

## **FOREWORD**

I am happy to present the revised curricula and syllabi of the following four M.Phil Chemistry courses of the School of Chemical Sciences (with effect from 2016 admission onwards) for favour of approval by the Faculty and Academic Council of the University.

1. M.Phil Chemistry (Inorganic Chemistry)
2. M.Phil Chemistry (Organic Chemistry)
3. M.Phil Chemistry (Physical Chemistry)
4. M.Phil Chemistry (Polymer Chemistry)

The BOS prepared draft proposals of revised curricula and syllabi for all the four M.Phil courses in Chemistry in conformity with the Revised CSS Regulations by the Mahatma Gandhi University to suit the Credit and Semester System. The draft curricula and syllabi for all the programmes were discussed in a very effective manner in the Board of Studies of the School of Chemical Sciences. The BOS feels that appreciable updating could be done in keeping with the current developments and trends in Chemistry education.

Prof. Suresh Mathew  
Chairman, Board of Studies of the School of Chemical Sciences

### **Members of the Board of Studies of School of Chemical Sciences**

1. Prof. Suresh Mathew (Chairman)
2. Prof. Sabu Thomas
3. Prof. A.S.Padmanabhan
4. Prof. Beena Mathew
5. Prof. K.S.Devaky
6. Dr. K. Pius
7. Prof. M.R. Prathapachandra Kurup
8. Dr. P.K. Radhakrishnan
9. Prof. K..K.Aravindakshan

## **MAHATMA GANDHI UNIVERSITY SCHOOL OF CHEMICAL SCIENCES**

|                                |   |
|--------------------------------|---|
| <b>PROGRAMME</b>               | <b>M.Phil Chemistry (Inorganic Chemistry)</b>       |
| <b>DURATION</b>                | <b>One Year (2016 Admission Onwards)</b>            |
| <b>Total credits required:</b> | <b>40 (for 2 semesters) [Core: 34; Elective: 6]</b> |

\* The student has to choose **three elective courses** for semester II

### SEMESTER I

| Course Code                | Course Title                           | Hours/Week |   |   | Credit |
|----------------------------|--|------------|---|---|--------|
|                            |  | L          | T | P |        |
| <b><u>Core Courses</u></b> |  |            |   |   |        |
| SCSPDIC1601                | Coordination Chemistry                 | 2          | 2 | - | 3      |
| SCSPDIC1602                | Organic Synthesis                      | 2          | 2 | - | 3      |
| SCSPDIC1603                | Computational Methods in Chemistry     | 2          | 2 | - | 3      |
| SCSPDIC1604                | Polymer Synthesis and Characterization | 2          | 2 | - | 3      |
| SCSPDIC1605                | Research Methodology                   | 4          | - | - | 4      |

### SEMESTER II

| Course Code                | Course Title            | Hours/Week |   |   | Credit |
|----------------------------|-------------------------|------------|---|---|--------|
|                            |                         | L          | T | P |        |
| <b><u>Core Courses</u></b> |                         |            |   |   |        |
| SCSPDIIC1606               | Research Project        | -          | - | - | 12     |
| SCSPDIIC1607               | Project Seminar         | -          | - | - | 3      |
| SCSPDIIC1608               | Comprehensive Viva-Voce | -          | - | - | 3      |

### **\*Elective Courses**

|             |                                    |   |   |   |   |
|-------------|------------------------------------|---|---|---|---|
| SCSPDIE1610 | Organometallics                    | 2 | - | - | 2 |
| SCSPDIE1611 | Chemistry of Materials             | 2 | - | - | 2 |
| SCSPDIE1612 | Asymmetric Catalysis               | 2 | - | - | 2 |
| SCSPDIE1613 | Supramolecular Chemistry           | 2 | - | - | 2 |
| SCSPDIE1614 | Environmental Chemistry            | 2 | - | - | 2 |
| SCSPDIE1615 | Computational Quantum Chemistry    | 2 | - | - | 2 |
| SCSPDIE1616 | Biopolymers                        | 2 | - | - | 2 |
| SCSPDIE1617 | Spectroscopic Methods in Chemistry | 2 | - | - | 2 |
| SCSPDIE1618 | Polymer Physics                    | 2 | - | - | 2 |

MAHATMA GANDHI UNIVERSITY  
SCHOOL OF CHEMICAL SCIENCES

PROGRAMME                    M.Phil **Chemistry** (Organic Chemistry)  
DURATION                    One Year (2016 Admission Onwards)  
Total credits required:      40 (for 2 semesters) [Core: 34; Elective: 6]

\* The student has to choose **three elective courses** for semester II

**SEMESTER I**

| Course Code                | Course Title                           | Hours/Week |   |   | Credit |
|----------------------------|--|------------|---|---|--------|
|                            |  | L          | T | P |        |
| <b><u>Core Courses</u></b> |  |            |   |   |        |
| SCSPDIC1601                | Coordination Chemistry                 | 2          | 2 | - | 3      |
| SCSPDIC1602                | Organic Synthesis                      | 2          | 2 | - | 3      |
| SCSPDIC1603                | Computational Methods in Chemistry     | 2          | 2 | - | 3      |
| SCSPDIC1604                | Polymer Synthesis and Characterization | 2          | 2 | - | 3      |
| SCSPDIC1605                | Research Methodology                   | 4          | - | - | 4      |

