Department of Chemistry
Davangere University, Shivaganogtri,
Davanagere - 577 007, Karnataka, India

Ph.D., Course Work Syllabus

				IA	Exam	Total
Course - I	:	Research Methodology	03 hr/Week	25	75	100
Course - II	:	Cognate Subject	03 hr/Week	25	75	100
Course - III	:	Field of Specialization	03 hr/Week	25	75	100
Coursse- IV	:	Research and Publication Ethics	02hr/Week	10	40	50

15/2/2020

15/2/2020

15/02/2020

15/02/2020

15/2/2020

Department of Chemistry
Ph.D., Course Work
Course-1: Research Methodology,

3hrs/week 48 hours

UNIT 1: Research sources 12 hrs

Selection of research problems and literature survey: primary sources- Journals periodicals, abstracts; Secondary listing of titles, reviews –annual Treatises, serials, monographs and text books, encyclopedia, catalogues, index of tabulated data- Science citation index- Searching the chemical literature-location of journal article- materials on a given topic- information about specific compound- Choosing a problem-abstract of a research paper.

Internet: Introduction to internet-web browsers-World Wide Web-Search engines-literature survey in Chemistry-popular website in chemistry-Database in chemistry. E-Mail: Introduction to e-mail- creating e-mail-Receiving and sending e-mail. Patent: Introduction, patentable subject

UNIT 2: Purification and safety measures 12 hrs

Purification of compounds: General methods of isolation and purification of chemicals. Solvent extraction both cold and hot methods of crystallization, fractional crystallization, sublimation, Distillation; fractional distillation, distillation under reduced pressure, steam distillation, drying methods of solvents.

Handling of chemicals; hazardous chemicals; air/water sensitive, corrosive, toxic, explosive, carcinogenic and radioactive materials. Safety measures in laboratory, Good laboratory practices (GLP)

UNIT 3: Error Analysis in Chemical Measurements and results 12 hrs

Classification of errors-Accuracy-Precision-Minimization of errors-Significant figures. Statistical treatment of data: Mean and Standard Deviation-distribution of random and normal errors-Reliability of results- Confidence interval- Comparison of mean results students t-distribution and t- tests-Comparison of mean with expected value, comparison of the results of the two different methods, comparison of precision of two methods- Linear regression, regression line, standard deviation, correlation coefficient – Multiple linear regression (one variable with two other variables).

UNIT 4: 12 hrs

Research manuscript preparation Full length research paper, short communication, letters, reviews, popular science articles in magazines, Few case studies with reference to journals and periodicals. Presentation of research papers: Oral and poster presentation in seminars, workshops and conferences etc.. Preparation of synopsis and Thesis, Preparation of research project proposals for various funding agencies like UGC, CSIR, DST, DBT, AICTE, state, central and foreign agencies.

J.B.P. 11/2/2020

15/02/2020

Department of Chemistry
Ph.D. Course work
Course -II : Cognate subject

3hrs/week 48 hours

UNIT-I : Analytical Chemistry 12 hrs

NMR, UV-Vis, IR, Mass Chromatogphy-Basics, TLC, Colum, HPLC GC.
Basic principles, Instrumentation, application.

UNIT-II 12 hrs

Review of VBT and CFT of bonding in coordination complex, shortcomings of CFT, evidences for covalency. MOT of complexes involving sigma and pi-bonding. MO energy level diagrams for octahedral and tetrahedral complexes with sigma and pi-bonding. Crystal field effects on ionic radii, lattice energy, heat of ligation (hydration), geometry, structure of spinels, Jahn Teller distortion, Templates and macrocylic effects, Chelates- chelate effect, condition for chelation, factors affecting stability of chelates, importance of chelates.

Electronic spectra of complexes: Spectra of transition metal ions-Spectroscopic terms, terms and microstates for the p2 and d2 configurations. Ground state terms for dn configuration, splitting of terms in weak crystal fields.

