

CURRICULUM OF CHEMISTRY

MPhil Program (2-Year, 4-Semester)



Department of Chemistry
Shaheed Benazir Bhutto Women University
Peshawar

SCHEME OF STUDIES
(Session 2019 onward)

MPhil Chemistry
SCHEME OF STUDIES

MPhil Two Years Program
Year 1 (Two Semesters): Course Work
Year 2 (Two Semesters): Research Work

Course Work	
Course	Credit Hours
Semester – I	
Course 1	3
Course 2	3
Course 3	3
Course 4*	3
Total	12
Semester – II	
Course 1	3
Course 2	3
Course 3	3
Course 4*	3
Total	12
Research Work	
Semester – III & IV	06
Thesis and Viva	

*One minor course of 03 credit hours borrowed from other department(s) i.e., Mathematics/Statistics/Computer Science should be offered in semester I and semester II.

MPhil Courses

I. Analytical Chemistry

CHM-710	Applied Chemometrics (Cr. 2 + 1)
CHMA-711	One- and Two-Dimensional NMR Spectroscopy (Cr. 3)
CHMA-712	Diffraction Methods of Analysis (Cr. 3)
CHMA-713	Applied Industrial Processes (Cr. 3)
CHMA-714	Advanced Applied Chemistry (Cr. 3)
CHMA-715	Advanced Analytical Instrumental Techniques (Cr. 3)
CHMA-716	Advanced Thermal Analysis (Cr. 3)
CHMA-717	Analysis and Characterization of Polymers (Cr. 3)
CHMA-718	Advanced Atomic Spectroscopy (Cr. 3)
CHMA-719	Chromatographic Methods of Analysis (Cr. 3)
CHMA-720	Special Topics in Analytical Chemistry (Cr. 3)
CHMA-721	X-Ray Methods of Analysis (Cr. 3)

II. Inorganic Chemistry

CHM-710	Applied Chemometrics (Cr. 2 + 1)
CHMI-711	Medicinal Inorganic Chemistry (Cr. 3)
CHMI-712	Inorganic Electronic Spectroscopy (Cr. 3)
CHMI-713	Kinetics and Mechanisms of Inorganic Reactions (Cr. 3)
CHMI-714	Organo-transition Metal Chemistry (Cr. 3)
CHMI-715	Bio-Inorganic Chemistry (Cr. 3)
CHMI-716	Physical Methods in Inorganic Chemistry (Cr. 3)
CHMI-717	Inorganic Material Chemistry (Cr. 3)
CHMI-718	Special Topics in Inorganic Chemistry (Cr. 3)
CHMI-719	Catalysis (Cr. 3)
CHMI-720	Composite Materials (Cr. 3)
CHMI-721	Water and Soil Chemistry (Cr. 3)
CHMI-722	Atmospheric Chemistry (Cr. 3)

III. Organic Chemistry

CHM-710	Applied Chemometrics (Cr. 2 + 1)
CHMO-711	Modern Name Reactions in Organic Synthesis (Cr. 3)
CHMO-712	Computational Chemistry/Molecular Modeling (Cr. 3)
CHMO-713	Protecting Groups in Organic Synthesis (Cr. 3)
CHMO-714	Organic Synthesis-Retrosynthetic Approach (Cr. 3)
CHMO-715	Advanced Stereochemistry (Cr. 3)
CHMO-716	Physical Organic Chemistry (Cr. 3)
CHMO-717	Nuclear Magnetic Resonance in Organic Chemistry (Cr. 3)
CHMO-718	Advances in Chromatographic Techniques (Cr. 3)
CHMO-719	Chemistry of Isoprenoids and Steroids (Cr. 3)
CHMO-720	Chemistry of Glycosides (Cr. 3)
CHMO-721	Biosynthesis of Natural Products (Cr. 3)
CHMO-722	Chemistry of Organometallic Compounds (Cr. 3)
CHMO-723	Reactive Intermediates in Organic Chemistry (Cr. 3)
CHMO-724	Advanced Heterocyclic Chemistry (Cr. 3)
CHMO-725	Advanced Mass Spectrometry (Cr. 3)
CHMO-726	Organic Photochemistry (Cr. 3)

- CHMO-727 Organic Polymer Chemistry (Cr. 3)
- CHMO-728 Pericyclic Reactions (Cr. 3)
- CHMO-729 Special Topics in Organic Chemistry (Cr. 3)
- CHMO-730 Medicinal Chemistry (Cr. 3)
- CHMO-731 Cheminformatics (Cr. 3)
- CHMO-732 Advanced Stereoselective Synthesis (Cr. 3)
- CHMO-733 Special Organic Materials (Cr. 3)
- CHMO-734 Aroma and Flavor Chemistry (Cr. 3)

IV. Physical Chemistry

- CHM-710 Applied Chemometrics (Cr. 2 + 1)
- CHMP-711 Physical Chemistry of High Polymers (Cr. 3)
- CHMP-712 Advanced Quantum Chemistry (Cr. 3)
- CHMP-713 Electrode Process (Cr. 3)
- CHMP-714 Magnetic Resonance Spectroscopy (Cr. 3)
- CHMP-715 Advanced Chemical Kinetics (Cr. 3)
- CHMP-716 Advanced Molecular Spectroscopy (Cr. 3)
- CHMP-717 Photochemistry (Cr. 3)
- CHMP-718 Advanced Photochemistry (Cr.3)
- CHMP-719 Advanced Surface Chemistry (Cr. 3)
- CHMP-720 Advanced Solution Chemistry (Cr. 3)
- CHMP-721 Chemistry of Advanced Composite Materials (Cr. 3)
- CHMP-722 Advanced Statistical Mechanics (Cr. 3)
- CHMP-723 Solid State and Semiconductors (Cr. 3)
- CHMP-724 Surfactant and Colloid Chemistry (Cr. 3)
- CHMP-725 Nuclear and Radiation Chemistry (Cr. 3)
- CHMP-726 Advanced Nuclear and Radiation Chemistry (Cr. 3)
- CHMP-727 Applied Chemical Thermodynamics (Cr. 3)
- CHMP-728 Introductory Biophysical Chemistry (Cr. 3)
- CHMP-729 Advanced Biophysical Chemistry (Cr. 3)
- CHMP-730 Physical Chemistry of Environment (Cr. 3)
- CHMP-731 Numerical Methods and Computational Chemistry (Cr. 3)
- CHMP-732 Theoretical and advanced Computational Chemistry (Cr. 3)
- CHMP-733 Chemistry of Superconductors (Cr. 3)
- CHMP-734 Material Chemistry (Cr. 3)
- CHMP-735 Advanced Techniques in Physical Chemistry (Cr. 3)
- CHMP-736 Electroanalytical Methods and Techniques (Cr. 3)

IV. CHMA/CHMI/CHMO/CHMP-799 Thesis and Viva Voce Exam

Details of MPhil Courses

I. Analytical Chemistry

CHM-710 Applied Chemometrics (Cr. 2 + 1)

Introduction: Basics of Chemometrics. **Multivariate structure of data:** Matrices, dimension, transposition, centering, covariance, correlation, pretreatment of the data, transformation of variables, handling of missing data. **Principal component analysis:** Loading plots, score plots, choice of principal components (rank analysis), both numerically and graphically (scree plot). **Clusters analysis:** Distance matrix, similarity matrix, Dendrograms. **Linear discriminant analysis:** Correlation matrix, covariance matrix, correlations, correlogram, Box tests, Kullback's test, Wilks' lambda test, Bartlett's test, loading plots, score plots Eigen values. **Calibration:** Linear regression, Regression coefficients, Correlation coefficient, Prediction coefficient, Standard error of the estimate, Principal Component Regression (PCR), Partial Least Squares Method (PLS). **Practical examples:** Working with spectroscopic instruments (NIR, FTIR, UV/Vis, NMR, MS, ICP-OES, ICP-MS), chromatography instruments (LC, GC, HPLC).

Teaching and Learning Methods/Tools

Lectures, video projector for explanation of spreadsheets, and Computer exercises (acquisition of specific informatics tools; software for mathematics and statistics including Microsoft Excel, XLSTAT, SPSS, R, MINITAB etc).

Assessment Methods

Individual report submission (Text Document) by students about a chemometric problem, relevant to a dataset provided by the teacher.

Viva Voce Examination about the final report and the theory explained in the class room lessons (definitions and demonstrations).

Final mark: Mark assigned to report + Mark assigned to oral exam

Recommended Books

1. H. Martens, M. Martens, *Multivariate Analysis of Quality: An Introduction*, John Wiley (2001).
2. H. Mark, *Principles and Practice of Spectroscopic Calibration*, John Wiley (1991).
3. M. Otto, *Chemometrics Statistics and Computer Application in Analytical Chemistry*, Wiley - VCH (1999).
4. J.W. Einax, H.W. Zwanziger, S. Geiss, *Chemometrics in Environmental Analysis*, VCH (1997).
5. J.C. Miller, J.N. Miller, *Statistics and Chemometrics for Analytical Chemistry*, Pearson Education (2010).
6. R.G. Brereton, *Applied Chemometrics for Scientists*, Wiley (2007).
7. R. Kramer, *Chemometric Techniques for Quantitative Analysis*, Marcel Dekker (1998).

CHMA-711 One- and Two-Dimensional NMR Spectroscopy (Cr. 3)

Introduction: Basic principle of NMR, instrumentation, sample preparation. **Chemical shifts:** ^1H , ^{13}C , ^{15}N , ^{31}P , ^{29}S and ^{11}B chemical shifts, factor affecting chemical shifts. **Spin-spin coupling:** Coupling constant, spin systems, H,H-coupling, C,H-coupling, C,C-coupling constants and chemical structures. **NMR Experiments:** Spin decoupling in ^1H and ^{13}C NMR, H,H-COSY, H,C-COSY, NOE and other experiments.

Recommended Books

1. H. Friebolin, *Basic One- and Two-Dimensional NMR Spectroscopy*, 4th ed., VCH Publishers, New York (2005).
2. A. Rehman, *Nuclear Magnetic Resonance Spectroscopy*, Press Manager, UGC Print Shop, Islamabad (1989).
3. J.K.M. Saunderson, *Modern NMR Spectroscopy*, Oxford University Press, London (1989).
4. R.S. Macomber, *A Complete Introduction to Modern NMR Spectroscopy*, John-Wiley and Sons (1998).

Supplementary Books

1. T.D.W. Claridge, *High Resolution NMR Techniques*, Elsevier Science, Amsterdam (1999).
2. R.J. Abraham, J. Fischer and P. Lotus, *Introduction of NMR Spectroscopy*, Wiley Chichester, USA (1988).

CHMA-712 Diffraction Methods of Analysis (Cr. 3)

Introduction: Principles and instrumentation of diffractive methods. **Applications:** Application of X-ray, electron and neutron diffraction methods in the determination of structure of compounds. **Geometry:** Determination of geometry and other related parameters for crystalline solids by X-ray method. **Pair distribution:** Determination of pair distribution function of solids and liquids.

Recommended Books

1. M. Ladd, R. Palmer, *Structure Determination by X-ray Crystallography*, 4th ed., Kluwer Academic/Plenum Publishers, (2003).
2. B.D. Cullity, S.R. Stock, *Elements of X-ray Diffraction*, 3rd ed., Prentice Hall, (2003).

