Sacred Heart College (Autonomous)

Department of Chemistry

MSc Applied Chemistry - Pharmaceutical

Course Plan

Academic Year 2015 – 16

Semester 2

COURSE PLAN					
ACADEMIC YEAR 2015-16					
PROGRAMME	**:**	*M.Sc. Applied Chemistry - Pharmaceutical*	**LECTURE HOURS**	**:**	*72*
SEMESTER	**:**	*2*	**CREDITS**	**:**	*4*
SUBJECT TITLE	**:**	**COORDINATION CHEMISTRY**	**SUBJECT CODE**	**:**	**P2CPHT05**
COURSE TEACHERS	**:**	***Dr. Joseph John (JJ), Mr. Midhun Dominic C D (MD), Mr. Senju Devassykutty, Dr. Ramakrishnan S (RKS)***			
Course Objectives	**:**	*1. Ability to understand the structure and bonding in coordination complexes* *2. To understand the spectral and magnetic properties of complexes* *3. To know about the Kinetics and Mechanism of Reactions in Metal Complexes* *4. To understand the Stereochemistry of Coordination Compounds* *5. To know about Coordination Chemistry of Lanthanides and Actinides*			

Teacher I – JJ : Unit 1: Structural Aspects and Bonding (18 Hours)			
No. of Session	**Session Topic and Discussion Theme**	**Method of Teaching**	**Remarks/Student Assignments**
1	Classification of complexes based on coordination numbers and possible geometries.	Conventional Lecture Chalk & Board	Assignment on coordination numbers and possible geometries
2	Sigma and pi bonding ligands such as CO, NO, CN^-.		
3	Sigma and pi bonding ligands such as R_3P, and Ar_3P.	Lecture With power point presentation	
4	Stability of complexes – factors affecting stability		
5	Stability of complexes, thermodynamic aspects of complex formation		
6	Irving William order of stability, chelate effect	Conventional Lecture	
7	**First Internal Test**		
8	Splitting of *d* orbitals in octahedral, tetrahedral, square planar	Lecture With Powerpoint presentation	Assignment on Crystal field theory
9	Splitting of *d* orbitals in square pyramidal and triagonal bipyramidal fields		
10	LFSE, *Dq* values, Jahn Teller (JT) effect		
11	Theoretical failure of crystal field theory, evidence of covalency in the metal ligand bond		
12	Nephelauxetic effect, ligand field theory		
13	Ligand field theory		
14	Introduction to Molecular orbital theory		
	Second Internal Test		
15	Molecular orbital theory-M.O energy level diagrams for octahedral complexes without and with π-bonding	Lecture with ICT	Assignment on Molecular orbital theory
16	M.O energy level diagrams for tetrahedral complexes without and with π-bonding,		
17	Experimental evidences for pi-bonding.		
18	Revision		

Reference Text Books
1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.
2. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.
5. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
7. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.
8. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008.

Teacher II – RKS	**Module Taken : Unit 2: Spectral and Magnetic Properties of Metal Complexes (Total – 18 Hrs)**		
No. of Session	**Session Topic and Discussion Theme**	**Method of Teaching**	**Remarks/Student Assignments**
1	Introduction to spectral and magnetic properties	Conventional Lecture Using Chalk and Board	Assignment on correlation diagrams
2	Electronic Spectra of complexes-Term symbols of dn system, Racah parameters		
3	Splitting of terms in weak and strong octahedral and tetrahedral fields.		
4	Correlation diagrams for dn in octahedral and tetrahedral fields (qualitative approach)		
5	Correlation diagrams for d10-n ions in octahedral and tetrahedral fields (qualitative approach)		
6	d-d transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.		
	First Internal Test		
7	Interpretation of electronic spectra of complexes-Orgel diagrams	Lecture With Chalk and board	Assignments based on Orgel diagrams
8	Demerits of Orgel diagrams		
9	Tanabe-Sugano diagrams		
10	Calculation of *Dq*, *B* and β (Nephelauxetic ratio) values		
11	Spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.		
12	Magnetic properties of complexes-paramagnetic and diamagnetic complexes		
13	molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment.		
	Second Internal Test		
14	Temperature dependence of magnetism-Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP)		

15	Spin state cross over, Antiferromagnetism-inter and intra molecular interaction.	Lecture with ICT	Seminar Based on Applications of radioactivity
16	Anomalous magnetic moments.		
17	Elucidating the structure of cobalt complexes using electronic spectra, IR spectra and magnetic moments.		
18	Elucidating the structure of nickel complexes using electronic spectra, IR spectra and magnetic moments.		