**SEMESTER II**

| Course Code                | Course Title            | Hours/Week |   |   | Credit |
|----------------------------|-------------------------|------------|---|---|--------|
|                            |                         | L          | T | P |        |
| <b><u>Core Courses</u></b> |                         |            |   |   |        |
| SCSPDIIC1606               | Research Project        | -          | - | - | 12     |
| SCSPDIIC1607               | Project Seminar         | -          | - | - | 3      |
| SCSPDIIC1608               | Comprehensive Viva-Voce | -          | - | - | 3      |

| <b><u>*Elective Courses</u></b> |                                    |   |   |   |   |
|---------------------------------|------------------------------------|---|---|---|---|
| SCSPDIE1610                     | Organometallics                    | 2 | - | - | 2 |
| SCSPDIE1611                     | Chemistry of Materials             | 2 | - | - | 2 |
| SCSPDIE1612                     | Asymmetric Catalysis               | 2 | - | - | 2 |
| SCSPDIE1613                     | Supramolecular Chemistry           | 2 | - | - | 2 |
| SCSPDIE1614                     | Environmental Chemistry            | 2 | - | - | 2 |
| SCSPDIE1615                     | Computational Quantum Chemistry    | 2 | - | - | 2 |
| SCSPDIE1616                     | Biopolymers                        | 2 | - | - | 2 |
| SCSPDIE1617                     | Spectroscopic Methods in Chemistry | 2 | - | - | 2 |
| SCSPDIE1618                     | Polymer Physics                    | 2 | - | - | 2 |

MAHATMA GANDHI UNIVERSITY  
SCHOOL OF CHEMICAL SCIENCES

PROGRAMME                    M.Phil **Chemistry** (Physical Chemistry)  
DURATION                    One Year (2016 Admission Onwards)  
Total credits required:     40 (for 2 semesters) [Core: 34; Elective: 6]

\* The student has to choose **three elective courses** for semester II

**SEMESTER I**

| Course Code                | Course Title                           | Hours/Week |   |   | Credit |
|----------------------------|--|------------|---|---|--------|
|                            |  | L          | T | P |        |
| <b><u>Core Courses</u></b> |  |            |   |   |        |
| SCSPDIC1601                | Coordination Chemistry                 | 2          | 2 | - | 3      |
| SCSPDIC1602                | Organic Synthesis                      | 2          | 2 | - | 3      |
| SCSPDIC1603                | Computational Methods in Chemistry     | 2          | 2 | - | 3      |
| SCSPDIC1604                | Polymer Synthesis and Characterization | 2          | 2 | - | 3      |
| SCSPDIC1605                | Research Methodology                   | 4          | - | - | 4      |

**SEMESTER II**

| Course Code                | Course Title            | Hours/Week |   |   | Credit |
|----------------------------|-------------------------|------------|---|---|--------|
|                            |                         | L          | T | P |        |
| <b><u>Core Courses</u></b> |                         |            |   |   |        |
| SCSPDIIC1606               | Research Project        | -          | - | - | 12     |
| SCSPDIIC1607               | Project Seminar         | -          | - | - | 3      |
| SCSPDIIC1608               | Comprehensive Viva-Voce | -          | - | - | 3      |

| <b><u>*Elective Courses</u></b> |                                    |   |   |   |   |
|---------------------------------|------------------------------------|---|---|---|---|
| SCSPDIE1610                     | Organometallics                    | 2 | - | - | 2 |
| SCSPDIE1611                     | Chemistry of Materials             | 2 | - | - | 2 |
| SCSPDIE1612                     | Asymmetric Catalysis               | 2 | - | - | 2 |
| SCSPDIE1613                     | Supramolecular Chemistry           | 2 | - | - | 2 |
| SCSPDIE1614                     | Environmental Chemistry            | 2 | - | - | 2 |
| SCSPDIE1615                     | Computational Quantum Chemistry    | 2 | - | - | 2 |
| SCSPDIE1616                     | Biopolymers                        | 2 | - | - | 2 |
| SCSPDIE1617                     | Spectroscopic Methods in Chemistry | 2 | - | - | 2 |
| SCSPDIE1618                     | Polymer Physics                    | 2 | - | - | 2 |

MAHATMA GANDHI UNIVERSITY  
SCHOOL OF CHEMICAL SCIENCES

PROGRAMME                    M.Phil **Chemistry** (Polymer Chemistry)  
DURATION                    One Year (2016 Admission Onwards)  
Total credits required :    40 (for 2 semesters) [Core: 34; Elective: 6]

\* The student has to choose **three elective courses** for semester II

**SEMESTER I**

| Course Code                | Course Title                           | Hours/Week |   |   | Credit |
|----------------------------|--|------------|---|---|--------|
|                            |  | L          | T | P |        |
| <b><u>Core Courses</u></b> |  |            |   |   |        |
| SCSPDIC1601                | Coordination Chemistry                 | 2          | 2 | - | 3      |
| SCSPDIC1602                | Organic Synthesis                      | 2          | 2 | - | 3      |
| SCSPDIC1603                | Computational Methods in Chemistry     | 2          | 2 | - | 3      |
| SCSPDIC1604                | Polymer Synthesis and Characterization | 2          | 2 | - | 3      |
| SCSPDIC1605                | Research Methodology                   | 4          | - | - | 4      |