3. J.P. Glusker, K.H. Trueblood, *Crystal Structure Analysis, A. Primer*, 2nd ed., Oxford University Press, (1985).

Supplementary Books

1. G.H. Stout, L.H. Jenson, *X-ray Structure Determination, A Practical Guide*, 2nd ed., John Wiley & Sons (1989).

CHMA-713 Applied Industrial Processes (Cr. 3)

The importance of chemical industries for the economic development of Pakistan; chemistry of ceramics and its processing; the agrochemical industry; chemistry of structural adhesives; dyes and pigments; chemistry of silicone technology; chemistry of fuel technology; corrosion; quality control (analytical and statistical).

Recommended Books

1. G.T. Austin, *Shreve's Chemical Processes Industries*, 5th ed., McGraw-Hill, International Editions, New York (1984).
2. R.J. Farrauto, *Fundamentals of Industrial Catalytic Processes*, Blackie Academic, London (1997).
3. K.H. Davis, *Hand Book of Industrial Chemistry*, Vol. 2, CBS Publishers, New Delhi (2004).

Supplementary Books

1. O. Levenspiel, *Chemical Reaction Engineering*, 3rd ed., John Wiley, New York (1999).
2. M.M. Uppal, *Engineering Chemistry (Chemical Technology)*, S.C. Bhatia (Ed.), Khanna Publishers, New Delhi (2005).

CHMA-714 Advanced Applied Chemistry (Cr. 3)

Various aspects of the energy and raw material supply, cost calculations to improve yield and to reduce pollution. Industrial techniques and quality control. Equipment for large-scale manufacturing. Conversion of a lab. process to a pilot plant and then plant procedure. Industrial catalysis. Inorganic and organic processes. Products of fermentation process. Preparation of chemical products from small molecules. Pesticides, herbicides and pharmaceuticals. The environmental impact of a process.

Recommended Books

1. G.T. Austin, *Shreve's Chemical Processes Industries*, 5th ed., McGraw-Hill, International Editions, New York (1984).
2. R.J. Farrauto, *Fundamentals of Industrial Catalytic Processes*, Blackie Academic, London (1997).

3. K.H. Davis, *Hand Book of Industrial Chemistry*, Vol. 2, CBS Publishers, New Delhi (2004).

Supplementary Books

1. O. Levenspiel, *Chemical Reaction Engineering*, 3rd ed., John Wiley, New York (1999).
2. M.M. Uppal, *Engineering Chemistry (Chemical Technology)*, S.C. Bhatia (Ed.), Khanna Publishers, New Delhi (2005).

CHMA-715 Advanced Analytical Instrumental Techniques (Cr. 3)

Principles of mass spectrometry and gas chromatography, instrumentation, application of mass spectrometry to organometallics, organosilicon and organophosphorous compounds. Mass spectrometry coupled with gas chromatography. Discussion on relevant research papers and review articles.

Recommended Books

1. D.A. Skoog, *Principles of Instrumental Analysis*, 3rd ed., Saunder College Publishing, Philadelphia (1984).
2. G.W. Ewing, *Instrumental Methods of Chemical Analysis*, McGraw-Hill, New York (1985).
3. D.A. Skoog, et al., West and Holler, *Fundamentals of Analytical Chemistry Office*, 8th ed., Thomson, Brooks/Cole, Australia (2004).

CHMA-716 Advanced Thermal Analysis (Cr. 3)

Theory and instrumentation: Thermogravimetry (TG), differential thermal analysis (DTA), differential scanning calorimetry (DSC). **Quantitative interpretation:** TGA, DTA and DSC curves. **Kinetic and thermodynamic parameters.** **Applications:** DTA, TGA in cements, catalysts, clays, minerals, biological materials, drugs, polymers and textiles. **High temperature reflectance spectroscopy (HTRS):** Instrumentation and applications to various inorganic compounds.

Recommended Books

1. T. Hatakeyama and F.X. Quinn, 2nd ed., *Thermal Analysis Fundamentals and Applications to Polymer Science*, John Wiley, New York (1999).
2. P.J. Haines, *Thermal Methods of Analysis*, Blackie Academic and Professional, London (1995).
3. W.W.M. Wendlandt, *Thermal Analysis*, 3rd ed., John Wiley, New York (1986).

Supplementary Books

1. T. Daniels, *Thermal Analysis*, Kogan Page, London (1973).

2. J.W. Dodd and K.H. Tonge, *Thermal Method: Analytical Chemistry by Open Learning*, John Wiley (1987).

CHMA-717 Analysis and Characterization of Polymers (Cr. 3)

The polymerization processes and techniques, molecular weight and its determination, polymer additives (plasticizers, stabilizers and fillers). Chemical analysis, GPC and other chromatographic methods of analysis. Mechanical, thermal, spectroscopic, microscopic and X-ray diffraction analyses. Synthetic and degradation reactions.

Recommended Books

1. J.M.G. Cowie, *Polymers: Chemistry and Physics of Modern Materials*, International Textbook Co., London (1973).
2. F.W. Billmeyer, *Textbook of Polymer Science*, 3rd ed., John Wiley & Sons, New York (1994).
3. C.E. Carraher, *Seymour/Carraher's Polymer Chemistry*, 5th ed., Revised and Expanded, Marcel Dekker, New York (2000).

Supplementary Books

1. C.E. Carraher, *Introduction to Polymer Chemistry*, CRC Taylor and Francis Group, New York (2007).
2. J.R. Fried, *Polymer Science and Technology*, Prentice Hall PTR (1995).
3. A. Rudin, *The Elements of Polymer Science and Engineering*, Academic Press (1999).
4. T.R. Crompton, *Analysis of Polymers: An Introduction*, Pergamon Press (1989).
5. C.E. Carraher, Jr., *Polymer Chemistry, An Introduction*, 4th ed., Marcel Dekker, Inc. (1992).

CHMA-718 Advanced Atomic Spectroscopy (Cr. 3)

Atomic spectroscopy: Quantitative and qualitative aspects, spectra from high energy sources. **Atomic absorption spectroscopy:** Flame and electrothermal atomization, cold vapour and hydride generation techniques, construction, working, advantages and limitations of instrumental components. **Optimization parameters:** interferences and applications of atomic absorption spectroscopy. **Atomic fluorescence spectroscopy:** Theory and applications, comparison of AFS with AAS. **Atomic emission spectroscopy:** Based on plasma sources, simultaneous and sequential systems, experimental considerations and performance characteristics, instrumentation and applications of ICP-AES. **Electric arc and spark emission spectrophotometric methods:** Lasers, analytical applications in atomic spectroscopy. **QA and QC in atomic spectroscopic methods:** Data handling and statistical manipulation.

Recommended Books

1. E.H. Evans, *An Introduction to Analytical Atomic Spectrometry*, John Wiley & Sons Ltd., New York (1998).
2. J.R. Dean, *Atomic Absorption and Plasma Spectroscopy*, 2nd ed., D.J. Ando, (Ed), John Wiley and Sons (1997).
3. A. Montaser and D.W. Goloightly, *Inductively Coupled Plasmas in Analytical Atomic Spectrometry*, VCH Publishers Inc., New York (1992).

Supplementary Books

1. M. Thompson, and J.N. Walsh, *Handbook of Inductively Coupled Plasma Spectrometry*, 2nd Edition, Blackie and Son Ltd., Glasgow and London (1989).
2. F. Rouessac and A. Rouessac, *Chemical Analysis – Modern Instrumental Methods and Techniques*, John Wiley & Sons, Ltd., UK (2000).
3. K.A. Rubinson and J.F. Rubinson, *Contemporary Instrumental Analysis*, Prentice-Hall, Inc., USA (2000).
4. D.A. Skoog and J.J. Leary, *Principles of Instrumental Analysis*, 4th ed., Saunders College Publishing, USA (1992).
5. R.D. Braun, *Introduction to Instrumental Analysis*, McGraw-Hill Book Company (1987).
6. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Analysis*, 6th ed., Pearson Education Ltd. (2000).
7. D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill Companies Inc. (2000).

CHMA-719 Chromatographic Methods of Analysis (Cr. 3)

Introduction: Classification of chromatographic methods, theory of separations and retention characteristics, descriptions of chromatograms. **Chromatographic parameters:** The van-Deemter equation, column efficiency, band broadening and resolution. **Quantitation techniques:** Sample loading, loss of material on column, column packing, flow rates, detector response, batch separations, symmetrical and asymmetrical peaks. **Types of liquid chromatography:** Working methodology, instrumentation and applications of adsorption, partition, ion-exchange, gel permeation, affinity and high performance liquid chromatography, effect of temperature, particle size, column size, pressure and HETP. **Detectors for liquid chromatography:** High performance thin layer chromatography. **Gas-Chromatography:** Sample introduction, splitters, columns and detectors in GC, optimization of gas-chromatographic separations. **Supercritical fluid Chromatography:** Working principle, instrumentation and applications. **Gel-electrophoresis:** Theory and applications.

Recommended Books

1. D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill Companies Inc. (2000).

2. K.A. Rubinson and J.F. Rubinson, *Contemporary Instrumental Analysis*, Prentice-Hall, Inc., USA (2000).
3. A. Braithwaite and F.J. Smith, *Chromatographic Methods*, Chapman and Hall, New York (1985).

Supplementary Books

1. J. Weiss, *Ion Chromatography*, 2nd ed., VCH Publishers Inc, New York (1995).
2. F. Rouessac and A. Rouessac, *Chemical Analysis – Modern Instrumental Methods and Techniques*, John Wiley & Sons, Ltd., UK (2000).
3. G.D. Christian, *Analytical Chemistry*, 6th ed., John Wiley & Sons Ltd., Singapore (2003).
4. D.A. Skoog and J.J. Leary, *Principles of Instrumental Analysis*, 4th ed., Saunders College Publishing, USA (1992).
5. D.C. Harris, *Quantitative Chemical Analysis*, 3rd ed., W.H. Freeman Company, New York (1991).
6. R.D. Braun, *Introduction to Instrumental Analysis*, McGraw-Hill Book Company (1987).
7. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2nd ed., Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004).

CHMA-720 Special Topics in Analytical Chemistry (Cr. 3)

Topics under recent investigation and of current interest (the choice will depend upon the interests of the teacher giving this course).

CHMA-721 X-Ray Methods of Analysis (Cr. 3)

Origin of X-ray spectra: Energy levels, Moseley's law. **The absorption spectrum:** Mass absorption coefficient. **Instrumentation:** X-ray generation, sources, wavelength dispersive devices, energy dispersive devices, detectors, sample preparation methods, working principle, analytical applications of X-ray absorption, X-ray fluorescence, particle induced X-ray emission, auger emission spectroscopy. **Electron microscopy:** Scanning electron microscopy for chemical analysis, quality control procedures, interferences and their remedial measures.

Recommended Books

1. C. Whiston, *X-Ray Methods*, John Wiley & Sons (1997).
2. H.H. Willard, L.L. Merritt, J.A. Dean, F.A. Settle, *Instrumental Methods of Analysis*, Wiley, New York (2003).
3. F. Rouessac and A. Rouessac, *Chemical Analysis – Modern Instrumental Methods and Techniques*, John Wiley & Sons, Ltd., UK (2000).