Reference Text Books

1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.
2. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.
5. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
7. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.
8. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008.

Teacher III– SD	**Module Taken : Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hours)**		
No. of Session	**Session Topic and Discussion Theme**	**Method of Teaching**	**Remarks/Student Assignmets**
1	Introduction	Conventional Lecture	**Seminar Assignment to Students on the nucleophilic substitution reactions**
2	Thermodynamic and kinetic stability	Conventional lecture using Chalk and Board and ICT-PPT	
3	Thermodynamic and kinetic stability		
4	Kinetics and mechanism of nucleophilic substitution reactions in square planar complexes		
5	Kinetics and mechanism of nucleophilic substitution reactions in square planar complexes		
6	*trans* effect-theory and applications.		
First Internal Test			
7	Kinetics and mechanism of octahedral substitution- water exchange	Conventional Lecture using Chalk and Board and ICT -PPT	**Assignment to Students on the general mechanism of octahedral substitution**
8	Kinetics and mechanism of octahedral substitution- dissociative and associative mechanisms		
9	Kinetics and mechanism of octahedral substitution- base hydrolysis		
10	Kinetics and mechanism of octahedral substitution- racemization reactions		
11	Kinetics and mechanism of octahedral substitution-solvolytic reactions (acidic and basic).		
Second Internal Test			
12	Electron transfer reactions: outer sphere mechanism-Marcus theory	Conventional Lecture using Chalk and Board and ICT -PPT	**Assignment on electron transfer reactions**

13	Electron transfer reactions: outer sphere mechanism-Marcus theory		
14	Electron transfer reactions: outer sphere mechanism-Marcus theory		
15	Electron transfer reactions: inner sphere mechanism-Taube mechanism.		
16	Electron transfer reactions: inner sphere mechanism-Taube mechanism.		
17	Electron transfer reactions: inner sphere mechanism-Taube mechanism.		
18	Revision		

1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.
2. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.
5. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
7. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.
8. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008

Teacher IV – MD	Module Taken : Unit 4: Stereochemistry of Coordination Compounds (9 Hrs)		
No. of Session	**Session Topic and Discussion Theme**	**Method of Teaching**	**Remarks/Student Assignments**
1	Introduction to stereochemistry	Conventional Lecture	**Preparation of Lecture Notes**
2	Geometrical and optical isomerism in octahedral complexes		
3	Resolution of optically active complexes		
4	Determination of absolute configuration of complexes by ORD and circular dichroism		
5	Stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds		
6	Linkage isomerism-electronic and steric factors affecting linkage isomerism.		
7	Symbiosis-hard and soft ligands		
8	Prussian blue and related structures, Macrocycles-crown ethers.		
9	**Revision**		
First Internal Test			

Reference Text Books

1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.
2. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.
5. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
7. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.
8. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008

Teacher IV – MD	Module Taken : Unit 5: Coordination Chemistry of Lanthanides and Actinides (9 Hrs)		
10	General characteristics of lanthanides-Electronic configuration	Conventional Lecture	**Preparation of Notes on characteristics of lanthanides**
11	Term symbols for lanthanide ions, Oxidation state		
12	Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes.		
13	Electronic spectra and magnetic properties of lanthanide complexes		
14	.Lanthanide complexes as shift reagents		
Second Internal Test			
15	General characteristics of actinides-difference between 4f and 5f orbitals	Conventional Lecture	**Preparation of Notes on characteristics of actinides**
16	Comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra properties.		
17	Comparative account of coordination chemistry of lanthanides and actinides with special reference to magnetic properties.		
18	Revision		