Ligand field spectra: d-d transition selection-spin and Laporte selection rules and their relaxation symmetry, spin orbital coupling and vibrionic coupling effects, spectral band widths. Orgel diagrams for octahedral and tetrahedral complexes (d1 – d9 states)

Tanabe-Sugano diagrams, Interpretation of electronic spectra. Calculation of Dq, B, and parameters for Cr(III), Co(II) and Ni(II) complexes, Spectrochemical series and Nephilauxetic series. Charge transfer transitions-Characteristics, types-LMCT &MLCT.

UNIT-III 12 hrs

Combined applications of spectroscopic techniques in structural elucidation of Organic Compounds: Combined applications of IR, UV-Visible, ^{1}H NMR, ^{13}C NMR and Mass spectroscopy in the structural elucidation of different types of compounds.

At least 12 problems to be solved involving the following functional groups

1.Alcohols,.Phenols,.Aldehydes, Ketones, –unsaturated aldehydes and ketones, Carboxyic acids, Esters, Amines, Anilides, Amides, Nitro compounds, Compounds containing halogen,. Heterocyclic compounds and Examples involving functional group introversions.

UNIT-IV 12 hrs

Brief review of quantum chemistry formulation of Scbroeling is equation-application to are and three –dimension box. Basic aspects of thermodynamics-laws of thermodynamics, Evaluation of thermodynamic parameters and their significance. Chemical dynamics-Kinetics of fast reactions. Surface chemistry, Theories of adsorption-Frendlich and langmeir theories BET theory. Catalysis: Basics of catalysis, Michael-mention equation. Electrochemistry: Review of basic principles, Electrochemical energy sources (primary, sending & Fuel cells). References.

Department of Chemistry
Ph.D. Course work
Course III Field of specialization - Inorganic chemistry
Revised regulations-2010

48 hrs (3 Hrs/week)

UNIT-1:

Spectral and Magnetic properties of complexes:

Term symbols for d^n ions, spectroscopic ground states, selection rules, nature of spectral bands-band shapes, band intensities, band widths, effect of spin-orbit coupling, Orgal diagrams, Tanabe-Sugano diagrams, Racah parameters, interpretation of spectra of octahedral, distorted octahedral, tetrahedral and square planar complexes, calculation of nephelauxetic parameter, Charge transfer bands, intervalence charge-transfer bands.

Types of magnetic behavior, classical magnetism, orbital contribution, orbital contribution reduction factor, spin orbit coupling, measurement of magnetic susceptibility-Gouy and Faraday methods, diamagnetic corrections, magnetically non-dilute compounds-ferro, antiferro and ferri magnetic, spin cross-over systems, correlation of magnetic and structural properties.

UNIT-2:

Reaction Mechanisms of Transition Metal Complexes:

Energy profile of a reaction, inert and labile complexes, kinetics of octahedral substitution and mechanistic aspects, Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism and evidence in its favour. Anation reactions, Substitution reactions in square planar complexes, trans effect mechanisms of substitution. Electron transfer reaction-inner sphere and outer sphere reactions, complimentary and non-complimentary reactions.

Photochemistry of metal complexes-types of photochemical reactions, photo substitution and photoredox reactions and solar energy conversion.

Metal ions in biological systems: Essential and trace metals, active transport of cations(Na and K) ionophores, Metalloproteins as enzymes-carboxy peptidase, catalyses, peroxides, cytochrome P450, superoxide dismutase, copper oxidases, vitamin B_{12} coenzyme. Synthetic model compounds. Metals in medicine-metal deficiency (Fe, Mn, Cu and Zn), chelation therapy and metal complexes as drugs.

