs phase rule, graphical representation of three component systems.	Chalk and board	Quiz	
7.	Solid-liquid equilibria, ternary solutions with common ions Hydrate formation, compound formation.	Chalk and board		
8.	Liquid-liquid equilibria-one pair of partially miscible liquids	Chalk and board		
9.	Two pairs of partially miscible liquids, three pairs of partially miscible liquids.	Chalk and board		
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	
11.	Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations.	Chalk and board		
12.	The Onsager reciprocal relations - principle of microscopic reversibility.	Chalk and board		
13.	Electrokinetic phenomena.	Chalk and board		
14.	Thermoelectric phenomena	Chalk and board	Quiz	
15.	Bioenergetics: Coupled reactions, ATP and its role in bioenergetics.	Power point presentation		
16.	High energy bond, free energy and entropy change in ATP hydrolysis.	Power point presentation		
17.	Thermodynamic aspects of metabolism and respiration	Power point presentation		
18.	Thermodynamic aspects of glycolysis and biological redox reactions.	Power point presentation		
19.	Revision	Power point presentation	Quiz	
Teacher III – KBJ : Unit 3 : STATISTICAL THERMODYNAMICS (27h)				
20.	Permutation, probability, apriori and thermodynamic probability.	Chalk and board		
21.	Stirlings approximation, macrostates and microstates.	Chalk and board		

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

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

INDIVIDUAL ASSIGNMENTS/SEMINAR – DETAILS & GUIDELINES

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	22/08/17	Solid-liquid equilibria, ternary solutions with common ions

GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	11/09/17	Different statistical models and comparison

REFERENCES:

- R.P. Rastogi, R.R. Misra, An introduction to Chemical Thermodynamics, Vikas publishing house, 2009.
- J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.
- M.C. Gupta, Statistical Thermodynamics, New age international, 2007.
- M.W. Zemansky, R.H. Dittman, Heat and Thermodynamics, Tata McGraw Hill, 1981.
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COURSE 4

PROGRAMME	**M.SC. CHEMISTRY**	**SEMESTER**	**1**
COURSE CODE AND TITLE	**16P1CHET04 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 OBJECTIVE
To understand the foundation and postulates of quantum mechanics.
To describe the use of simple models for predictive understanding of different molecular systems and phenomena.
To illustrate the concept of atomic orbitals by quantum mechanics.
To explain the fundamentals of group theory.
To apply the principles of group theory in chemical bonding.

UNIT 1: POSTULATES OF QUANTUM MECHANICS (9H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
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		
7.	Commuting and non-commuting operators	Lecture method		
8.	Problems based on the topics discussed	Interaction/Discussion	Q & A Session	
9.	Problems based on the topics discussed	Interaction/Discussion	Q & A Session	
UNIT 2: APPLICATION TO EXACTLY SOLVABLE MODEL PROBLEMS (18H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
10.	Translational motion: free particle in one-dimension, particle in a one dimensional box with infinite potential walls	Lecture method		
11.	Particle in a one-dimensional box with finite potential walls-tunnelling	Lecture method		
12.	Particle in a three dimensional box separation of variables, degeneracy.	Lecture method		
13.	Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation	Lecture method		
14.	Wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.	Lecture method		
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		
16.	Particle on a ring, the phi equation and its solution, wave functions in the real form	Lecture method		
17.	Non-planar rigid rotor (or particle on a sphere)- separation of variables, the phi and the theta equations	Lecture method		
18.	Legendre and associated Legendre equations, Legendre and associated Legendre polynomials.	Lecture method		

