SACRED HEART COLLEGE (AUTONOMOUS)

DEPARTMENT OF CHEMISTRY

MASTER OF SCIENCE IN APPLIED CHEMISTRY - PHARMACEUTICAL

Course plan

Academic Year 2018-19

Semester 2

PROGRAMME OUTCOMES

PO1	The students are capable of exercising their critical thinking in creating new knowledge leading to innovation, entrepreneurship and employability.
PO2	The students are able to effectively communicate the knowledge of their study and research in their respective disciplines to their employers and to the society at large.
PO3	The students are able to make choices based on the values upheld by the college, and have the readiness and know-how to preserve environment and work towards sustainable growth and development.
PO4	The students possess an ethical view of life, and have a broader (global) perspective transcending the provincial outlook.
PO5	The students possess a passion for exploring new knowledge independently for the development of the nation and the world and are able to engage in a lifelong learning process.

PROGRAM SPECIFIC OUTCOMES

Knowledge and Understanding	
PSO 1	Demonstrate an in-depth knowledge and understanding of the principles of Inorganic, Organic, Physical and Theoretical Chemistry.
PSO 2	Demonstrate an awareness of the relevance of chemistry in a wider multi-disciplinary context.
Intellectual Abilities	
PSO 3	Apply their understanding in Chemistry to design solutions to unfamiliar problems in Chemistry and those involving other related disciplines.
PSO 4	Use their knowledge and understanding to conceptualize appropriate models and representations.
Practical Skills	
PSO 5	Design and conduct analytical, modelling and experimental investigations in Inorganic, Organic, Physical and Theoretical Chemistry.
Professional Skills	

PSO 6	Ability to identify, design and conduct appropriate experiments, interpret data obtained, draw pertinent conclusions and communicate all these effectively.

Course Structure

Course Code	Title Of The Course	No. Hrs./Week	Credits	Total Hrs./Sem
16P2CPHT05	Inorganic Chemistry II	4	4	72
16P2CPHT06	Organic Reaction Mechanism	4	4	72
16P2CPHT07	Physical Chemistry II	3	3	54
16P2CPHT08	Theoretical and Computational Chemistry	4	3	72

COURSE PLAN

PROGRAMME	**M.SC. APPLIED CHEMISTRY - PHARMACEUTICAL**	**SEMESTER**	**2**
COURSE CODE AND TITLE	**16P2CPHT05 , 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 OUTCOMES	POs / PSOs	*CL*
CO 1	Understand the structural and bonding aspects of co-ordination compounds.	PO1 PSO1	U
CO 2	Explain the spectral and magnetic properties of metal complexes.	PO1 PSO3	U
CO 3	Explain the thermodynamic and kinetic aspects of reactions of metal complexes.	PO1 PSO1	U
CO 4	Understand the stereochemistry of co-ordination compounds.	PO1 PSO1	U

CO 5	Describe the co-ordination chemistry of lanthanoids and actinoids	PO1 PSO3	U

CL* Cognitive Level

Teacher I – SD : Unit 1: Structural Aspects and Bonding (18h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**COURSE OUTCOME**
1.	Classification of complexes based on coordination numbers and possible geometries.	Conventional Lecture Chalk & Board	Quiz	CO1
2.	Sigma and pi bonding ligands such as CO, NO, CN^-.	Lecture With power point presentation		CO1
3.	Sigma and pi bonding ligands such as R_3P, and Ar_3P.	Lecture With power point presentation		CO1
4.	Macrocycles-crown ethers, cryptands, macrocyclic effect, applications of crown ethers, template synthesis, Inverse crown ether complexes.	Lecture With power point presentation		CO 1
5.	Stability of complexes – factors affecting stability	Lecture With power point presentation	Q & A Session	CO 1
6.	Stability of complexes, thermodynamic aspects of complex formation	Lecture With power point presentation		CO 1
7.	Irving William order of stability, chelate effect	Conventional Lecture		CO 1
8.	Splitting of *d* orbitals in octahedral, tetrahedral, square planar	Lecture With power point presentation		CO 1
9.	Splitting of *d* orbitals in square pyramidal and triagonal bipyramidal fields	Lecture With power point presentation		CO 1
10.	LFSE, *Dq* values, Jahn Teller (JT) effect	Lecture With power point presentation		CO 1
11.	Theoretical failure of crystal field theory, evidence of covalency in the metal ligand bond	Lecture With power point presentation		CO 1
12.	Nephelauxetic effect, ligand field theory	Lecture With power point presentation		CO 1
13.	Ligand field theory	Lecture With power point		CO 1

