SACRED HEART COLLEGE (AUTONOMOUS)

Department of Chemistry

MSc Chemistry

Course Plan

Academic Year 2018-19

Semester Three

PROGRAMME	MSc Chemistry	SEMESTER	3
COURSE CODE AND TITLE	**16P3CHET09: INORGANIC CHEMISTRY-III**	CREDIT	4
HOURS/WEEK	4	HOURS/SEM	72
FACULTY NAME	Dr. Midhun Dominic C D, Dr. Ramakrishnan S, Mr. Senju Devassykutty		

Course Objectives
To describe the structure, reactions and phase transitions of solid state
To interpret the electrical, magnetic and optical properties of solids.
To illustrate the structure and applications of inorganic chains, rings, cages and clusters, and organometallic polymers.
To categorize different metal clusters
To describe the synthesis, classification and applications of ceramics and refractories

SESSION	TOPIC	LEARNING RESOURCES	VALUE ADDITIONS	REMARKS
MODULE I (Solid state Chemistry) (18 h)				
1	Close Packing. Imperfections in solids-point defects, Stoichiometric and non-stoichiometric defects	PPT	video	
2	Non stoichiometric defects in the monoxides of 3d series, Vegard's rule. Line defects and plane defects	PPT/Lecture		
3	Structure of solids:. Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), ABX_3 (Perosvskite, Ilmenite).	PPT/Lecture		
4	Spinels. Inverse spinel structures.	PPT/Lecture	e-resource	
5	Diffusion in solids. Mechanisms- vacancy	PPT/Lecture		

	diffusion, Interstitial diffusion, Interstitialcy diffusion, Ring mechanism.			
6	Diffusion equation- Coefficient of diffusion atomic approach.	PPT/Lecture		
7	Solid state reactions-Factors affecting the rate of solid state reactions- Reaction condition, Structural factor, Nucleation and growth	Lecture		
8	Surface area of solids, Surface structure and reactivity, Wagner reaction mechanism, Kirkendall effect, Nucleation and reactivity, Topotactic and epitactic reaction	Lecture		
9	Synthesis of solids- Direct reactions (Shake n bake method) Examples $L_{i4}Si_{O4}$,$YB_{a2}C_{u3O7}$ and Na β/β'', Sol-gel method	Lecture		
10	(Synthesis of Silica glass,Indium tin oxide, Zeolites),Intercalation and deintercalation, Vapour phase transport, and Chemical vapour deposition.	Lecture		
11	Phase transition in solids- Buerger's Classification of phase transitions, Reconstructive and Displacive Transitions	PPT/Lecture		
12	Thermodynamic Classification-first and second order phase transitions (Brief study only).Nucleation, growth and critical size in phase transition. Order-disorder transitions and Martensitic transformations.	PPT/Lecture		
13	Crystal Growth.Growth of Single crystal. Various Techniques-Crystal growth from melt-Czohralski method, Bridgman and Stockbarger method, Zone melting.	PPT/Lecture		
14	Crystallization from solution-Hydro thermal method, gel method. Crystal growth from Vapour- Chemical Vapour Deposition.	PPT/Lecture		
15	Solid Electrolytes- Solid cationic electrolytes, Solid anionic electrolytes	PPT/Lecture		

16	Mixed ionic electronic conductors.	Lecture		
17	Solid solution-Substitutional Solid Solution, Requirments for formation,Interstitial Solid Solution,	Lecture		
18	Metal alloys,Engel-Brewer rule, Intermetallic compounds, Hume-Rothery Compounds, Zintal Phase.	Lecture		
MODULE II (Electrical, Magnetic and Optical Properties of Solids) (18 h)				
19	Classical free electron theory of metals(Lorentz-Drude theory)-Drift velocity-current density J-mobility of charge carriers-conductivity-advantages and disadvantages of classical free electron theory	Lecture		
20	Quantum free electron theory(Sommerfield)-Fermilevel and calculation of Fermi energy-Density of states	PPT/Lecture		
21	Calculation of average energy of free electrons-specific heat in quantum free electron theory-Lorenz number in Quantum free electron theory	PPT/Lecture		
22	Zone theory of solids (Quantum mechanical approach)-Kronig-Penney model	PPT/Lecture		
23	K space-Wigner Seitz cell- K space- Brillouin Zone-Extended Zone scheme	PPT/Lecture		
24	MO theory of solids. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors	Lecture		
	CIA-I			
25	Hall Effect- Significance of Hall coefficient	Lecture		
26	Pyroelectricity- Piezo electricity	Lecture		
27	Ferro electricity	Lecture		
28	Eectronic and Magnetic properties of monoxides of elements in 3d series. Higher oxide and complex oxides of Transition	Lecture		

