

**SACRED HEART COLLEGE (AUTONOMOUS)**

**DEPARTMENT OF CHEMISTRY**

**MASTER OF SCIENCE IN APPLIED CHEMISTRY - PHARMACEUTICAL**

**Course plan**

**Academic Year 2018 - 19**

**Semester 3**

PROGRAMME	MSC APPLIED CHEMISTRY - PHARMACEUTICAL	SEMESTER	3
COURSE CODE AND TITLE	16P3CPHT09: PHARMACEUTICAL CHEMISTRY - I	CREDIT	4
HOURS/WEEK	4	HOURS/SEM	72
FACULTY NAME	DR. JINU GEORGE, DR. GRACE THOMAS, DR. IGNATIUS ABRAHAM, DR. RAMAKRISHNAN S		

<b>Course Objectives</b>
To describe the Drug design, Pharmacology, mechanism of action of drugs
To interpret the receptor theories and bio-transformation of drugs.
To know the structure, synthesis, pharmacological and mechanism of action and SAR of Antiinfective agents.
To know the structure, synthesis, pharmacological and mechanism of action and SAR of Drugs acting on CVS
To know the structure, synthesis, pharmacological and mechanism of action and SAR of Chemotherapeutic agents
To know the structure, synthesis, pharmacological and mechanism of action and SAR of Antipyretics and NSAIDs

SESSION	TOPIC	LEARNING RESOURCES	VALUE ADDITIONS	REMARKS
<b>MODULE I : Pharmacology (12h)</b>				
1	Drugs and Drug targets. Enzymes: active sites, mechanism of catalysis	PPT	video	
2	Enzyme inhibitors, Enzyme selectivity, Receptors ligand gated ionic channels	PPT/Lecture		
3	G-Protein coupled receptors, Kinase linked receptors	PPT/Lecture		
4	Carrier Proteins, Structural Proteins, Nucleic acids, Lipids and carbohydrates and DNA as drug targets	PPT/Lecture	e-resource	
5	Structure activity relationship, Binding interactions, Functional groups as binding	PPT/Lecture	Q & A Session	

	groups			
6	Concept and definition of pharmacophore Pharmacokinetic principles: absorption	PPT/Lecture		
7	Distribution, metabolism and excretion of drugs.	Lecture		
8	Dose of drugs and routes of administration. Drug dosing, drug half life, Steady state concentration, Drug tolerance, Bioavailability, Drug delivery	Lecture		
<b>First Internal Examination</b>				
9	Pharmacodynamic principles : Examples of agonists, allosteric modulators, Antagonists, Partial agonists, Inverse agonists	Lecture		
10	Desensitization and sensitization, Tolerance and dependence, Affinity, efficacy and potency.	Lecture		
11	Dose response relationships, unusual and adverse responses of drugs	PPT/Lecture		
12	Structurally specific and nonspecific drugs. Ferguson's principle.	PPT/Lecture	Q & A Session	
<b>Second Internal Examination</b>				
<b>MODULE II : Toxicology and Biotransformations (12h)</b>				
13	Receptor theories and receptor models- rate theory	PPT/Lecture		
14	Occupancy and induced fit theory	PPT/Lecture		
15	Activation-aggregation and molecular perturbation theories	PPT/Lecture		
16	General concepts of toxicity, Acute, subacute & chronic toxicity tests	Lecture	Q & A Session	
17	Teratogenicity & carcinogenicity,, LD50, ED50	Lecture		
18	MIC- anti infectives, habituation & addiction	Lecture		
19	Factors affecting biotransformation, site of biotransformations	Lecture		
20	Effect of biotransformation on the biological activity of drugs	PPT/Lecture		
<b>First Internal Examination</b>				
21	Biotransformation- Oxidation, reduction,	PPT/Lecture		

