SACRED HEART COLLEGE (AUTONOMOUS)

DEPARTMENT OF CHEMISTRY

MASTER OF SCIENCE IN CHEMISTRY

Course plan

Academic Year 2017 – 18

Semester 2

Course Code	Title Of The Course	No. Hrs./Week	Credits	Total Hrs./Sem
16P2CHET05	Inorganic Chemistry II	4	4	72
16P2CHET06	Organic Reaction Mechanism	4	4	72
16P2CHET07	Physical Chemistry II	3	3	54
16P2CHET08	Theoretical and Computational Chemistry	4	3	72

COURSE PLAN

PROGRAMME	**M.SC. CHEMISTRY**	**SEMESTER**	**2**
COURSE CODE AND TITLE	**16P2CHET05 , INORGANIC CHEMISTRY II**	**CREDIT**	**4**
HOURS/WEEK	**4**	**HOURS/SEM**	**72**
FACULTY NAME	**MR. MIDHUN DOMINIC C D (MDCD), MR. SENJU DEVASSYKUTTY (SD), DR. RAMAKRISHNAN S (RKS)**		

COURSE OBJECTIVES
To understand the structural and bonding aspects of co-ordination compounds.
To explain the spectral and magnetic properties of metal complexes.
To know the thermodynamic and kinetic aspects of reactions of metal complexes.
To understand the stereochemistry of co-ordination compounds.
To describe the co-ordination chemistry of lanthanoids and actinoids

Teacher I – SD : Unit 1: Structural Aspects and Bonding (18h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
1.	Classification of complexes based on coordination numbers and possible geometries.	Conventional Lecture Chalk & Board	Quiz	
2.	Sigma and pi bonding ligands such as CO, NO, CN^-.	Lecture With power point presentation		
3.	Sigma and pi bonding ligands such as R_3P, and Ar_3P.	Lecture With power point presentation		

4.	Macrocycles-crown ethers, cryptands, macrocyclic effect, applications of crown ethers, template synthesis, Inverse crown ether complexes.	Lecture With power point presentation		
5.	Stability of complexes – factors affecting stability	Lecture With power point presentation	Q & A Session	
6.	Stability of complexes, thermodynamic aspects of complex formation	Lecture With power point presentation		
7.	Irving William order of stability, chelate effect	Conventional Lecture		
8.	Splitting of *d* orbitals in octahedral, tetrahedral, square planar	Lecture With power point presentation		
9.	Splitting of *d* orbitals in square pyramidal and triagonal bipyramidal fields	Lecture With power point presentation		
10.	LFSE, *Dq* values, Jahn Teller (JT) effect	Lecture With power point presentation		
11.	Theoretical failure of crystal field theory, evidence of covalency in the metal ligand bond	Lecture With power point presentation		
12.	Nephelauxetic effect, ligand field theory	Lecture With power point presentation		
13.	Ligand field theory	Lecture With power point presentation		
14.	Introduction to Molecular orbital theory	Lecture With power point presentation		
15.	Molecular orbital theory-M.O energy level diagrams for octahedral complexes without and with π-bonding	Lecture With power point presentation		
16.	M.O energy level diagrams for tetrahedral complexes without and with π-bonding,	Lecture With power point presentation		
17.	Experimental evidences for pi-bonding.	Lecture With power point presentation		
18.	Revision	Lecture With power point presentation	Q & A Session	