**SEMESTER II**

| Course Code                | Course Title            | Hours/Week |   |   | Credit |
|----------------------------|-------------------------|------------|---|---|--------|
|                            |                         | L          | T | P |        |
| <b><u>Core Courses</u></b> |                         |            |   |   |        |
| SCSPDIIC1606               | Research Project        | -          | - | - | 12     |
| SCSPDIIC1607               | Project Seminar         | -          | - | - | 3      |
| SCSPDIIC1608               | Comprehensive Viva-Voce | -          | - | - | 3      |

| <b><u>*Elective Courses</u></b> |                                    |   |   |   |   |
|---------------------------------|------------------------------------|---|---|---|---|
| SCSPDIE1610                     | Organometallics                    | 2 | - | - | 2 |
| SCSPDIE1611                     | Chemistry of Materials             | 2 | - | - | 2 |
| SCSPDIE1612                     | Asymmetric Catalysis               | 2 | - | - | 2 |
| SCSPDIE1613                     | Supramolecular Chemistry           | 2 | - | - | 2 |
| SCSPDIE1614                     | Environmental Chemistry            | 2 | - | - | 2 |
| SCSPDIE1615                     | Computational Quantum Chemistry    | 2 | - | - | 2 |
| SCSPDIE1616                     | Biopolymers                        | 2 | - | - | 2 |
| SCSPDIE1617                     | Spectroscopic Methods in Chemistry | 2 | - | - | 2 |
| SCSPDIE1618                     | Polymer Physics                    | 2 | - | - | 2 |

## SCSPDIC1601 COORDINATION CHEMISTRY

**Credit: 3**

**Contact Hours: 4**

Crystal Field Theory(CFT) of bonding in complexes-its merits and demerits, evidences of covalency in metal ligand bond, Ligand Field Theory(LFT), Molecular Orbital Theory(MOT)-MO energy level diagram for octahedral complexes without and with  $\pi$ -bonding, two-dimensional spectrochemical series.

Electronic spectra of complexes: d-d transition and charge transfer transition, selection rules for electronic transition, effect of spin-orbit coupling and vibronic coupling on electronic transition, Orgel and Tanabe Sugano diagrams.

Magnetic studies of complexes: thermal population of different energy levels-large and small multiplet widths, orbital contribution to magnetic moment, antiferromagnetism, Temperature Independent Paramagnetism(TIP), Spin State Cross Overs.

Coordination chemistry of lanthanides: factors limiting the formation of lanthanide complexes, coordination numbers and geometries, electronic spectra, covalency parameters, hypersensitive transitions, magnetic properties, bonding in lanthanide complexes.

Coordination chemistry of actinides: comparison of electronic structures of actinide with those of lanthanides, stereochemistry, absorption spectra and magnetic properties. A comparative account of the complexes of lanthanides and actinides.

Applications of the following physico-chemical methods in the structural elucidation of complexes.

1. Vibrational, electronic and ESR spectra
2. Magnetic studies
3. Thermal (TG, DTG, DTA) studies
4. Single crystal XRD studies

### References

01. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 3<sup>rd</sup>Edn., Wiley, 1972.
02. J.E. Huheey, R.A. Keiter, R.L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, 4<sup>th</sup> Edn., Prentice Hall, 1997.
03. T. Moeller, International Reviews of Sciences, Inorganic Chemistry, Series-I, Vol.VII, Butterworth, 1972.
04. K. Nakamoto, Infrared and Raman spectroscopy of Inorganic and Coordination Compounds, 6<sup>th</sup> Edn., John Wiley & Sons, 2008.
05. R.S. Drago, Physical Methods in Chemistry, 2<sup>nd</sup> Edn., Saunders College, 1992.
06. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.
07. W.W. Wendlandt, Thermal Analysis, Elsevier, 1981.
08. E.A.V. Ebsworth, D.W.H. Rankin, S. Craddock, Structural Methods in Inorganic Chemistry, 2<sup>nd</sup> Edn., CRS Press, 1991.

## SCSPDIC1602 ORGANIC SYNTHESIS

**Credit: 3**

**Contact Hours: 4**

Retrosynthesis: general survey of organic reactions, comparison and selection of appropriate reactions-designing synthesis. Retrosynthetic analysis, disconnection approach-one group, two group and illogical disconnections. Functional group interconversion, protection of functional groups, synthetic equivalent groups, multistep synthesis, convergent synthesis, formation of C-C bonds, carbon-heteroatom bonds, ring closure and ring opening reactions, retro syntheses of aromatic heterocycles.

Synthesis of natural products: chemistry of alkaloids, terpenes, steroids, prostaglandins, vitamins, plant hormones, insect pheromones, germination stimulants and insect control agents. Synthesis of strychnine, epimyrine, epibatidine, juvabione, longifolene, taxol, ephedrine, cholesterol, lanosterol, prostaglandin E, vitamin A, gibberellic acid, grandisol, strigol, orobanchol and pyrethrins.

Synthetic methods: macrolactonization, metathesis-Pd catalyzed coupling reactions in organic synthesis, N-heterocyclic carbenes in catalysis, asymmetric conjugate addition, chiral dienes in synthesis, chiral dienes in catalysis.

Drug Synthesis: basic principles, IC<sub>50</sub>, LogP, LogD, MIC, efficacy, adsorption, distribution, metabolism and excretion, stages in drug discovery, natural and synthetic drugs. Synthesis of the following drugs: antiviral drug-Tamiflu, antibacterial drugs (Cipro or Zyxon),  $\beta$ -lactam antibiotics, penicillins, quinolones and fluoroquinolones, opium analgesics, cimetidine, antiinflammatory drugs (Celebrex), non steroid anti inflammatory drugs (Ibuprofen and Naproxen), ATPase inhibitor, esomeprazole, cardiovascular drugs, statin drugs, atorvastatin, sulfonamides, central nervous system (CNS) drugs.