Supplementary Books

1. J.D. Ingle and S.R. Crouch, *Spectrochemical Analysis*, Prentice-Hall International, Inc. (1998).
2. K.A. Rubinson and J.F. Rubinson, *Contemporary Instrumental Analysis*, Prentice-Hall, Inc., USA (2000).
3. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2nd ed., Wiley-VCH Verlag, GmbH & Co. KGaA, Weinheim (2004).
4. R.D. Braun, *Introduction to Instrumental Analysis*, McGraw-Hill Book Company (1987).
5. D.A. Skoog and J.J. Leary, *Principles of Instrumental Analysis*, 4th ed., Saunders College Publishing, USA (1992).

II. Inorganic Chemistry

CHM-710 Applied Chemometrics (Cr. 2 + 1)

Introduction: Basics of Chemometrics. **Multivariate structure of data:** Matrices, dimension, transposition, centering, covariance, correlation, pretreatment of the data, transformation of variables, handling of missing data. **Principal component analysis:** Loading plots, score plots, choice of principal components (rank analysis), both numerically and graphically (scree plot). **Clusters analysis:** Distance matrix, similarity matrix, Dendrograms. **Linear discriminant analysis:** Correlation matrix, covariance matrix, correlations, correlogram, Box tests, Kullback's test, Wilks' lambda test, Bartlett's test, loading plots, score plots Eigen values. **Calibration:** Linear regression, Regression coefficients, Correlation coefficient, Prediction coefficient, Standard error of the estimate, Principal Component Regression (PCR), Partial Least Squares Method (PLS). **Practical examples:** Working with spectroscopic instruments (NIR, FTIR, UV/Vis, NMR, MS, ICP-OES, ICP-MS), chromatography instruments (LC, GC, HPLC).

Teaching and Learning Methods/Tools

Lectures, video projector for explanation of spreadsheets, and Computer exercises (acquisition of specific informatics tools; software for mathematics and statistics including Microsoft Excel, XLSTAT, SPSS, R, MINITAB etc).

Assessment Methods

Individual report submission (Text Document) by students about a chemometric problem, relevant to a dataset provided by the teacher.

Viva Voce Examination about the final report and the theory explained in the class room lessons (definitions and demonstrations).

Final mark: Mark assigned to report + Mark assigned to oral exam

Recommended Books

1. H. Martens, M. Martens, *Multivariate Analysis of Quality: An Introduction*, John Wiley (2001).

2. H. Mark, *Principles and Practice of Spectroscopic Calibration*, John Wiley (1991).
3. M. Otto, *Chemometrics Statistics and Computer Application in Analytical Chemistry*, Wiley - VCH (1999).
4. J.W. Einax, H.W. Zwanziger, S. Geiss, *Chemometrics in Environmental Analysis*, VCH (1997).
5. J.C. Miller, J.N. Miller, *Statistics and Chemometrics for Analytical Chemistry*, Pearson Education (2010).
6. R.G. Brereton, *Applied Chemometrics for Scientists*, Wiley (2007).
7. R. Kramer, *Chemometric Techniques for Quantitative Analysis*, Marcel Dekker (1998).

CHMI-711 Medicinal Inorganic Chemistry (Cr. 3)

Introduction: General introduction to medicinal inorganic chemistry. **Radiotherapy:** Emitter therapy and radiopharmaceuticals. **Metal complexes as pharmaceuticals:** Anticancer drugs in chemotherapy, arthritis treatment, insulin mimics. **Chelate Compounds:** Chelation therapy for metal-related diseases and toxicity, nanotechnology in biomedicine.

Recommended Books

1. S.J. Lippard and J.M. Berg, *Principle of Bioinorganic Chemistry*, University Science Books (1994).
2. R.W. Hay, *Bioinorganic Chemistry*, Ellis, Harwood, London (1991).
3. K.S. Coleman, *Annu. Rep. Prog. Chem., Sect. A*, 103, 392-406 (2007) (Review).

Supplementary Books

1. P.C. McGown, *ibid*, 101, 631-648 (2005) (Review).
2. D.S. Urch and M.J. Welch, *ibid*, 101, 585-606 (2005) (Review).

CHMI-712 Inorganic Electronic Spectroscopy (Cr. 3)

Term symbols, Russel Saunders, coupling scheme, development of correlation and Tanabe-Sugano diagrams, crystal field diagrams. Energy level calculations; selection rules, band intensities and band assignments. Interpretation of crystal field and charge transfer spectra. Spectra of low symmetry complexes. Application of group theory to vibrational spectra of simple and coordination compounds.

Recommended Books

1. A.B.P. Lever, *Introduction to Electronic Spectroscopy*, Elsevier, Amsterdam (1968).

2. J.P. Facler, *Symmetry in Coordination Chemistry*, Academic Press, New York (1971).
3. Alan and Vincent, *Molecular Symmetry and Group Theory*, John Wiley, London (1977).

Supplementary Books

1. F.A. Cotton, *Chemical Applications of Group Theory*, 3rd ed., John Wiley, New York (1990).
2. J. Huheey, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th ed., Addison-Wesley, Reading/Singapore (1993).

CHMI-713 Kinetics and Mechanisms of Inorganic Reactions (Cr. 3)

Principles of kinetics. Steady state approximation. Determination of rate law. Inert and labile complexes. Substitution reactions of octahedral, square planer and tetrahedral complexes. Oxidation-reduction reactions of metal ions. Organo-transition metal compounds. Free radical reactions.

Recommended Books

1. D. Benson, *Mechanisms of Inorganic Reaction in Solution: An Introduction*, McGraw-Hill, London (1968).
2. F. Basolo and R.G. Pearson, *Mechanisms of Inorganic Reactions: A Study of Metal Complexes in Solutions*, 2nd ed., John Wiley, New York (1967).
3. D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, Wiley-Interscience, New York (1987).

Supplementary Books

1. S.R. Logan, *Fundamentals of Chemical Kinetics*, Longman, London (1996).
2. J.O. Edwards, *Inorganic Reaction Mechanism: An Introduction*, W.A. Benjamin, New York (1965).
3. R.C. Henderson, *The Mechanisms of Reactions of Transition Metals*, 5th ed., Oxford University Press (1993).

CHMI-714 Organo-transition Metal Chemistry (Cr. 3)

Classification of organometallic compounds; transition metal to carbon sigma bonded compounds, complexes with metal-carbon pi bonds such as η^2 - η^7 . Synthesis, properties and nature of bonding in pi complexes. Complexes of molecular nitrogen, oxygen and carbon disulphide. Fundamental processes in organometallics, fluxional and dynamic equilibrium, oxidative addition and reductive elimination, insertion and deinsertion, reactions of coordinated ligands. Catalysis by organometallic (stoichiometric and catalytic processes) compounds. Polymerization and oligomerization, synthesis with CO hydrogenation of olefin etc.

Recommended Books

1. A. Yamamoto, *Organotransition Metal Chemistry Fundamental Concepts and Applications*, John Wiley & Sons (1986).
2. M.L.H. Green, G.E. Coates and K. Wades, *Organometallic Compounds*, Methuen & Co. Ltd., (1968).
3. M. Bochmann, *Organometallic 1 and 2*, Oxford Science Publications (1994).

Supplementary Books

1. F.A. Cotton, G. Wilkenson, *Advanced Inorganic Chemistry*, 6th Ed. John Wiley & Sons, (1999).

CHMI-715 Bio-Inorganic Chemistry (Cr. 3)

Introduction: Development and importance of bio-inorganic chemistry. **Metals and Complexes:** Metals of biological importance. Function of metals in enzyme catalysis. Metalloproteins and enzymes containing a transition metal centre at their active site. Oxygen carriers; uptake and transport activation and utilization; synthetic dioxygen carriers; nitrogen fixation; vitamin B₆ and B₁₂. Importance of nonmetals in biological systems. Metal ions and chelating agents in biological systems.

Recommended Books

1. S.J. Lippard and J.M. Berg, *Principles of Bioinorganic Chemistry*, Panima Publishing Corporation, New Delhi (1997).
2. R.W. Hay, *Bioinorganic Chemistry*, Ellis Horwood, London (1984).
3. I. Bertim, H.B. Gray, S.J. Lippard and J.S. Valentine, *Bioinorganic Chemistry*, Viva Book Private Ltd. New Delhi (1998).

Supplementary Books

1. B.K. Keppler, *Metal Complexes in Cancer Chemotherapy*, VCH, Weinheim (1993).
2. M.F. Gielen, *Metal Based Anti-tumor Drugs*, Freund Publishing House Ltd. London (1988).

CHMI-716 Physical Methods in Inorganic Chemistry (Cr. 3)

Infrared and Raman spectroscopy and their applications. Group theory and vibrational analysis. Application of ORD, CD, NMR, ESR and Mass Spectrometry to inorganic systems.

Recommended Books

1. J.B. Lambert and E.P. Mazzola, *Nuclear Magnetic Resonance Spectroscopy*, Prentice Hall, New Jersey, (2003).

2. D.L. Pavia, G.M. Lamp and G.S. Kriz, *Introduction to Spectroscopy*, 3rd ed., Thomson Learning, Inc., U.K. (2001).
3. R. Davis, M. Frearson, *Mass Spectrometry, Analytical Chemistry by Open Learning*, John Wiley and Sons, New York (1987).

Supplementary Books

1. C.G. Herbert, R.A.W. Johnstone, *Mass Spectrometry, Basics*, CRC Press London (2002).
2. M. Yonus, *Organic Spectroscopy*, AHP International (Pvt.) Ltd. Lahore, (1998).

CHMI-717 Inorganic Material Chemistry (Cr. 3)

Introduction to inorganic materials, Application and interpretation of powder X-ray diffraction data of materials, The synthesis of inorganic materials – Solid state reactions, Precursor, solution and sol-gel methods, Solid-gas reactions, Hydrothermal method, CVD, Aerosol process, Low temperature method, Transition metal oxides, Electronic, magnetic and optical properties of inorganic materials, Nonstoichiometric compounds, Zeolites, intercalation in layer materials and solid electrolytes, Some recent developments in inorganic material chemistry.

Recommended Books

1. M.T. Weller, *Inorganic Material Chemistry*, Oxford University Press, Inc., New York (1994).
2. L. Smart and E. Moore, *Solid State Chemistry*, 2nd ed., Chapman & Hall (2004).
3. A.R. West, *Basic Solid State Chemistry*, 2nd ed., John Wiley & Sons, Ltd. (2000).

CHMI-718 Special Topics in Inorganic Chemistry (Cr. 3)

Topics under recent investigation and of current interest (the choice will depend upon the interests of the teacher giving this course).

CHMI-719 Catalysis (Cr. 3)

Physical adsorption, Chemisorption of gases on metals and metal oxides, textural and structural characterization of catalysts, Synthesis of porous solids, Kinetics of catalytic reactions, Catalysis and theoretical concepts, Catalytic process such as oxidation reactions, production of petrochemicals, environmental catalysis, polymerization and photocatalysis, Catalyst deactivation, Fuel cells.

Recommended Books

1. B. Viswanath, S. Sivasanker and A.V. Ramaswamy, *Catalysis Principles and Applications*, Narosa Publishing House, New Delhi, India (2006).
2. J. Hagen, *Industrial Catalysis: A Practical Approach*, 2nd rev. ed., Wiley-VCH, Weinheim, Germany (2006).

