SACRED HEART COLLEGE (AUTONOMOUS)

Department of Chemistry

MSc Chemistry - Pharmaceutical

Course Plan

Academic Year 2018-19

Semester One

PROGRAMME OUTCOMES

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

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

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 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 PSO 1	U
CO3	Demonstrate a systematic understanding of the key aspects of nuclear chemistry and their analytical applications.	PO 1 PSO 1	U
CO4	Recognize and explain the interaction of different metal ions with biological ligands.	PO 1 PSO 1	U

CL* Cognitive Level

UNIT 1: ORGANOMETALLIC COMPOUNDS-SYNTHESIS, STRUCTURE AND BONDING (18H)				
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 carbonyls. Preparation, properties, structure, bonding in metal carbonyls	Conventional Lecture using Chalk and Board		CO1
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	Conventional Lecture using Chalk and Board		CO1

	dihydrogen complexes	and ICT -PPT		
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
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
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,	Conventional Lecture		CO3

	variation of neutron cross section with energy(1/V law)			
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
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
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

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- 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.
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- 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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- P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988.
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- B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

COURSE 2

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 PSO 1	R
CO2	Illustrate the principles of physical organic chemistry.	PO 1 PSO 1	U
CO3	Demonstrate the reactivity and stability of organic molecules based on structure, including conformation and stereochemistry.	PO 1 PSO 3	U
CO4	Recognize the importance of organic photochemical reactions.	PO 1 PSO 4	U

CL* Cognitive Level

UNIT 1: BASIC CONCEPTS IN ORGANIC CHEMISTRY (12H)				
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
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
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
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. 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. 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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COURSE 3

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 PSO 3	A
CO2	Explain the relationship between microscopic properties of molecules with macroscopic thermodynamic observables.	PO 1 PSO 2	U

CO3	Explain the kinetic behaviour of gases and their transport properties.	PO 1 PSO 4	U

CL* Cognitive Level

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 functions	Chalk and board		CO 1
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
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
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

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.
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- P.W. Atkins, Physical Chemistry, ELBS, 1994.
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- J. Kestin, J. R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971

COURSE 4

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

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	Lecture method		CO 2

	walls			
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	Q & A	CO 1

		presentation	Session	
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
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
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

REFERENCES:

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- P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, 4th Edition, Oxford University Press, 2005
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- K.Veera Reddy, Symmetry & Spectroscopy of Molecules 2nd Edn., New Age International 2009