Reference Text Books

1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.
2. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.
5. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
7. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.
8. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008

COURSE PLAN					
ACADEMIC YEAR 2015-16					
PROGRAMME	**:**	*M.Sc. Applied Chemistry - Pharmaceutical*	**LECTURE HOURS**	**:**	*72*
SEMESTER	**:**	*2*	**CREDITS**	**:**	*4*
SUBJECT TITLE	**:**	*Organic Reaction Mechanism*	**SUBJECT CODE**	**:**	*P2CPHT06*
COURSE TEACHERS	**:**	*Dr. Joseph .T. Moolayil, Dr. V.S Sebastian, Dr. June Cyriac*			
Instructional Hours	**:**	*Four Hours per Week*			

	No. of Session	Session Topic and Discussion Theme	Value additions	COs
JTM				
Unit 7: Concerted reactions (18 Hours)	1.	Classification	Assignment No: 1	
	2.	Electrocyclic reactions.		
	3.	Sigmatropic reactions.		
	4.	Cycloaddition reactions.		
	5.	Chelotropic reactions.		
	6.	Ene reactions.		
	7.	Woodward Hoffmann rules	Power Point	
	8.	Frontier orbital and orbital symmetry correlation approaches -	Power Point	
	9.	Continued	Power Point	
	10.	PMO method.	Power Point	
	11.	Pericyclic reactions in organic synthesis such as Claisen rearrangement		
	12.	Cope rearrangement		
	13.	Wittig rearrangement, Mislow-Evans rearrangement		
	14.	Sommelet-Hauser rearrangements, Diels-Alder and Ene reactions (with stereochemical aspects)		
	15.	Dipolar cycloaddition (introductory).		
	16.	Pyrolytic elimination reactions: cheletropic elimination.	Power Point	
	17.	Decomposition of cyclic azo compounds.		
	18.	β-eliminations involving cyclic transition states such as N-oxides, Acetates and xanthates.		
Text	R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*,7thEdn., Pearson, New Delhi, 2011.			

	J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004. Fleming, Wiley, *Frontier Orbitals and Organic Chemical Reactions*, London, 1976. S. Sankararaman, *Pericyclic Reactions-A Text Book*, Wiley VCH, 2005.

JUC				
Unit2: Chemistry of Carbanions (9 Hours)	19.	Formation, structure and stability of carbanions	Assignment No.3	
	20.	Reactions of carbanions: C-X bond (X = C, O, N)		
	21.	Formations through the intermediary of carbanions.		
	22.	Chemistry of enolates and enamines.		
	23.	Kinetic and Thermodynamic enolates-lithium and boron enolates in aldol alkylation and acylation of enolates.		
	24.	Electrophilic additions to alkenes, Kinetics, effect of structure, orientation and stereochemistry.	Power Point	
	25.	Ozonolysis and hydroboration. Nucleophilic additions to carbonyls groups. Named reactions under carbanion chemistry –Mechanism of Claisen,		
	26.	Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations. Shapiro reaction and Julia elimination. Favorski rearrangement.		
	27.	Ylids: Chemistry of Phosphorous and Sulphur ylids - Wittig and related reactions, Peterson olefination.		
		J. March and M. B. Smith, March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6thEdn., Wiley, 2007. http://www.organic-chemistry.org/namedreactions. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*,7thEdn., Pearson, New Delhi, 2011. J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.		

VSS				
Unit5: Radical Reactions (9 Hours)	28.	Generation of radical intermediates		
	29.	Its (a) addition to alkenes, alkynes (inter & intramolecular)		
	30.	For C-C bond formation - Baldwin's		
	31.	Fragmentation and rearrangements		
	32.	Hydroperoxide: formation, rearrangement and reactions.	Assignment No:2	
	33.	Continued		
	34.	Auto-oxidation.		
	35.	Named reactions involving radical intermediates: Barton deoxygenation		
	36.	Decarboxylation, McMurry coupling.		
Text Books		J. March and M. B. Smith, March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure,* 6thEdn., Wiley, 2007. http://www.organic-chemistry.org/namedreactions. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*,7thEdn., Pearson, New Delhi, 2011. J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.		
Unit4: Carbenes, Carbenoids, Nitrenes and Arynes	37.	Structure of carbenes (singlet and triplet) - generation of carbenes -		
	38.	Addition and insertion reactions.		
	39.	Rearrangement reactions of carbenes such as Wolff rearrangement -		
	40.	Generation and reactions of ylids by carbenoid decomposition.		
	41.	Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.		
	42.	Continued		