3. R. Richards, *Surfaces and Nanomolecular Catalysis*, CRC, Taylor/Frances, Boca Raton (2006).

Supplementary Books

1. K. Bucholz and V. Kasche, *Biocatalysis and Enzyme Technology*, Wiley-VCH, New York (2005).
2. I. Chorkendorff and J.W. Niemantsverdriet, *Concepts of Modern Catalysis and Kinetics*, Wiley-VCH, Weinheim, Germany, New York (2003).
3. A. Weichkowsky et al., *Catalysis and Electrocatalysis at Nanoparticles Surfaces*, Marcel Dekker, New York (2003).
4. B.K. Hodnett, *Heterogeneous Catalysis Oxidation*, John Wiley and Sons, New York (2000).
5. S. Bhaduri and D. Mukesh, *Homogenous Catalysis: Mechanisms and Industrial Applications*, John Wiley-Interscience, New York (2000).
6. J. Tsuji, *Transition Metal Reagents and Catalysis: Innovation in Organic Synthesis*, John Wiley and Sons, Chichester/New York (2000).
7. S.M. Robert, *Biocatalysts for Fine Chemical Synthesis*, John Wiley and Sons, Chichester (1999).
8. R.J. Farrauto and C.H. Bartholomew, *Fundamentals of Industrial Catalytic Processes*, Blackie Academic Professional, London (1997).
9. B.C. Gates, *Catalytic Chemistry*, John Wiley & Sons, New York (1992).
10. Bond, *Heterogeneous Catalysis: Principles and Applications*, Clarendon Press, Oxford (1986).
11. J.M. Thomas and R.M. Lambert (Eds.), *Characterization of Catalysis*, John Wiley & Sons, Chichester (1980).
12. G.C. Bond, *Catalysis by Metals*, Academic Press, London (1962).

CHMI-720 Composite Materials (Cr. 3)

Materials, composite materials and their classification, matrices and reinforcements for composites. Reinforcements-matrix interface properties and processing of composites with metallic, ceramic and polymeric matrices. Mechanical, dynamic mechanical and thermal properties of composite materials. Toughening mechanisms and mechanical failure in polymeric composites. Spectroscopic and microscopic analyses.

Recommended Books

1. D.D.L. Chung, *Composite Materials: Functional Material of Modern Technologies*, Springer-Verlag, London (2003).

2. F.L. Mathews and R.D. Rawlings, *Composite Materials: Engineering and Science*, Chapman and Hall, London (1994).
3. T.L. Vigo and B.J. Kinzig, *Composite Applications: The role of Matrix, Fiber and Interface*, VCH, New York (1992).

Supplementary Books

1. B.C. Hoskin and A.A. Baker, *Composite Materials for Aircraft Structures*, American Institute of Aeronautics and Astronautics, Inc. New York (1986).
2. M.M. Schwartz, *Composite Materials: Processing, Fabrication and Applications*, Prentice Hall, PTR, New Jersey (1997).
3. L. Nicolais and G. Carotenuto, *Metal-Polymer, Nanocomposites*, Wiley Interscience (2005).
4. T.S. Pinnavaia and G.W. Beall, *Polymer-Clay Nanocomposites*, John Wiley & Sons (2000).

CHMI-721 Water and Soil Chemistry (Cr. 3)

Aquatic environment: hydrological cycle, water quality criteria, physical, chemical and biological characteristics of water, utilization, contamination and protection of water resources, collection and preservation of water samples. **Physico-chemical analysis of water:** Fresh water bodies, stratification and turn-over. **Eutrophication:** Causes and control. **Water pollution:** Soap, detergents and agricultural sprays. **Water management:** Policies and tools. **Deposition of sediments:** Trace metals in the hydrocycle and sediments, quantification of environmental impact in sediments. **Formation and composition of soil:** Soil types and their properties, soil degradation and pollution, soil management for sustainable agriculture. **Contamination of soils:** Analysis of physical and chemical characteristics of soils, effects of mining on geoenvironment. **Geological hazards and geotechnology:** Standards and guidelines for water and soil quality by national and international organizations/agencies.

Recommended Books

1. R.M. Harrison, *An Introduction to Pollution Science*, The Royal Society of Chemistry, UK (2006).
2. D. Langmuir, *Aqueous Environmental Geochemistry*, Prentice Hall, New Jersey (1997).
3. S.E. Manahan, *Environmental Science and Technology*, Lewis Publishers, New York (1997).

Supplementary Books

1. H.L. Bohn, *Soil Chemistry*, John Wiley & Sons, New York (1985).
2. P. Evangelou, *Environmental Science and Water Chemistry*, John Wiley & Sons, Inc., New York (1998).

3. L. Friberg, G.F. Nordberg and V.B. Vouk, *Handbook on the Toxicology of Metals*, Volume 1, Elsevier Science Publishers, Amsterdam (1986).
4. P. Patnaik, *Handbook of Environmental Analysis*, CRC Press Inc., Florida, USA. (1997).
5. B.J. Alloway, *Heavy Metals in Soils*, John Wiley & Sons Inc., New York (1990).
6. APHA, AWWA and WPCF, *Standard Methods for the Examination of Water and Wastewater*, 20th ed., Washington DC, USA (1998).
7. R.A. Bailey, H.M. Clark, J.P. Ferris, S. Krause and R.L. Strong, *Chemistry of the Environment*, 2nd Edition, Academic Press, London (2002).

CHMI-722 Atmospheric Chemistry (Cr. 3)

Atmospheric structure: Natural constituents, anthropogenic emissions and atmospheric pollution. **Air quality criteria pollutants:** Sources, dispersion models and sinks of atmospheric pollutants. **Measurement and monitoring methods:** Gaseous pollutants and particulate matter in the atmosphere, dry and wet depositions. **Effects:** Effects of air pollutants on humans, animals, plants, materials and visual range, controlling the anthropogenic pollutants. **Photochemical smog-formation:** Types and effects. **Acid rain:** Causes, effects and control. **Ozone Chemistry:** Stratospheric ozone production and depletion, causes and significance of ozone hole, catalytic and non-catalytic processes, effects of UV on the biosphere. **Global warming:** Green house gases, production, control and future trends of green house gases, consequences of global warming. **Control management:** Standards and legislation regarding the atmospheric pollution.

Recommended Books

1. J. Colls, *Air Pollution-An Introduction*, SPON Press, Taylor & Francis Group, London (1997).
2. S.E. Manahan, *Environmental Science and Technology*, Lewis Publishers, New York (1997).
3. R. Miroslav and N.B. Vladimir, *Practical Environmental Analysis*, The Royal Society of Chemistry, UK (1999).

Supplementary Books

1. J.H. Seinfeld, *Atmospheric Chemistry and Physics of Air Pollution*, John Wiley & Sons, New York (1986).
2. J.H. Seinfeld and S.N. Pandis, *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change*, John Wiley & Sons, New York (1998).
3. WHO, *Guidelines for Air Quality*, World Health Organization, Geneva (2000), ([www.who.int/environmental information/Air/Guidelines/aqguide7pdf](http://www.who.int/environmental_information/Air/Guidelines/aqguide7pdf))
4. P. Patnaik, *Handbook of Environmental Analysis*, CRC Press Inc., Florida, USA

(1997).

5. R.A. Bailey, H.M. Clark, J.P. Ferris, S. Krause and R.L. Strong, *Chemistry of the Environment*, 2nd ed., Academic Press, London (2002).
6. R.M. Harrison, *An Introduction to Pollution Science*, The Royal Society of Chemistry, UK (2006).
7. S.T. Holgate, J.M. Samet, H.S. Koren and R.L. Maynard, *Air Pollution and Health*, Academic Press, New York (1999).

III. Organic Chemistry

CHM-710 Applied Chemometrics (Cr. 2 + 1)

Introduction: Basics of Chemometrics. **Multivariate structure of data:** Matrices, dimension, transposition, centering, covariance, correlation, pretreatment of the data, transformation of variables, handling of missing data. **Principal component analysis:** Loading plots, score plots, choice of principal components (rank analysis), both numerically and graphically (scree plot). **Clusters analysis:** Distance matrix, similarity matrix, Dendrograms. **Linear discriminant analysis:** Correlation matrix, covariance matrix, correlations, correlogram, Box tests, Kullback's test, Wilks' lambda test, Bartlett's test, loading plots, score plots Eigen values. **Calibration:** Linear regression, Regression coefficients, Correlation coefficient, Prediction coefficient, Standard error of the estimate, Principal Component Regression (PCR), Partial Least Squares Method (PLS). **Practical examples:** Working with spectroscopic instruments (NIR, FTIR, UV/Vis, NMR, MS, ICP-OES, ICP-MS), chromatography instruments (LC, GC, HPLC).

Teaching and Learning Methods/Tools

Lectures, video projector for explanation of spreadsheets, and Computer exercises (acquisition of specific informatics tools; software for mathematics and statistics including Microsoft Excel, XLSTAT, SPSS, R, MINITAB etc).

Assessment Methods

Individual report submission (Text Document) by students about a chemometric problem, relevant to a dataset provided by the teacher.

Viva Voce Examination about the final report and the theory explained in the class room lessons (definitions and demonstrations).

Final mark: Mark assigned to report + Mark assigned to oral exam

Recommended Books

1. H. Martens, M. Martens, *Multivariate Analysis of Quality: An Introduction*, John Wiley (2001).
2. H. Mark, *Principles and Practice of Spectroscopic Calibration*, John Wiley (1991).
3. M. Otto, *Chemometrics Statistics and Computer Application in Analytical Chemistry*, Wiley - VCH (1999).

4. J.W. Einax, H.W. Zwanziger, S. Geiss, *Chemometrics in Environmental Analysis*, VCH (1997).
5. J.C. Miller, J.N. Miller, *Statistics and Chemometrics for Analytical Chemistry*, Pearson Education (2010).
6. R.G. Brereton, *Applied Chemometrics for Scientists*, Wiley (2007).
7. R. Kramer, *Chemometric Techniques for Quantitative Analysis*, Marcel Dekker (1998).

CHMO-711 Modern Name Reactions in Organic Synthesis (Cr. 3)

Recent modifications and advancements in classical name reactions: Evans Aldol Condensation, Mukaiyama Aldol, Barton-McCombie Reaction, Baylis-Hillman Reaction, Biginelli Reaction, Bishler-Napieralski Reaction, Blanc Reaction, Brook Rearrangement, Castro-Stephens Coupling, Cory-Kim Oxidation, Dakin-West Reaction, Hetero-Diels-Alder Reaction, Eschenmoser Fragmentation, Friedlander Synthesis, Horner-Wadsworth-Emmons reaction, Milas Hydroxylation Reaction, Pictet-Spengler Ritter Reaction, Doebner Modification. **Recent name reactions and their application:** Sharpless Dihydroxylation, reactions, CBS reduction, Dess-Martin Oxidation, Swern Oxidation, Stephen aldehyde synthesis, Corey-Fuchs reaction, Fukuyama, Sonogashira, Stille Suzuki, McMurry and Heck coupling, Ugi reaction, Wittig Rearrangement, Mitsunobu Reaction, McMurry coupling, Fujimoto-Belleau reaction, Tebbe olefination, Tamao oxidation, Weinreb synthesis..

Recommended Books

1. L. Kurti and B. Czako, *Strategic Applications of Name Reactions in Organic Synthesis*, Academic Press, New York (2005).
2. L. Kurti and B. Czako, *Name Reactions and Reagents in Organic Synthesis*, 2nd ed., Elsevier, Amsterdam (2005).
3. B. P. Mundy, M. G. Eller, et al., *Name Reactions and Reagents in Organic Synthesis*, John Wiley, New York (2005).