	hydroxylation, hydrolysis			
22	Reactions and mechanism with specific drug molecules	PPT/Lecture		
23	Phase II biotransformations -glucosidation, sulfation, conjugation with glutathione acetylation methylation- illustrate with suitable drug molecules	PPT/Lecture		
24	Chemical and pharmacological roles of Phase I & phase II transformations.	Lecture	Q & A Session	
<b>Second Internal Examination</b>				
<b>MODULE III : Anti-Infective agents (12h)</b>				
25	Sulphonamides- structure, chemistry, SAR and mechanism of action Sulfadiazine	Lecture		
26	Sulfamethoxole, sulfones, cotrimoxazole(sulfamethoxole+ trimethoprim.) Zwitter ion.	Lecture		
27	Sulfonamides: Synthesis of: Sulfadiazine, sulfamethoxole	Lecture		
28	Synthesis of pyrimethamine, Dapsone	Lecture		
29	Antifungal agents: study of Amphotericin B, griseofulvin physical and chemical properties	PPT/Lecture		
30	Study of nystatin, ketoconazole, clotrimazole, fluconazole, 5-flucytosine	PPT/Lecture		
31	Antiprotozoal agents: Chemistry, mechanism of action and therapeutic uses of Anti Amoebic and Anthelmintics	PPT/Lecture		
32	Antiviral drugs- mode of action and therapeutic uses	PPT/Lecture		
<b>First Internal Examination</b>				
33	Chemistry and mechanism of action of amantadine, Ribavirin.	PPT/Lecture	Q & A Session	
34	Chemistry and mechanism of action of Abacavir, acyclovir, oseltamivir, vidarabine	PPT/Lecture		
35	Chemistry and mechanism of action of Ganciclovir, fosfovir, zalcitabine. Synthesis of -, Sulphanilamide, Dapsone, Griseofulvin	PPT/Lecture		

36	Synthesis of 5-flucytosine, acyclovir, Adefovir, Combivir, Didanosine, ganciclovir	Lecture	Quiz	
<b>Second Internal Examination</b>				
<b>MODULE IV : Drugs Acting on CVS (12 h)</b>				
37	Pharmacology and SAR of Cardiotonic drugs: cardiac glycosides chemistry of digoxin and digitoxin	PPT/Lecture	Q & A Session	
38	Synthesis of Dobutamide, milrinone Antiarrhythmic drugs:quinidine, disopyramide, lidocaine, phenytoin and procainamide	PPT/Lecture		
39	$\beta$ -blockers-propranolol. Calcium channel blockers-verapamil synthesis of lidocaine , phenytoin, bretilium. Neurone blockers - bretilium	PPT/Lecture		
40	Antihypertensive Drugs: peripheral antiadrenergics-prazosin and terazosin. Reserpine, clonidine and methyldopa. $\beta$ -atenolol and labetalol	PPT/Lecture		
41	Calcium channel blockers-nifedipine and amlodipine. ACE inhibitors-captopril	PPT/Lecture		
42	Angiotensin receptor blockers-losartan. Diuretics-thiazide diuretics	Lecture		
43	Synthesis of: captopril, methyl DOPA, amlodipine. Antianginal drugs: vasodilators-nitrites and nitrates, $\beta$ -blockers-propranolol	PPT/Lecture		
44	Calcium channel blockers-verapamil and nifedipine. Miscellaneous-dipyridamoland aspirin	PPT/Lecture		
<b>First Internal Examination</b>				
45	Synthesis : verapamil. Anticoagulants: heparin	PPT/Lecture		
46	Coumarin derivatives and indanedione derivatives	PPT/Lecture		
47	Antilipidemic agents: Statins- lovastatin,simvastatin, fluvastatin	PPT/Lecture	Quiz	
48	Synthesis of fluvastatin. Fibrates-clofibrate, and cholestyramine resin.	PPT/Lecture		

<b>Second Internal Examination</b>				
<b>MODULE V : Chemotherapeutic Agents (12 h)</b>				
49	Antibiotics- Classification, mechanism of action and therapeutic uses.- penicillin	PPT/Lecture		
50	Cephalosporins, Quinolones, Aminoglycosides, Carbapenems, macrolide and others	PPT/Lecture		
51	Antibiotic resistance mechanism and implications in therapeutics	PPT/Lecture		
52	Synthetic studies of :Penicillin V, Cefotaxim, Meropenem, Streptomycin, Ciprofloxacin, Trimethoprim	PPT/Lecture	Video	
53	Chemotherapy of Tuberculosis: First line Drugs and second line drugs- chemistry Pharmacology	PPT/Lecture		
54	The problem of MDR tuberculosis. Recent innovations. Synthesis of isoniazid	PPT/Lecture		
55	Synthesis of pyrazinamide, ethionamide, paraaminosalicylic acid.	PPT/Lecture		
56	Antimalarials : Chemotherapy of Malaria, mode of action of the various classes of drugs used, Chemistry, SAR and Drug resistance	Lecture		
57	Study of the following drugs in the treatment , efficacy , problem of side effects of Quninesulphate, Chloroquine, primaquine	PPT/Lecture	Quiz	
58	Mephloquine, quinacrine ,proguanil, plaquenil	PPT/Lecture		
<b>Second Internal Examination</b>				
59	Drug combinations in the therapy of Malarial parasite. Treatment of drug resistant malaria, recent progress	PPT/Lecture		
60	Synthetic studies of chloroquine, primaquine, proguanil, malarone.	PPT/Lecture		
CIA-II				
<b>MODULE VI : Analgesics, Antipyretics &amp; Anti inflammatory drugs (12h)</b>				
61	Mechnism of action and SAR of: Different types of analgesia	PPT/Lecture		
62	Narcotic analgesics - morphine and codeine,	PPT/Lecture		