		presentation		
14.	Introduction to Molecular orbital theory	Lecture With power point presentation		CO 1
15.	Molecular orbital theory-M.O energy level diagrams for octahedral complexes without and with π-bonding	Lecture With power point presentation		CO 1
16.	M.O energy level diagrams for tetrahedral complexes without and with π-bonding,	Lecture With power point presentation		CO 1
17.	Experimental evidences for pi-bonding.	Lecture With power point presentation		CO 1
18.	Revision	Lecture With power point presentation	Q & A Session	CO 1
Teacher II – RKS : Unit 2: Spectral and Magnetic Properties of Metal Complexes (18h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**COURSE OUTCOME**
19.	Introduction to spectral and magnetic properties	Conventional Lecture Using Chalk and Board	Q & A Session	CO 2
20.	Electronic Spectra of complexes-Term symbols of dn system, Racah parameters	Conventional Lecture Using Chalk and Board		CO 2
21.	Splitting of terms in weak and strong octahedral and tetrahedral fields.	Conventional Lecture Using Chalk and Board		CO 2
22.	Correlation diagrams for dn in octahedral and tetrahedral fields (qualitative approach)	Conventional Lecture Using Chalk and Board		CO 2
23.	Correlation diagrams for d10-n ions in octahedral and tetrahedral fields (qualitative approach)	Conventional Lecture Using Chalk and Board		CO 2
24.	d-d transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.	Conventional Lecture Using Chalk and Board		CO 2

25.	Interpretation of electronic spectra of complexes-Orgel diagrams	Conventional Lecture Using Chalk and Board		CO 2
26.	Demerits of Orgel diagrams	Conventional Lecture Using Chalk and Board		CO 2
27.	Tanabe-Sugano diagrams	Conventional Lecture Using Chalk and Board		CO 2
28.	Calculation of *Dq*, *B* and *β* (Nephelauxetic ratio) values, Spectra of complexes with lower symmetries	Conventional Lecture Using Chalk and Board		CO 2
29.	Charge transfer spectra, luminescence spectra. Intra Valence charge transfer transition Prussian blue.	Conventional Lecture Using Chalk and Board		CO 2
30.	Magnetic properties of complexes-paramagnetic and diamagnetic complexes	Conventional Lecture Using Chalk and Board	Quiz	CO 2
31.	Molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment.	Conventional Lecture Using Chalk and Board		CO 2
32.	Temperature dependence of magnetism-Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP)	Lecture with ICT		CO 2
33.	Spin state cross over, Antiferromagnetism-inter and intra molecular interaction.	Lecture with ICT		CO 2
34.	Anomalous magnetic moments and quenching of magnetic moment	Lecture with ICT		CO 2
35.	Elucidating the structure of cobalt complexes using electronic spectra, IR spectra and magnetic moments.	Lecture with ICT		CO 2
36.	Elucidating the structure of nickel complexes using electronic spectra, IR spectra and magnetic moments.	Lecture with ICT		CO 2
Teacher III – SD : Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes (18h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**COURSE OUTCOME**
37.	Introduction	Conventional Lecture using	Quiz	CO 3