UNIT-3: Research work-1(to be given by concerned Guide) **12 hrs**

UNIT-4: Research work-2(to be given by concerned Guide) **12 hrs**

Department of Chemistry
Ph.D. Course work
Course –III- Field of Specialization - Organic Chemistry
-Revised Regulations [2015]

48 Hrs
[3Hrs/Week]

UNIT-I

12 Hrs

A. **Separation and Purification Techniques:**

Principle of:

1. Re crystallization : using various solvents and mixture of solvents
2. Fractional crystallization: e.g. Separation of naphthalene and diphenyl
3. Fractional distillation: e.g. Separation of Benzene, acetone, ethyl alcohol etc.
4. Steam distillation
5. Soxhlet Extraction

B. **Synthetic Organic Chemistry:**

1. Disconnection approach
2. Retrosynthesis
3. Protecting groups
4. Functional Group Inter conversions

C. **Biological and Pharmacological Screening of compounds**

Principle, material and methodology for the following activities:

1. Antimicrobial (Antibacterial, antifungal and antiviral)
2. Analgesic
3. Anti-inflammatory
4. Anthelmintic
5. Mechanism of action

UNIT-II

12 Hrs

A. **Oxidations and Reductions in Organic Synthesis**

Oxidation reactions involving – Chromium and manganese compounds, air, ozone, hydrogen peroxide, per acids, periodic acid, N-Bromo succinimide
Reduction reactions involving- Catalytic hydrogenation, Complex metal hydrides, dissolving metals.

B. **Reagents in Organic Synthesis**

1. Gilman reagent
2. Lithium diisopropyl amide (LDA)
3. Dicyclohexyl carbodiimide (DCC)
4. 1,3-Dithiane
(Reactivity umpolung)
5. Trimethyl silyl iodide
6. Tri-n-butyl hydride (TNBH)
7. DDQ
8. Woodward-Prevost hydroxylation

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9. Osmium tetroxide
10.Stannic chloride
11.Selenium dioxide
12.Phase transfer catalyst
13.Crown ether
14.Merrifield resin
15.Bakers yeast
16.Peterson synthesis

C. Stereochemistry

Topocity and prochirality
Asymmetric synthesis and asymmetric induction.
Double diastereoselection and double asymmetric induction.
Diastereoselection in cyclic systems
Enantioselective alkylation of ketones via hydrazones.

Specificity of enzymes towards D &L and E & Z isomers

UNIT-III

Substitution Reaction **12 hrs**

Nucleophilic substitution reactions: Introduction to nucleophiles, hard and soft nucleophiles. Nucleophilic substitution at saturated carbon - S_N1, S_N2 and S_Ni reactions and mechanisms. Factors affecting substitution reaction – substrate (neighbouring group participation and conjugation), nucleophile, leaving group, solvent, steric and strain effect on substitution and ionization rates.

Reactivity of benzylic, allylic, vinylic and aryl halides. Mitsunobu reaction. Nucleophilic substitution on epoxides, esters and ethers. Introduction to nitrogen and sulphur nucleophiles in S_N2 reactions.

Nucleophilic substitution at aromatic compounds: Addition-elimination mechanism, nucleophilic substitution via aryne intermediate, nucleophilic substitution by unimolecular mechanism, preparation of aryl halides through radical mechanism. Nucleophilic substitution by rearrangements.

Electrophilic substitution reactions: General mechanism in aromatic electrophilic substitution reaction, nitration, halogenations, sulphonation, Friedal Craft alkylation and acylation. Orientation effect of substituents, theory of reactivity and orientation, ortho-para ratio, competition between substituents for third group. Side chain reactions of benzene derivatives.

UNIT-IV

12hrs

Electro-organic Chemistry

General introduction, Electro-synthesis: anodic oxidation reactions, cathodic reduction reactions, Electrochemical fluorination, Kolbe oxidation, Non-Kolbe oxidation, Shono Oxidation, Marko-Lam Reduction, Tafel rearrangement.

Electrosyntheis using hydrophobic electrode, natural product synthesis using anodic oxidation, indirect electro-synthesis using mediator, electro-synthesis of conducting polymers, Electro-polymerization of pyrrole.

Industrial Electro-synthesis: electro-synthesis of adiponitrile, electrochemical perfluorination, synthesis of 3, 6-dichloropicolic acid and β-lactam derivative.

Department of Chemistry
Ph.D. Course work
Course-III: Field of Specialization –Physical Chemistry

48 hrs

UNIT-I: ELECTROANALYTICAL TECHNIQUES

12 hrs

Introduction, electrochemical cells, faradic and non-faradic current, mass transfer in cells, galvanic and electrolytic cells, anodes and cathodes, liquid junction potential, schematic representation of cells.