	Phenyl(ethyl) piperidines, Diphenylheptanones, fentanyl analogues, nalfurafine			
63	Antipyretics and NSAIDs: Basic idea of COX I & II inhibitors	Lecture	Demo video	
64	Salicylates - aspirin, p-aminophenol derivatives-paracetamol, phenacetin	Lecture		
66	Pyrazolidinediones - Phenylbutazone, Anthranilic acid derivatives - Flufenamic acid	Lecture		
67	Indoleacetic acid derivatives-indomethacin, Arylacetic/ Propionic acid derivatives - ibuprofen and Ketoprofen)	PPT/Lecture		
68	Arylacetic/ Propionic acid derivatives flubiprofen and diclofenac	PPT/Lecture		
69	Oxicams - tenoxicam, Drugs used for gout - allopurinol, Colchicine, Pegloticase	PPT/Lecture		
70	Antiinflammatory: Sulindac, Naproxen, Novel Analgesics: Funapide, Raxatrigine (Structure only).	Lecture	Quiz	
<b>Second Internal Examination</b>				
71	Synthesis of the following drugs-levorphanol, pethidine, methadone, phenyl butazone, flufenamic acid	PPT/Lecture		
72	Synthesis of Diclofenac, tenoxicam, allopurinol and Codeine, Ketoprofen, Naproxen	PPT/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	08/10/2018	Synthesis of Anti-infective agents
2	07/11/2018	SAR of drugs used as antipyretics

### GROUP ASSIGNMENTS/ACTIVITIES – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	06/11/2018	Previous CSIR questions (Group activity)

### References

01. G. Patrick, Medicinal Chemistry, BIOS. 2001.
02. T. Nogrady, D.F. Weaver, Medicinal Chemistry, Oxford University Press, 2005.
03. W.O. Foye, T.L. Lemke, D.A. Williams, Principles of Medicinal Chemistry, 4thEdn., Williams & Wilkins, 1995.
04. J.P. Remington, Remington's Pharmaceutical Sciences, Vol.13, , 19th Edn., Mack,1990.
05. D. Sriram , P. Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.
06. K. D. Tripathi, Essentials of Medical Pharmacology, 6th Edn.,Jaypee, 2008
07. L.S. Goodman, A. Gillman, The Pharmacological Basis of Therapeutics, 10thEdn., McGraw Hill, 2001.
08. S.S. Kadam, Principles of Medicinal Chemistry, Vol.I& II, Pragati Books, 2008.
09. A. Kar, Medicinal Chemistry, New Age International, 2007.
10. C.O. Wilson, J.M. Beale, J.H. Block, Textbook of Organic Medicinal and Pharmaceutical Chemistry, 12th Edn., Lippincott Williams and Wilkins, 2010



PROGRAMME	MSC APPLIED CHEMISTRY - PHARMACEUTICAL	SEMESTER	3
COURSE CODE AND TITLE	16P3CPHT10 and ORGANIC SYNTHESSES	CREDIT	4
HOURS/WEEK	4	HOURS/SEM	72
FACULTY NAME	DR. JOSEPH T MOOLAYIL, DR. V.S SEBASTIAN, DR. FRANKLIN J, DR.GRACE THOMAS		

<b>Course Objectives</b>
To describe the applications of oxidation and reduction techniques in organic syntheses.
To illustrate modern synthetic methods and applications of reagents.
To explain different methods for the construction of carbocyclic and heterocyclic ring systems.
To understand the principles and applications of protecting groups in chemistry.
To apply retrosynthetic analysis to design the synthesis of a target molecule.
To understand the concept of molecular recognition and supramolecular chemistry

SESSION	TOPIC	LEARNING RESOURCES	VALUE ADDITIONS	REMARKS
<b>Unit 1 : Organic Synthesis via Oxidation and Reduction (18 hours)</b>				
1	Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction.	PPT	video	
2	Metal based and non-metal based oxidations of alcohols to carbonyls (Chromium, Manganese)	PPT/Lecture		
3	Metal based and non-metal based oxidations of alcohols to carbonyls(aluminium and DMSO based reagents)	PPT/Lecture		
4	Alkenes to epoxides (peroxides/per acids based)-	PPT/Lecture	Assignment	
5	Sharpless asymmetric epoxidation.	PPT/Lecture		
6	Jacobsen epoxidation, Shi epoxidation	PPT/Lecture		