Supplementary Books

1. T. Laue and A. Plagens, *Name Organic Reactions*, John Wiley and Sons: Chichester, England, New York (1998).
2. J. J. Li, *Name Reactions: A Collection of Detailed Reaction Mechanisms*, 3rd ed., Springer-Verlag, Berlin (2006).

CHMO-712 Computational Chemistry/Molecular Modeling (Cr. 3)

Basic concepts: Wave function and Schrödinger wave equation, probability distribution of wave function. **Molecular mechanics:** Single point energy calculations, geometry optimization and molecular modeling. **Semiempirical and ab initio molecular orbital methods:** Prediction of molecular properties, spectra and reactivity of organic compounds. **Molecular docking and QSAR:** Use of available software packages e.g.,

Hyperchem and Gaussian for MO calculations, MOE and Autodock for QSAR and molecular docking.

Recommended Books

1. A. Hinchcliffe, *Modelling Molecular Structures*, John Wiley and Sons, England (2000).
2. H.J. Cremer, *Essentials of Computational Chemistry*, 2nd ed., Theories and Models (2004).

Supplementary Books

1. A. Frisch and J.B. Foresman, *Exploring Chemistry with Electronic Structure Methods (Paperback)*, Gaussian Publishers (1993).
2. A.R. Leach, *Molecular Modelling: Principles and Applications*, Prentice Hall (2001).
3. A.K. Rappé and C.J. Casewit, *Molecular Mechanics across Chemistry*, University Science Books, Sausalito CA (1997).

CHMO-713 Protecting Groups in Organic Synthesis (Cr-3)

Introduction: characteristics of good protecting groups. **Protection of various functional groups:** Hydroxyl, thiols, carbonyl, amino and carboxylic groups. **Synthetic applications:** Protection and deprotection of the various functionalities in organic synthesis including peptide bond formation.

Recommended Books

1. P.J. Kocienski, *Protecting Groups*, George Thieme Verlag, Stuttgart Germany (2003).
2. A.J. Person and W.R. Roush, *Activating Agents and Protecting Groups*, John Wiley and Sons, New York (1999).
3. T.W. Greene and P.G.M. Wuts, *Protective Groups in Organic synthesis*, John Wiley and Sons New York (1999).

Supplementary Books

1. J.R. Hanson, *Protecting Groups in Organic Synthesis*, Blackwell Science Ltd. (1999).

CHMO-714 Organic Synthesis-Retrosynthetic Approach (Cr.3)

Introduction: Basic definitions of retrosynthesis and disconnection approach. **Synthesis of aromatic compounds:** One and two group C-X disconnections. **Synthons:** Definitions and different types of donor and acceptor synthons, concept of “Umpolung”. **C-C disconnections of difunctionalised compounds:** Dicarbonyl compounds such as 1,2; 1,3; 1,4; 1,5 and 1,6 diO compounds. **Synthesis of ring compounds:** Three, four,

five six, seven and eight membered carbocycles and heterocycles. **Devising synthetic schemes:** Joint application of the concepts to unknown molecules and some natural products.

Recommended Books

1. S. Warren, *Organic Synthesis: the Disconnection Approach*, John Wiley & Sons Ltd. (1992).
2. J. Clayden, N. Greeves. S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press (2001).
3. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Blackie Academic and Professional, London, 1993.

Supplementary Books

1. W. Carruthers, *Modern Method of Organic Synthesis*, Cambridge University Press (1971).
2. S. Warren, *Designing Organic Syntheses*, J. Wiley & Sons, Chichester (1982).
3. T.W. Greene and P.G.M. Wuts, *Protective Group in Organic Synthesis*, John Wiley & Sons, Inc (1999).
4. J. Fuhrhop and G. Penzlin, *Organic Synthesis*, 2nd Edition, VCH, Weinheim, Germany (1994).

CHMO-715 Advanced Stereochemistry (Cr. 3)

Configuration and conformation of cyclic molecules: Stereochemistry and conformational analysis of cyclohexane systems, six-membered sp²-hybridized cyclic systems, six-membered saturated heterocycles. **Stereochemistry and conformational effects in ring systems:** Small, common and medium bicyclic and polycyclic fused rings; bridged rings and stereochemical restrictions. **Chiroptical properties:** Optical rotatory dispersion (ORD) and circular dichroism (CD).

Recommended Books

1. E.L. Eliel, S.H. Wilen and M.P. Doyle, *Basic Organic Stereochemistry*, Wiley Interscience, New York (2003).
2. D. Nasipuri, *Stereochemistry of Organic Compounds-Principles and Applications*, New Age international Publishers (P) Limited, New Delhi, India (1991).
3. P.S. Kalsi, *Stereochemistry and Mechanism Through Solved Problems*, New Age International Publishers, New Delhi, India (2001).

Supplementary Books

1. J. Eames (Queen Mary and Westfield College, University of London) and J.M. Peach, *Stereochemistry at a Glance*, Blackwell Publishing (2003).
2. D.G. Morris, *Stereochemistry*, Royal Society of Chemistry, U.K. (2001).
3. R. Gabba, *Stereochemistry*, Campus Books International, New Delhi, India (2002).

CHMO-716 Physical Organic Chemistry (Cr. 3)

History and development: Evolution of a hybrid discipline, energy changes during chemical reactions, theory and principles related to kinetics and equilibrium processes. **Correlation of structure and reactivity:** Hammett equation and other linear free energy relationships. **Hückel molecular orbital (HMO) method:** Correlation of HMO parameters with molecular properties, alternant and nonalternant hydrocarbons and their properties. **Correlation of structure and activity:** Use of molecular descriptors, Hansch analysis, Craig plots, Topliss scheme in establishing SAR. **FMO method:** Concept of Frontier orbitals and its application for explaining chemical reactivity.

Recommended Books

1. Miller, *Advanced Mechanisms in Organic Chemistry*, Pearson Education (2004).
2. T.H. Lowry and K.H. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd ed., Harper & Row Publisher (1987).
3. N.S. Issacs, *Physical Organic Chemistry*, Longman Group (1995).
4. A. Streitwieser, Jr., *Molecular Orbital Theory for Organic Chemists*, Wiley, New York (1961).

Supplementary Books

1. E.V. Anslyn, *Modern Physical Organic Chemistry*, University Science Books, US (2006).
2. F.L. Ansari, R. Qureshi and M.L. Qureshi, *Electrocyclic Reactions-from Fundamentals to Research*, Wiley-VCH (1999).
3. C. Hansch and A. Leo and D.H. Hoekman, *Exploring QSAR: Fundamentals and Applications in Chemistry and Biology*, ACS (1995).
4. A. Pross, *Theoretical & Physical Principles of Organic Reactivity*, Wiley Interscience (1995).

CHMO-717 Nuclear Magnetic Resonance in Organic Chemistry (Cr. 3)

Spin couplings: Spin coupling in different spin systems. **Double resonance experiments:** Spin decoupling in ¹H- and ¹³C-NMR spectroscopy, suppression of solvent signal, ¹H BB decoupling, gated decoupling, ¹H off-resonance decoupling. **1D NMR**

experiments with complex pulse sequence: The *J*-modulated spin echo, SPI, INEPT and DEPT experiments. **2D NMR Spectroscopy:** Introduction, theory and presentation of 2D spectrum. **2D *J*-resolved NMR spectroscopy:** Homo- and hetero-nuclear 2D *J*-resolved NMR spectroscopy. **2D shift-correlated NMR spectroscopy:** H,H-COSY, H,C-COSY, NOESY, ROESY, HMBC, HMQC and TOCSY experiments. **Applications:** NMR use as a tool for structure elucidation and stereochemical assignments.

Recommended Books

1. H. Friebolin, *Basic one-and two-dimensional NMR spectroscopy*, 4th ed., Wiley-VCH, New York (2005).
2. D. Canet, *Nuclear magnetic resonance: concepts and methods*, John Wiley & Sons, Chichester, England (1996).
3. Atta-ur-Rehman and M.I. Chaudhry, *Solving problems with NMR spectroscopy*, Academic Press, California (1996).
4. R. M. Silverstein, F. X. Webster and D. J. Kiemle, *Spectrometric identification of organic compounds*, John Wiley & sons Inc., USA (2005).

Supplementary Books

1. R.S. Macomber, *NMR spectroscopy: basic principles and applications*, Harcourt Brace Jovanovich Publishers, San Diego (1988).
2. S. Berger and S. Braun, *200 and more NMR experiments*, Wiley-VCH, Weinheim, Germany (2004).
3. *Handbook of proton-nmr spectra and data*, Asahi Research Center Co., Academic Press, New York (1985).
4. J.K.M. Sanders, et al., *Modern NMR spectroscopy: a guide for chemists*, The University Press, Oxford (1993).
5. Breitmaier and Eberhard, *Structure elucidation by NMR in organic chemistry: a practical guide*, John Wiley, West Sussex (2002).
6. Y.C. Ning, *Spectral Identification of organic compounds with spectroscopic techniques*, Wiley-VCH, Weinheim (2005).

CHMO-718 Advances in Chromatographic Techniques (Cr. 3)

Introduction: Principles of chromatographic separation. **Conventional chromatographic techniques:** Paper, thin layer, and column chromatography. **Pressure chromatographic techniques:** High performance-, medium pressure-, high pressure thin layer liquid-, vacuum liquid-, flash-, centrifugal thin layer- and gas chromatography. **Liquid-liquid chromatography:** Droplet counter current, counter current distribution, and rotation locular counter current chromatography. **Miscellaneous chromatographic techniques:** Paper electrophoresis and capillary zone electrophoresis. **Hyphenated chromatographic techniques:** Gas chromatography- mass spectrometry and liquid

chromatography-mass spectrometry. **Application of chromatographic techniques:** Separation of natural products and mixtures of other organic compounds.

Recommended Books

1. K. Hosttettman, A. Marston and M. Hostettmann, *Preparative chromatography Techniques*, Springer (1997).
2. Richard J. P. Canel (editor), *Natural products isolation*, Humana press, New Jersey, USA (1998).
3. W.M.A Niessen and J. Van der Greef, *Liquid Chromatography-mass spectrometry: principles and applications*, Marcel Dekker, New York (1992).

Supplementary Books

1. H.M. McNair and J.M. Miller, *Basic Gas Chromatography*, John Wiley & Sons, Inc. (1998).
2. D. Hage, *Handbook of Affinity Chromatography*, Hage David Saylor & Francis, Inc. (2005).
3. B. Kolb and L.S. Ettre, *Static Headspace-Gas Chromatography: Theory and Practice*, Wiley, John & Sons, Inc. (2006).
4. P.R. Brown, *Advances in Chromatography*, Vol. 41, E. Grushka (Ed.), Marcel Dekker (2001).
5. P.R. Brown, *Advances in Chromatography*, Vol. 40, E. Grushka (Ed.), Marcel Dekker (2000).
6. P.R. Brown, *Advances in Chromatography*, Vol. 37, E. Grushka (Ed.), Marcel Dekker (1997).
7. R.E. Ardrey, *Liquid Chromatography – Mass Spectrometry: An Introduction*, John Wiley & Sons (2003).

CHMO-719 Chemistry of Isoprenoids and Steroids (Cr. 3)

Introduction, classification, isolation, structure elucidation, reactions and biological activity: Terpenes, bile acids, cholesterol, ergosterol, vitamin D, estrogens, gastrogens, androgens, adrenocortical hormones, cardiac steroids and bufadienolides. **Total synthesis:** Equilinen, cholesterol, oestrone and epiandrosterone.

