

RAJAH SERFOJI GOVT. COLLEGE (AUTONOMOUS), THANJAVUR – 613 005

CBCS PATTERN FOR ALL M.PHIL. COURSES

SUBJECT: CHEMISTRY

(Applicable to the Candidates admitted from the Academic Year 2015 – 2016 onwards)

PART	CODE	COURSE	TITLE	MARKS		TOTAL	HOURS	CREDIT
				IA	WE			
			I SEMESTER					
III	RR1MCH1	CC1	Research Methodology and Laboratory Techniques	40	60	100		4
III	RR1MCH2	CC2	Physical Methods in Chemistry - I	40	60	100		4
III	RR1MCH3	CC3	Physical Methods in Chemistry II	40	60	100		4
III	RR1MCH4*	CC4	Principles and Advances in Medicinal Chemistry (ELECTIVE)	40	60	100		4
		TOTAL				400		16
			II SEMESTER					
				v.v	Dis.	TOTAL		
III	RR2MCHT	CC5	Dissertation and viva voce	50	150	200		8
		GRAND TOTAL				600		24

No of Papers

Core Courses	4 (each of 4 credits)
Project	1 (8 credits)
Total	5 (24 credits)

***Optional Paper**

Rajah Serfoji Govt. College (Autonomous), Thanjavur – 613 005
CBCS Pattern M.Phil. - CHEMISTRY – PROGRAMME
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Code: RR1MCH1

SEMESTER – I

(For students admitted from 2015 onwards)

Paper 1: Research Methodology and Laboratory Techniques

UNIT I

Literature Survey

Source of information: primary, secondary and tertiary – sources: Journals, Abstracts, Current Tiles, Reviews, Monographs and Dictionaries – Information retrievals: using internet and other electronic medias (preparing a review article related to problem of research of the student) E journals and data bases – search engines: Google and Yahoo search and Wikipedia. Reports and research work – laboratory observation – preparation of records and manuscripts – Research paper formats in Indian Journal of Chemistry, Journal of Indian Chemical Society, Journal of American Chemical Society, Tetrahedron Letters, Journal of Chemical Education, etc., - Writing of the project reports of thesis – IUPAC nomenclature of organic & inorganic Compounds.

UNIT II

Error Analysis

Types of Error – Accuracy, precision, significant figures, use of calculus in the estimation of errors – Frequency distributions, the binomial distribution, the Poisson distribution and normal distribution – Describing Data, population and sample, mean, variance, standard deviation, way of quoting uncertainty, robust estimators, repeatability and reproducibility of measurements – Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t-Test, Paired t-Test – Analysis of variance (ANOVA) – Correlation and Regression– Curve fitting, Fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – General polynomial equation fitting, linear zing transformations, exponential function fit – r and its abuse – Multiple linear regression analysis, elementary aspects – Applications of some computer packages like MS-Excel, Origin.

UNIT III

X-ray Spectroscopy

Introduction, Mosley's law, X-ray instrumentation, X-ray absorption X-ray emission methods, X-ray emission vs X-ray absorption, X-ray diffraction, Bragg's law. Automated X-ray diffractometry, Determination of crystal structure, Interpretation of X-ray diffraction pattern, Applications.

Molecular luminescence, Fluorometry and phosphorimetry

Introduction, Principles of fluorescence phosphorescence, Interpretation of fluorescence spectra, Factors, fluorescence intensity and concentration, instrumentation for fluorometry, Types of filter fluorometry, Reporting fluorescence spectra, Applications of fluorometry – Some special determinations.

UNIT IV

Chromatography and Separation Techniques

Solvent extraction – Principles of ion exchange, paper, thin layer and column chromatography – Gas Chromatography techniques – Columns, adsorbents, methods, Rf values, McReynold's constants and their uses – HPTLC, HPLC techniques – Adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques: methods, principles and uses. Electrophoresis: Principles, factors affecting ionic migration – Effect of pH and ionic strength – Gel electrophoresis.