Teacher II – RKS : Unit 2: Spectral and Magnetic Properties of Metal Complexes (18h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
19.	Introduction to spectral and magnetic properties	Conventional Lecture Using Chalk and Board	Q & A Session	
20.	Electronic Spectra of complexes-Term symbols of dn system, Racah parameters	Conventional Lecture Using Chalk and Board		
21.	Splitting of terms in weak and strong octahedral and tetrahedral fields.	Conventional Lecture Using Chalk and Board		
22.	Correlation diagrams for dn in octahedral and tetrahedral fields (qualitative approach)	Conventional Lecture Using Chalk and Board		
23.	Correlation diagrams for d10-n ions in octahedral and tetrahedral fields (qualitative approach)	Conventional Lecture Using Chalk and Board		
24.	d-d transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.	Conventional Lecture Using Chalk and Board		
25.	Interpretation of electronic spectra of complexes-Orgel diagrams	Conventional Lecture Using Chalk and Board		
26.	Demerits of Orgel diagrams	Conventional Lecture Using Chalk and Board		
27.	Tanabe-Sugano diagrams	Conventional Lecture Using Chalk and Board		
28.	Calculation of *Dq*, *B* and *β* (Nephelauxetic ratio) values, Spectra of complexes with lower symmetries	Conventional Lecture Using Chalk and Board		
29.	Charge transfer spectra, luminescence spectra. Intra Valence charge transfer transition Prussian blue.	Conventional Lecture Using		

		Chalk and Board		
30.	Magnetic properties of complexes- paramagnetic and diamagnetic complexes	Conventional Lecture Using Chalk and Board	Quiz	
31.	Molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment.	Conventional Lecture Using Chalk and Board		
32.	Temperature dependence of magnetism- Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP)	Lecture with ICT		
33.	Spin state cross over, Antiferromagnetism-inter and intra molecular interaction.	Lecture with ICT		
34.	Anomalous magnetic moments and quenching of magnetic moment	Lecture with ICT		
35.	Elucidating the structure of cobalt complexes using electronic spectra, IR spectra and magnetic moments.	Lecture with ICT		
36.	Elucidating the structure of nickel complexes using electronic spectra, IR spectra and magnetic moments.	Lecture with ICT		
Teacher III – SD : Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes (18h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
37.	Introduction	Conventional Lecture using Chalk and Board	Quiz	
38.	Thermodynamic and kinetic stability	Chalk and Board and ICT - PPT		
39.	Kinetics and mechanism of nucleophilic substitution reactions in square planar complexes	Conventional Lecture using Chalk and Board		
40.	Factors affecting the reactivity of square planar complexes of Pt(II)	Chalk and Board and ICT - PPT		
41.	Factors affecting the reactivity of square planar complexes of other d^8 metal ions	Conventional Lecture using Chalk and Board		

42.	*trans* effect-theory and applications.	Chalk and Board and ICT - PPT		
43.	Kinetics and mechanism of octahedral substitution- water exchange reactions	Conventional Lecture using Chalk and Board		
44.	Dissociative and associative mechanisms	Chalk and Board and ICT - PPT		
45.	Hydrolysis under acidic conditions, rate and stereochemistry of aquation of cis and trans isomers of Co(III) complexes	Conventional Lecture using Chalk and Board		
46.	Base hydrolysis – conjugate base mechanism, base hydrolysis of different isomers of $[Co(tren)(NH_3)Cl]^{2+}$	Chalk and Board and ICT - PPT		
47.	Racemization reactions.	Conventional Lecture using Chalk and Board		
48.	Electron transfer reactions: outer sphere mechanism-Marcus theory	Chalk and Board and ICT - PPT		
49.	Electron transfer reactions: outer sphere mechanism-Marcus theory	Conventional Lecture using Chalk and Board		
50.	Electron transfer reactions: outer sphere mechanism-Marcus theory	Chalk and Board and ICT - PPT		
51.	Electron transfer reactions: inner sphere mechanism-Taube mechanism.	Conventional Lecture using Chalk and Board		
52.	Electron transfer reactions: inner sphere mechanism-Taube mechanism.	Chalk and Board and ICT - PPT		
53.	Electron transfer reactions: inner sphere mechanism-Taube mechanism. Nature of bridging ligand	Conventional Lecture using Chalk and Board		
54.	Revision	Chalk and Board and ICT –PPT	Q & A Session	
Teacher IV – MDCD : Unit 4: Stereochemistry of Coordination Compounds (9h)				