		Chalk and Board		
38.	Thermodynamic and kinetic stability	Chalk and Board and ICT - PPT		CO 3
39.	Kinetics and mechanism of nucleophilic substitution reactions in square planar complexes	Conventional Lecture using Chalk and Board		CO 3
40.	Factors affecting the reactivity of square planar complexes of Pt(II)	Chalk and Board and ICT - PPT		CO 3
41.	Factors affecting the reactivity of square planar complexes of other d^8 metal ions	Conventional Lecture using Chalk and Board		CO 3
42.	*trans* effect-theory and applications.	Chalk and Board and ICT - PPT		CO 3
43.	Kinetics and mechanism of octahedral substitution- water exchange reactions	Conventional Lecture using Chalk and Board		CO 3
44.	Dissociative and associative mechanisms	Chalk and Board and ICT - PPT		CO 3
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		CO 3
46.	Base hydrolysis – conjugate base mechanism, base hydrolysis of different isomers of $[Co(tren)(NH_3)Cl]^{2+}$	Chalk and Board and ICT - PPT		CO 3
47.	Racemization reactions.	Conventional Lecture using Chalk and Board		CO 3
48.	Electron transfer reactions: outer sphere mechanism-Marcus theory	Chalk and Board and ICT - PPT		CO 3
49.	Electron transfer reactions: outer sphere mechanism-Marcus theory	Conventional Lecture using Chalk and Board		CO 3
50.	Electron transfer reactions: outer sphere mechanism-Marcus theory	Chalk and Board and ICT -		CO 3

		PPT		
51.	Electron transfer reactions: inner sphere mechanism-Taube mechanism.	Conventional Lecture using Chalk and Board		CO 3
52.	Electron transfer reactions: inner sphere mechanism-Taube mechanism.	Chalk and Board and ICT - PPT		CO 3
53.	Electron transfer reactions: inner sphere mechanism-Taube mechanism. Nature of bridging ligand	Conventional Lecture using Chalk and Board		CO 3
54.	Revision	Chalk and Board and ICT –PPT	Q & A Session	CO 3
Teacher IV – MDCD : Unit 4: Stereochemistry of Coordination Compounds (9h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**COURSE OUTCOME**
55.	Introduction to stereochemistry	Conventional Lecture using Chalk and Board	Quiz	CO 4
56.	Geometrical and optical isomerism in octahedral complexes	Conventional Lecture using Chalk and Board		CO 4
57.	Resolution of optically active complexes	Conventional Lecture using Chalk and Board		CO 4
58.	Determination of absolute configuration of complexes by ORD and circular dichroism	Conventional Lecture using Chalk and Board		CO 4
59.	Stereoselectivity and conformation of chelate Rings	Conventional Lecture using Chalk and Board		CO 4
60.	Asymmetric synthesis catalyzed by coordination compounds.	Conventional Lecture using Chalk and Board		CO 4
61.	Linkage isomerism-electronic and steric factors affecting linkage isomerism	Conventional Lecture using Chalk and		CO 4

		Board		
62.	Symbiosis-hard and soft ligands	Conventional Lecture using Chalk and Board		CO 4
63.	Revision	Conventional Lecture using Chalk and Board	Q & A Session	CO 4
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	CO 5
65.	Term symbols for lanthanide ions, Oxidation state	Conventional Lecture		CO 5
66.	Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes.	Conventional Lecture		CO 5
67.	Electronic spectra and magnetic properties of lanthanide complexes	Conventional Lecture		CO 5
68.	Lanthanide complexes as shift reagents and separation of lanthanides	Conventional Lecture		CO 5
69.	General characteristics of actinides-difference between 4f and 5f orbitals	Conventional Lecture		CO 5
70.	Comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra properties.	Conventional Lecture		CO 5
71.	Comparative account of coordination chemistry of lanthanides and actinides with special reference to magnetic properties.	Conventional Lecture		CO 5
72.	Revision	Conventional Lecture	Q & A Session	CO 5

INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

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

GROUP ASSIGNMENTS/ACTIVITES – DETAILS & GUIDELINES

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)	Course Outcome
1	02/12/18	Orgel diagrams & Tanabe-Sugano diagrams	CO 2

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. APPLIED CHEMISTRY - PHARMACEUTICAL**	**SEMESTER**	**2**
COURSE CODE AND TITLE	**16P2CPHT06 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)**		