7	Alkenes to diols (Manganese and Osmium based)-	Lecture		
8	Prevost reaction	Lecture		
9	Woodward modification	Lecture		
10	Alkenes to carbonyls with bond cleavage (Manganese and lead based, ozonolysis)	Lecture		
11	Alkenes to alcohols/carbonyls without bond cleavage	PPT/Lecture		
12	Hydroboration-oxidation, Wacker oxidation, selenium/chromium based allylic oxidation.	PPT/Lecture	Quiz	
13	Ketones to ester/lactones- Baeyer-Villiger oxidation	Lecture		
14	Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson).	Lecture		
15	Metal based reductions- Birch reduction, pinacol formation, acyloin formation	Lecture		
16	Hydride transfer reagents from Group III and Group IV in reductions - LiAlH <sub>4</sub> .	Lecture		
17	DIBAL-H, Red-Al, NaBH <sub>4</sub> and NaCNBH <sub>3</sub> , selectrides	PPT/Lecture		
18	Trialkylsilanes and trialkylstannane. Meerwein-Ponndorf-Verley reduction. Baker's yeast	PPT/Lecture		
<b>Unit 2 : Modern Synthetic Methods and Reagents (15 Hours)</b>				
19	Baylis-Hillman reaction.	PPT/Lecture		
20	Henry reaction, Nef reaction	PPT/Lecture		
21	Kulinkovich reaction, Ritter reaction	PPT/Lecture		
First Internal Examination				
22	Sakurai reaction, Tishchenko reaction, Ugi	PPT/Lecture		

	reaction			
23	Noyori reaction. Brook rearrangement	PPT/Lecture		
24	Tebbe olefination.	PPT/Lecture	Assignment	
25	Metal mediated C-C and C-X coupling reactions: Heck Reaction	PPT/Lecture		
26	Stille Reaction	PPT/Lecture		
27	Suzuki, Suzuki-Miyaura,	PPT/Lecture		
28	Negishi-Sonogashira, Nozaki-Hiyama	PPT/Lecture		
29	Buchwald-Hartwig, Ullmann and Glaser coupling reactions.	PPT/Lecture		
30	Wohl-Ziegler reaction.	PPT/Lecture		
31	Reagents such as NBS	Lecture		
32	DDQ and DCC	Lecture		
33	Gilman reagent.	Lecture		
<b>Unit 3: Construction of Carbocyclic and Heterocyclic Ring Systems (12 Hours)</b>				
34	Different approaches towards the synthesis of three, four, five and six-membered rings.	Lecture		
35	Photochemical approaches for the synthesis of four membered rings- oxetanes and cyclobutanes			
36	Ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction,	PPT/Lecture		
37	Volhardt reaction, Bergman cyclization,	PPT/Lecture		
38	Nazarov cyclization, Mitsunobu reaction,	PPT/Lecture		
39	Cation-olefin cyclization and radical-olefin cyclization.			
40	Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction	PPT/Lecture		

41	Reformatsky reaction. Construction of Macrocylic rings-ring closing metathesis.	PPT/Lecture		
42	Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more than one hetero atom like N, S	PPT/Lecture		
43	Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more than one hetero atom like O -	Lecture	Quiz	
44	Pyrrole, furan, thiophene,	PPT/Lecture		
45	Imidazole, thiazole and oxazole	PPT/Lecture		
<b>Unit 4: Protecting group Chemistry (9 Hours)</b>				
46	Protection and deprotection of hydroxy, carboxyl	PPT/Lecture		
47	Carbonyl, and amino groups. Chemo and regio selective protection and deprotection.	PPT/Lecture		
48	Illustration of protection and deprotection in synthesis.	Lecture		
49	Protection and deprotection in peptide synthesis.	PPT/Lecture		
50	common protecting groups used in peptide synthesis	PPT/Lecture		
51	protecting groups used in solution phase	PPT/Lecture		
52	solid phase peptide synthesis (SPPS).	PPT/Lecture		
53	Functional equivalence and reactivity Umpolung.	PPT/Lecture		
54	Role of trimethyl silyl group in organic synthesis	PPT/Lecture		
<b>Unit 5: Retrosynthetic Analysis(9 Hours)</b>				
55	Basic principles and terminology of reterosynthesis: method.	PPT/Lecture		