SESSION	TOPIC	LEARNING RESOURCES	VALUE ADDITIONS	REMARKS
55.	Introduction to stereochemistry	Conventional Lecture using Chalk and Board	Quiz	
56.	Geometrical and optical isomerism in octahedral complexes	Conventional Lecture using Chalk and Board		
57.	Resolution of optically active complexes	Conventional Lecture using Chalk and Board		
58.	Determination of absolute configuration of complexes by ORD and circular dichroism	Conventional Lecture using Chalk and Board		
59.	Stereoselectivity and conformation of chelate Rings	Conventional Lecture using Chalk and Board		
60.	Asymmetric synthesis catalyzed by coordination compounds.	Conventional Lecture using Chalk and Board		
61.	Linkage isomerism-electronic and steric factors affecting linkage isomerism	Conventional Lecture using Chalk and Board		
62.	Symbiosis-hard and soft ligands	Conventional Lecture using Chalk and Board		
63.	Revision	Conventional Lecture using Chalk and Board	Q & A Session	
Teacher V – MDCD : Unit 5: Coordination Chemistry of Lanthanides and Actinides (9h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**COURSE OUTCOME**
64.	General characteristics of lanthanides-Electronic configuration	Conventional Lecture	Quiz	
65.	Term symbols for lanthanide ions, Oxidation state	Conventional Lecture		

INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

66.	Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes.	Conventional Lecture		
67.	Electronic spectra and magnetic properties of lanthanide complexes	Conventional Lecture		
68.	Lanthanide complexes as shift reagents and separation of lanthanides	Conventional Lecture		
69.	General characteristics of actinides-difference between 4f and 5f orbitals	Conventional Lecture		
70.	Comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra properties.	Conventional Lecture		
71.	Comparative account of coordination chemistry of lanthanides and actinides with special reference to magnetic properties.	Conventional Lecture		
72.	Revision	Conventional Lecture	Q & A Session	

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	18/12/17	Assignment on Crystal field theory

GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**
1	02/12/17	Orgel diagrams & Tanabe-Sugano diagrams

REFERENCES

1. 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.
9. G.L. Miessler, D. A. Tarr, Inorganic Chemistry 3rd Ed., Pearson Education, 2007

COURSE PLAN

PROGRAMME	**M.SC. CHEMISTRY**	**SEMESTER**	**2**
COURSE CODE AND TITLE	**16P2CHET06 AND ORGANIC REACTION MECHANISM**	**CREDIT**	**4**
HOURS/WEEK	**4**	**HOURS/SEM**	**72**
FACULTY NAME	**DR. V.S SEBASTIAN(VSS) , DR. GRACE THOMAS (GT), DR. JUNE CYRIAC (JUC)**		

COURSE OBJECTIVES
To know the mechanisms of different types organic reactions.
To explain the chemistry of carbanions, carbocations, carbenes, carbenoids, nitrenes and arynes.
To understand the chemistry of radical reactions and its applications.
To explain the basics and applications of concerted reactions

Teacher I – JUC : Unit 1: Review of substitution reaction Mechanisms (11h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
1.	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)	Power point	Q & A Session	
2.	Continued	Power point		
3.	Continued	Power point		
4.	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		
5.	Continued	Power point		

6.	Stereochemistry of E_2 reaction, Intramolecular pyrolytic elimination, Cope elimination. Elimination *vs* substitution.	Power point		
7.	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).	Power point		
8.	Substitution at the aromatic centre, unimolecular mechanism, bimolecular mechanism. Kinetics of SE_2-Ar reaction. Ortho-para selectivity ratio.	Power point	Quiz	
9.	Electrophilic substitution via enolization and stork-enamine reaction.	Power point		
10.	Benzyne mechanism. Von Ritcher	Power point		
11.	Vilsmeyer formylation, Jacobson and Gatterman-Koch reactions.	Power point		
Teacher II – GT : Unit 2: Chemistry of Carbanions (10h)				
12.	Formation, structure and stability of carbanions	Power point	Quiz	
13.	Reactions of carbanions: C-X bond (X = C, O, N)	Power point		
14.	Formations through the intermediary of carbanions.	Power point		
15.	Chemistry of enolates and enamines.	Power point		
16.	Kinetic and Thermodynamic enolates-lithium and boron enolates in aldol alkylation and acylation of enolates.	Power point		
17.	Electrophilic additions to alkenes, Kinetics, effect of structure, orientation and stereochemistry.	Power point		
18.	Ozonolysis and hydroboration. Nucleophilic additions to carbonyls groups. Named reactions under carbanion chemistry –Mechanism of Claisen	Power point	Q & A Session	
19.	Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations	Power point		
20.	Shapiro reaction and Julia elimination. Favorski rearrangement.	Power point		
21.	Ylids: Chemistry of Phosphorous and Sulphur ylids - Wittig and related reactions, Peterson olefination.	Power point		