	elements			
29	Oxides with M_2O_3 Corundum structure, Rhenium trioxide and related oxides. Conductivity in mixed oxides, Isomorphous Substitution, Principles and applications.	PPT/Lecture		
30	Spinels and inverse spinels, LFSE and spinel structure	PPT/Lecture		
31	Cooperative magnetism-Ferromagnetic materials, Curie temperature, Anti ferromagnetism, Neel temperature, Super exchange, Ferrimagnetisms.	PPT/Lecture		
32	Perovskite and related Phases. Perovskite structure-Optical properties-photoconductivity, photovoltaic effects, luminescence	PPT/Lecture		
33	Applications of optical properties.TiO_2 as Photocatalyst	PPT/Lecture		
34	Super conductivity-Type I and Type II superconductors- Meisner effect and its applications Cooper pairs- theory of low temperature super conductors, BCS theory of superconductivity (derivation not required	PPT/Lecture		
35	Josephson Tunneling- Super conducting cuprates – Preparation, properties and application of-YBaCu oxide system	PPT/Lecture		
36	Meisner effect and its applications-conventional superconductors, high temperature superconductors.	Lecture	Quiz	
MODULE III Inorganic Chains, Rings and Cages (24 h)				
37	Chains - catenation, heterocatenation			
38	Silicate minerals	PPT/Lecture		
39	Structure of silicates- common silicates, silicates containing discrete anions, silicates containing infinite chains	PPT/Lecture		
40	silicates containing sheets, framework silicates.	PPT/Lecture		

41	Silicones	PPT/Lecture		
42	Zeolites	Lecture		
43	.Isopoly acids of vanadium	PPT/Lecture		
44	Isopoly acids of molybdenum and tungsten.	PPT/Lecture		
45	Heteropoly acids of Mo and W.	PPT/Lecture		
46	Condensed phosphates-preparation, structure and applications.	PPT/Lecture		
47	Polythiazyl – one dimensional conductor	PPT/Lecture		
48	Rings-topological approach to boron hydrides, Styx numbers.	PPT/Lecture		
49	Synthesis, structure and bonding in borazines	PPT/Lecture		
50	Synthesis, structure and bonding in ring silicates and silicones	PPT/Lecture		
51	phosphazenes	PPT/Lecture		
52	Synthesis, structure and bonding of phosphazenes	PPT/Lecture	Video	
53	Heterocyclic inorganic ring systems	PPT/Lecture		
54	Synthesis, structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds	PPT/Lecture		
55	Homocyclic inorganic ring systems	PPT/Lecture		
56	synthesis, structure and bonding in sulphur, selenium and phosphorous compounds	Lecture		
57	Cages: synthesis, structure and bonding of cage like structures of phosphorous – phosphorous-oxygen compounds.	PPT/Lecture		
58	Boron cage compounds	PPT/Lecture		
59	Wade Mingos Lauher rules, MNO rule, boranes	PPT/Lecture		
60	carboranes, metallacarboranes	PPT/Lecture		
CIA-II				

MODULE IV Metal clusters (5h)				
61	Halide Clusters: Dinuclear compounds of Re	PPT/Lecture		
62	Dinuclear compounds of Cu and Cr	PPT/Lecture		
63	Metal- metal multiple onding in $(Re_2X_8)^{2-}$	Lecture	Demo video	
64	trinuclear clusters, tetranuclear clusters, hexanuclear clusters.	Lecture		
66	Glasses-glassy state	Lecture		
67	Glass formers, glass modifiers	PPT/Lecture		
68	Ceramics-ceramic structures- mechanical properties	PPT/Lecture		
69	Refractories-characterisations, properties and applications.	PPT/Lecture		
70	One dimensional Solids. Magnetic, Electrical and optical properties of the following Solids. KCP and other Pt compounds	Lecture		
71	$Hg_{3-x}AsF_6$, $[(CH_3)_4N]MnCl_6$,$KCuF_3$,and,RbF_3.	PPT/Lecture		
72	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	15/10/2018	Wade Mingos rules : Problems
2	27/11/2018	Classification and applications of ceramics and refractories

GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	6/11/2018	Previous CSIR questions (Group activity)

References

1. Shiver & Atkins, Inorganic Chemistry, 4th Edn. Oxford University Press,2006.
2. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers,1993.
3. G.L. Miessler,D. A. Tarr, Inorganic Chemistry 3rd Ed., Pearson Education, 2007.Further Reading.
4. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
5. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.
6. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.
7. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.
8. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.
9. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley & sons, 2006.
10. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.
11. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience,1999.
12. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
13. P.C. Jain, M. Jain, Engineering Chemistry, 12th Edn., Dhanpat Rai Pub., 2006.
14. C.V. Agarwal, Chemistry of Engineering Materials, 9th Edn., B.S. Pub., 2006.
15. W.L Jolly, Modern Inorganic Chemistry, 2nd Edn. Tata McGraw Hill,2007.
16. C. N. R. Rao and J. Gopalakrishnan, New directions in Solid state Chemistry, 2nd Edition, Cambridge University Press1997.