PROGRAMME OUTCOMES

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	COURSE OUTCOMES	**PO / PSO**	***CL***
CO1	Describe the mechanisms of different types organic reactions.	PO1 PSO1	U
CO2	Explain the chemistry of carbanions, carbocations, carbenes, carbenoids, nitrenes and arynes.	PO2 PSO2	U
CO3	Understand the chemistry of radical reactions and its applications.	PO3 PSO3	U
CO4	Explain the basics and applications of concerted reactions	PO4 ,PO5 PSO4	U

CL* Cognitive Level

Teacher I – JUC : Unit 1: Review of substitution reaction Mechanisms (11h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**COURSE OUTCOME**
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	CO 1
2.	Continued	Power point		CO 1
3.	Continued	Power point		CO 1

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		CO 1
5.	Continued	Power point		CO 1
6.	Stereochemistry of E_2 reaction, Intramolecular pyrolytic elimination, Cope elimination. Elimination *vs* substitution.	Power point		CO 1
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		CO 1
8.	Substitution at the aromatic centre, unimolecular mechanism, bimolecular mechanism. Kinetics of SE_2-Ar reaction. Ortho-para selectivity ratio.	Power point	Quiz	CO 1
9.	Electrophilic substitution via enolization and stork-enamine reaction.	Power point		CO 1
10.	Benzyne mechanism. Von Ritcher	Power point		CO 1
11.	Vilsmeyer formylation, Jacobson and Gatterman-Koch reactions.	Power point		CO 1
Teacher II – GT : Unit 2: Chemistry of Carbanions (10h)				
12.	Formation, structure and stability of carbanions	Power point	Quiz	CO 2
13.	Reactions of carbanions: C-X bond (X = C, O, N)	Power point		CO 2
14.	Formations through the intermediary of carbanions.	Power point		CO 2
15.	Chemistry of enolates and enamines.	Power point		CO 2
16.	Kinetic and Thermodynamic enolates-lithium and boron enolates in aldol alkylation and acylation of enolates.	Power point		CO 2
17.	Electrophilic additions to alkenes, Kinetics, effect of structure, orientation and stereochemistry.	Power point		CO 2
18.	Ozonolysis and hydroboration. Nucleophilic additions to carbonyls groups. Named reactions under carbanion chemistry –Mechanism of Claisen	Power point	Q & A Session	CO 2
19.	Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations	Power point		CO 2

20.	Shapiro reaction and Julia elimination. Favorski rearrangement.	Power point		CO 2
21.	Ylids: Chemistry of Phosphorous and Sulphur ylids - Wittig and related reactions, Peterson olefination.	Power point		CO 2
Teacher III – GT : Unit 3: Chemistry of Carbocations (9h)				
22.	Formation, structure and stability of carbocations.	Power point	Quiz	CO 2
23.	Classical and non-classical carbocations.	Power point		CO 2
24.	C-X bond (X = C, O, N) formations through the intermediary of carbocations.	Power point		CO 2
25.	Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol	Power point		CO 2
26.	Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.	Power point		CO 2
27.	C-C bond formation involving carbocations: Oxymercuration, halolactonisation.	Power point		CO 2
28.	Structure and reactions of α, β- unsaturated carbonyl compounds – electrophilic addition	Power point	Q & A Session	CO 2
29.	Nucleophilic addition - Michael addition	Power point		CO 2
30.	Mannich reaction and Robinson annulation.	Power point		CO 2
Teacher IV – VSS : Unit 4: Carbenes, Carbenoids, Nitrenes and Arynes (9h)				
31.	Structure of carbenes (singlet and triplet) - generation of carbenes	Power point	Quiz	CO 2
32.	Addition and insertion reactions.	Power point		CO 2
33.	Rearrangement reactions of carbenes such as Wolff rearrangement	Power point		CO 2
34.	Generation and reactions of ylids by carbenoid decomposition.	Power point		CO 2
35.	Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.	Power point		CO 2
36.	Continued	Power point		CO 2
37.	Hoffmann, and Curtius reactions.	Power point		CO 2