	43.	Hoffmann, and Curtius reactions.		
	44.	Lossen,, Schmidt and Beckmann rearrangement reactions		
	45.	Arynes: Generation, structure, stability and reactions. Orientation effect-amination of haloarenes.		
	J. March and M. B. Smith, March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure,* 6thEdn., Wiley, 2007. http://www.organic-chemistry.org/namedreactions. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*,7thEdn., Pearson, New Delhi, 2011. J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.		

JUC				
Unit1: Review of substitution reaction Mechanisms (9 Hours)	46.	A comprehensive study on the effect of substrate, reagent, leaving group, solvent, ambident nucleophile and neighbouring group on nucleophilic substitution(SN_1 and SN_2)		
	47.	Contiued		
	48.	Contiued		
	49.	Study on the effect of substrate, reagent, leaving group, solvent, ambident nucleophile and neighbouring group on elimination (E_1, E_2andE_{1CB}) reactions.	Power Point	
	50.	Continued		
	51.	Stereochemistry of E_2 reaction, Intramolecular pyrolytic elimination, Cope elimination. Elimination *vs* substitution.	Power Point	
	52.	Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (SN^i, SE_1, SE_2 and SE^i).		
	53.	Continued		
	54.	Markovnikovs and anti Markovnikovs addition		
	F. A. Carey, R. A. Sundberg,*Advanced Organic Chemistry*, Part B: Reactions and Synthesis, 5thEdn.,, Springer, New York, 2007. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, First South Asian Edition, Cambridge University Press, 2005. J. March and M. B. Smith, March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6thEdn., Wiley, 2007. http://www.organic-chemistry.org/namedreactions. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*,7thEdn., Pearson, New Delhi, 2011. J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.			

Unit 3: Chemistry of Carbocations (9Hours)	55.	Formation, structure and stability of carbocations.		
	56.	Classical and non-classical carbocations.	Power Point	
	57.	C-X bond (X = C, O, N) formations through the intermediary of carbocations.		
	58.	Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol,		
	59.	Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.		
	60.	C-C bond formation involving carbocations: Oxymercuration, halolactonisation.		
	61.	Structure and reactions of α, β- unsaturated carbonyl compounds – electrophilic addition		
	62.	Nucleophilic addition - Michael addition,		
	63.	Mannich reaction and Robinson annulation.		

R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanism*, Academic Press,2002.

F. A. Carey, R. A. Sundberg,*Advanced Organic Chemistry*, Part B: Reactions and Synthesis, 5thEdn.,, Springer, New York, 2007.

W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, First South Asian Edition, Cambridge University Press, 2005.

J. March and M. B. Smith, March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6thEdn., Wiley, 2007.

http://www.organic-chemistry.org/namedreactions.

R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*,7thEdn., Pearson, New Delhi, 2011.

J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.

	64.	Reactions of carbonyl compounds		
Unit 6: Chemistry of Carbonyl Compounds (9 Hours)	65.	Oxidation, reduction addition		
	66.	Continued		
	67.	Cannizzaro reaction		
	68.	Grignard reagent		
	69.	Structure and reactions of α,β unsaturated carbonyl compounds		
	70.	Michael addition		
	71.	Mannich reaction		
	72.	Robinson annulation		
	J. March and M. B. Smith, March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure,* 6thEdn., Wiley, 2007. http://www.organic-chemistry.org/namedreactions. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry,*7thEdn., Pearson, New Delhi, 2011. J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.			

