HAJEE KARUTHA ROWTHER HOWDIA COLLEGE (AUTONOMOUS) UTHAMAPALAYAM

M. Phil CHEMISTRY SYLLABUS 2015-2016

I Semester

Three theory	Code		
Core:	Paper I	Research Methodology	15MCHC11
Core:	Paper II	Course Work	15MCHC12
Elective:	Paper III	Advanced Inorganic chemistry	15MCHE11

For each paper- Internal 40 marks and external 60 marks

Mark splitting pattern (Internal)

Conducting three tests (Average of best two)	25 marks
Seminar	15 marks
Total	40 marks

Question pattern (External)

Max. marks: 60

Time 3 hrs.

Part A (5 x 6 = 30 marks)

Answer ALL questions choosing either (a) or (b)

(One question from each unit with internal choice)

Part B (3 x 10 = 30 marks)

Answer ANY THREE questions (out of five questions)

(One question from each unit)

II Semester

Dissertation only- 200 marks

Evaluation of dissertation	150 marks
(Average of internal and external examiners)	
Viva- voce	50 marks
Total	200 marks

DETAILS OF COURSE CATEGORY, CODE, TITLE & CREDITS

Course Category	Course Code	Course Title	Hrs/ Week	CIAE Marks	TEE Marks	Max. Marks	Credits
		SEM	ESTER -	I			
Core - I	15MCHC11	Research Methodology	5	40	60	100	4
Core - II	15MCHC12	Course Work	5	40	60	100	4
Elective	15MCHE11	Advanced Inorganic chemistry	5	40	60	100	4
15						300	12
SEMESTER - II							
	15MCHCE V	Project	Project Internal	mal	Externa		
		rioject	Internal		1		
Core		Dissertation	<u> </u>		150	150	
							8
		Viva- voce		-	50	50	
						200	8
Grand Total					500	20	

UNIT 1- Literature search

Searching the chemical literature, primary sources- journals and patents, secondary sources-Beilstein, reviews, periodicals-serials-monograph and text booksdictionaries, encyclopedias, catalogues and index of tabulated data, location data, location of published and comprehensive account of research with special reference to physical, organic and inorganic chemistry. Inductive and deductive reasoning-role of experimentation-interpretation of results-formation-testing and rejection of hypothesis- Getting idea on impact factor of journals-Leading funding agencies in India- Submission of research project proposals.

UNIT 2 - Thesis writing

Thesis layout: Format of title page, certificates, declaration, Preface, acknowledgements and table contents. Text of the thesis: Chapter division and subdivision-use of centered reading, side heading and paragraph heading. Quotations: When, what and how to use quotations, interpolation of quotations. Footnotes, tables and figures: Format, conventions and referencing. Documentation: Methodology of writing references-MLA and APA style. Editing and evaluating: Basic idea of editing, revising and evaluating the thesis. Ethics and research Plagiarism.

UNIT 3 - Error in chemical analysis and statistics

Classification of errors-accuracy-precision-minimization of errors-mean-standard deviation-Normal or Gaussian distribution-Reliability of results-Confidence interval-comparisionofresults-Student's t-test,F test, paired t-test-correlation and regression-the least square method for deriving calibration plots like straight line-Analysis of variance (ANOVA)- Pearson correlation coefficient-r value.

UNIT 4 - Computers in chemistry

Data types: int, short, long int, float, double and long double; variable and scope. Global caching, automatic register and static operators: assignment, precedence and associatively:programselection:if-else logical operators-ternary operator switch statement:Repetition:while.do-while and for loops, gotostatement;functions, void. Return statement, invoking functions, passing arguments-protyping.

Array: Single dimensional arrays, accessing arrays, initializing and copying arrays-array as function arguments-multidimensional arrays.

Simple C programming applications in chemistry such as van der waals equation, pH titration, kinetics, radioactive decay, evaluation of lattice energy and ionic radii from experimental data. Use of computer in literature search, significance of chemdraw-drawing chemical structure-paste them in the text.

UNIT 5 - Analytical Chemistry

Electro Chemical methods: Voltammetry – principles-linear sweapvoltammetry-cyclic voltammetry, differential pulse voltammetry-electrodes and electrolytes- pulse polarographic methods-applications.