38.	Lossen, Schmidt and Beckmann rearrangement reactions	Power point		CO 2
39.	Arynes: Generation, structure, stability and reactions. Orientation effect- amination of haloarenes.	Power point	Q & A Session	CO 2
Teacher V – VSS : Unit 5: Radical Reactions (9h)				
40.	Generation of radical intermediates	Power point	Q & A Session	CO 3
41.	Its addition to alkenes, alkynes (inter & intramolecular)	Power point		CO 3
42.	For C-C bond formation - Baldwin's reaction	Power point		CO 3
43.	Fragmentation and rearrangements	Power point		CO 3
44.	Hydroperoxide: formation, rearrangement and reactions.	Power point		CO 3
45.	Continued	Power point		CO 3
46.	Auto-oxidation.	Power point		CO 3
47.	Named reactions involving radical intermediates: Barton deoxygenation	Power point	Quiz	CO 3
48.	Decarboxylation, McMurry coupling.	Power point		CO 3
Teacher VI – JUC : Unit 6: Concerted reactions (24h)				
49.	Classification	Power point	Q & A Session	CO 4
50.	Electrocyclic reactions.	Power point		CO 4
51.	Sigmatropic reactions.	Power point		CO 4
52.	Cycloaddition reactions.	Power point		CO 4
53.	Chelotropic reactions.	Power point		CO 4
54.	Ene reactions.	Power point		CO 4
55.	Woodward Hoffmann rules	Power point		CO 4
56.	Frontier orbital and orbital symmetry correlation approaches	Power point		CO 4
57.	Continued	Power point		CO 4
58.	PMO method.	Power point		CO 4

59.	Pericyclic reactions in organic synthesis such as Claisen rearrangement	Power point	Quiz	CO 4
60.	Cope rearrangement	Power point		CO 4
61.	Wittig rearrangement	Power point		CO 4
62.	Mislow-Evans rearrangement	Power point		CO 4
63.	Sommelet-Hauser rearrangements.	Power point		CO 4
64.	Diels-Alder and Ene reactions (with stereochemical aspects)	Power point		CO 4
65.	Continued	Power point		CO 4
66.	Dipolar cycloaddition (introductory).	Power point		CO 4
67.	Pyrolytic elimination reactions: cheletropic elimination.	Power point	Q & A Session	CO 4
68.	Decomposition of cyclic azo compounds.	Power point		CO 4
69.	β-eliminations involving cyclic transition states such as N-oxides	Power point		CO 4
70.	Acetates and xanthates.	Power point		CO 4
71.	Introduction to Click reactions -Mechanism of the Huisgen Azide-Alkyne 1, 3-Dipolar Cycloaddition.	Power point		CO 4
72.	Staudinger ligation and Staudinger reduction.	Power point		CO 4

INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**	**Course Outcome**
1.	02/12/2018	Hydroperoxide: formation, rearrangement and reactions.	CO 3

GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**	**Course Outcome**
2.	03/02/2019	Classifications of concerted reactions	CO 4

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. APPLIED CHEMISTRY - PHARMACEUTICAL**	**SEMESTER**	**2**
COURSE CODE AND TITLE	**16P2CPHT07 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)**		

PROGRAMME OUTCOMES

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	COURSE OUTCOME	**POs / PSOs**	***CL***
CO1	Ability to understand theory and application to Microwave, Infrared and Raman Spectroscopy	PO1,PO2 PSO1, PSO2	U
CO2	Analyze the various aspects of Electron & Electronic Spectroscopy & Lasers	PO3, PO4 PSO3,PSO4	AN
CO3	Understand the fundamental concepts of atomic, molecular and spin resonance spectroscopy.	PO5 PSO5, PSO 6	U

CL* Cognitive Level

Teacher I – KBJ : Unit 1 : Microwave, Infrared and Raman Spectroscopy (14h)				
SESSION	**TOPIC**	**LEARNING RESOURCES**	**VALUE ADDITIONS**	**COURSE OUTCOME**
1.	Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption	Chalk and board	Q & A Session	CO 1
2.	influencing factors, signal to noise ratio, natural line width, contributing factors	Chalk and board		CO 1
3.	Doppler broadening, Lamb dip spectrum	Chalk and board		CO 1
4.	Born Oppenheimer approximation, energy dissipation from excited states (radiative and non radiative processes), and relaxation time.	Chalk and board		CO 1