COURSE PLAN					
ACADEMIC YEAR 2015-16					
PROGRAMME	**:**	*M.Sc. Applied Chemistry - Pharmaceutical*	**LECTURE HOURS**	**:**	*54*
SEMESTER	**:**	*2*	**CREDITS**	**:**	*3*
SUBJECT TITLE	**:**	*MOLECULAR SPECTROSCOPY*	**SUBJECT CODE**	**:**	*P2CPHT08*
COURSE TEACHERS	**:**	*Dr Franklin J, Dr. Jinu George, Dr KB Jose*			
COURSE OBJECTIVES	**:**	*Ability to understand the basics spectroscopy* *Ability to interpret the spectroscopic properties in simple systems, selection rules, derivations of related mathematical expressions* *Ability to explore and reflect about the wide range of possibilities and applications of spectroscopy*			
Instructional Hours	**:**	**3 hours/week**			

	No. of Sessions	Session Topic and Discussion Theme	Value additions	Web URL/additional resources
Unit 2: Resonance Spectroscopy	1	Resonance Raman scattering and resonance fluorescence.		
	2	Principle of SERS, selection rules, application. Comparison of IR and Raman.		https://youtu.be/H6_GgJN39vY
	3	Unit 2 Electron & Electronic Spectroscopy & Lasers : Introduction	ICT	
	4	Electron Spectroscopy: Basic principles		
	5 6	Photoelectron spectra of simple molecules, selection rules-Electron spectroscopy for chemical analysis (ESCA)-UPS		
	7	Applications		
	1st Internal Examination			
	8	X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES).		
	9	Electronic spectroscopy: Electronic spectra of diatomic molecules, Franck-Condon principle	Power Point Presentation	

Text Books

1. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.
3. P.W. Atkins, Physical Chemistry, ELBS,1994
4. R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965.
5. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
6. K.J. Laidler, J.H. Meiser, Physical Chemistry, 2ndEdn. CBS, 1999.
7. W. Kemp, NMR in chemistry-A Multinuclear Introduction, McMillan, 1986.
8. H. Kaur, Spectroscopy, 6thEdn. Pragati Prakashan, 2011.
9. H. Gunther, NMR Spectroscopy, Wiley, 1995.
10. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.
11. D.N. Sathyanarayan, Electronic Absorption Spectroscopy and Related Techniques, Universities Press, 2001.
12. D.N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2007.

	13. D.N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, IK International, 2009. 14. J. D. Graybeat. Molecular Spectroscopy, McGraw-Hill International Edition, 1988			
Unit II	**No. of Sessions**	**Session Topic and Discussion Theme**	**Value additions**	
Unit 2: Resonance Spectroscopy	10	Vibronic transitions, Spectra of organic compounds, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition.		
	11	Lasers: Laser action, population inversion, properties of laser radiation	Power Point Presentation	
	12	Two stage, three stage-examples of simple laser systems.	Power Point Presentation	
	13	Unit 3: Resonance Spectroscopy: Introduction		
	14	Discussions related to new gen Lasers	Group Discussion	
	2nd Internal Examination			
	15	3.1 NMR spectroscopy : interaction between nuclear spin and applied magnetic field		
	16	Nuclear energy levels, population of energy levels		
	17	Larmor precession, relaxation methods, chemical shift	Individual Assignment: Various intermolecular forces	
	18	Representation, examples of AB, AX and AMX types, exchange phenomenon		
Text Books				

	No. of Sessions	**Session Topic and Discussion Theme**	**Method**	
Unit 1: Foundations of Spectroscopic Techniques	1	**1.1 Origin of spectra**: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption		
	2	influencing factors, signal to noise ratio, natural line width, contributing factors		
	3	Doppler broadening, Lamb dip spectrum	ICT	
	4	Born Oppenheimer approximation, energy dissipation from excited states (radiative and non radiative processes), and relaxation time.		
	5 6	**1.2 Microwave spectroscopy***:* Classification of molecules;		
	7	rigid rotor model; rotational spectra of diatomics and polyatomics;		
	1st Internal Examination			
	8	effect of isotopic substitution and nonrigidity; selection rules and intensity distribution.		
	9	**1.3 Vibrational spectroscopy**: Vibrational spectra of diatomics;	Power Point Presentation	
Text Books				
Unit III	**No. of Sessions**	**Session Topic and Discussion Theme**	**Value additions**	