56	Synthesis of aromatic compounds, one group	PPT/Lecture		
57	two group C-X disconnections, one group C-C and two group C-C disconnections.	PPT/Lecture		
58	Amine and alkene synthesis: important strategies of retrosynthesis,	PPT/Lecture	Video	
59	Functional group transposition, important functional group interconversions.	PPT/Lecture		
60	Important functional group interconversions,	PPT/Lecture		
61	Enantioselective synthesis of Corey lactone	PPT/Lecture		
62	longifolene and luciferin.	PPT/Lecture		
63	Umpolung equivalent – Peterson olefination, enolate formation, Ireland	Lecture		
Second Internal examination				
<b>Unit 6: Molecular Recognition and Supramolecular Chemistry(9 Hours )</b>				
64	Concept of molecular recognition- host-guest complex formation-	PPT/Lecture		
65	Forces involved in molecular recognition. Molecular receptors:	Lecture	Quiz	
66	Cyclodextrins, crown ethers, cryptands, spherands	PPT/Lecture		
67	Tweezers, carcerands	PPT/Lecture		
68	cyclophanes, calixarenes.	PPT/Lecture		
69	Importance of molecular recognition in nucleic acids and protein.	PPT/Lecture		
70	Applications of supramolecular complexes in medicine-	PPT/Lecture		
71	targeted drug delivery	PPT/Lecture		
72	Revision	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	2/10/2018	Retrosynthetic analysis- problems
2	28/10/2018	Seminar on Reagents

### GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	05/11/2018	Protecting groups (Group Discussion)

### References

- ❖ M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.
- ❖ F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.
- ❖ W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.
- ❖ J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.
- ❖ R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

PROGRAMME	MSC APPLIED CHEMISTRY - PHARMACEUTICAL	SEMESTER	3
COURSE CODE AND TITLE	16P3CPHT11: Physical Chemistry III	CREDIT	4
HOURS/WEEK	4	HOURS/SEM	72
FACULTY NAME	Dr. K B Jose, Dr. Thommachan Xavier, Dr Jorphin Joseph, Dr Jinu George		

<b>COURSE OBJECTIVES</b>
To apply the principles of chemical kinetics in different types of reactions.
To apply the principles of chemical kinetics in different types of solutions and enzyme catalysis.
To analyze the theories of electrochemistry with its applications in measurements.
To describe the chemistry of surfaces and its applications in colloids and macromolecules.
To explain the chemistry of light

SESSION	TOPIC	LEARNING RESOURCES	VALUE ADDITIONS	REMARKS
<b>MODULE I : CHEMICAL KINETICS I (14h)</b>				
1.	Theories of reaction rates: Collision theory-steric factor, potential energy surfaces.	PPT	video	
2.	Conventional transition state theory-Eyring equation, Comparison of the two theories.	PPT/Lecture		
3.	Thermodynamic formulation of the two theories, Thermodynamic formulation of the reaction rates.	PPT/Lecture		
4.	Significance of $\Delta G^*$ , $\Delta H^*$ and $\Delta S^*$ . Volume of activation. Effect of pressure and volume on velocity of gas reactions.	PPT/Lecture	e-resource	

5.	Introduction to Molecular Reaction Dynamics	PPT/Lecture		
6.	Various types of reaction theories	PPT/Lecture		
7.	Lindemann-Hinshelwood mechanism	Lecture		
8.	Qualitative idea of RRKM theory	Lecture		
9.	Fast reactions: relaxation, Flow and Shock methods, Flash photolysis.			
10.	NMR and ESR a methods of studying fast reactions.	Lecture		
11.	Chain reactions, free radical and chain reactions, Steady state treatment,	PPT/Lecture		
12.	kinetics of $H_2-Cl_2$ and $H_2-Br_2$ reactions	PPT/Lecture		
13.	Rice –Herzfeld mechanism, Branching chains $H_2-O_2$ , Semenov-Hinshelwood mechanism of explosive reactions.	PPT/Lecture		
14.	Kinetics of polymerization: mechanism of step growth Ionic and addition polymerization Kinetics of anionic and cationic polymerization.	Lecture		
	REVISION			
<b>MODULE II: CHEMICAL KINETICS II (14h)</b>				
15.	Reactions in solution: factors determining reaction rates in solutions	PPT	video	
16.	effect of dielectric constant and ionic strength	PPT/Lecture		
17.	cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect,	PPT/Lecture		
18.	Influence of solvent on reaction rates, significance of volume of activation linear free energy relationship	PPT/Lecture	e-resource	
19.	kinetic isotope effect	PPT/Lecture		