Polarography: Theory, principle and applications classical polarography, dropping mercury electrode, polarogram, polarographic measurements, polarographic current, Ilkovic equation, current and concentration relationship, half wave potential, oxygen interference- advantages and limitations. Qualitative and quantitative analysis. Derivative polarography.

Amperometry, Coulometry at controlled potential and at constant current. Cyclic voltammetry-basic principles, instrumentation and applications.

Electrogravimetry-theory, electrode reactions, over-voltage, characteristics of a good deposit, completeness of deposition, separation of metals at controlled cathode potential. Determination of copper and nickel in Cu-Ni alloy.

UNII-II: Nanomaterials:

12 hrs

Introduction: Fundamentals and importance, Metal nanoclusters, magic numbers, theoretical modeling of nano particles, Geometric structure, electronic structure, reactivity, fluctuations, magnetic clusters, Bulk to nano transitions. Semi conducting nanoparticles- optical properties, photofragmentation, coulombic explosion.

Carbon nano particles: Introduction, Carbon molecules, Nature of the carbon bond, New carbon structures. Carbon clusters: small carbon clusters, C_{60}; Discovery , structure, crystal, alkali doping , super conductivity, Fullerens, other Bulkyballs. Carbon nano-tubes: Fabrication, structure, electrical properties, vibrational properties, mechanical properties, application of nano materials.

Methods of preparation: Plasma arcing, chemical vapour deposition, sol-gel, silica-gel, hydrolysis, Condensation and polymerization of monomers to form particles, Electrodeposition, ball milling, Chemical methods, Thermolysis, Pulsed laser methods.

UNIT-III : Research Work – 1. **(to be given by concerned Guide)** **12 hrs**

UNIT-IV : Research Work – 2. **(to be given by concerned Guide)** **12 hrs**

Department of Chemistry
Ph.D. Course work
Title: Field of Specialization-Analytical Chemistry

48 hrs (3 Hrs/week)

UNIT-1 **12 hrs**

Thermal Methods Of Analysis (TGA): Types of thermo gravimetric analysis, Principles. Factors affecting the results - heating rate, furnace, instrument control /data handling. Applications - purity and thermal stability, evaluation of correct drying temperature, analysis of complex mixture and determination of kinetic parameters of thermal degradation.

Differential Thermal Analysis (DTA): Theory – Variables affecting the DTA curves. Differences between TGA and DTA. General principles, Instrumentation. Applications – analysis of the physical mixture and thermal behavior study. Determination of melting point, boiling point and decomposition point.

Differential Scanning Calorimetry (DSC): Basic principles. Differences between DTA and DSC. Instrumentation – power compensated DSC, Heat flux DSC. Applications - Studies of thermal transitions and isothermal crystallization. Pharmaceutical industry for testing the purity of the samples.

Thermo mechanical analysis. Dynamic mechanical analysis.

UNIT-2 **12 hrs**

Chromatographic Methods of Analysis:

Gas-liquid chromatography and Gas-solid chromatography: Principles, Instrumentation and applications.

High performance liquid chromatography (HPLC): Principle, Instrumentation-columns (analytical and guard columns). Stationary phases, choosing a mobile phase. isocratic vs. gradient elution, HPLC plumbing, sample introduction. Detectors for HPLC. Spectroscopic, electrochemical and other quantitative applications.

Supercritical fluid chromatography (SFC): Properties of supercritical fluids, instrumentation and operating variables, comparisons of SFC with other types of chromatography, applications.

Supercritical fluid extraction: Advantages of supercritical fluid extraction Instrumentation. Supercritical fluid choice, off-line and on-line extractions, typical applications of supercritical fluid extraction.

Principle and applications of HPTLC: (High performance thin layer chromatography) UPLC (Ultrafast performance liquid Chromatography) GC-MS, LC-MS and LC-NMR.

UNIT-3: Research work-1 (to be given by concerned Guide) **12 hrs**

UNIT-4: Research work-2 (to be given by concerned Guide) **12 hrs**

Course IV : Research and publication Ethics 02hr/week.