UNIT V

Electro analytical Techniques

Voltammetry – Polarography – Principles and introduction, Current – voltage relationship, Polarogram interpretation. Half wave potential, Reversible and Irreversible waves – residual, Migration and Diffusion currents, the Dropping Mercury Electrode (DME), Advantages of DME – Advantages and Applications of polarography. Amperometric Titrations – Principles, Titrations with two indicators – Instrumentation, Titration procedure, Advantages and Disadvantages, Applications. Ion selective electrodes – Glass – Membrane, Liquid – Membrane, Solid state Membrane, and their applications

References

UNIT I

1. <http://www.virtualref.com/govdocs/s189.htm>
2. <http://www.inflibnet.ac.in>
3. <http://www.springerlink.com>
4. <http://rsc.org>
5. <http://www.pubs.acs.org>
6. <http://dspace.org>
7. <http://dspace.bdu.ac.in>

UNIT II

1. D. B. Hibbert and J. J. Gooding, Data Analysis for Chemistry, Oxford University Press, 2006.
2. J. Topping, Errors of Observation and Their Treatment, Fourth Edn., Chapman Hall, London, 1984.
3. S. C. Gupta, Fundamentals of Statistics, Sixth Edn., Himalaya Publ. House, Delhi, 2006.
4. H. E. Solbers, Inaccuracies in Computer Calculation of Standard Deviation, Anal. Chem. 55, 1611 (1983).
5. P. M. Wanek et al., Inaccuracies in the Calculation of Standard Deviation with Electronic Calculators, Anal. Chem. 54, 1877 (1982).

UNIT III

1. A. Sharma, S. G. Schulman, Introduction to Fluorescence Spectroscopy, Wiley-Interscience, New York, 1999.
2. F. Rouessac and A. Rouessac, Chemical Analysis, John Wiley and Sons, Chichester, 2000.
3. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th edn., Tata McGraw-Hill, New Delhi, 1994.
4. Nicolo Omemetto, Analytical Laser Spectroscopy, Vol.50, John-Wiley and Sons, New York, 1979

UNIT IV

1. R. Stock and C. B. F. Rice, Chromatographic Methods, Chapman and Hall, New York. , 1963
2. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, a. R. Tatchell, Vogel's Text Book of Practical Organic Chemistry, 5th Edition, Pearson, New Delhi, 1989
3. V. K. Srivastava and K. K. Srivastava, Introduction to Chromatography, S. Chand & Co., New Delhi, 2nd edition, 1981.

UNIT V

1. C. H. Hamann, A. Hamnett and W. Vilelstich, Electrochemistry, Wiley-VCH, 1998.
2. A. J. Bard and L. F. Faulkner, Electrochemical methods – Fundamentals and Applications, 2nd Edn., Wiley-VCH, 1998.
3. A. C. Fisher, Electrode Dynamics, Oxford University Press, 1996.
4. J. Koryta and K. Stulik, Ion-Selective Electrodes, Cambridge University Press, 1983.
5. J. Janata, Principles of Chemical Sensors, Plenum Press, New York, 1989.

QUESTION PAPER PATTERN

Maximum: External: 60 Internal: 40 Exam Duration: Three Hours

Section – A: Either or Type Questions (5X6 =30 Marks) 1 pair from each unit.

Section – B: Out of 5 (3X10 = 30Marks) 1 questions from each unit.

Signature of the HOD

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Code: RR1MCH2

SEMESTER – I

(For students admitted from 2015 onwards)

PAPER II: PHYSICAL METHODS IN CHEMISTRY – I

UNIT I

Electronic Absorption Spectroscopy

Principles of absorption spectroscopy – Chromophore – UV-Visible Spectroscopy – Application to organic compounds – Woodward–Fieser and Scott rules for conjugated dienes and polymers – Ketones, aldehydes, α,β -unsaturated acids, esters, nitriles, and amides. Woodward's rule for enones – Differentiation of geometrical isomers and positional isomers – disubstituted benzene derivatives – Study of steric effect on aromaticity.

Microstates – Term symbols and energy levels for d1 – d9 ions in cubic and square fields – Intensity of bands – Group theoretical approach to selection rules – Effects of distortion and spin-orbit coupling on spectra – Evaluation of $10Dq$ and Δ values for octahedral complexes of cobalt and nickel – Applications to simple coordination compounds – Charge transfer spectra.

UNIT II

Infrared Spectroscopy

Vibrations in simple molecules (H_2O , CO_2) and their symmetry notation for molecular vibrations – Group vibrations and the limitations – Combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like N_2O , ClF_3 , NO_3^- , ClO_4^- – Effect of coordination on ligand vibrations – Uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide – Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment). The modes of stretching and bonding – FT-IR – Sampling techniques – Correlation tables for functional groups – Alkanes, alkenes, alkynes, aromatic rings, alcohols, carbonyl compounds – Factors that influence C=O stretching vibration – Hydrogen bonding (inter, intramolecular).