5.	Microwave spectroscopy*:* Classification of molecules	Chalk and board		CO 1
6.	Rigid rotor model; rotational spectra of diatomics and polyatomics	Chalk and board		CO 1
7.	Effect of isotopic substitution and nonrigidity; selection rules and intensity distribution.	Chalk and board		CO 1
8.	Vibrational spectroscopy: Vibrational spectra of diatomics	Chalk and board	Quiz	CO 1
9.	Effect of anharmonicity; Morse potential	Chalk and board		CO 1
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		CO 1
11.	Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum	Chalk and board		CO 1
12.	Rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra	Chalk and board		CO 1
13.	Polarized and depolarized Raman lines	Chalk and board		CO 1
14.	Revision	Chalk and board	Q & A Session	CO 1
Teacher II – FJ : Unit 2 : Electron & Electronic Spectroscopy & Lasers (13h)				
15.	Electron Spectroscopy: Basic principles	Chalk and board		CO 2
16.	Photoelectron spectra of simple molecules, selection rules	Chalk and board	Quiz	CO 2
17.	Electron spectroscopy for chemical analysis (ESCA)-UPS	Chalk and board		CO 2
18.	X-ray photoelectron spectroscopy (XPS)	Chalk and board		CO 2
19.	Auger electron spectroscopy (AES).	Chalk and board		CO 2
20.	Electronic spectroscopy: Electronic spectra of diatomic molecules	Chalk and board	Q & A Session	CO 2
21.	Franck-Condon principle.	Chalk and board		CO 2
22.	Vibronic transitions, Spectra of organic compounds	Chalk and board		CO 2
23.	$\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition.	Power Point Presentation	Quiz	CO 2
24.	Lasers: Laser action	Power Point Presentation		CO 2
25.	Population inversion, properties of laser radiation, two stage	Power Point Presentation		CO 2

26.	Three stage-examples of simple laser systems	Power Point Presentation		CO 2
27.	Revision	Power Point Presentation	Q & A Session	CO 2
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		CO 3
29.	Nuclear energy levels, population of energy levels	Power Point Presentation		CO 3
30.	Larmor precession, relaxation methods	Power Point Presentation		CO 3
31.	Chemical shift, representation	Power Point Presentation		CO 3
32.	Examples of AB, AX and AMX types	Power Point Presentation	Q & A Session	CO 3
33.	Exchange phenomenon, factors influencing coupling	Power Point Presentation		CO 3
34.	Karplus relationship.	Power Point Presentation		CO 3
35.	FTNMR, second order effects on spectra	Power Point Presentation	Quiz	CO 3
36.	Spin systems (AB, AB_2)	Power Point Presentation		CO 3
37.	Simplification of second order spectra	Power Point Presentation		CO 3
38.	Chemical shift reagents	Power Point Presentation	Q & A Session	CO 3
39.	High field NMR	Power Point Presentation		CO 3
40.	Double irradiation, selective decoupling, double resonance, NOE effect	Power Point Presentation		CO 3
41.	Two dimensional NMR, COSY	Power Point Presentation		CO 3
42.	HETCOR	Power Point Presentation		CO 3
43.	^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, ^{19}F, ^{31}P, NMR spectroscopy.	Power Point Presentation		CO 3
44.	EPR spectroscopy: electron spin in molecules	Power Point Presentation		CO 3
45.	Interaction with magnetic field, g factor, factors affecting g values	Power Point Presentation		CO 3
46.	Determination of g values ($g_{\parallel}$ and $g^{\perp}$)	Power Point Presentation	Quiz	CO 3
47.	Fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.	Power Point Presentation		CO 3