### References

01. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry, 5<sup>th</sup> Edn., Springer, 2007.
02. S. Warren, Organic Synthesis: The Disconnection Approach, John Wiley, 1984.
03. S.V. Bhat, B.A. Nagasampagi, M. Sivakumar, Chemistry of Natural Products, Springer, 2005.
04. J. Tsuji, Palladium in Organic Synthesis, Springer, 2005.
05. G. Thomas, Fundamentals of Medicinal Chemistry, John Wiley & Sons, 2003
06. A. Kar, Medicinal Chemistry, 3<sup>rd</sup> Edn., New Age International, 2005

## SCSPDIC1603 COMPUTATIONAL METHODS IN CHEMISTRY

**Credit: 3**

**Contact Hours: 4**

Introduction to programming languages, C programming language, variables, logical variables, loops-for loop and while loop, arrays, pointers, structures, recursion.

Numerical analysis: polynomial equations, equations of fifth degree or greater polynomials, Newton Raphston method of iteration, finding the inverse and determinant of a square matrix, numerical solution of differential equations.

Non numerical algorithms: towers of Hanoi, search methods such as binary search, sorting methods such as heap sort and merge sort.

Application of programming, principles to numerical and non numerical algorithms: factorial,  $\sin(x)$ ,  $\cos(x)$ ,  $\log(x)$ ,  $\tan(x)$ , estimation of determinant of a square matrix, inverse of a square matrix, solution of simultaneous equations using Krammer's rule, method of least squares, Newton Raphston method of the solution of equations, towers of Hanoi, binary search.

Stochastic programming, Monte Carlo methods, random number generators.

### References

01. B.W. Kernigan, D.M. Ritchie, The C Programming Language(ANSI C), 2<sup>nd</sup> Edn., Prentice Hall, 1988.
02. E. Kreyszig, Advanced Engineering Mathematics, 10<sup>th</sup> Edn., John Wiley and Sons, 2011.



## SCSPDIC1604 POLYMER SYNTHESIS AND CHARACTERIZATION

**Credit: 3**

**Contact Hours: 4**

Polymer synthesis:, Introduction to polymerization techniques: bulk, solution, suspension and emulsion polymerizations, melt and solution poly condensation, interfacial condensation, addition and condensation polymerization, co-ordination polymerization, polymerization initiated by metal catalysts, Ziegler-Natta polymerization, free radical ring opening polymerization, polymerization of cyclic organic molecules such as cyclic ethers, lactones, lactams, cycloalkenes etc, ring opening metathesis polymerization (ROMP), ADMET polymerization, controlled radical polymerization (ATRP, RAFT & NMP), group transfer polymerization (GTP) and aldol group transfer polymerization, photolytic polymerization, radiation polymerization, electrolytic polymerization and plasma polymerization. Reactions of synthetic polymers: side chain and main chain modifications.

Polymer characterization: Determination of molecular weights by various methods such as End group analysis, Viscometry, Osmometry, Gel Permeation Chromatography (GPC), Light scattering method, ultracentrifugation etc. Applications of following techniques to polymers. UV-visible spectroscopy, IR and Raman spectroscopy, NMR (proton & carbon) spectroscopy, Solid state NMR of polymers, tacticity studies, sequence determination of polymers by NMR. MALDI-TOF. Microscopy, optical diffraction, diachronic. Birefringence dielectric properties. Details of techniques such as SEM, TEM, AFM, etc. X-ray diffraction analysis. Introduction, instrumentation and applications of Thermal analysis such as TGA, DTA/DSC, TMA. Mechanical testing: tensile strength, elongation, modulus, flexural, impact strength and hardness

### References.

1. H.R. Alcock, F.W. Lampe, J.E. Mark, Contemporary Polymer Chemistry, 3rd Edn., Prentice Hall, 2003.
2. J.M.G. Cowie, V. Arighi, Polymers: Chemistry and Physics of Modern Materials, 3<sup>rd</sup> Edn., CRC Press, 2008.
3. R.P. Brown, Handbook of Plastics Test Methods, 3rd Edn., Longman, 1988.
4. M. Chanda, S.K. Roy, Plastic Technology Handbook, 4th Edn., Taylor and Francis, 2006.
5. J.R. Fried, Polymer Science and Technology, 2nd Edn., Prentice Hall, 2003.

## SCSPDIC1605 RESEARCH METHODOLOGY

Credit: 4

Contact Hours: 4

### Unit I

Research methods: identification of a problem, determination of the mode of attack, literature survey, mode of approach of actual investigation, abstraction of the research paper, drawing influences from data, qualitative and quantitative analysis, internet and its applications, e-journals, assessing the status of the problem, results and conclusions, presenting a scientific seminar, publication of research paper, art of writing a thesis.

### Unit II

Survey of literature including patents: chemical nomenclature, primary and secondary sources including reviews, treatise and monographs, literature searching, review of work relevant to the chosen problem.

### Unit III

Hypothesis: characteristics of a good hypothesis. Methods and design of the research-different types of variables and research methods. Sampling-characterization of a good sample, sample errors and ways to reduce them. Collection, analysis and interpretation of data- procedure of data collection, scoring of data, tabulation, editing and analysis.