Unit 1: Foundations of Spectroscopic Techniques	10	effect of anharmonicity; Morse potential;		
	11	Vibration-rotational spectra of diatomics, polyatomic molecules-	Power Point Presentation	
	12	P,Q,R branches, normal modes of vibration, overtones, hot bands drawbacks of dispersive IR, FTIR	Power Point Presentation	
	13	**1.4 Raman spectroscopy**: scattering of light, polarizability and classical theory of Raman spectrum		
	14	rotational and vibrational Raman spectrum,	Group Discussion	
	2nd Internal Examination			
	15	complementarities of Raman and IR spectra,		
	16	mutual exclusion principle,		
	17	polarized and depolarized Raman lines,	Individual Assignment	
	18	Revision		
Text Books	2. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994. 3. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001. 4. P.W. Atkins, Physical Chemistry, ELBS,1994 5. R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965. 6. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.			

	No. of Sessions	**Session Topic and Discussion Theme**	**Value additions**	
	1	Factors influencing coupling, Karplus relationship.		
	2	FTNMR, second order effects on spectra, spin systems (AB, AB2)		
	3	Simplification of second order spectra, chemical shift reagents	ICT	
	4	High field NMR, double irradiation, selective decoupling		
	5 6	Double resonance		
	7	NOE effect, two dimensional NMR		
	1st Internal Examination			
	8	COSY and HETCOR		
	9	^{13}C NMR, natural abundance, sensitivity	Power Point Presentation	
Text Books	**References** 1. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994. 2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001. 3. P.W. Atkins, Physical Chemistry, ELBS,1994 4. R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965. 5. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992. 6. K.J. Laidler, J.H. Meiser, Physical Chemistry, 2ndEdn. CBS, 1999. 7. W. Kemp, NMR in chemistry-A Multinuclear Introduction, McMillan, 1986. 8. H. Kaur, Spectroscopy, 6thEdn. Pragati Prakashan, 2011.			
	No. of Sessions	**Session Topic and Discussion Theme**	**Value additions**	
Unit 2: Resonance Spectroscopy	10	^{19}F, ^{31}P, NMR spectroscopy.		
	11	3.2 EPR spectroscopy: Introduction	Power Point Presentation	
	12	Electron spin in molecules, interaction with magnetic field	Power Point Presentation	
	13	g factor, factors affecting g values, determination of g values ($g_{\parallel}$ and $g_{\perp}$)		
	14	Fine structure and hyperfine structure, Kramers' degeneracy	Group Discussion	
	2nd Internal Examination			
	15	McConnell equation. An elementary study of NQR spectroscopy.		
	16	3.3 Mossbauer spectroscopy: Introduction, principle		
	17	Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift	Individual Assignment:	
	18	Application to the structural elucidation of metal complexes		

Text Books	9. H. Gunther, NMR Spectroscopy, Wiley, 1995. 10. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997. 11. D.N. Sathyanarayan, Electronic Absorption Spectroscopy and Related Techniques, Universities Press, 2001. 12. D.N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2007. 13. D.N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, IK International, 2009. 14. J. D. Graybeat. Molecular Spectroscopy, McGraw-Hill International Edition, 1988

COURSE PLAN					
ACADEMIC YEAR 2015-16					
PROGRAMME	**:**	*M.Sc. Applied Chemistry - Pharmaceutical*	**LECTURE HOURS**	**:**	*72*
SEMESTER	**:**	*2*	**CREDITS**	**:**	*4*
SUBJECT TITLE	**:**	**CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY**	**SUBJECT CODE**	**:**	**P2CPHT07**
COURSE TEACHERS	**:**	***Dr. M George (MG), Dr. Jorphin Joseph(JRJ) & Dr Ignatious Abraham (IGA)***			
Course Objectives	**:**	*1. Ability to understand the basics of approximate methods in quantum chemistry such as variation method, perturbation method and Hartree Fock Method* *2. Apply the approximate methods in quantum chemistry and extend the concepts for understanding the principles of chemical bonding.* *3. Understand, identify and analyze the strengths and limitations of VB and MO methods for explaining the chemical bonding in molecules.*			