48.	An elementary study of NQR spectroscopy.	Power Point Presentation		CO 3
49.	Mossbauer spectroscopy: principle	Power Point Presentation		CO 3
50.	Doppler effect, recording of spectrum	Power Point Presentation		CO 3
51.	Chemical shift, factors determining chemical shift	Power Point Presentation		CO 3
52.	Application to the structural elucidation of metal complexes	Power Point Presentation		CO 3
53.	Revision	Power Point Presentation	Q & A Session	CO 3
54.	Revision	Power Point Presentation		CO 3

INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)	Course Outcome
1	22/01/2019	Vibration-rotational spectra of diatomics, polyatomic molecules- P,Q,R branches	CO 1

GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)	Course Outcome
1	11/02/19	Application to the structural elucidation of metal complexes	CO 2

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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.
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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. APPLIED CHEMISTRY - PHARMACEUTICAL**	**SEMESTER**	**2**
COURSE CODE AND TITLE	**16P2CPHT08 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)**		

PROGRAMME OUTCOMES

PO1	The students are capable of exercising their critical thinking in creating new knowledge leading to innovation, entrepreneurship and employability.
PO2	The students are able to effectively communicate the knowledge of their study and research in their respective disciplines to their employers and to the society at large.
PO3	The students are able to make choices based on the values upheld by the college, and have the readiness and know-how to preserve environment and work towards sustainable growth and development.
PO4	The students possess an ethical view of life, and have a broader (global) perspective transcending the provincial outlook.
PO5	The students possess a passion for exploring new knowledge independently for the development of the nation and the world and are able to engage in a lifelong learning process.

PROGRAM SPECIFIC OUTCOMES

Knowledge and Understanding	
PSO 1	Demonstrate an in-depth knowledge and understanding of the principles of Inorganic, Organic, Physical and Theoretical Chemistry.
PSO 2	Demonstrate an awareness of the relevance of chemistry in a wider multi-disciplinary context.
Intellectual Abilities	
PSO 3	Apply their understanding in Chemistry to design solutions to unfamiliar problems in Chemistry and those involving other related disciplines.

PSO 4	Use their knowledge and understanding to conceptualize appropriate models and representations.
Practical Skills	
PSO 5	Design and conduct analytical, modelling and experimental investigations in Inorganic, Organic, Physical and Theoretical Chemistry.
Professional Skills	
PSO 6	Ability to identify, design and conduct appropriate experiments, interpret data obtained, draw pertinent conclusions and communicate all these effectively.

	COURSE OUTCOME	**POs / PSOs**	***CL***
CO1	Explain the approximation methods in quantum mechanics.	PO 1 PSO 1	U
CO2	Describe the quantum mechanical explanation of chemical bonding.	PO 1 PSO 1	A
CO3	Explain the methods of computational quantum chemistry.	PO 1 PSO 3	U
CO4	Explain Model Chemistry and Molecular Simulations	PO 1 PSO 3	U

CL* Cognitive Level

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

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

27.	MO theory of H_2^+ ion	Chalk & Board and ICT		CO 2
28.	MO theory of H_2 molecule	Conventional Lecture		CO 2
29.	MO Theory of homo nuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2	Chalk & Board and ICT		CO 2
30.	MO Theory of hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order	Conventional Lecture		CO 2
31.	Correlation diagrams, non-crossing rule	Chalk & Board and ICT		CO 2
32.	Spectroscopic term symbols for diatomic molecules	Conventional Lecture		CO 2
33.	Comparison of MO and VB theories.	Chalk & Board and ICT		CO 2
34.	Hybridization	Conventional Lecture	Q & A Session	CO 2
35.	Quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation	Chalk & Board and ICT		CO 2
36.	Semiempirical MO treatment of planar conjugated molecules	Conventional Lecture		CO 2
37.	Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene.	Chalk & Board and ICT		CO 2
38.	Calculation of charge distributions, bond orders and free valency	Conventional Lecture		CO 2
39.	Froniter Molecular Orbitals	Chalk & Board and ICT		CO 2
40.	Woodward-Hoffmann rule	Conventional Lecture		CO 2
41.	Introduction to global and local reactivity descriptors - electrophilicity index	Chalk & Board and ICT	Quiz	CO 2
Teacher III – ATG : Unit 3: Computational Quantum Chemistry (18h)				
42.	Introduction and scope of computational chemistry.	Conventional Lecture	Q & A Session	CO 3
43.	Potential energy surface - Conformational search	Chalk & Board and ICT		CO 3
44.	Global minimum, Local minima, saddle points.	Conventional Lecture		CO 3
45.	Conformational analysis of ethane and butane	Chalk & Board and ICT		CO 3
46.	Ab initio methods	Conventional Lecture	Quiz	CO 3
47.	A review of Hartee-Fock method. Self Consistent Field Procedure	Chalk & Board and ICT		CO 3