### Unit IV

Writing a thesis or paper: general information, page and chapter formation, the use of quotation, footnotes, tables and figures, referencing, appendixes, revision of a paper or thesis-editing and evaluating the final product, proof reading, final typed copy.

### Unit V

Probability: embedding discrete probability spaces into the real line especially the  $[0,1]$  interval. Stochastic Process: (a) process with independent variables, (b) Markov process, (c) Martingales, (d) Brownian Motion

### Unit VI

Data Analysis: errors in chemical analysis, classification of errors, determination of accuracy of methods, improving accuracy of analysis, significant figures, mean and standard deviation, comparison of results: "t" test, "f" test and "chi" square test, rejection of results, presentation of data. Sampling: theory and techniques of sampling, statistical criteria of good sampling and required size, stratified sampling vs random sampling, minimization of variance in stratified sampling, transmission and storage of samples.

## References

01. C.R. Kothari, Research Methodology, 2nd Edn., New Age International, 2004.
02. N. Moore, How to do Research: The Practical Guide to Designing and Managing Research Projects, 3rd Edn., Facet Publishing, 2006.
03. J. Anderson, Assignment and Thesis Writing, 4th Edn., John Wiley and Sons, 2002.
04. P. Billingsley, Probability and Measures, 3rd Edn., Wiley Interscience, 1995.
05. S. Karlin, H.M. Taylor, A First Course in Stochastic Processes, 2nd Edn., Academic Press, 1975.
06. N. Madras, G. Slade, The Self Avoiding Walk, Birkhauser, 1991.
07. G.F. Lawler, Intersection of Random Walks, G.F. Lawler, Birkhauser, 1996.
08. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, Brooks Cole, 2003.

## **SCSPDIIC1607 RESEARCH PROJECT**

### **Credit: 12**

The candidate has to do a project of original research on a relevant topic under the guidance of a Supervising Teacher of the School of Chemical Sciences during the second semester and submit the dissertation at the end of the second semester.

The dissertation shall be evaluated both by the Internal Examiner (Supervising Teacher) and the External Examiner. The content, literature survey, subject grasp and current interest will be considered for evaluation.

## **SCSPDIIC1608 PROJECT SEMINAR**

**Credit: 3**

The candidate shall give a seminar (30 minutes) on the research project submitted as per course SCS 631 Research Project. This follows discussion with the Examination Board consisting of the Chairman, the Internal Examiner and the External Examiner.

## **SCSPDIIC1609 COMPREHENSIVE VIVA-VOCE**

### **Credit: 3**

The comprehensive viva-voce shall be conducted by the Examination Board consisting of the Chairman, the Internal Examiner and the External Examiner.

Thorough understanding of all the M.Phil. level course contents and recent trends in the broad area of chemical sciences are evaluated. If candidate's performance is found unsatisfactory, he/she has to reappear for the viva-voce.

## SCSPDIE1610 ORGANOMETALLICS

**Credit: 2**

**Contact Hours: 2**

Nomenclature of organometallic compounds, classification, hapticity and electron contribution of ligands,  $\eta^1$ ,  $\eta^2$ ,  $\eta^3$ ,  $\eta^4$ ,  $\eta^5$  and  $\eta^6$ -type hapticities,  $\mu$ -type organic ligands, 18- and 16-electron rules, structure prediction through electron counts. Metal carbonyls, terminally bound and bridging type metal carbonyls and its distinction by IR spectra, polynuclear carbonyls. Structure and bonding in metal nitrosyls, metal cyanides and metal phosphines.

Organometallic compounds containing metal-metal bonds and metal clusters, metal-metal multiple bonds with  $\sigma$ -,  $\pi$ - and  $\delta$ -type of bonds. Structure and bonding in metal-olefins, metal-acetylenes, metal-allyls, metal-carbenes, metal-carbynes, metal-polyenes, metal-cyclooctatetraenes, metal-norbornadiene. Donor and acceptor properties of the ligands in the above compounds. A-frame complexes and their special features.

Fragment molecular orbitals (FMO) of various organic and inorganic moieties/fragments: IFMO's of  $C_3H_5$ ,  $C_4H_4$ ,  $C_4H_6$ ,  $C_5H_5$ ,  $C_6H_6$ ,  $C_8H_8$ ,  $ML_5$ ,  $ML_4$ ,  $ML_3$  type fragments. Isolobal concept, isolobal relationships between organic and inorganic ( $ML_n$ ) fragments. Structure and bonding in metallocenes, half-sandwich compounds,  $ML_n$ -cyclobutadiene and  $ML_n$ -carbenes based on FMOs and MO diagrams.

Stereochemical non-rigidity and fluxional nature of organometallic compounds, characterization of different types of fluxional nature by variable temperature NMR spectroscopy. Reactions involving various organometallic compounds-oxidative addition reactions and reductive elimination reactions, migratory insertion reactions, CO and alkene insertion reactions, 1,1- and 1,2-insertion,  $\beta$ -hydride elimination reactions, cyclometallation reactions.

Alkene hydrogenation (Wilkinson's catalyst), water-gas shift reaction, hydroformylation reactions, catalytic addition of molecular oxygen to alkenes (Wacker process), synthetic gasoline, Ziegler-Natta polymerization of alkenes, Fischer-Tropsch process, alkene metathesis, oligomerisation of alkynes, metallacycles, ortho-metallation, Suzuki coupling.

Organometallics in industry, medicine, agriculture and environmental science.