Teacher III – GT : Unit 3: Chemistry of Carbocations (9h)				
22.	Formation, structure and stability of carbocations.	Power point	Quiz	
23.	Classical and non-classical carbocations.	Power point		
24.	C-X bond (X = C, O, N) formations through the intermediary of carbocations.	Power point		
25.	Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol	Power point		
26.	Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.	Power point		
27.	C-C bond formation involving carbocations: Oxymercuration, halolactonisation.	Power point		
28.	Structure and reactions of α, β- unsaturated carbonyl compounds – electrophilic addition	Power point	Q & A Session	
29.	Nucleophilic addition - Michael addition	Power point		
30.	Mannich reaction and Robinson annulation.	Power point		
Teacher IV – VSS : Unit 4: Carbenes, Carbenoids, Nitrenes and Arynes (9h)				
31.	Structure of carbenes (singlet and triplet) - generation of carbenes	Power point	Quiz	
32.	Addition and insertion reactions.	Power point		
33.	Rearrangement reactions of carbenes such as Wolff rearrangement	Power point		
34.	Generation and reactions of ylids by carbenoid decomposition.	Power point		
35.	Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.	Power point		
36.	Continued	Power point		
37.	Hoffmann, and Curtius reactions.	Power point		
38.	Lossen, Schmidt and Beckmann rearrangement reactions	Power point		
39.	Arynes: Generation, structure, stability and reactions. Orientation effect- amination of haloarenes.	Power point	Q & A Session	
Teacher V – VSS : Unit 5: Radical Reactions (9h)				

40.	Generation of radical intermediates	Power point	Q & A Session	
41.	Its addition to alkenes, alkynes (inter & intramolecular)	Power point		
42.	For C-C bond formation - Baldwin's reaction	Power point		
43.	Fragmentation and rearrangements	Power point		
44.	Hydroperoxide: formation, rearrangement and reactions.	Power point		
45.	Continued	Power point		
46.	Auto-oxidation.	Power point		
47.	Named reactions involving radical intermediates: Barton deoxygenation	Power point	Quiz	
48.	Decarboxylation, McMurry coupling.	Power point		
Teacher VI – JUC : Unit 6: Concerted reactions (24h)				
49.	Classification	Power point	Q & A Session	
50.	Electrocyclic reactions.	Power point		
51.	Sigmatropic reactions.	Power point		
52.	Cycloaddition reactions.	Power point		
53.	Chelotropic reactions.	Power point		
54.	Ene reactions.	Power point		
55.	Woodward Hoffmann rules	Power point		
56.	Frontier orbital and orbital symmetry correlation approaches	Power point		
57.	Continued	Power point		
58.	PMO method.	Power point		
59.	Pericyclic reactions in organic synthesis such as Claisen rearrangement	Power point	Quiz	
60.	Cope rearrangement	Power point		
61.	Wittig rearrangement	Power point		
62.	Mislow-Evans rearrangement	Power point		

63.	Sommelet-Hauser rearrangements.	Power point		
64.	Diels-Alder and Ene reactions (with stereochemical aspects)	Power point		
65.	Continued	Power point		
66.	Dipolar cycloaddition (introductory).	Power point		
67.	Pyrolytic elimination reactions: cheletropic elimination.	Power point	Q & A Session	
68.	Decomposition of cyclic azo compounds.	Power point		
69.	β-eliminations involving cyclic transition states such as N-oxides	Power point		
70.	Acetates and xanthates.	Power point		
71.	Introduction to Click reactions -Mechanism of the Huisgen Azide-Alkyne 1, 3-Dipolar Cycloaddition.	Power point		
72.	Staudinger ligation and Staudinger reduction.	Power point		

INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**
1.	02/12/2017	Hydroperoxide: formation, rearrangement and reactions.

GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**
2.	03/02/2018	Classifications of concerted reactions

References

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1. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, Organic Chemistry,7thEdn., Pearson, New Delhi, 2011.
2. J. Clayden, N. Greeves, S.Warren, P.Wothers, Organic Chemistry, Oxford University Press, New York, 2004.
3. Fleming, Wiley, Frontier Orbitals and Organic Chemical Reactions, London, 1976.
4. S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005.
5. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6thEdn., Wiley, 2007.
6. http://www.organic-chemistry.org/namedreactions.

7. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, Organic Chemistry,7thEdn., Pearson, New Delhi, 2011.
8. F. A. Carey, R. A. Sundberg,Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5thEdn.,, Springer, New York, 2007.
9. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, First South Asian Edition, Cambridge University Press, 2005.
10. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

COURSE PLAN

PROGRAMME	**M.SC. CHEMISTRY**	**SEMESTER**	**2**
COURSE CODE AND TITLE	**16P2CHET07 AND PHYSICAL CHEMISTRY – II**	**CREDIT**	**3**
HOURS/WEEK	**3**	**HOURS/SEM**	**54**
FACULTY NAME	**DR FRANKLIN J (FJ) , DR. JINU GEORGE (JG) DR. K. B. JOSE (KBJ), DR. THOMMACHAN XAVIER (TX)**		

COURSE OBJECTIVE
To understand theory and application to Microwave, Infrared and Raman Spectroscopy
To know the various aspects of Electron & Electronic Spectroscopy & Lasers
To know the fundamental concepts of atomic, molecular and spin resonance spectroscopy.

Teacher I – KBJ : Unit 1 : Microwave, Infrared and Raman Spectroscopy (14h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
1.	Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption	Chalk and board	Q & A Session	
2.	influencing factors, signal to noise ratio, natural line width, contributing factors	Chalk and board		
3.	Doppler broadening, Lamb dip spectrum	Chalk and board		

4.	Born Oppenheimer approximation, energy dissipation from excited states (radiative and non radiative processes), and relaxation time.	Chalk and board		
5.	Microwave spectroscopy*:* Classification of molecules	Chalk and board		
6.	Rigid rotor model; rotational spectra of diatomics and polyatomics	Chalk and board		
7.	Effect of isotopic substitution and nonrigidity; selection rules and intensity distribution.	Chalk and board		
8.	Vibrational spectroscopy: Vibrational spectra of diatomics	Chalk and board	Quiz	
9.	Effect of anharmonicity; Morse potential	Chalk and board		
10.	Vibration-rotational spectra of diatomics, polyatomic molecules- P,Q,R branches, normal modes of vibration, overtones, hot bands drawbacks of dispersive IR, FTIR	Chalk and board		
11.	Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum	Chalk and board		
12.	Rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra	Chalk and board		
13.	Polarized and depolarized Raman lines	Chalk and board		
14.	Revision	Chalk and board	Q & A Session	
Teacher II – FJ : Unit 2 : Electron & Electronic Spectroscopy & Lasers (13h)				
15.	Electron Spectroscopy: Basic principles	Chalk and board		
16.	Photoelectron spectra of simple molecules, selection rules	Chalk and board	Quiz	
17.	Electron spectroscopy for chemical analysis (ESCA)-UPS	Chalk and board		
18.	X-ray photoelectron spectroscopy (XPS)	Chalk and board		
19.	Auger electron spectroscopy (AES).	Chalk and board		
20.	Electronic spectroscopy: Electronic spectra of diatomic molecules	Chalk and board	Q & A Session	
21.	Franck-Condon principle.	Chalk and board		
22.	Vibronic transitions, Spectra of organic compounds	Chalk and board		
23.	$\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition.	Power Point Presentation	Quiz	

INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

24.	Lasers: Laser action	Power Point Presentation		
25.	Population inversion, properties of laser radiation, two stage	Power Point Presentation		
26.	Three stage-examples of simple laser systems	Power Point Presentation		
27.	Revision	Power Point Presentation	Q & A Session	
Teacher III – TX and JG : Unit 3: Resonance Spectroscopy (27h)				
28.	^{1}H NMR spectroscopy : interaction between nuclear spin and applied magnetic field	Power Point Presentation		
29.	Nuclear energy levels, population of energy levels	Power Point Presentation		
30.	Larmor precession, relaxation methods	Power Point Presentation		
31.	Chemical shift, representation	Power Point Presentation		
32.	Examples of AB, AX and AMX types	Power Point Presentation	Q & A Session	
33.	Exchange phenomenon, factors influencing coupling	Power Point Presentation		
34.	Karplus relationship.	Power Point Presentation		
35.	FTNMR, second order effects on spectra	Power Point Presentation	Quiz	
36.	Spin systems (AB, AB_2)	Power Point Presentation		
37.	Simplification of second order spectra	Power Point Presentation		
38.	Chemical shift reagents	Power Point Presentation	Q & A Session	
39.	High field NMR	Power Point Presentation		
40.	Double irradiation, selective decoupling, double resonance, NOE effect	Power Point Presentation		
41.	Two dimensional NMR, COSY	Power Point Presentation		
42.	HETCOR	Power Point Presentation		
43.	^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, ^{19}F, ^{31}P, NMR spectroscopy.	Power Point Presentation		
44.	EPR spectroscopy: electron spin in molecules	Power Point Presentation		
45.	Interaction with magnetic field, g factor, factors affecting g values	Power Point Presentation		

46.	Determination of g values ($g_{\parallel}$ and $g_{\perp}$)	Power Point Presentation	Quiz	
47.	Fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.	Power Point Presentation		
48.	An elementary study of NQR spectroscopy.	Power Point Presentation		
49.	Mossbauer spectroscopy: principle	Power Point Presentation		
50.	Doppler effect, recording of spectrum	Power Point Presentation		
51.	Chemical shift, factors determining chemical shift	Power Point Presentation		
52.	Application to the structural elucidation of metal complexes	Power Point Presentation		
53.	Revision	Power Point Presentation	Q & A Session	
54.	Revision	Power Point Presentation		

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	22/01/2018	Vibration-rotational spectra of diatomics, polyatomic molecules- P,Q,R branches

GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)
1	11/02/18	Application to the structural elucidation of metal complexes

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.
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

PROGRAMME	**M.SC. CHEMISTRY**	**SEMESTER**	**2**
COURSE CODE AND TITLE	**16P2CHET08 AND THEORETICAL AND COMPUTATIONAL CHEMISTRY**	**CREDIT**	**3**
HOURS/WEEK	**4**	**HOURS/SEM**	**72**
FACULTY NAME	**DR. JORPHIN JOSEPH (JRJ), DR. ABI T.G. (ATG), DR. IGNATIOUS ABRAHAM (IGA)**		

COURSE OBJECTIVE
To explain the approximation methods in quantum mechanics.
To describe the quantum mechanical explanation of chemical bonding.
To explain the methods of computational quantum chemistry.
To explain Model Chemistry and Molecular Simulations

Teacher I – JRJ : Unit 1: Approximate Methods in Quantum Mechanics (21h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**REMARKS**
1.	Many-body problem and the need of approximation methods	Conventional Lecture Chalk & Board and ICT	Q & A Session	
2.	Independent particle model.	Conventional Lecture		
3.	Variation method, variation theorem with proof	Chalk & Board and ICT		
4.	Illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box	Conventional Lecture		
5.	Using the trial function e-ar for the hydrogen atom,	Chalk & Board and ICT		