ANNEXURE

Course Title:

- **Research and Publication Ethics (RPE)**-Course for awareness about the publication ethics and publication misconducts.

Course Level:

- 2 Credit course (30 hrs.)

Eligibility:

- M.Phil., Ph.D. students and interested faculty members (It will be made available to post graduate students at later date)

Fees:

- As per University Rules

Faculty:

- Interdisciplinary Studies

Qualifications of faculty members of the course:

- Ph.D. in relevant subject areas having more than 10 years' of teaching experience

About the course

Course Code: CPE- RPE

Overview

- This course has total 6 units focusing on basics of philosophy of science and ethics. research integrity, publication ethics. Hands-on-sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.) and plagiarism tools will be introduced in this course.

Pedagogy:

- Class room teaching, guest lectures, group discussions, and practical sessions.

Evaluation

- Continuous assessment will be done through tutorials, assignments, quizzes, and group discussions. Weightage will be given for active participation. Final written examination will be conducted at the end of the course.

Course structure

- The course comprises of six modules listed in table below. Each module has 4-5 units.

		Teaching hours
Theory		
RPE 01	Philosophy and Ethics	4
RPE 02	Scientific Conduct	4
RPE 03	Publication Ethics	7
Practice		
RPE 04	Open Access Publishing	4
RPE 05	Publication Misconduct	4
RPE 06	Databases and Research Metrics	7
	Total	**30**

Syllabus in detail

THEORY

- **RPE 01: PHILOSOPHY AND ETHICS (3 hrs.)**

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgements and reactions

- **RPE 02: SCIENTIFICCONDUCT (5hrs.)**

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data

- **RPE 03: PUBLICATION ETHICS (7 hrs.)**

1. Publication ethics: definition, introduction and importance
2. Best practices / standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
5. Violation of publication ethics, authorship and contributorship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

PRACTICE

- **RPE 04: OPEN ACCESS PUBLISHING(4 hrs.)**

1. Open access publications and initiatives

I.B.B. 15/1/2020

15/02/2020

15/02/2020

2. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

- **RPE 05: PUBLICATION MISCONDUCT (4hrs.)**

A. Group Discussions (2 hrs.)

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools (2 hrs.)

Use of plagiarism software like Turnitin, Urkund and other open source software tools

- **RPE 06: DATABASES AND RESEARCH METRICS (7hrs.)**

A. Databases (4 hrs.)

1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs.)

1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
2. Metrics: h-index, g index, i10 index, altmetrics

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REGISTRAR
SAVITRIBAI PHULE PUNE UNIVERSITY

15/02/2020

ज्ञान-विज्ञान विमुक्तये

प्रो. रजनीश जैन
सचिव

Prof. Rajnish Jain
Secretary

सत्यमेव जयते

विश्वविद्यालय अनुदान आयोग
University Grants Commission
(मानव संसाधन विकास मंत्रालय, भारत सरकार)
(Ministry of Human Resource Development, Govt. of India)
बहादुरशाह जफ़र मार्ग, नई दिल्ली-110002
Bahadur Shah Zafar Marg, New Delhi-110002
Ph :. 011-23236288/23239337
Fax : 011-2323 8858
E-mail : secy.ugc@nic.in

D.O.No.F.1-1/2018(Journal/CARE)

December, 2019

Respected Sir/Madam,

University Grants Commission in its 543rd meeting held on 9th August, 2019 approved two Credit Courses for awareness about publication ethics and publication misconducts entitled **"Research and Publication Ethics (RPE)"** to be made compulsory for all Ph.D. students for pre-registration course work (**attached as Annexure**).

In view of the above, you are requested to ensure that the above two Credit courses may be made compulsory for all Ph.D. students for pre-registration course work undertaken in your University from the forthcoming academic session.

With regards,

Yours sincerely,

(Rajnish Jain)

TO THE VICE-CHANCELLORS OF ALL UNIVERSITIES

ANNEXURE

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15/1/2020