### References

01. J.E. Huheey, R.A. Keiter, R.L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, 4<sup>th</sup> Edn., Prentice Hall, 1997.
02. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6<sup>th</sup> Edn., Wiley-Interscience, 1999.
03. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver and Atkins Inorganic Chemistry, 4<sup>th</sup> Edn., Oxford University Press, 2006.
04. J.D. Atwood, Inorganic and Organometallic Reaction Mechanism, 2<sup>nd</sup> Edn., Wiley-VCH, 1997.
05. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> Edn., Wiley-India, 2007.
06. J.P. Collman, L.G. Hegedus, J.R. Norton, R.G. Finke, Principles and Applications of Organotransition Metal Chemistry, 2<sup>nd</sup> Edn., University Science Books, 1987.

## SCSPDIE1611 CHEMISTRY OF MATERIALS

**Credit: 2**

**Contact Hours: 2**

Materials: classification, synthesis and characterization of materials, formation of bulk materials-direct synthesis methods, solution methods, chemical deposition methods.

High-Tc oxide superconductors: structural features of cuprate superconductors, type I and type II superconductors, mechanism of superconductivity in cuprates, applications of high Tc cuprates.

Colossal magneto-resistance, rechargeable battery materials, oxide glasses-formation, composition, production and applications.

Metal Oxides, nitrides and fluorides, chalcogenides, intercalation compounds and metal rich phases, frame work structures.

Hydrides and hydrogen-storage materials: metal hydrides, magnesium-based metal hydrides.

Semiconductor materials: inorganic pigments-coloured solid materials, white and black pigments, Photocatalysis of nanotitania and hydrides.

Molecular materials and fullerides: one-dimensional metals, molecular magnets, inorganic liquid crystals, fullerides, Structure of grapheme. Materials property at the nanoscale, ferrofluids synthesis, properties and applications.

### References

01. A.R. West, Solid State Chemistry and its Applications, John-Wiley, 1984.
02. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5<sup>th</sup> Edn., Oxford University Press, 2010.
03. C.N. R. Rao, J. Gopalakrishnan, New Directions in Solid State Chemistry, 2<sup>nd</sup> Edn., Cambridge University Press, 2004.
04. R.C. Buchanan, T. Park, Materials Crystal Chemistry, Marcel Dekker, 1997.
05. J.I. Gersten, F.W. Smith, The Physics and Chemistry of Materials, Wiley-Interscience, 2001.
06. Y. Gogotsi, Nanomaterials Handbook, CRC Press, 2006.
07. Odenbach S. (Ed). Ferrofluids: Magnetically Controllable Fluids and Their Applications, Springer Verlag, 2002.
08. Harry R Allcock, Introduction to Materials Chemistry, Wiley 1<sup>st</sup> Edn. 2008

## SCSPDIE1612 ASYMMETRIC CATALYSIS

**Credit: 2**

**Contact Hours: 2**

Asymmetric hydrogenation: ligand design for catalytic hydrogenation, enantioselective hydrogenation of prochiral olefins, asymmetric reduction of ketones using chiral organometallic compounds, asymmetric reduction of ketones using non metallic catalysts, contributions of Brown, Kagan, and Noyori in hydrogenation reactions, different hydrogenation catalysts.

Asymmetric hydrogenation of C-C double bonds: ligand design for C-C bond formation, asymmetric hydrogenation of C-C double bonds using organometallic catalysts, asymmetric aldol and Michael reactions, enantioselective allylation.

Asymmetric oxidation: ligand design for oxidation, asymmetric epoxidation using Binol-Ph<sub>3</sub>PO/cumene hydroperoxide, asymmetric epoxidation using chiral titanium complexes, Sharpless epoxidation, Jacobsen Katzuki epoxidation, Shi epoxidation, Aggarwal epoxidation, contributions of Backvall, Beller, Bolm and Burgess in asymmetric oxidation, asymmetric epoxidation of unfunctionalized olefins.

Green catalysis: catalysis by solid acids and bases, heterogeneous catalysis, basic principles of enzyme catalyzed reactions. Asymmetric reduction of ketones using Baker's yeast.

Non linear effects in asymmetric catalysis, asymmetric C-H bond activation, organo catalysis- Hajos Parish reaction.

### References

01. K. Mikami, M. Lautens, *New Frontiers in Asymmetric Catalysis*, Wiley, 2007.
02. S.M. Roberts, G. Poignant, *Catalysis for Fine Chemical Synthesis: Hydrolysis, Oxidation and Reduction Vol 1*, John Wiley 2002
03. J.E. Backvall, *Modern Oxidation Methods*, Wiley VCH, 2004
04. R. A. Sheldon, I. Arends, U. Hanefeld, *Green Chemistry and Catalysis*, Wiley-VCH, 2007.



## SCSPDIE1613 SUPRAMOLECULAR CHEMISTRY

**Credit: 2**

**Contact Hours: 2**

Introduction: Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p and van der Waals interactions.

Design of Supramolecular Systems: Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands. Host-Guest interactions, pre-organization and complementarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules.

Self-assembly and Molecular Devices: design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots. molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic. Examples of recent developments in supramolecular chemistry from current literature: catenanes and rotaxanes, nonlinear optical materials, dendrimers.

Supramolecular Catalysis: Relevance of supramolecular chemistry to mimic biological systems, cyclodextrins as enzyme mimics, ion channel mimics and supramolecular catalysis.