20.	Homogenous catalysis -Acid-base catalysis: van't Hoff and Arrhenius intermediates for prototropic and protolytic mechanisms with examples specific and general catalysis.	PPT/Lecture		
21.	Skrabal diagram, Bronsted catalysis law	Lecture		
22.	Acidity function.	Lecture		
23.	Enzyme catalysis and its mechanism			
24.	Michelis-Menten equation	Lecture		
25.	Effect of pH and temperature on enzyme catalysis.	PPT/Lecture		
26.	Heterogeneous catalysis Mechanisms of: unimolecular and bimolecular surface reactions, Langmuir-Hinshelwood and Langmuir-Rideal mechanism-	PPT/Lecture		
27.	ARRT of surface reactions-mechanisms of catalyzed reactions like ammonia synthesis,	PPT/Lecture		
28.	hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.	Lecture		
	REVISION			
<b>MODULE III : ELECTROCHEMISTRY I (12h)</b>				
29.	Theories of ions in solution, Ion activity, Ion-ion and ion-solvent interaction	Lecture		
30.	Born's model, Debye-Huckel theory, Ionic atmosphere.	Lecture		
31.	The Debye-Huckel-Onsager conductance equation-its derivation and experimental verification	Lecture		
32.	Validity of DHO equation for aqueous and non-aqueous solutions.	Lecture		
33.	Deviations from DHO conductance equation.	Lecture		

34.	Extension of DHO equation to ion solvent interactions.	PPT/Lecture		
35.	Derivation of Debye-Huckel limiting law.	PPT/Lecture		
36.	Conductance measurements Results of conductance measurements Factors affecting conductance	PPT/Lecture		
37.	Debye Falkenhagen and Wein effects,	PPT/Lecture		
38.	Walden rule, abnormal ionic conductance.	PPT/Lecture		
39.	Electro kinetic effects - electrophoresis, electro osmosis, streaming potential	Lecture		
40.	sedimentation potential – Donnan membrane equilibrium.	Lecture		
	REVISION			
<b>MODULE IV : SURFACE CHEMISTRY AND COLLOIDS (18h)</b>				
41.	Gas adsorption at solid surface - influencing factors	PPT/Lecture		
42.	Bonding of adsorbate to solid – adsorption isotherms –	PPT/Lecture		
43.	Langmuir (derivation)	PPT/Lecture		
44.	BET (derivation) Determination of surface area.	Lecture	Quiz	
45.	Spectroscopic techniques for probing solid surfaces	Lecture	Q &Ans Session	
46.	Temperature programmed desorption (TPD)	PPT/Lecture		
47.	Reflection absorption infrared spectroscopy (RAIRS)	PPT/Lecture		
48.	High resolution electron energy loss spectroscopy (HREELS).	PPT/Lecture		
49.	Surface films -Introduction film pressure	PPT/Lecture		

50.	criteria for spreading of one liquid on another	Lecture		
51.	Adsorption from solutions	PPT/Lecture		
52.	Electrostatic adsorption, Gibbs adsorption isotherm (derivation) - verifications.	PPT/Lecture		
53.	Colloids & Micellar systems Types of colloids, Electrical properties of colloids	PPT/Lecture		
54.	Electrical double layer, zeta potential	PPT/Lecture		
55.	Miscelles, and miscellisation	PPT/Lecture		
56.	Structure of miscelles - ionic miscelles.	PPT/Lecture		
57.	Adsorption from solutions - electrostatic adsorption	PPT/Lecture		
58.	Gibbs adsorption isotherm (derivation) - verifications.	PPT/Lecture		
	REVISION			
<b>MODULE V : PHOTOCHEMISTRY (14h)</b>				
59.	Laws of Photochemistry	PPT/Lecture		
60.	Grothus –Draper Law, Stark-Einstein’s Law, Laws of light absorption, Quantum yield. Chemical actinometry	PPT/Lecture		
61.	Excimers and exciplexes, photosensitization	PPT/Lecture	Video	
62.	chemiluminescence, bioluminescence, thermo luminescence	PPT/Lecture		
63.	Applications in daily life	PPT/Lecture		
64.	pulse radiolysis, hydrated electrons			
65.	photo stationary state, dimerization of anthracene.	Lecture	Debate	
66.	Photo physical processes in electronically excited molecules	PPT/Lecture		

67.	Jablonsky diagram Fluorescence and Phosphorescence.	PPT/Lecture		
68.	Quenching of fluorescence and its kinetics	PPT/Lecture		
69.	Stern-Volmer equation, static and dynamic quenching pulse radiolysis, hydrated electrons, photo stationary state, dimerization of anthracene..	PPT/Lecture		
70.	Concentration quenching, E-type and P-type. Effect of temperature on emissions,	PPT/Lecture		
71.	Two photon absorption spectroscopies Principle of utilization of solar energy	Lecture	video	
72.	Solar cells and their working. Photochemistry of vision. delayed fluorescence	Lecture		
	Revision			

#### INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	I CIA	Imaging in medicine
2	II CIA	Surface studies relevance in current research

#### GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	I INT	Chemistry of vision (Group Discussion)
2	II INT	Adsorption in industry

#### References

1. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
2. K.J. Laidler, Chemical kinetics, 3<sup>rd</sup>Edn. Harper & Row, 1987.
3. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and

- Applications, New Age International, 2005.
- J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.
  - P.W. Atkins, Physical Chemistry, ELBS, 1994.
  - D.A. McQuarrie, J.D. Simon, Physical chemistry: A Molecular Approach, University Science Books, 1997
  - K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2<sup>nd</sup> Edn. New Age International, 1986.
  - G. Aruldas, Molecular structure and Spectroscopy, PHI Learning, 2007.
  - M.R Wright, An Introduction to Chemical Kinetics, John Interscience-2007
  - A.W & Sons, Adamson, A.P. Gast, Physical chemistry of surfaces, 6<sup>th</sup> Edn, John Wiley, 1997
  - D.O. Cowan, R.L. Drisko, Elements of Organic Photochemistry, Plenum Press, 1976

PROGRAMME	MSC APPLIED CHEMISTRY - PHARMACEUTICAL	SEMESTER	3
COURSE CODE AND TITLE	16P3CPHT12- SPECTROSCOPIC METHODS IN CHEMISTRY	CREDIT	3
HOURS/WEEK	3	HOURS/SEM	54
FACULTY NAME	DR. JOSEPH T MOOLAYIL, Dr. JUNE CYRIAC		

#### COURSE OBJECTIVES

To describe the principles of UV-visible, Chiro-optical, IR, NMR and Mass spectroscopic techniques.

To illustrate various spectroscopic techniques using simple problems.

To elucidate the structure of an unknown organic compound using data from various spectroscopic techniques.

SESSION	TOPIC	LEARNING RESOURCES	VALUE ADDITIONS	REMARKS
<b>MODULE I : Ultraviolet-Visible and Chiroptical Spectroscopy (9h)</b>				
1	Energy levels and selection rules	PPT	video	
2	Woodward-Fieser Rule	PPT/Lecture		
3	Fieser-Kuhn Rule	PPT/Lecture		
4	Solvent effect, Stereochemical effect-non-conjugated interactions.	PPT/Lecture	e-resource	

5	Applications, Chiroptical properties- ORD	PPT/Lecture		
6	CD, octant rule	PPT/Lecture		
7	Chiroptical properties- ORD	Lecture		
8	Axial haloketone rule, Cotton effect.	Lecture		
9	Problems based on the above topics.	Lecture		
<b>MODULE II : Infrared Spectroscopy (9h)</b>				
10	Fundamental vibrations	PPT/Lecture		
11	Characteristic regions of the spectrum	PPT/Lecture		
12	Continued	PPT/Lecture		
13	Influence of substituents, ringsize, hydrogen bonding, vibrational coupling and field effect on frequency.	PPT/Lecture		
14	Continued	PPT/Lecture		
15	Determination of stereochemistry by IR technique.	Lecture		
16	IR spectra of olefins and arenes, - C=C bonds and C=O bonds.	Lecture		
17	Problems-spectral interpretation with examples.	Lecture		
18	Continued			
CIA-1				
<b>MODULE III : Nuclear Magnetic Resonance Spectroscopy (18h)</b>				
19	A comparison of the NMR phenomena of $^1\text{H}$ and $^{13}\text{C}$ nuclei.	Lecture		
20	Factors affecting chemical shift -	PPT/Lecture		
21	Relaxation processes, chemical and magnetic	PPT/Lecture		

	non-equivalence			
22	local diamagnetic shielding and magnetic anisotropy.	PPT/Lecture		
23	Proton and <sup>13</sup> C NMR scales	PPT/Lecture		
24	Spin-spin splitting:AX, AX <sub>2</sub>	Lecture		
25	Scheduling criteria, Scheduling Algorithms AX <sub>3</sub> , A <sub>2</sub> X <sub>3</sub> , AB, ABC, AMX type coupling	Lecture		
26	First order and non-first order spectra - Pascal's triangle	Lecture		
27	Coupling constant - mechanism of coupling, heteronuclear couplings-Karplus curve	Lecture		
28	Quadrupole broadening and decoupling - diastereomeric protons - virtual coupling	PPT/Lecture		
29	Long range coupling-epi, peri, bay effects. NOE - NOE and cross polarization.	PPT/Lecture		
30	Simplification non-first order spectra: shift reagents-mechanism	PPT/Lecture		
31	Spin decoupling-double resonance and off resonance decoupling.	PPT/Lecture		
32	2D NMR, HOMOCOSY and HETEROCOSY	PPT/Lecture		
33	Continued	PPT/Lecture		
34	Polarization transfer.	PPT/Lecture		
35	Problems-Spectral interpretation with examples.	Lecture	Quiz	
36	Problems-Spectral interpretation with examples.	Lecture	Q &Ans Session	
<b>MODULE IV : Mass Spectrometry (9h)</b>				
37	Molecular ion: ion production methods (EI).	PPT/Lecture		
38	Soft ionization methods: SIMS, FAB, CI, MALDI, Electrospray ionization.	PPT/Lecture		