Principles and instrumentations of Atomic Force Microscopy(AFM), powder XRD,Scanning Electron Microscopy(SEM), Transmission Electron Microscopy (TEM)and HRTEM, Scanning Tunneling Spectroscopy(STS), Scanning Tunneling Microscopy(STM), Thermo gravimetric Analysis(TGA), Differential Thermal Analysis(DTA), Differential Scanning Colorimetry(DSC)

4

REFERENCES:

UNIT 1

- 1. Advanced organic chemistry, Jerry March, 4th edition.
- 2. How to find chemical information? A guide for practicing chemistry teachers and students, Robert E Maizll.

UNIT 2

- 1. Vogel's textbook of Quantitative Chemical Analysis, 5th Edn., Longman scientific and Industrial, UK, 1989.
- 2. Fundamentals of Analytical Chemistry, VII Edn., D.A.Skoog, D.M.West & F.J.Holler, Saunder's College of publishing, Newyork.

UNIT 3

- 1. Computers in chemistry, K.V.Raman Tata McGraw-Hill publishing Co., Ltd., New Delhi (1993).
- 2. Programming in ANSI-C, II Edn., E.Balagurusamy, Tata McGraw-Hill publishing Co.,Ltd., New Delhi (1998).

UNIT 4

- 1. Advanced organic chemistry, Jerry March, 4th Edn.,
- 2. Reaction Mechanisms : A guide book, P.Sykes.
- 3. Structure and mechanism in organic chemistry, E.S.Goulg.
- 4. Chemical kinetics, Frost and Pearson.
- 5. Electron transfer reaction, R.D.Canon, Butterworth.
- Inventions of rate and mechanism of reactions: part 1,2nd edn., S.L.Fuess, E.S.Lewis and A.Weissberger.
- 7. Fast reactions, Bradley.
- 8. Advances in free energy relationships, N.B.Chapmann & J.Shorter.
- 9. Correlation analysis in organic chemistry: An introduction to LFER, J.Shorter.
- 10. Correlation analysis in organic chemistry:, N.B.Chapmann& J.Shorter.

UNIT 5

- 1. H.V.Malmstadt, C.G.Enkes and S.R.Crouch, Instrumentation for scientists series Modulas 1-4-Benhamin Inc.
- 2. Instrumental methods of analysis, Williard, Merrit & Dean.
- 3. Principles of Instrumentalanalysis, D.A.Skoog & D.M.West.
- 4. NMR and chemistry, J.M.Akitt, II Edn.,
- 5. Fourier transform NMR techniques: A practical approach, K.Mullie & P.S.Pregosin.
- 6. Data reduction and error analysis for physical sciences,
- 7. Applications of organic spectroscopy of organic compounds, J. R. Dyer.
- 8. Spectroscopic identification of organic compounds, R. M. Silverstein, G.O. Bassder & T.C. Murrell.
- 9. Organic spectroscopy, W.Kemp.
- 10. Physical methods in chemistry, R. S. Drago.

Core Paper I1Code: 15MCHC12COURSE WORKHours-5 / Credit

Unit I – Organic synthesis and organometallic reagent in synthesis:

Types of (carbon to carbon bond forming) reactions – key intermediates – starting materials – sandheimer synthesis – stork approach. Use of reterosynthetic analysis for the synthesis of simple cyclic molecules – Gabriel synthesis. A schematic analysis of the total synthesis of Υ – caprolactone, 6-methoxy tryptamine, 6, 6 – ethylenedioxy -1 (9) octalin – 2-one, α – onocerin and quinotoxine. Organo copper reagents – vinyl Grignard reagents – carboalumination – nucleophilic addition of alkenylalanates to carbonyl compounds – ortholithiation – use of formamidines – lithiated dithianes and nitroalkanes in synthesis.

Unit II – Group Theory

Projection operators – symmetry adopted linear combination (SALC) – construction of MO wave functions for allyl, butadiene, cyclopropenyl, benzene and tetramethylcyclobutane calculation of delocalization of hybrid orbitals and wave functions of hybrid orbitals for molecules having tetrahedral, trigonal triangular and square planar geometry (SP², SP³ and dSP² hybridizations).