Recommended Books

1. D.F. Cane, D.H.R. Barton, K. Nakanishi and O. Meth-Cohn, *Comprehensive Natural Products Chemistry: Isoprenoids Including Carotenoids and Steroids*, Vol. 2, Elsevier Science Ltd. (1999).
2. K. Nakanishi, T. Goto, S. Ioto, S. Natori, S. Nozone, et al., *Natural Products Chemistry*, Vol. 1, Academic Press Inc, New York (1974).

3. F.L. Ansari, R. Quershi and M.L. Quershi, *Electrocyclic Reactions*, John Wiley & Sons (1999).

Supplementary Books

1. F.J. Leeper, *Biosynthesis: Aromatic Polyketides, Isoprenoids, Alkaloids*, Springer Verlag (2000).
2. S.V. Bhat, B.A. Nagasampagi and S. Minakshi, *Chemistry of Natural Products*, Narosa Publishing House (2005).
3. J.H. Fuhrhop and C. Endisch, *Molecular and Supramolecular Chemistry of Natural Products and Their Model Compounds*, Macel Dekker, Inc. New York (2000).

CHMO-720 Chemistry of Glycosides (Cr. 3)

Introduction: Glycosides of flavonoids, coumarins and saponins, isolation, detection and chromatographic separation, biological importance of glycosides. **Chemical reactions:** Acid, alkaline and enzymatic hydrolysis to aglycones, derivatization. **Structure elucidation:** Identification of sugar residue, spectroscopic determination of aglycones and glycosides.

Recommended Books

1. R. Ikan (Ed.), *Naturally Occurring Glycosides*, Wiley, John & Sons, Inc. (1999).
2. B.A. Bohm, *Introduction to Flavonoids*, Harwood Academic Publishers, Canada (1998).
3. K.R. Markham, *Techniques of Flavonoid Identification*, Academic Press, London (1982).
4. J.B. Harborn, *The Flavonoids – Advances in Research Since 1986*, Chapman & Hall, London (1994).

Supplementary Books

1. J. Mann, R.S. Davidson and J.B. Hobbs, *Natural Products: Their Chemistry and Biological Significance*, Longman Group UK Limited (1994).
2. D. Crich, *Reagents for Glycoside, Nucleotide and Peptide Synthesis*, John Wiley & Sons (2005).
3. D.E. Levy and C. Tang, *The Chemistry of C-glycosides*, Pergamon Press (1995).
4. K. Hostettmann and A. Marston, *Saponins*, Cambridge University Press (2005).
5. V. Ahmed and A. Basha, *Spectroscopic Data of Saponins*, Vol. III, CRC Press (2000).

6. R. O'Kennedy, R.D. Thornes, *Coumarins: Biology, Applications and Mode of Action*, John Wiley & Sons (1997).
7. R. Douglas, H. Murray and J. Méndez, *The Natural Coumarins: Occurrence, Chemistry, and Biochemistry*, Stewart Anglin Brown (1982).

CHMO-721 Biosynthesis of Natural Products (Cr. 3)

Introduction: Classification of natural products, primary and secondary metabolites, enzymes and coenzymes. **Biosynthesis:** Fatty acids, polyketides, isoprenoids, amino acids and alkaloids. **Metabolites from shikimic acid:** ArC₁, ArC₂ and ArC₃ metabolites. **Mixed biosynthesis:** Metabolites derived from acetate and mevalonate, shikimate and mevalonate, acetate and shikimate, tryptophan and mevalonate.

Recommended Books

1. S.P. Stanforth, *Natural Product Chemistry at a Glance*, Oxford: Blackwell (2006).
2. J. Mann, *Secondary Metabolism*, Oxford Science Publications, (1987).
3. J.D. Bu'Lock, *The Biosynthesis of Natural Products*, McGraw-Hill, London (1965).

Supplementary Books

1. S. Ranganathan, *Art in Biosynthesis*, Academic Press, New York (1976).
2. R.H. Thomson (Ed.), *The Chemistry of Natural Products*, 2nd ed., Springer-Verlag New York, LLC (1993).
3. R.B. Herbert, *The Biosynthesis of Secondary Metabolites*, Springer-Verlag, New York, LLC (1989).
4. K. Nakanishi, T. Goto, S. Ioto, S. Natori, S. Nozone, et al., *Natural Products Chemistry*, Vol. 1, Academic Press Inc, New York (1974).

CHMO-722 Chemistry of Organometallic Compounds (Cr. 3)

Introduction, synthesis, reactivity and reactions: Grignard's reagents and alkyllithium. **Applications:** Alkyllithium as metallating agents in organic synthesis. **Organotransition metal compounds:** Organo palladium compounds, cupperates and organo zinc compounds, their synthesis and applications.

Recommended Books

1. M.Gielen, R. Willem and B. Warckmeyer (Eds.), *Physical Organometallic Chemistry*, Vol.3, John Willey and Sons, New York (2002).
2. L.S. Heqedus and L.G. Wade, *Transition Metals in the Synthesis of Complex Organic Molecules*, 2nd ed., John Willey and Sons. Ltd., New York (1999).

3. M. Schlosser, *Organometallics in Synthesis*, John Willey and Sons, Ltd. New York (1996).
4. A.W. Parking and R.C. Poller, *An Introduction to Organometallic Chemistry*, McMillian Education Ltd., New York (1987).
5. E.I. Negishi, *Organometallics in Organic Synthesis*, Vol.1, John Willey and Sons, New York (1980).

Supplementary Books

1. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University (2001).
2. G.M. Loudon, *Organic Chemistry*, 4th ed., Oxford University Press, New York (2002).

CHMO-723 Reactive Intermediates in Organic Chemistry (Cr. 3)

Introduction: Reactive intermediates and transition states. **Carbocations:** Classical and non-classical carbocations, reactions of non-classical carbocations with stereochemical aspects, pericyclic reactions involving carbocations. **Carbanions:** Generation of carbanions, kinetic and thermodynamic control, stability and reactions, carbanions stabilized by heteroatoms, rearrangements. **Free radicals, carbenes, nitrenes and arynes:** Generation and reactions, relative stability and stereochemical aspects of reactions.

Recommended Books

1. R. A. Moss, M. S. Platz and Maitland Jr. (Eds.), *Reactive Intermediate Chemistry*, Jones. Wi (2004).
2. N. Issac, *Reactive Intermediate in Organic Chemistry*, John Wiley and Sons (1974).
3. M. Jones and R. A. Moss, *Reactive Intermediates*, John Wiley and Sons, New York (1978).

Supplementary Book

1. M.B. Smith and J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, John Wiley & Sons (2007).

CHMO-724 Advanced Heterocyclic Chemistry (Cr. 3)

Oxygen, nitrogen and sulphur containing heterocycles: Synthesis, reactions, stereochemistry and spectroscopy. **Heterocycles with more than one heteroatom:** Synthesis, reactions and spectroscopy of five - seven membered heterocycles. **Fused ring systems:** Benzofused five - seven membered heterocycles.

Recommended books

1. H. El-Syed, *Heterocyclic Chemistry*, Blackwell Publishing (2006).
2. J. Joule, *Synthesis of Naturally Occurring Heterocycles from Carbohydrates*, Blackwell Publishing (2006).
3. R.K. Bansel, *Heterocyclic Chemistry*, New Age International, New Delhi (1996).

Supplementary Books

1. R.H. Acheson, *An Introduction to Chemistry of Heterocycles Compounds*, 3rd ed., John Wiley, New York (1976).
2. J.M. Loudon, *Organic Chemistry*, Oxford University Press (2002).
3. F.A. Carey, R.J. Sandberg, *Advance Organic Chemistry*, Kulver Academic/Plenum Publisher (2000).

CHMO-725 Advanced Mass Spectrometry (Cr. 3)

Introduction: Aims and scope, theory and basic terminology. **Instrumentation:** Instrumental design, ionization techniques, types of analyzers and detectors. **Applications:** Modes of fragmentation of various organic compounds, interpretation of mass spectra of unknown organic compounds.

Recommended Books

1. C.G. Herbert and D.P. Schulz, *Mass Spectrometry Basics*, Taylor & Francis, New York (2003).
2. F.W. McLafferty, F. Turecek and J. Choi, *Interpretation of Mass Spectra*, University Science Books, California (1993).
3. E. De Hoffmann, J. Charette and V. Stroobant, *Mass Spectrometry, Principles & Applications*, John Willey & sons (1996).

Supplementary Books

1. J.H. Gross, *Mass Spectrometry*, Springer-Verlag New York (2004).
2. A.Frigerio, *Essential Aspects of Mass Spectrometry*, Spectrum Publications Inc. New York (1974).
3. H.E. Duckworth, R.C. Barber and V.S. Venkatasubramanian, *Mass Spectroscopy*, Cambridge University Press, London (1986).
4. R.E. Ardrey, *Liquid Chromatography – Mass Spectrometry: An Introduction*, John Wiley & Sons (2003).
5. S.M. Nelms, *Inductively Coupled Plasma Mass Spectrometry Handbook*, Taylor & Francis, New York (2005).

CHMO-726 Organic Photochemistry (Cr. 3)

Introduction: Electronic structure of molecules, electronic transitions, radiative and non-radiative processes, energy transfer and sensitization, hydrogen abstraction. **Photochemical reactions:** Photo-elimination, photo-substitution, photo-oxidation and photo-reduction of carbonyl compounds and olefins. **Pericyclic reactions:** Photochemical dimerization, cycloadditions and rearrangements. **Applications:** Photochemical organic industrial processes.

Recommended Books

1. J.D. Coyle, *Introduction to Organic Photochemistry*, Wiley & Sons Inc. (1986).
2. J. Kopecky, *Organic Photochemistry*, John Wiley & Sons Inc. (1991).
3. A.G. Griesbeck, *Synthetic Organic Photochemistry*, Marcel Dekker Inc. (2004).
4. V. Ramamurthy, *Organic Photochemistry*, Marcel Dekker Inc. (1997).

Supplementary Books

1. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Chapman Hall, London (1993).
2. M.B. Smith and J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, John Wiley & Sons (2007).

CHMO-727 Organic Polymer Chemistry (Cr.3)

Fundamental concepts: types of polymers, classification. **Mechanism and kinetics:** Step growth, free radical addition polymerization, ionic polymerization, Ziegler-Natta polymerization. **Stereochemistry:** Definition and examples of Isotactic, atactic, syndiotactic polymers and their stereoregulation. **Molecular weight determination:** Different methods used to determine the absolute and relative molecular weights of polymers. **Structure-property relationship. Reactions of synthetic polymers. Polymer degradation and stability:** Special emphasis on thermal and photo-degradation.

Recommended Books

1. H.R. Allcock, F.W. Lampe and J.E. Mark, *Contemporary Polymer Chemistry*, 3rd ed., Pearson Education mc, Pearson Prentice Hall (2003).
2. F.W. Billmeyer Jr., *A Textbook of Polymer Science*, J. Wiley & Sons, Pte. Ltd., Singapore (1994).
3. G. Odian, *Principles of Polymerization*, 4th ed., John Wiley & Sons, Inc. (2004).