39	Mass Analysis- Magnetic and electric fields, Quadrupole	PPT/Lecture		
40	TOF and ion trap mass analysers	Lecture		
41	Fragmentation patterns in EI MS	PPT/Lecture		
42	Continued	PPT/Lecture		
43	Nitrogen and ring rules- McLafferty rearrangement - applications.	PPT/Lecture		
44	HRMS, MS-MS, MIKES,CAD, FTMS,LC-MS, GC-MS.	PPT/Lecture		
45	Problems-Spectral interpretation with examples.	PPT/Lecture		
<b>MODULE V : Structural Elucidation Using Spectroscopic Techniques (9h)</b>				
46	Identification of structures of unknown organic molecules based on the data from IR, <sup>1</sup> HNMR and <sup>13</sup> CNMR spectroscopy and mass spectroscopy	PPT/Lecture		
47	Identification of structures of unknown organic molecules based on the data from IR, <sup>1</sup> HNMR and <sup>13</sup> CNMR spectroscopy and mass spectroscopy	PPT/Lecture		
48	Identification of structures of unknown organic molecules based on the data from IR, <sup>1</sup> HNMR and <sup>13</sup> CNMR spectroscopy and mass spectroscopy	PPT/Lecture		
49	Identification of structures of unknown organic molecules based on the data from IR, <sup>1</sup> HNMR and <sup>13</sup> CNMR spectroscopy and mass spectroscopy	PPT/Lecture	Video	
50	Interpretation of the given UV-Vis, IR NMR and mass spectra.	PPT/Lecture		
51	Interpretation of the given UV-Vis, IR NMR and mass spectra.	PPT/Lecture		
52	Interpretation of the given UV-Vis, IR NMR and			



	mass spectra.			
53	Interpretation of the given UV-Vis, IR NMR and mass spectra.	Lecture		
54	Interpretation of the given UV-Vis, IR NMR and mass spectra.	PPT/Lecture		
CIA II				

### INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
2/9/2018	Problems on Spectral interpretation
28/10/2018	Identification of structures of unknown organic molecules based on the data from IR, <sup>1</sup> HNMR and <sup>13</sup> CNMR spectroscopy and mass spectroscopy

### GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	09/11/2018	Interpretation of the given UV-Vis, IR NMR and mass spectra.

### References

1. D.L. Pavia, G.M. Lampman, G.S.Kriz, *Introduction to Spectroscopy: A Guide for Students of Organic Chemistry* (3<sup>rd</sup> Ed.), Thomson. 2004.
2. W. Kemp, *Organic Spectroscopy*, 2nd edition, ELBS-Macmillan, 1987.
3. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, Third Edition, New Age Publications, New Delhi, 2010.
4. D.F.Taber, *Organic Spectroscopic Structure Determination: A Problem Based Learning Approach*, Oxford University Press, 2009.
5. R. M. Silverstein, G.C. Bassler, T. C. Morrill, *Spectroscopic Identification of Organic Compounds*, John Wiley, 1991.

6. D. H. Williams, I. Fleming, *Spectroscopic Methods in Organic Chemistry*, Tata McGraw Hill, 1988.
7. F. Bernath, *Spectra of Atoms and Molecules*, 2nd Edition, Oxford University Press, 2005.
8. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, *Molecular Vibrations: The Theory of Infrared and Raman Spectra*, Dover Publications, 1980.
9. Atta-Ur-Rahman, M.I. Choudhary, *Solving Problems with NMR Spectroscopy*, Academic Press, New York, 1996.
10. L. D. Field, S. Sternhell, J. R. Kalman, *Organic Structures from Spectra* (fourth edition), Wiley, 2008.
11. Online spectroscopy problems and solutions like  
[www.orgchem.collarado.edu/Spectroscopy/Problems](http://www.orgchem.collarado.edu/Spectroscopy/Problems)  
[www.chem.ucla.edu/webSpectra](http://www.chem.ucla.edu/webSpectra)