Supramolecular Material Chemistry: Crystal engineering, noncovalent interactions in crystals, polymorphism, cocrystals, physic-chemical aspects of inclusion compounds, clathrate hydrates, synthetic clathrate hydrates, coordination polymers, metal organic frame works, gas storage and separation.

Soft Matter: Self-healing polymers, assembly of block copolymers, polymer networks, molecularly imprinted polymers, dendrimer chemistry, stimuli-responsive materials, supramolecular gels.

### References

01. P.A. Gale, J. W. Steed, *Supramolecular Chemistry: From Molecules to Nanomaterials*, J. Wiley, 2012
02. J.W. Steed, J.L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, 2000.
03. H. Dodziuk, *Introduction to Supramolecular Chemistry*, Springer, 2001.
04. F. Vogtle, E. Webner, *Host Guest Complex Chemistry: Macrocycles: Synthesis, Structures, applications*, 2<sup>nd</sup> Edn., Springer, 1985
05. P.D. Beer, P.A. Gale, D.K. Smith, *Supramolecular Chemistry*, Oxford University Press, 1999.
06. K. Ariga, T. Kunitake, *Supramolecular Chemistry: Fundamentals and Applications*, Springer, 2006

## SCSPDIE1614 ENVIRONMENTAL CHEMISTRY

**Credit: 2**

**Contact Hours: 2**

### **Unit 1**

Global warming-ozone hole, Environmental segments-The hydrological cycle-The oxygen cycle-The nitrogen cycle-The sulphur cycle-Composition of atmosphere-Earth's radiation balance-Green house effect.

### **Unit 2**

Air pollution-Primary pollutants, Acid rain-Air quality standards-Sampling-Monitoring-Analysis of CO, nitrogen oxides, sulphur oxides, hydrocarbons and particulate matter-Control of air pollution.

### **Unit 3**

Soil pollution-Inorganic and organic components in soil-Acid-Base and ion exchange reactions in soils-Micro and macro nutrients-Wastes and pollutants in soil.

### **Unit 4**

Water pollution-Water pollutants-Eutrophication-Water quality criteria for domestic and industrial uses-Trace elements in water-Determination of quality parameters-Total hardness, TDS, pH, chloride, heavy metals, etc.

Principles of water and waste water treatment-Aerobic and anaerobic treatment-Industrial waste water treatment-Removal of organic and inorganic materials from water and waste water.

### **Unit 5**

Instrumental techniques in environmental analysis-Use of neutron activation analysis-ASV, AAS, GC, HPLC, ion selective electrodes and ion chromatography in environmental chemical analysis.

## **References**

01. Environmental Chemistry, Gary W.VanLoon, Stephen J.Duffy, Oxford University Press, 2005
02. Principles of Environmental Chemistry, James Girard, Jones&Bartlett Learning, 2005.
03. Environmental Chemistry, Seventh Edition, Stanley E. Manahan, CRC Press, 2010
04. Applications of Environmental Chemistry, Eugene R.Weiner, CRC Press, 2010.
05. Environmental Chemistry, Ian Williams, J.Wiley 2001.
06. The essential guide to environmental chemistry, Georg Schwedt, John Wiley, 2001.

## SCSPDIE1615 COMPUTATIONAL QUANTUM CHEMISTRY

**Credit: 2**

**Contact Hours: 2**

Introduction to theoretical methods in chemistry, the tools of computational quantum chemistry.

The concept of the potential energy surface: stationary points, the Born-Oppenheimer approximation, geometry optimization, stationary points and normal mode vibrations, zero point energy corrections.

The Huckel Molecular Orbital(HMO) and Extended Huckel Molecular Orbital (EHMO) methods: principles and simple applications.

Introduction to *ab initio* methods: basis sets, the Hartree Fock method, electron correlation, post-Hartree Fock methods.

Semi-empirical methods: introduction, applications, strengths and weaknesses of semi-empirical methods.

Density functional calculations, basic principles of density functional theory(DFT), applications of DFT, strengths and weaknesses of DFT.

### References

01. D. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problem, John Wiley & Sons, 2001.
02. E.G. Lewars, Computational Chemistry, Springer, 2003.
03. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley & Sons, 2004.
04. S.M. Bachrach, Computational Organic Chemistry, John Wiley & Sons, 2007.

## SCSPDIE1616 BIOPOLYMERS

**Credit: 2**

**Contact Hours: 2**

Significance of biopolymers and its classification.

Polysaccharides: homopolysaccharides and heteropolysaccharides, starch, cellulose and chitin-structure and biological functions. Peptidoglycans, proteoglycans and glycoproteins.

Peptides and proteins: different structural levels-primary, secondary, tertiary and quaternary structures. Ramachandran plot, protein folding. Sequence determination by Edman method. Synthesis of peptides-different steps involved. Solid phase synthesis of peptides. Enzymes and enzyme kinetics.

Nucleic acids: structure, properties and functions of DNA and RNA. Base-pairing, double helical structure of DNA. Secondary and tertiary level organization, Various DNA forms(A,B&Z), DNA replication-transcription and translation. Recombinant DNA techniques.

Biodegradable polymer: sugar based biodegradable polymers, poly lactic acid(PLA) and polyhydroxyalkanoates (PHA), applications of biodegradable polymers.

### References

01. I.L. Finar, Organic Chemistry, Vol. 2, 5<sup>th</sup> Edn., ELBS, 1995
02. R. Chandra, R. Rustgi, Biodegradable Polymers-Progress in Polymer Science, Vol. 23, 1998
03. M. Johnson, L.Y. Mwaikambo, N. Tucker, Biopolymers, Rapra Technology, 2003
04. D.K. Platt, Biodegradable Polymers, Rapra Technology, 2006.