6.	Variation treatment for the ground state of helium atom.	Conventional Lecture		
7.	Perturbation method	Chalk & Board and ICT		
8.	Time-independent perturbation method (non-degenerate case only)	Conventional Lecture	Q & A Session	
9.	First order correction to energy and wave function	Chalk & Board and ICT		
10.	Illustration by application to particle in a 1D-box with slanted bottom	Conventional Lecture		
11.	Perturbation treatment of the ground state of the helium atom.	Chalk & Board and ICT		
12.	Hartree-Fock method. Multi-electron atoms.	Conventional Lecture		
13.	The antisymmetry principle and the Slater determinant	Chalk & Board and ICT		
14.	Hartree-Fock equations (no derivation).	Conventional Lecture		
15.	The Fock operator. Core Hamiltonian. Coulomb operator and exchange operator	Chalk & Board and ICT		
16.	Slater-type orbitals (STOs) as basis functions.	Conventional Lecture		
17.	Orbital energies and total energy. Helium atom example.	Chalk & Board and ICT		
18.	Koopman's theorem. Electron correlation energy.	Conventional Lecture	Quiz	
19.	The Hartree-Fock method for molecules.	Chalk & Board and ICT		
20.	Restricted and unrestricted HF calculations.	Conventional Lecture		
21.	The Roothan equations.	Chalk & Board and ICT		
Teacher II – IGA : Unit 2: Chemical Bonding (21h)				
22.	Schrödinger equation for molecules.	Conventional Lecture	Q & A Session	
23.	Born-Oppenheimer approximation.	Chalk & Board and ICT		
24.	Valence Bond (VB) theory	Conventional Lecture	Quiz	
25.	Singlet and triplet state functions (spin orbitals) of H_2.	Chalk & Board and ICT		
26.	Molecular Orbital (MO) theory	Conventional Lecture		
27.	MO theory of H_2^+ ion	Chalk & Board and ICT		
28.	MO theory of H_2 molecule	Conventional Lecture		

29.	MO Theory of homo nuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2	Chalk & Board and ICT		
30.	MO Theory of hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order	Conventional Lecture		
31.	Correlation diagrams, non-crossing rule	Chalk & Board and ICT		
32.	Spectroscopic term symbols for diatomic molecules	Conventional Lecture		
33.	Comparison of MO and VB theories.	Chalk & Board and ICT		
34.	Hybridization	Conventional Lecture	Q & A Session	
35.	Quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation	Chalk & Board and ICT		
36.	Semiempirical MO treatment of planar conjugated molecules	Conventional Lecture		
37.	Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene.	Chalk & Board and ICT		
38.	Calculation of charge distributions, bond orders and free valency	Conventional Lecture		
39.	Froniter Molecular Orbitals	Chalk & Board and ICT		
40.	Woodward-Hoffmann rule	Conventional Lecture		
41.	Introduction to global and local reactivity descriptors - electrophilicity index	Chalk & Board and ICT	Quiz	
Teacher III – ATG : Unit 3: Computational Quantum Chemistry (18h)				
42.	Introduction and scope of computational chemistry.	Conventional Lecture	Q & A Session	
43.	Potential energy surface - Conformational search	Chalk & Board and ICT		
44.	Global minimum, Local minima, saddle points.	Conventional Lecture		
45.	Conformational analysis of ethane and butane	Chalk & Board and ICT		
46.	Ab initio methods	Conventional Lecture	Quiz	
47.	A review of Hartee-Fock method. Self Consistent Field Procedure	Chalk & Board and ICT		
48.	Roothan concept of basis functions. Basis sets	Conventional Lecture		
49.	Slater type and Gaussian type basis sets, Minimal basis set	Chalk & Board and ICT		
50.	Pople style basis sets - Classification - double zeta, triple zeta, split valence,	Conventional Lecture		