Raman Spectroscopy

Theory – Selection rule – Mutual exclusion principle – Structural elucidation – Application to organic compounds – Factors affecting vibrational frequencies – Finger print region – functional groups and their characteristic vibrations – Resonance Raman Spectroscopy.

UNIT III

Optical Rotary Dispersion and Circular Dichroism

ORD and CD – Cotton effect – Octant rule, alpha – haloketone rule – applications to determining absolute configuration of simple monocyclic ketones and metal complexes.

Photoelectron Spectroscopy: Principles – Auger Electron spectroscopy – Electron spectra for chemical analysis.

Mass Spectrometry

Instrumentation – Resolution, EI and CI methods – base peak, isotopic peaks, metastable peak, parent peak – determination and use of molecular formula, recognition of molecular ion peak – FAB – Fragmentation – General rules – Pattern of fragmentation for various classes of compounds – McLafferty rearrangement – Importance of metastable peaks – Inorganic Applications – Molecular fragmentations – Ion reactions.

UNIT IV

Diffraction Methods

Crystal symmetry – combination of symmetry elements – crystal classes – screw axis and glide planes – space group – crystal axes - crystal systems, unit cell, Bravais lattices, asymmetric unit – space group – Equivalent positions – X-ray-diffraction by single crystals – Structure factor – Phase problem in structure analysis – Heavy atom method – Fourier synthesis – refinement of structure. Neutron diffraction – Applications and comparison with X-ray diffraction. Electron diffraction by gases – Basic principles and applications to simple molecules – XeF₆, Be(BH₄)₂, ferrocene, Cr(II) acetate.

UNIT V

Techniques in Nano Chemistry

Techniques for Characterization of nano scale materials (Basic aspects): Atomic force microscopy (AFM) – Transmission electron microscopy (TEM) – Resolution and scanning transition electron microscopy (STEM). Scanning Tunneling Microscopy (STM) – Scanning near field optical microscopy (SNOM) and surface Plasmon spectroscopy.

References

UNIT I

1. A. B. P. Lever, Inorganic Electronic Spectroscopy, American Elsevier, 1968, 1986.
2. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern company

UNIT II

1. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern company.
2. N. B. Clothup, L. H. Daly and S. E. Wiberly, Introduction to Infrared and Raman Spectroscopy, Academic Press, New York, 1975.

3. R. S. Drago, Physical Methods in Chemistry, W. B. Saunders company, Philadelphia, London.
4. D. N. Sathiyarayanan, Vibrational Spectroscopy, New Age International Publishers, New Delhi.
5. K. Nakamoto, Infrared Spectra of Inorganic and Coordination Compounds, 2nd Ed, Wiley-Inter Science, New York.
6. D. L. Pavia, G. M. Lampmann, G. S. Kriz, Introduction to Spectroscopy, Thomson, 3rd edition, 2001.

UNIT III

1. J. E. Eland, Photoelectron Spectroscopy, Wiley, 1974.
2. P. K. Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley and Sons, New York, 1983.
3. D. L. Pavia, G. M. Lampmann, G. S. Kriz, Introduction to Spectroscopy, Thomson, 3rd edition, 2001.

UNIT IV

1. P. J. Wheatley, The Determination of Molecular Structure, (Unit V).
2. E. A. V. Ebsworth, David W. H. Rankin and Stephen Craddock, Structural Methods in Inorganic Chemistry, Blackwell Scientific Publications, U. K. 1987.

UNIT V

1. Kenneth J. Klabunde (Ed), Nanoscale Materials in Chemistry, Wiley - Interscience, New York, 2001.
2. T. Pradeep, Nano: The Essentials in Understanding Nanoscience and Nanotechnology, Tata McGraw Hill, New Delhi, 2007.
3. William Clegg, Crystal Structure Determination, Oxford University Press, 1998.

QUESTION PAPER PATTERN

Maximum: External: 60 Internal: 40 Exam Duration: Three Hours

Section – A: Either or Type Questions (5X6 =30 Marks) 1 pair from each unit.

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Code: RR1MCH3

SEMESTER – I

(For students admitted from 2015 onwards)

PAPER III: PHYSICAL METHODS IN CHEMISTRY – II

UNIT I

NMR Spectroscopy: Principles

Definition of nuclear angular momentum and the nuclear magnetic moment Idea about the rotating axis system – Bloch equations – Quantum mechanical description of the NMR experiment, transition probabilities – Relaxation effects – Fourier transform NMR – Measurement of T_1 and T_2 - Effect of quadrupolar nuclei evaluation of thermodynamic and kinetic data using NMR techniques – Second order spectra – Quantum mechanical treatment of coupling effects of relative magnitudes of J on the spectrum of an AB molecule - Spectral simplification and determination of signs of coupling constants.