Application of group theory to IR, Raman and UV spectroscopy - selection rules for fundamental vibrations – symmetry of normal vibrations of molecules belonging to C₂h, C₂v, C₃v, C₄v, D₃h, D₄h, D ∞ h and C ∞ v point groups, stretching mode analysis of metal carbonyls and metal complexes.

Unit III – Bio – inorganic chemistry:

Metalloproteins and enzymes – blue copper proteins - copper proteins as oxidases/reductases – nickel containing enzymes structure of DNA – types of nucleic acid interactions – coordination, intercalation and hydrogen bonding – interactions of metal ions with nucleic acid – redox chemistry, hydrolytic chemistry – monitoring the DNA binding by UV, IR, NMR and CV spectral techniques. Applications of different metal complexes that bind nucleic acid – conformational probes – metallo foot printing reagents. Nature's use of metal/ nucleic acid interactions. Metal ion toxicity – detoxication using chelating agents. Inorganic compounds as therapeutic agents. Anticancer drugs – antiarthritis drugs. Treatment of essential trace metal deficiencies and excess.

Unit IV - Fundamentals of Medicinal Chemistry:

Definitions of Medicinal Chemistry, Pharmacology and Molecular Pharmacology-Major process involved in drug action-Pharmacokinetics phase –Quantitative structure –Activity relationship (QSAR)-Hansch approach –Concept of bio-isoterism- Pharmacodynamics phase – Receptors and classification of membrane bound receptors-Enzyme inhibitors as drugs (illustrated with one example). The concept of allosterism – Agonist and antagonists – neurotransmitters in peripheral nervous system – cholinergic and adrenergic nerve nerve transmission – relationship between drug metabolism and drug design – prodrugs and soft drugs.

Unit V – Nanochemistry and Photochemistry

Nanoparticles and nanostructural materials – introduction – methods of preparation – physical properties – metallic behavior – magnetic behavior – optical and electronic properties – chemical properties of surfaces: metals – semiconductors – metal oxides – application of nanoparticles: water purification – catalysis – sensors – information storage – solar cells – environmental clean up.

Solar energy conversion – photo electrochemical cells – water splitting – semiconductor solar cells.

References

Unit I

- 1. R.E. Ireland, Organic Synthesis, Prentice-Hall of India Pvt. Ltd., 1969.
- 2. The Synthesis and characterization of Inorganic compounds, W. L. Jolly.
- 3. Advanced practical Inorganic chemistry, D. M. Adams & J. B. Raynor.

Unit II

- 1. Chemical Applications of Group Theory, F.A.Cotton.
- 2. Introduction to Group Theory, G.Davidson.
- 3. Physical Methods in Chemistry R. S. Drago.
- 4. V. Ramakrishnan and Gopinath, Group Theory in Chemistry.

Unit III

- 1. Bioinorganic chemistry, lavano Bertini, Harry B. Gray, Stephen J. Lippard and Joan Selverstone valentine, Viva Books Pvt. Ltd., 1998.
- 2. James E. Hugheey, Ellen A. Keitler and Richard L. Keitler, Inorganic Chemistry, 4th Edn, Harper COllins COllege Publishes, New York, 1993.
- 3. J. Chem. Edn., November 1985.
- 4. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5th Edition, John Wiley & Sons, Singapore, 1998.
- 5. A text book on medicinal aspects of bioinorganic chemistry, A.K. Das, CBS Publishers.
- 6. A. K. De, Environmental chemistry, Wiley Eastern Ltd., Meerut, 1994.
- 7. Bioinorganic chemistry, G.R. Chatwal and Ajay Kumar Bhagi, Himalaya Publishing House.