19.	Spherical harmonics (imaginary and real forms) - polar diagrams of spherical harmonics.	Lecture method		
20.	Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (Lx, Ly, Lz and L2)-commutation relations between these operators.	Lecture method		
21.	Spherical harmonics as eigen functions of angular momentum operators Lz and L^2	Lecture method		
22.	Ladder operator method for angular momentum. Space quantization.	Lecture method		
23.	Problems based on the above topics	Interaction/Discussion		
24.	Problems based on the above topics	Interaction/Discussion		
25.	Revision	PowerPoint presentation		
26.	Revision	PowerPoint presentation	Q & A Session	
UNIT 3: QUANTUM MECHANICS OF HYDROGEN-LIKE ATOMS (9H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
27.	Potential energy of hydrogen-like systems	Lecture method		
28.	The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions	Lecture method		
29.	The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions	Lecture method		
30.	Wave functions and energies of hydrogen-like atoms. Orbitals-radial functions	PowerPoint presentation		
31.	Radial distribution functions, angular functions and their plots.	PowerPoint presentation		
32.	The postulate of spin by Uhlenbeck and Goudsmith	Lecture method		
33.	Discovery of spin-Stern Gerlach experiment	Lecture method		
34.	Spin orbitals-construction of spin orbitals from orbitals and spin functions.	Lecture method		
35.	Revision	PowerPoint presentation	Quiz	&

UNIT 4 : GROUP THEORY AND MOLECULAR SYMMETRY (18H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
36.	Symmetry elements, symmetry operations	PowerPoint presentation	Q & A Session	
37.	Symmetry elements, symmetry operations	PowerPoint presentation		
38.	Point groups and their symbols	PowerPoint presentation		
39.	Subgroups, classes, abelian and cyclic groups	PowerPoint presentation		
40.	Group multiplication tables	PowerPoint presentation		
41.	Classes in a group and similarity transformation	PowerPoint presentation		
42.	Matrices: addition and multiplication of matrices	Lecture method		
43.	Inverse and orthogonalmatrices, character of a matrix	Lecture method		
44.	Block diagonalisation, matrix representation of symmetry operations	PowerPoint presentation		
45.	Representation of groups by matrices,	Power Point Presentation		
46.	Construction of representation using vectors and atomic orbitals as basis	Power Point Presentation		
47.	Construction of representation using vectors and atomic orbitals as basis	Power Point Presentation		
48.	Statement of Great OrthogonalityTheorem (GOT)	Power Point Presentation		
49.	Properties of irreducible representations.	Power Point Presentation		
50.	Construction of irreducible representation using GOT	Power Point Presentation		
51.	Construction of character tables for C2v, C2h, C3, C3v and C4v	Power Point Presentation		
52.	Direct product of representations	Power Point Presentation		
53.	Revision	Power Point Presentation	Quiz	
UNIT 5: APPLICATION OF GROUP THEORY IN SPECTROSCOPY AND CHEMICAL BONDING (18H)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
54.	Applications in vibrational spectra	PowerPoint presentation		
55.	Transition moment integral	Power Point Presentation		

56.	Vanishing of integrals	Power Point Presentation		
57.	Symmetry aspects of molecular vibrations,	Power Point Presentation	Q & A Session	
58.	Vibrations of polyatomicmolecules-selection rules for vibrational absorption.	Power Point Presentation		
59.	Determination of thesymmetry of normal modes of H_2O, C_2H_4,	Power Point Presentation		
60.	Trans N_2F_2,$CHCl_3$and NH_3 using Cartesian coordinates and internal coordinates	PowerPoint presentation		
61.	Complementary character of IR and Raman spectra-determination of the IR and Raman active vibrational modes.	Power Point Presentation		
62.	Applications in chemical bonding	PowerPoint presentation		
63.	Applications in chemical bonding	PowerPoint presentation		
64.	Construction of hybrid orbitals with (1)H_2O (2), NH_3	Power Point Presentation		
65.	(3) BF_3 (4) CH_4	Power Point Presentation		
66.	PCl_5	Power Point Presentation		
67.	Transformation properties of atomic orbitals	Power Point Presentation		
68.	Symmetry adapted linear combinations (SALC).	Power Point Presentation	Q & A Session	
69.	Revision	Power Point Presentation		
70.	MO diagram for water and ammonia	Power Point Presentation		
71.	Revision	Power Point Presentation		
72.	Revision	Power Point Presentation	Quiz	

INDIVIDUAL ASSIGNMENTS/SEMINAR – DETAILS & GUIDELINES

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**
1.	29/07/17	Wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.
2.	16/08/17	construction of character tables for C2v,C2h, C3, C3v and C4v

GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1.	03/09/17	Radial distribution functions, angular functions and their plots.

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