Supplementary Books

1. M.S. Bhatnagar, *A Textbook of Polymers*, Vol. I, II, III, S. Chand & Co. Ltd. (2004).

2. L.H. Sperling, *Introduction to Physical Polymer Science*, 2nd ed., John Wiley & Sons (1992).
3. J.R. Fried, *Polymer Science & Technology*, Prentice Hall, Inc. (1995).

CHMO-728 Pericyclic Reactions (Cr. 3)

Introduction and significance: Concerted and nonconcerted processes, pericyclic reactions, their classification and examples. **Mechanism and analysis:** Analysis of pericyclic reactions based on orbital symmetry conservation, frontier orbital method, Möbius-Hückel approach and theoretical & computational approach. **Synthetic application:** Synthesis of carbocycles and heterocycles through pericyclic reactions.

Recommended Books

1. F.L. Ansari, R. Qureshi and M.L. Qureshi, *Electrocyclic Reactions from Fundamentals to Research*, Wiley – VCH (1999).
2. T.H. Lowry and K.H. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd ed., Harper & Row Publisher (1987).
3. F.A. Carey and R.J. Sandberg, *Advance Organic Chemistry*, Kulver Academic/Plenum Publisher (2000).

Supplementary Books

1. G.M. Loudon, *Organic Chemistry*, 3rd ed., The Benjamin/Cummings Publishing Company (1995).
2. E.A. Halevi, *Orbital Symmetry and Reaction Mechanism*, Springer Verlag (1992).
3. T. Rauk, *Orbital Interaction Theory of Organic Reaction*, John Wiley (1994).
4. R.T. Morrison and R.N. Boyd, *Organic Chemistry*, 6th ed., Prentice Hall, New Jersey (1992).
5. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University (2001).
6. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Chapman Hall, London (1993).

CHMO-729 Special Topics in Organic Chemistry (Cr. 3)

Topics under recent investigation and of current interest (the choice will depend upon the interests of the teacher giving this course).

CHMO-730 Medicinal Chemistry (Cr. 3)

Introduction: Historical perspectives of drug targets, pharmacokinetics and pharmacodynamics. **Biological screening:** Different types of bioassays, *in vitro* and *in*

in vivo testing of different compounds. **Drug discovery:** The lead compound, natural and synthetic sources of lead compounds. **Drug synthesis:** Combinatorial and solid phase synthesis of drug like compounds. **Structure activity relationship:** Calculation of molecular descriptors using different available software, Hansch analysis and use of Craig plots and Topliss scheme for the synthesis of lead analogs. **Binding interactions:** Different types of receptor-ligand interaction, functional group as binding groups and their bioisosters. **Computer assisted drug designing:** Generation of pharmacophore, receptor- and ligand-based drug designing.

Recommended Books

1. J.N. Delgado and W.A. Remens, *Textbook of Organic and Medicinal Chemistry*, 10th ed., Lippincott William and Wilkins (1998), 11th ed. (2004).
2. C.L. Patrick, *Introduction to Medicinal Chemistry*, OUP (2001).
3. P.K. Larsen, *Drug Design and Development*, 2nd ed., Harward Academic Publishers (1996).

Supplementary Books

1. G. Thomas, *Fundamentals of Medicinal Chemistry*, John Wiley (2003).
2. *Advanced Pharmaceutics*, C.J CRC. Press (2004).
3. P. Sencer, *Solid Phase Synthesis and Combinatorial Technologies*, Wiley Intense (2000).
4. C.G. Wenments, *Medicinal Chemistry*, Academic Press (2004).
5. B. Yan, *Analytical Methods in Combinatorial Chemistry*, Technomic Publishers (2000).
6. R.B. Silverman, *The Organic Chemistry of Drug Design and Drug Action*, 2nd ed., Academic Press (2004).

CHMO-731 Cheminformatics (Cr. 3)

Basic concepts: Introduction, evolution, history and prospects. **Database design & their management:** Database concept and architecture, Structured Query Language (SQL), chemical database design & their tools, structure-based searches. **Chemical information sources:** History and future of scientific internet, chemical literature, communication in chemistry. **Cheminformatics for drug discovery:** Representation and manipulation of 2-D and 3-D molecular structures, computational models, similarity methods, analysis of high throughput screening data, virtual screening, combinatorial library designing, computing physical-chemical data and chemical registration systems.

Recommend Books

1. A.R. Leach and V.J. Gillet, *An Introduction to Cheminformatics*, Kluwer Academic Publishers (2003).

2. R.B. Siverman, *The Organic Chemistry of Drug Design and Drug Action*, Academic Press (2004).
3. P.K. Larson, *A Textbook of Drug design and Development*, Overseas Publishers Associations OPA (1996).

Supplementary Book

1. C.M. Bladen, *Pharmaceutical Chemistry*, John Wiley (2002).

CHMO-732 Advanced Stereoselective Synthesis (Cr. 3)

Biological significance of chirality: Stereogenic units and types of chirality, chiral natural products, need for stereoselective synthesis. **Strategies for synthesis of chiral compounds:** First and second generation methods: chiral starting materials and chiral auxiliaries; third and fourth generation methods: asymmetric reactions, reagents and catalysts. **Asymmetric total synthesis:** Diastereoselective and enantioselective syntheses.

Recommended Books

1. M. Nogradi, *Stereoselective Synthesis: A Practical Approach* Wiley VCH (1994).
2. R.S. Atkinson, *Stereoselective Synthesis*, Wiley, Chichester, (1995).
3. E.M. Carreira and O. Reiser, *Classics in Stereoselective Synthesis*, Wiley-VCH, Weinheim (2007).

Supplementary Books

1. A. Koskinen, *Asymmetric Synthesis of Natural Products*, Wiley (1993).
2. Guo-Qiang Lin, Yue-Ming Li, Albert S. C. Chan, *Principles and Applications of Asymmetric Synthesis*, Wiley-Interscience (2001).
3. G.R. Stephenson, *Advanced Asymmetric Synthesis*, Springer; 1st edition (1996).

CHMO-733 Special Organic Materials (Cr. 3)

Organic dyes: Chromophore structure, synthesis of azodyes and cyanins, reactive vs. direct textile dyes, Chemiluminescence, photochromocs, color photography. **Liquid Crystals:** definition, classification: thermotropic/lyotropic, calamitic/discotic, nematic/smectic columnar, synthesis and orientation, liquid crystal displays (LCD's), liquid crystal polymers. **Electronic materials:** Types of organic semi-conductors, polyacetylenes, and polyparaphenylenes, band structure, synthesis, electroluminescence and light emitting diodes (LED's).

Recommended Books

1. K.H. Klaus (Ed.), *Industrial Dyes*, Wiley-VCH, Verlag, GmbH & Co. (2003).

2. V.P. Shibaev and L. Lam (Eds.), *Liquid Crystalline and Mesomorphic Polymers*, Springer-Verlag, Inc., New York (1994).
3. P.J. Collings and M. Hird, *Introduction to Liquid Crystals: Chemistry and Physics*, Taylors and Francis (1997).

Supplementary Books

1. Dierking, *Textures of Liquid Crystals*, Wiley-VCH, Verlag, GmbH & Co. (2003).
2. J.W. Goodby and G.W. Gray, *Structures and Textures of Liquid Crystals*, Taylors and Frances (2006).
3. H. Zollinger, *Color Chemistry: Synthesis, Properties and Applications of Organic Dyes*, 3rd ed., Wiley-VCH (2003).
4. S.H. Kim (Ed.), *Functional Dyes*, Elsevier (2006).
5. T.S. Chung (Ed.), *Thermotropic Liquid Crystal Polymers: Thin-Film Polymerization, Characterization, Blends and Applications* (2001).

CHMO-734 Aroma and Flavor Chemistry (Cr. 3)

Introduction: Aroma and flavor, properties of a compound and its flavor. **Nature of flavor compounds:** Precursors and mechanisms for the formation of flavor compounds, classification of food flavors, natural and synthetic flavorings. **Flavor determination techniques:** Modern techniques for determination of food flavor, impacts of ionizing radiations on flavor. **Recent publications on the chemistry of flavor compounds in SCI journals of good reputation.**

Recommended Books

1. T.E. Acree, R. Teranishi, *Flavor Science: Sensible Principles and Techniques*, American Chemical Society, Washington, D.C. (1993).
2. A. Gabelman, *Bioprocess Production of Flavor, Fragrance, and Color Ingredients*, John Wiley & Sons, New York (1994).
3. R. Ikan, *The Maillard Reaction: Consequences for the Chemical and Life Sciences*, John Wiley & Sons, New York (1996).
4. D.B. Min, T.H. Smouse. *Flavor Chemistry of Fats and Oils*, The American Oil Chemists' Society, Champaign, Illinois (1985).

IV. Physical Chemistry

CHM-710 Applied Chemometrics (Cr. 2 + 1)

Introduction: Basics of Chemometrics. **Multivariate structure of data:** Matrices, dimension, transposition, centering, covariance, correlation, pretreatment of the data, transformation of variables, handling of missing data. **Principal component analysis:** Loading plots, score plots, choice of principal components (rank analysis), both numerically and graphically (scree plot). **Clusters analysis:** Distance matrix, similarity

matrix, Dendrograms. **Linear discriminant analysis:** Correlation matrix, covariance matrix, correlations, correlogram, Box tests, Kullback's test, Wilks' lambda test, Bartlett's test, loading plots, score plots Eigen values. **Calibration:** Linear regression, Regression coefficients, Correlation coefficient, Prediction coefficient, Standard error of the estimate, Principal Component Regression (PCR), Partial Least Squares Method (PLS). **Practical examples:** Working with spectroscopic instruments (NIR, FTIR, UV/Vis, NMR, MS, ICP-OES, ICP-MS), chromatography instruments (LC, GC, HPLC).

Teaching and Learning Methods/Tools

Lectures, video projector for explanation of spreadsheets, and Computer exercises (acquisition of specific informatics tools; software for mathematics and statistics including Microsoft Excel, XLSTAT, SPSS, R, MINITAB etc).

Assessment Methods

Individual report submission (Text Document) by students about a chemometric problem, relevant to a dataset provided by the teacher.

Viva Voce Examination about the final report and the theory explained in the class room lessons (definitions and demonstrations).

Final mark: Mark assigned to report + Mark assigned to oral exam

Recommended Books

1. H. Martens, M. Martens, *Multivariate Analysis of Quality: An Introduction*, John Wiley (2001).
2. H. Mark, *Principles and Practice of Spectroscopic Calibration*, John Wiley (1991).
3. M. Otto, *Chemometrics Statistics and Computer Application in Analytical Chemistry*, Wiley - VCH (1999).
4. J.W. Einax, H.W. Zwanziger, S. Geiss, *Chemometrics in Environmental Analysis*, VCH (1997).
5. J.C. Miller, J.N. Miller, *Statistics and Chemometrics for Analytical Chemistry*, Pearson Education (2010).
6. R.G. Brereton, *Applied Chemometrics for Scientists*, Wiley (2007).
7. R. Kramer, *Chemometric Techniques for Quantitative Analysis*, Marcel Dekker (1998).