		4. Understanding the basics of advanced computational quantum chemistry methods such as ab initio methods, density functional theory methods and semiempirical methods *5. Explore the computational quantum chemistry methods for model chemistry calculations and understanding the principle of molecular mechanics and molecular simulations*

Teacher I – JRJ Module Taken : Unit 1: Approximate Methods in Quantum Mechanics (Total – 18 Hrs)
Instructional Hours : *One Hour Per Week*

No. of Session	Session Topic and Discussion Theme	Method of Teaching	Remarks/Student Assignments
1	Many-body problem and the need of approximation methods, Independent particle model.	Conventional Lecture Chalk & Board	Assignment on Problems Related to Variation Method
2	Variation method, variation theorem with proof,		
3	Illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box	Lecture With Mathematical Treatment	
4	Variation method using the trial function e^{-ar} for the hydrogen atom,		
5	Variation treatment for the ground state of helium atom.		
6	Perturbation method	Conventional Lecture	
7	Time-independent perturbation method, Perturbation of non-degenerate case only		

	First Internal Test		
8	First order correction to energy and wave function,	Lecture With Mathematical Treatment	Assignment on Problems Related to Perturbation Method
9	Illustration by application to particle in a 1D-box with slanted bottom,		
10	Perturbation treatment of the ground state of the helium atom		
11	Qualitative idea of Hellmann-Feynman theorem.		
12	Hartree Self-Consistent Field method for atoms.		
13	Spin orbitals for many electron atoms Multi-electron		
14	Symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants		
	Second Internal Test		
15	Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method.	Lecture with ICT	Assignment Related to Whole approximation methods
16	Roothan's concept of basis functions,		
17	Slater-type orbitals (STOs) as basis functions		
18	Gaussian type orbitals (GTO), sketches of STO and GTO.		

Reference Text Books

1. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.
2. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
3. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.
4. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books Pvt. Ltd., 1998.
5. F.L. Pilar, *Elementary Quantum Chemistry* , McGraw-Hill, 1968.

Teacher II – IGA **Module Taken : Unit 2: Chemical Bonding (Total – 18 Hrs)** **Instructional Hours :** *One Hour Per Week*			
No. of Session	**Session Topic and Discussion Theme**	**Method of Teaching**	**Remarks/Student Assignments**
1	Schrödinger equation for molecules.	Conventional Lecture Using Chalk and Board	Assignment for Preparing Class Notes
2	Born-Oppenheimer approximation.		
3	Valence Bond (VB) theory,		
4	VB theory of H2 molecule,		
5	Singlet and triplet state functions (spin orbitals) of H2.		
6	Molecular Orbital (MO) theory,		
7	MO theory of H_2^+ ion,		
8	MO theory of H_2 molecule		
	First Internal Test		
9	MO Theory of homo nuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2	Lecture With Mathematical Treatment	Assignments based on MO Calculations
10	MO Theory of hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order.		
11	Correlation diagrams, non-crossing rule.		
12	Spectroscopic term symbols for diatomic molecules.		
13	Comparison of MO and VB theories.		
14	Hybridization,		
15	quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation		
16	Semiempirical MO treatment of planar conjugated molecules,		
	Second Internal Test		

17	Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene.	Lecture with ICT	Seminar Based on HMO Theory
18	Calculation of charge distributions, bond orders and free valency.		

Reference Text Books

1. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.
2. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
3. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.
4. Frontier Orbitals and Organic Chemical Reactions, I. Fleming, Wiley, London, 1976.
5. Density functional theory of atoms and molecules, R G Parr and W Yang;
6. Chemical hardness: Applications from Molecules to Solids, R G Pearson.