	polarization and diffuse basis sets, contracted basis sets			
51.	Hartree-Fock limit and Post Hartree-Fock methods	Chalk & Board and ICT		
52.	Introduction to Møller Plesset Perturbation Theory, Configuration Interaction and Coupled Cluster	Conventional Lecture	Quiz	
53.	Semi empirical methods	Chalk & Board and ICT		
54.	Introduction to Density Functional Theory (DFT) methods	Conventional Lecture		
55.	Hohenberg-Kohn theorems. Kohn-Sham orbitals.	Chalk & Board and ICT		
56.	Exchange correlation functional. Local density approximation	Conventional Lecture		
57.	Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).	Chalk & Board and ICT		
58.	Comparison of ab initio, semi empirical and DFT methods	Conventional Lecture	Q & A Session	
Teacher IV – ATG : Unit 4: Model Chemistry and Molecular Simulations (12h)				
59.	Introduction to computational chemistry software packages. Generating molecular structures	Conventional Lecture And ICT with Power Point Presentation	Quiz	
60.	Cartesian coordinates, internal coordinates and Z-matrix of simple molecules	Conventional Lecture		
61.	Introduction to computational chemistry calculations using simple molecular structures of water, ammonia, methane, butane, benzene.	Conventional Lecture And ICT with Power Point Presentation		
62.	Input file format - Method, Basis Set, Calculation type, Spin Multiplicity, Coordinate format.	Conventional Lecture And ICT with Power Point Presentation		
63.	Single Point Energy, Geometry Optimization, Frequency Analysis.	Conventional Lecture		
64.	Computational Chemistry using Statistical mechanics.	Conventional Lecture And ICT with Power Point Presentation	Quiz	
65.	Features of molecular mechanics force field-bond stretching, angle bending, torsional terms, non-bonded interactions and electrostatic interactions.	Conventional Lecture And ICT with Power Point Presentation		
66.	Commonly used force fields AMBER and CHARMM.	Conventional Lecture		

67.	Molecular dynamics simulations.	Conventional Lecture And ICT with Power Point Presentation		
68.	Introduction to simulation softwares. Protein data bank (PDB) and Protein structure file (PSF) formats.	Conventional Lecture And ICT with Power Point Presentation	Quiz	
69.	Practical aspects of computer simulation.	Conventional Lecture		
70.	Analyzing the results of a simulation.	Conventional Lecture And ICT with Power Point Presentation		
71.	Revision	Conventional Lecture And ICT with Power Point Presentation	Q & A Session	
72.	Revision	Conventional Lecture And ICT with Power Point Presentation		

INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**
1	29/12/17	Assignment on Problems Related to Variation Method
2	16/01/18	Assignments based on MO Calculations

GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**
1	03/02/18	Seminar on the topic Molecular Mechanics

References

For Unit 1 & 2

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.

6. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics* , 4th Edition, Oxford University Press, 2005.
7. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.
8. Horia Metiu, *Physical Chemistry – Quantum Mechanics*, Taylor & Francis, 2006.
9. A.K. Chandra, *Introduction to Quantum Chemistry*, 4th Edition, Tata McGraw-Hill,1994.
10. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for many derivations).
11. Frontier Orbitals and Organic Chemical Reactions, I. Fleming, Wiley, London, 1976.
12. Density functional theory of atoms and molecules, R G Parr and W Yang;
13. Chemical hardness: Applications from Molecules to Solids, R G Pearson.

For Unit 3 & 4

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. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008.
7. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.
8. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*,
9. Gaussian Inc., 2000.
10. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.
11. D. Rogers *Computational Chemistry Using the PC, 3rd Edition*, John Wiley & Sons (2003).
12. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn., Longman, 2001.
13. J. M. Haile (2001) *Molecular Dynamics Simulation: Elementary Methods*.
14. 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.
    (For pdb,psf file formats and molecular dynamics simulations)
15. http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-win.pdf
16. http://www.ks.uiuc.edu/Training/Tutorials/vmd/vmd-tutorial.pdf
17. List of some Free and Commercial Computational Chemistry Softwares

    Drawing & Visualization

    Chem Draw, Avagadro, Discovery Studio Client, Gabedit, Open Babel, Gauss view, Pymol, VMD

    Quantum Chemistry Softwares

    Firefly, Gamess, Spartan, Molpro, Gaussian, Dmol3, Turbomole

    Molecular Mechanics and Dynamics Softwares

    NAMD, Tinker, DL-POLY, CHARMM, AMBER