Unit IV

- 1. G.L. Patrick, An introduction to Medicinal chemistry, II Edn. Oxford University Press, 2001.
- 2. T. Nagradi, Medicinal Chemistry A Biochemical Approach, Oxford University Press-2004.
- 3. J. B. Taylor and P.D. Kennewall, Introductory Medicinal Chemistry, Ellisworth Publishers, 1985.
- 4. Burger's Medicinal Chemistry, M. E. Wolf(Ed), 5th edn., John Wiley & Sons, 1995.
- 5. Medicinal Chemistry (Instant Notes), G. Patrick, Viva Books Pvt. Ltd., 2002 (Indian edition).
- 6. Principles of Medicinal Chemistry, W. O. Foye, Lee & Febiger, 1975.

Unit V

1. Nanoscale materials in chemistry, Kenneth J. Klabunde, John Wiley & Sons, Inc., Publication, 2001.s

I Semester

Elective Paper I1I	Code: 15MCHE11	ADVANCED INORGANIC CHEMISTRY	Hours-5 / Credits – 4
-----------------------	----------------	---------------------------------	-----------------------

Unit I – Inorganic polymers

General properties of inorganic polymers – classification – homoatomic – heteroatomic – condensation – addition polymers – coordination polymers. Glass transition temperature – phosphorous based polymers – polydimethoxy and polydiethoxy phosphazines – polyphosphoryl chlorides – polyphosphates – metaphosphates – poly phosphates cross linked phosphates – ultra phosphate glasses – borophosphate glasses – uses of phosphorous polymers – polymeric sulphur nitride – chalogenide glasses – coordination polymers – chain polymers – twodimensional polymers – synthetic coordination polymers – polymers having phthalocyanide and related structure – polymers with bis chelating agents.

Unit II – Molecular rearrangement and reactions of coordinated ligands:

Molecular rearrangement of four coordinated complexes – six coordinated complexes – reaction at coordinated ligands – reaction due to metal ion polarization of coordinated ligands – hydrolysis of amino acid esters and amides and of peptides – Aldol condensation – imine formation, hydrolysis and substituent exchange – the template effect and macrocyclic ligands.

Unit III - Organometallic compounds:

Alkylidene and alkylidyne complexes – synthesis of alkylidene complexes in low oxidation state and higher oxidation state of metals – synthesis of alkylidyne complexes – reactivity and bonding in alkylidene and alkylidyne complexes – alkyne complexes – synthesis reactivity and bonding – cobalt catalysed alkyne cycloaddition reactions.

Unit IV – Metal ion in medicine

Introduction – trace elements – metal deficiency and disease – toxic effect of metals (Pb, Cd, Hg and As) and their detoxification – metals used for diagnosis and chemotherapy – platinum anticancer drugs: discovery, principles and development of drug – clinical picture of cisplatin and carbopltin – Bioinorganic chemistry of platinum anticancer drugs – design of new inorganic anticancer drugs.

Unit V – Energy and environment

Sources of energy – fossil fuels – nuclear fission – nuclear fusion – solar energy in space heating and water heating – production of electricity using solar energy – solar trough collectors – power tower – solar bond – solar energy for driving vehicles – power from indirect solar energy – hydropower, wind power, biomass energy – product of ethanol, methane from biomass – photosynthesis – photoelectrochemical cells – geothermal energy – ocean thermal energy conversion – tidal power, air energy.

References

Unit I

- 1. Principles of inorganic chemistry, B.R.Puri, L.R.Sharma and K.C.Kalia, Milestone publishers, Delhi, 30th edition.
- 2. Advanced inorganic chemistry, Gurdeepraj, Goel publishing House.

Unit II

1. Inorganic chemistry, K.F.Purcel and J.C.kotz

Unit III

- 1. Organometallic chemistry, R.C.Mehotra and A.Singh.
- 2. Organometallics I Complexes with transiton metal carbon s-bonds Manfred Bochmann.

Unit IV

- 1. Bioinorganic chemistry, Ivano Bertini, Harry B.Gray, Stephen J. Lippard and Joan Selverstone Valentine, Viva Books Pvt.Ltd., 1998.
- 2. Environmental chemistry, A.K.De, Wiley Eastern Ltd.,
- 3. A text book of Medicinal aspects of Bioinorganic chemistry, A.K.Das, CBS publishers.

Unit V

1. A textbook of environmental chemistry and pollution control, S.S.Dara, S.Chand & Co., 7th edition.