Systems with chemical exchange – Evaluation of thermodynamic parameters in simple systems – Study of fluxional behaviour of molecules an elementary treatment of second order spectra – examples.

NMR Spectroscopy: Applications to Inorganic Systems ^1H , ^{19}F , ^{31}P , ^{13}C – Applications in probing inorganic structures, study of fluxional behavior in organometallics, evaluation of thermodynamic parameters – NMR of paramagnetic molecules – isotropic shifts – Contact and pseudo-contact shifts – Lanthanide shift reagents.

UNIT II

NMR Spectroscopy: Proton and Carbon NMR

Examples for different spin systems – Chemical shifts and coupling constants (Spin-spin coupling) involving different nuclei (^1H , ^{19}F , ^{31}P , ^{13}C) – interpretation and applications to inorganic compounds – Effect of quadrupole nuclei (^2H , ^{10}B , ^{11}B) on the proton NMR spectra – Satellite spectra.

^1H NMR Spectroscopy – Coupling constant – First order and second order splitting – Spin-spin splitting – Dependence of J on dihedral angle – Vicinal and geminal coupling constants – Karplus equation – Long range coupling constants - Influence of stereochemical factors on chemical shift of protons – Simplification of complex spectra – Double resonance techniques – Shift reagents – Chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOH, NH, NH_2) – An elementary treatment of NOE phenomenon – 2D Techniques (COSY, NOESY and ROESY)

Application of Proton NMR in MRI - ^{13}C NMR spectroscopy – Basic theory of FT-NMR – Relaxation – Broad band decoupling – Off resonance decoupling and chemical shift correlations (CH, CH_2 , CH_3 , aromatic). Identification of structure based on NMR data – Problems.

UNIT III

NQR Spectroscopy

Introduction – Characteristics of quadrupolar nuclei – Effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – Applications of NQR spectroscopy.

Mossbauer Spectroscopy

Introduction – Isomer shift – Magnetic interactions – Mossbauer emission spectroscopy – Applications to iron and tin Compounds.

UNIT IV

Electron Spin Resonance Spectroscopy

Basic concepts of ESR spectroscopy – Spin densities and McConnell equation – Hyperfine splitting – Factors affecting the magnitude of g and A values – Anisotropy in g and A values – ESR spectra of free radicals in solution: methyl, allyl, vinyl and related radicals, benzene anion, p-benzo-semiquinone, p-nitrobenzoate dianion – naphthalene dianion, – Spin-trapping – CINDNP and CIDEP techniques – Double resonance in ESR – Advantages of ENDOR spectroscopy.

UNIT V

Electron Paramagnetic Resonance Spectroscopy

Applications of EPR to some simple inorganic systems such as Xe^{2+} – Factors affecting the magnitude of g and A tensors in metal complexes – Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – EPR spectra of dinuclear Cu(II) complexes - Applications of EPR to a few metalloproteins containing Cu(II) and Fe(III) ions. Basic principles of ENDOR spectroscopy and its applications in inorganic Chemistry.

References

UNIT I

1. E. A. V Ebsworth, David W. H. Rankin and Stephen Craddock, Structural Methods in Inorganic Chemistry, Blackwell Scientific Publications, U. K. 1987

UNIT II

1. W. Kemp, NMR in Chemistry – A Multinuclear Introduction, McMillan, 1986.
2. C. D. Becker, High Resolution NMR – Theory and Applications, Academic Press, 2nd Edition, 1980.
3. Silverstein and Webster, Spectrometric Identification of Organic Compounds, Sixth Edition, Wiley, 1998.
4. B. P. Straughan and S. Walker, Spectroscopy Vol. I, Chapman and Hall, 1976.
5. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd Edition, Wiley Eastern Company.
6. D. L. Pavia, G. M. Lampmann, G. S. Kriz, Introduction to Spectroscopy, Thomson, 3rd edition, 2001.

UNIT III

1. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern company.
2. T. C. Gibbs, Principles of Mössbauer Spectroscopy, Chapman and Hall, 1976.
3. T. P. Das and E. L. Hah, NQR Spectroscopy, Acad. Press, Ny, 1958.

UNIT IV

1. B. P. Straughan and S. Walker, Spectroscopy, Chapman and Hall, London, vol.1 and 2, 1976.
2. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 3rd edition, Tata- McGraw Hill, New Delhi, 1983.12
3. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw-Hill, New York, 1964.
4. R. S. Drago, Physical Methods in Chemistry, Saunders, 1977.