Teacher III– MG Module Taken : Unit 3: Applications of Group Theory in Chemical Bonding
(Total – 9 Hrs) Instructional Hours : *One Hour Per Week*

No. of Session	Session Topic and Discussion Theme	Method of Teaching	Remarks/Student Assignmets
1	Applications of Group Theory in Chemical Bonding	Conventional Lecture	**Seminar Assignment to Students on the Topic "**Applications of Group Theory in Chemical Bonding"
2	Construction of hybrid orbitals in CH_4 & BF_3	Conventional lecture using Chalk and Board and ICT-PPT	
3	PCl_5 as example.		
4	Transformation properties of atomic orbitals.		
5	Symmetry adapted linear combinations (SALC)		
6	SALC of C2v, C2h,		

7	SALC of C3, C3v and D3h point groups. and ammonia.		
8	MO diagram for water		
9	MO diagram for Ammonia		
	First Internal Test		

References

1. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.
2. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.
3. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010

Teacher III – MG **Module Taken : Unit 4 & 5 : Computational Chemistry and Computational Chemistry Calculations (Total – 27 Hrs) Instructional Hours :** *Two Hours Per Week*			
No. of Session	**Session Topic and Discussion Theme**	**Method of Teaching**	**Remarks/Student Assignments**
1	**Unit 4 :** Introduction: computational chemistry as a tool and its scope.		
2	Potential energy surface:		
3	Stationary point, transition state or saddle point, local and global minima.		
4	Molecular mechanics methods:		

5	Force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions.	Conventional Lecture And ICT with Power Point Presentation	**Preparation of Lecture Notes**
6	Mathematical expressions. Parameterisation from experiments or quantum chemistry.		
7	Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM		
8	Ab initio methods: A review of Hartee-Fock method.		
9	Basis set approximation. Slater and Gaussian functions.		
10	Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets,		
11	Pople style basis sets and their nomenclature, correlation consistent basis sets		
First Internal Test			
12	Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods-variational method		
13	Basic principles of Configuration Inetraction(CI). Perturbational methods-basic principles of Møller Plesset Perturbation Theory		
14	General introduction to semiempirical methods: basic principles and terminology.		

15	Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional.	Conventional Lecture And ICT with Power Point Presentation 2. Visual Display of Computational Calculations Using Gamess / Gaussian	**1. Seminar on the topic** Comparison of molecular mechanics, ab initio, semiempirical and DFT methods. 2. Exercises using GAMESS/Gaussian in the Computer Lab
16	Local densityapproximation. Generalized gradient approximation. Hybrid functionals		
17	Model Chemistry-notation, effect on calculation time (cost).		
18	Comparison of molecular mechanics, ab initio, semiempirical and DFT methods.		
19	**Unit 5 :** Computational Chemistry Calculations Molecular Geometry - input-cartesian coordinates and internal coordinate- Z matrix		
20	Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane.		
21	General format of GAMESS / Firefly input file. GAMESS / Firefly key word for: basis set selection, method selection, charge, multiplicity,		
22	Single point energy calculation, geometry optimization,		
Second Internal Test			
23	Constrained optimization and frequency calculation.Identifying a successful GAMESS/ Firefly calculation-	. Conventional Lecture	

24	Locating local minima and saddle points, characterizing transition states	And ICT with Power Point Presentation 2. Visual Display of Computational Calculations Using Gauss View	Practicing and Visualization of Computational Chemistry Exercises.
25	Calculation of ionization energies, Koopmans' theorem, electron affinities and atomic charges.		
26	Identifying HOMO and LUMO-		
27	Visualization of molecular orbitals and normal modes of vibrations using suitable packages		

Reference Text Books

1. E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.
2. F. Jensen, Introduction to computational chemistry, 2nd Edn., John Wiley & Sons, 2007.
3. Michael Springborg, Methods of Electronic-Structure Calculations: From Molecules to Solids John Wiley & Sons, 2000.
4. W. Koch, M.C. Holthausen, "A Chemist's Guide to Density Functional Theory", Wiley-VCH Verlag 2000
5. K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008.
6. Stote, R. H., Dejaegere, A. and Karplus, M. (1997). Molecular Mechanics and Dynamics Simulations of Enzymes. Computational Approaches to Biochemical Reactivity. Netherlands, Kluwer Academic Publishers.