Web resource references:

- http //solid-state.com

PROGRAMME	MSC CHEMISTRY	SEMESTER	3
COURSE CODE AND TITLE	16P3CHET10 and ORGANIC SYNTHESES	CREDIT	4
HOURS/WEEK	4	HOURS/SEM	72
FACULTY NAME	DR. JOSEPH T MOOLAYIL, DR. V.S SEBASTIAN, DR. FRANKLIN J, DR.GRACE THOMAS		

Course Objectives

- 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
Unit 1 : Organic Synthesis via Oxidation and Reduction (18 hours)				
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 - LiAlH4,.	Lecture		
17	DIBAL-H, Red-Al, NaBH4 and NaCNBH3, selectrides	PPT/Lecture		
18	Trialkylsilanes and trialkylstannane. Meerwein-Pondorff-Verley reduction. Baker's yeast	PPT/Lecture		
Unit 2: Modern Synthetic methods and Reagents (15h)				
19	Baylis-Hillman reaction.	PPT/Lecture		
20	Henry reaction, Nef reaction	PPT/Lecture		
21	Kulinkovich reaction, Ritter reaction	PPT/Lecture		
22	Sakurai reaction, Tishchenko reaction, Ugi reaction	PPT/Lecture		
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	Gilmann reagent.	Lecture		
Unit 3: Construction of Carbocyclic and Heterocyclic Ring Systems (12 Hours)				
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 Macrocyclic 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		
Unit 4: Protecting group Chemistry (9 Hours)				
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		
Unit 5: Retrosynthetic Analysis(9 Hours)				
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				
Unit 6: Molecular Recognition and Supramolecular Chemistry(9 Hours)				
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 CHEMISTRY	SEMESTER	3
COURSE CODE AND TITLE	16P3CHET11: 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		

COURSE OBJECTIVES
To know the principles of chemical kinetics in different types of reactions.
To understand 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**
MODULE I : CHEMICAL KINETICS I (14h)				
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, Thermodynamicformulation of the reaction rates.	PPT/Lecture		
4.	Significance of ΔG*, ΔH* andΔS*.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			
MODULE II: CHEMICAL KINETICS II (14h)				
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			
MODULE III : ELECTROCHEMISTRY I (12h)				
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	PPT/Lecture		

	conductance			
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			
MODULE IV : SURFACE CHEMISTRY AND COLLOIDS (18h)				
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			
MODULE V : PHOTOCHEMISTRY (14h)				
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, 3rd Edn. Harper & Row, 1987.
3. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.
4. J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.
5. P.W. Atkins, Physical Chemistry, ELBS, 1994.
6. D.A. McQuarrie, J.D. Simon, Physiacl chemistry: A Molecular Approach, University Science Books,1997
8. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2nd Edn. New Age International, 1986.
9. G. Aruldhas, Molecular structure and Spectroscopy, PHI Learning, 2007.
10. M.R Wright, An Introduction to Chemical Kinetics, John Interscience-2007
11. A.W &Sons, Adamson, A.P. Gast, Physical chemistry of sufaces,6thEdn,John Wiley, 1997
12. D.O. Cowan ,R.L. Drisko , Elements of Organic Photochemistry, Plenum Press,.1976

PROGRAMME	MSC CHEMISTRY	SEMESTER	3
COURSE CODE AND TITLE	16P3CHET12- 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**
MODULE I : Ultraviolet-Visible and Chiroptical Spectroscopy (9h)				
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		
MODULE II : Infrared Spectroscopy (9h)				
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				
MODULE III : Nuclear Magnetic Resonance Spectroscopy (18h)				
19	A comparison of the NMR phenomena of ^{1}H and ^{13}C nuclei.	Lecture		
20	Factors affecting chemical shift -	PPT/Lecture		
21	Relaxation processes, chemical and magnetic non-equivalence	PPT/Lecture		
22	local diamagnetic shielding and magnetic anisotropy.	PPT/Lecture		
23	Proton and ^{13}C NMR scales	PPT/Lecture		
24	Spin-spin splitting:AX, AX_2	Lecture		
25	Scheduling criteria, Scheduling Algorithms AX_3, A_2X_3, 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	PPT/Lecture		

	- NOE and cross polarization.			
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	
MODULE IV : Mass Spectrometry (9h)				
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		
MODULE V : Structural Elucidation Using Spectroscopic Techniques (9h)				
46	Identification of structures of unknown organic molecules based on the data from IR, ^{1}HNMR and ^{13}CNMR spectroscopy and mass	PPT/Lecture		

	spectroscopy			
47	Identification of structures of unknown organic molecules based on the data from IR, ^{1}HNMR and ^{13}CNMR spectroscopy and mass spectroscopy	PPT/Lecture		
48	Identification of structures of unknown organic molecules based on the data from IR, ^{1}HNMR and ^{13}CNMR spectroscopy and mass spectroscopy	PPT/Lecture		
49	Identification of structures of unknown organic molecules based on the data from IR, ^{1}HNMR and ^{13}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, ^{1}HNMR and ^{13}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* (3rd 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. Morril, *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 Specroscopy*, 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

    www.chem.ucla.edu/webSpectra