UNIT V

1. R. S. Drago, Physical Methods in Inorganic Chemistry, Third Edition, Wiley Eastern,
2. M. C. R. Symons, Chemical and Biochemical Aspects of Electron Spin Resonance Spectroscopy, Van Nostrand Reinhold Co., 1978.
3. J. A. Weil, J. R. Bolton and J. E. Wertz, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, John Wiley and sons, 1994.
4. F. E. Mabbs and D. Collison, Electron Paramagnetic Resonance of d Transition Metal Compounds, Elsevier, 1992

QUESTION PAPER PATTERN

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SEMESTER – I

(For students admitted from 2015 onwards)

PAPER IV: PRINCIPLES AND ADVANCES IN MEDICINAL CHEMISTRY

UNIT I

Nomenclature and Mechanism of Drugs

Introduction – Study of drugs – Important terminologies in pharmaceutical chemistry – Classification and nomenclature of drugs – Nomenclature of some heterocyclic systems – Mechanism of action of drugs – metabolism of drugs – Absorption of drugs – Assay of drugs.

UNIT II

Drug Discovery and Development

Introduction – Choosing a drug target – Identifying a bioassay – Finding a lead compound – Structure-activity relationship(SAR) – Identification of a pharmacophore – Drug metabolism – Manufacture-synthetic issues – Toxicity – Clinical trials – Patents.

UNIT III

Drug Design and Pharmacokinetics

Drug design: Variation of substituents, chain extension, ring expansions/contractions, ring variations, ring fusions, isosteres, rigidification of the structure, conformational blockers.

Pharmacokinetics: Pharmacokinetics issues in drug design – Solubility and membrane permeability – Resistant to hydrolysis and metabolism – Targeting drugs – Reducing toxicity – Prodrugs – Methods of administration – Formulation.

UNIT IV

Combinatorial Synthesis

Introduction – Combinatorial synthesis for drug discovery – Solid phase techniques – Methods of parallel synthesis – Mixed combinatorial synthesis – Deconvolution – Structure determination of the active compound – Limitations – Examples – Designing a combinatorial synthesis – Testing for activity.

UNIT V

Application of Drugs for Treatment

Structure, properties and mechanism of action of the following: Antibacterial drugs – Sulpha drugs: Sulphanilamide, Sulphadiazine, Sulfapyridine. Antibiotics – Chloramphenicol, Penicillin, Streptomycin. Antiseptics and disinfectants: Phenol and its derivatives, Halogen compounds and organic mercurials. Analgesics: Morphine, Heroin, Pethidine, Morphine. Anticonvulsant: Barbiturates, Oxazolindiones. Diabetes: Control of diabetes, Insulin. Cancer and anti neo plastic drugs: Alkylating agents, Anti metabolites, Plant products. Cardio vascular drugs: Anti arrhythmic drugs, Anti hypertension drugs.

Textbooks and Reference books

1. G. L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, 2nd Edition, 2001.
2. J. Ghosh, Fundamental Concepts of Applied Chemistry, S. Chand and Co., New Delhi, 2006.
3. A. Kar, Medicinal Chemistry, New Age International (P) Ltd, Delhi, 1997.

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RAJAHSERFOJIGOVERNMENTCOLLEGE(AUTONOMOUS)

THANJAVUR – 613 005

(Accredited by NAAC – B⁺⁺)

M.Phil., CHEMISTRY - SYLLABUS

(Under Choice Based Credit System - CBCS)

For Candidates admitted from the year 2015 – 16 onwards



**Finalized (for the I semester) in the
BOARD OF STUDIES MEETING HELD ON -----
&**

APPROVED BY THE ACADEMIC COUNCIL ON _____

PG & RESEARCH DEPARTMENT OF CHEMISTRY

CBCS GENERAL STRUCTURE OF M.Phil., CHEMISTRY

For Candidates admitted from the year 2015 – 16 onwards

SEM	SUB CODE	PAPER	HOURS	MARKS		TOTAL	CREDITS
				INT	EXT		
I	RMCH1	Research Methodology and Laboratory Techniques		40	60	100	
I	RMCH2	Physical Methods in Chemistry - I		40	60	100	
I	RMCH3	Physical Methods in Chemistry II		40	60	100	
I	RMCH4	Principles and Advances in Medicinal Chemistry (ELECTIVE)		40	60	100	
II	DISSERTATION						