48.	Roothan concept of basis functions. Basis sets	Conventional Lecture		CO 3
49.	Slater type and Gaussian type basis sets, Minimal basis set	Chalk & Board and ICT		CO 3
50.	Pople style basis sets - Classification - double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets	Conventional Lecture		CO 3
51.	Hartree-Fock limit and Post Hartree-Fock methods	Chalk & Board and ICT		CO 3
52.	Introduction to Møller Plesset Perturbation Theory, Configuration Interaction and Coupled Cluster	Conventional Lecture	Quiz	CO 3
53.	Semi empirical methods	Chalk & Board and ICT		CO 3
54.	Introduction to Density Functional Theory (DFT) methods	Conventional Lecture		CO 3
55.	Hohenberg-Kohn theorems. Kohn-Sham orbitals.	Chalk & Board and ICT		CO 3
56.	Exchange correlation functional. Local density approximation	Conventional Lecture		CO 3
57.	Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).	Chalk & Board and ICT		CO 3
58.	Comparison of ab initio, semi empirical and DFT methods	Conventional Lecture	Q & A Session	CO 3
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	CO 4
60.	Cartesian coordinates, internal coordinates and Z-matrix of simple molecules	Conventional Lecture		CO 4
61.	Introduction to computational chemistry calculations using simple molecular structures of water, ammonia, methane, butane, benzene.	Conventional Lecture And ICT with Power Point Presentation		CO 4
62.	Input file format - Method, Basis Set, Calculation type, Spin Multiplicity, Coordinate format.	Conventional Lecture And ICT with Power Point Presentation		CO 4
63.	Single Point Energy, Geometry Optimization, Frequency Analysis.	Conventional Lecture		CO 4
64.	Computational Chemistry using Statistical mechanics.	Conventional Lecture And ICT with Power Point Presentation	Quiz	CO 4

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		CO 4
66.	Commonly used force fields AMBER and CHARMM.	Conventional Lecture		CO 4
67.	Molecular dynamics simulations.	Conventional Lecture And ICT with Power Point Presentation		CO 4
68.	Introduction to simulation softwares. Protein data bank (PDB) and Protein structure file (PSF) formats.	Conventional Lecture And ICT with Power Point Presentation	Quiz	CO 4
69.	Practical aspects of computer simulation.	Conventional Lecture		CO 4
70.	Analyzing the results of a simulation.	Conventional Lecture And ICT with Power Point Presentation		CO 4
71.	Revision	Conventional Lecture And ICT with Power Point Presentation	Q & A Session	CO 4
72.	Revision	Conventional Lecture And ICT with Power Point Presentation		CO 4

INDIVIDUAL ASSIGNMENTS/SEMINAR – Details & Guidelines

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**	**Course Outcome**
1	29/12/18	Assignment on Problems Related to Variation Method	CO 2
2	16/01/19	Assignments based on MO Calculations	CO 2

GROUP ASSIGNMENTS/ACTIVITES – Details & Guidelines

	Date of completion	**Topic of Assignment & Nature of assignment (Individual/Group – Written/Presentation – Graded or Non-graded etc)**	**Course Outcome**
1	03/02/19	Seminar on the topic Molecular Mechanics	CO 4

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.
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6. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics* , 4th Edition, Oxford University Press, 2005.
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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.
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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