## SCSPDIE1617 SPECTROSCOPIC METHODS IN CHEMISTRY

**Credit: 2**

**Contact Hours: 2**

Infrared Spectroscopy: fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), effect of H-bonding and solvent effect on vibrational frequency. Vibrational frequencies of various functional groups.

Nuclear Magnetic Resonance Spectroscopy:  $^1\text{H}$  NMR spectroscopy, chemical shift and chemical equivalence, factors affecting the chemical shift values, approximate chemical shift values of various protons bonded to aliphatic, olefinic, aldehydic and aromatic carbons, anisotropic effects, effect of hydrogen bonding, proton exchange and effect of deuteration, spin-spin interaction and splitting of spectral signals, magnetic equivalence, Pople notations-AX, AB, AMX and ABC spectra, coupling constant J, first-order and non first-order spectra, enantiotopic and diastereotopic protons, Karplus curve, variation of coupling constant with dihedral angle, simplification of complex spectra using NMR shift reagents, double resonance and Nuclear Overhauser Effect (NOE).

$^{13}\text{C}$  NMR Spectroscopy: chemical shift values of aliphatic, olefinic, alkyne, aromatic, hetero-aromatic and carbonyl carbons, coupling constants, two-dimensional NMR spectroscopy, NOESY, DEPT and INEPT terminologies. Application of 2D-NMR in macromolecules.

EPR spectroscopy: electron spin interaction with magnetic field, g factor, determination of  $g_{\parallel}$  and  $g_{\perp}$ , fine and hyperfine structures, Kramers' degeneracy, McConnell equation.

Mass Spectroscopy: mass spectral fragmentation of compounds of common functional groups, molecular ion peak, McLafferty rearrangements, different methods of fragmentation.

Applications of IR, NMR, EPR and mass spectroscopic techniques for structure elucidation of inorganic and organic compounds.

### References

01. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3<sup>rd</sup> Edn., Brooks Cole, 2000.
02. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
03. W. Kemp, Organic Spectroscopy, 2<sup>nd</sup> Edn., Macmillan, 1987.
04. R.M. Silverstein, G.C. Bassler, T.C. Morrill, Spectroscopic Identification of Organic Compounds, 5<sup>th</sup> Edn., Wiley, 1991.
05. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Edn., Tata McGraw-Hill, 1994.
06. P.S. Kalsi, Spectroscopy of Organic Compounds, 6<sup>th</sup> Edn., New Age International, 2007.
07. D. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6<sup>th</sup> Edn., McGraw-Hill, 2008.

## SCSPDIE1618 POLYMER PHYSICS

**Credit: 2**

**Contact Hours: 2**

Polymer structure and properties: solubility and cohesive energy density, structural factors influencing chain flexibility, mechanical, thermal, chemical, optical and electrical properties.

Transition phenomena in polymers: glass transition temperature and crystalline melting points, principles of corresponding temperature, molecular motion and transitions, the Boyer-Berman rule, molecular interpretation of the glassy state of polymers, types of mechanical deformation, polymer structure and transition behaviour..

Polymer viscoelasticity: types of mechanical deformation, introduction to the viscoelastic properties of polymers, simple linear viscoelastic models-Maxwell and Voigt models, the Boltzman principle, linear viscoelastic behavior of polymer solids, creep, stress relaxation, stress-strain and oscillatory experiments, the elastic modulus, time temperature equivalence, time-temperature superposition principle, Payne and Mullins effects.

Polymer rheology: Newtonian fluids, non-Newtonian fluids, pseudoplastic materials, bingham plastics, dilatants, viscoelastic fluids, time dependent fluids, rheopectic and thixotropic fluids, rheological models, elastic effects: die swell, melt fracture, Barus effect, shark skin, Weissenberg effect.

Theory of rubber elasticity, molecular and mechanical requirements for a material to be rubber, load-deformation, rubber elasticity of ideal rubber, thermodynamics of ideal rubber, statistical approach to rubber elasticity, rubber like elasticity of real rubbers, Mooney-Rivillian equation, crosslink density.

Crystallization of polymers: structural requirements for crystallinity, Fringed miscelle model, Lamellar model, configurations of polymer chain, crystallization and melting, strain-induced crystallization, representative crystal structures, polymer single crystals, growth from solutions, hollow pyramids, morphology of polymer crystallized from the melt, interlamellar ties, orientation and drawing, characterization of crystallinity and crystal structure, spherulites, long period, lamellar thickness, interplanar distance.

### References

01. P.J. Flory, Principles of Polymer Chemistry, Cornel University Press, 1953.
02. H.G. Elias, Macromolecules: Structure and Properties, Springer, 1977.
03. A. Tager, Physical Chemistry of Polymer, 2<sup>nd</sup> Edn., Mir Publishers, 1978.
04. R.P. Brown, Physical Testing of Rubber, 3<sup>rd</sup> Edn., Springer, 1996.
05. F.W. Billmeyer, Text Book Of Polymer Science, 3<sup>rd</sup> Edn., Wiley, 1984.
06. D.I. Bower, An Introduction to Polymer Physics, Cambridge University Press, 2002.
07. L.H. Sperling, Introduction to Physical Polymer Science, 4<sup>th</sup> Edn., John Wiley & Sons, 2006.