CHMP-711 Physical Chemistry of High Polymers (Cr. 3)

Polymer interactions: Molecular forces and chemical bonding in polymers; configuration and conformation of polymer chains. Dimensions of polymer chain; RMS unperturbed end-to-end displacement length. **Polymer solutions:** Expansion factor in solutions; physical parameters affecting the chain dimensions; theta conditions. Theories of polymer solutions; phase separation and fractionation; solubility parameters; criteria for solubility. Plasticisation. **Molecular weights of polymers:** Molecular size measurement. Techniques for measuring: number-average; weight-average; z-average and viscosity-average molecular mass; universal curve. **Spectroscopic analysis:** UV,

FTIR and NMR techniques. **Thermal analysis:** TGA; DSC; DMA; glass transition temperature. **Morphology:** Amorphous and crystalline structures; semicrystalline nature; viscoelasticity; models and predictions; time-temperature dependency; polymer rheology; electrical and magnetic properties of polymers.

Recommended Books

1. A. Ravve, *Principles of Polymer Chemistry*, 2nd ed., Plenum Publishers, New York (2000).
2. F.W. Billmeyer, Jr., *Textbook of Polymer Science*, John Wiley & Sons, New York (1994).

Supplementary Books

1. J.R. Fried, *Polymer Science and Technology*, Prentice Hall/PTR (1995).
2. C.E. Carraher, *Seymour/Carraher's Polymer Chemistry*, 5th ed., Marcel Dekker, New York (2000).
3. J. Furnkaw, *Physical Chemistry of Polymer Rheology*, Springer-Verlag, Berlin (2003).
4. C. Tanford, *Physical Chemistry of Macromolecules*, John-Wiley and Sons, New York (1961).

CHMP-712 Advanced Quantum Chemistry (Cr. 3)

A brief overview of basic concepts and solution of four representative systems: Particle in a box, simple harmonic oscillator, rigid rotor and hydrogen atom. **Appropriate methods:** Variation and perturbation methods; application of variation method to molecular orbitals. **Many electron atoms:** Slater's determinants, electron spin and spin orbit interaction. **Molecular orbital (MO) and valence bond (VB) theory:** Homonuclear and homonuclear diatomic molecules. **Semiempirical and ab-initio:** MO treatment of molecules.

Recommended Books

1. I.N. Levine, *Quantum Chemistry*, 5th ed., Prentice Hall, New Jersey (2000).
2. A. Szabo, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Revised 1st ed., McMillan, New York (1996).

Supplementary Book

1. A. Szabo and N.S. Ostund, *Modern Quantum Chemistry*, McMillan, New York (1982).

CHMP-713 Electrode Process (Cr. 3)

Overview of electrode processes: Kinetics of electrode reactions. Mass transfer by migration and diffusion. **Electroanalytical techniques:** potential step and potential sweep methods. **Electrochemical impedance spectroscopy:** Effects of solution resistance and double layer capacitance. Electrode reactions with coupled homogeneous chemical reactions. **Industrial electrochemistry:** Corrosion study: detection, measurement, monitoring and remedial. **Energy conversion systems:** fuel cells and batteries. Digital simulation of cyclic voltammograms.

Recommended Books

1. A.J. Bard and L.R. Faulkner, *Electroanalytical Chemistry*, Marcel Dekker (1993).
2. D. Pletcher and F.C. Walsh, *Industrial Electrochemistry*, 2nd ed., Blackie Academic & Publisher (1993).

Supplementary Books

1. J.O'M. Bockriss, A.K.N. Reddy, and M.F. Gomboa, *Modern Electrochemistry: Electrodes in Chemistry, Engineering, Biology and Environmental Science*, 2nd ed., Springer (2000).
2. M. Mohammad and M. Amjad, *Principles of Electrode Kinetics*, Rooha Printers, Lahore (2000).
3. P.H., Reiger, *Electrochemistry*, Chapman and Hall, New York (1994).

CHMP-714 Magnetic Resonance Spectroscopy (Cr. 3)

Introduction to magnetic resonance: Principles of magnetic resonances spectroscopy; physical basis of nuclear magnetic resonance (NMR) spectroscopy; pulsed NMR methods. **NMR spectral parameters:** Chemical shift spin-spin coupling and its various types, treatment and analyses of AX_n, AMX and AB systems. NMR of nuclei other than ¹H and ¹³C. **NMR relaxation:** Mechanisms and their applications. **Other applications:** Dynamic NMR; two-dimensional NMR spectroscopy and its various types. NMR applications in structure elucidation. **Electron Spin Resonance (ESR) spectroscopy:** Principles; applications to solids and solutions.

Recommended Books

1. H. Friebolin, *One- and Two-Dimensional NMR Spectroscopy*, VCH, Weinheim (1993).
2. J.K.M. Sanders and B.X. Hunter, *Modern NMR Spectroscopy*, 2nd ed., Oxford University Press, UK (1993).
3. R.S. Alger, *Electron Paramagnetic Resonance*, John Wiley, New York (1968).

Supplementary Books

1. E.D. Becker, *High Resolution NMR: Theory & Chemical Applications*, New York, Academic Press (1980).
2. W.R. Groasmun and R.M.K. Carlson, *Two Dimensional NMR Spectroscopy*, VCH Publishers, New York (1987).
3. J.A. Pople, *High-Resolution Nuclear Magnetic Resonance*, McGraw-Hill, New York (1959).
4. C.P. Pople, *Electron Spin Resonance*, John Wiley, New York (1967).
5. P.B. Ayscough, *Electron Spin Resonance in Chemistry*, Methuen & Co., London (1967).

CHMP-715 Advanced Chemical Kinetics (Cr. 3)

Reactions in solutions: Diffusion-controlled reactions; applications of transition state theory; solvent effects on polar and ionic reactions; salt effects on reactions. Kinetic isotope effects. **Chain reactions:** Features of chain mechanisms; branching chain and oscillating reactions. **Determination of reaction orders:** Methods when the infinity reading is unknown; 0th-order or fractional order reactions with respect to a single concentration; rate expression and method of flooding; reactions with complex dependence on a single concentration variable. **Product catalyzed reactions:** Dual solution in consecutive reactions; series reaction with reversible step; prior-equilibrium and improved steady-state approximation. Concentration-jump methods for opposing reactions. **Methods of data analysis:** Linear free energy relation (LFER). Hammett correlation; acid-base catalysis; the Bronsted catalysis law; mechanisms of acid-base catalyzed reactions, reactivity-selectivity principle and iso-selectivity rule; intrinsic barrier and Hammond's postulate. Marcus equations and its applications.

Recommended Books

1. J.H. Espenson, *Chemical Kinetics and Reaction Mechanisms*, 2nd ed., McGraw-Hill, Singapore (1995).

Supplementary Books

1. A.A.M. Frost and R.G. Pearson, *Kinetics and Mechanism*, 3rd ed., Butterworths, London (1969).
2. R.A. Alberty and R.J. Silby, *Physical Chemistry*, John Wiley, New York (1995).

CHMP-716 Advanced Molecular Spectroscopy (Cr. 3)

General: Introduction of molecular spectroscopy; molecular symmetry and group theory. **Vibrators:** Rigorous treatment of microwave and IR spectra of non-rigid and polyatomic molecules. **Raman spectroscopy:** Principles; applications to diatomic and simple molecules; normal coordinate analysis. **Electronic spectroscopy:** Introduction to theories of molecular bonding; classification of molecular orbitals and electronic transitions; selection rules; electronic spectra of diatomic and simple polyatomic

molecules; dissociation and dissociation products; the Birge-Sponer method for characterization of the excited species; high resolution electronic spectra and rotational energy interaction; the Fortrat diagram and application.

Recommended Books

1. C.N. Banwell, *Fundamentals of Molecular Spectroscopy*, 3rd ed., McGraw-Hill, UK (1983).
2. J.D. Graybeal, *Molecular Spectroscopy*, International Edition, McGraw-Hill Book Company, New York (1988).
3. J.M. Hollas, *High Resolution Spectroscopy*, 2nd ed., Wiley, USA (1998).

CHMP-717 Photochemistry (Cr.3)

Fundamentals: Light and nature of electromagnetic radiations, electronic structure of atoms, interaction of light with atoms and molecules, term symbols, absorption and emission of radiations. Fluorescence, phosphorescence, Jablonski diagram, chemiluminescence, quantum yields of photochemical reactions, actinometry, kinetics of photochemical reactions. **Laws of photochemistry:** Photo excited molecules, monophotonic and multiphotonic processes, photodissociation. Photo-electrochemistry, photochemical reactions in gas phase and in solutions, photophysics and photochemistry of metal complexes. **Applied Photochemistry:** Photography, Photo-imaging, photochromism, vision, photochemistry of polymers, solar energy storage, photochemistry in synthesis, optical brighteners and photo-medicine.

Recommended Books

1. P. Suppan, *Chemistry and Light*, The Royal Society of Chemistry, London (1994).
2. R.P. Wayne, *Principles and Applications of Photochemistry*, Oxford University Press (1988).
3. Wayne and Richard P., *Photochemistry*, Macmillan (1988).
4. J.G. Calvert, and J.N. Pitts, *Photochemistry*, John Wiley and Sons Inc., New York (1966).
5. C.E. Wayne, *Photochemistry*, Oxford University Press, London (1996).
6. M. Bhaskaram, S. Sriram and K. Iniewski, *Energy Harvesting with Functional Materials and Microsystems*, CRC Publisher, Taylor and Francis group, UK (2014).
7. J. N. Pitts, G. S. Hammond, K. Gollnick. *Advances in Photochemistry*, Volume 12, John Wiley & Sons (2009).

CHMP-718 Advanced Photochemistry (Cr.3)

Principles of photochemistry: Primary and secondary chemical processes. **Electron transfer in photochemistry:** Collisional and coulombic modes; effect of temperature; eximers and exiplexes, the SET photochemistry, quantum yields. **Kinetics and energetic of photochemical reactions:** Mechanism of photochemical reactions; intersystem crossing; flash photolysis; mass spectrometric methods. **Experimental methods in photochemistry:** Low, medium and high pressure mercury lamps; resonance lamps; actinometers, phototubes; sources of high intensity flashes of light; laser and synchrotron radiations. **Photolytic studies:** Aqueous and non aqueous systems; effects of radiations on solids. **Applications in daily life and industry:** Picosecond and femtosecond flash photolysis, Supramolecular photochemistry.

Recommended Books

1. P. Suppan, *Chemistry and Light*, The Royal Society of Chemistry, London (1994).
2. R.P. Wayne, *Principles and Applications of Photochemistry*, Oxford University Press (1988).

Supplementary Books

1. J.G. Calvert, and J.N. Pitts, *Photochemistry*, John Wiley and sons Inc. New York (1966).
2. A. Cox and T.J. Kemp, *Introduction of Photochemistry*, McGraw-Hill, London (1971).

CHMP-719 Advanced Surface Chemistry (Cr. 3)

Solid-liquid interface: Wetting; heat of wetting; thermodynamic description of an interface; Gibbs-Duhem equation for an interphase, Gibbs adsorption isotherm, adsorption from solutions (dilute, liquid mixtures, non-electrolytes, electrolytes, etc.) at solid-liquid interface; detergency and flotation. **Study of liquid interfaces:** Kelvin's and Laplace equations. **Technical catalysis:** Catalyst preparation techniques; catalytic reactors; supported metal catalysts; industrial applications of heterogeneous catalysts. Catalysis for steam-reforming, CO- & CO₂-methanation; water-gas shift; Fischer-Tropsch synthesis reactions. Catalysts for syntheses of: ammonia; nitric acid; chemical fertilizers etc.

Recommended Books

1. S.J. Gregg and K.S.W. Sing, *Adsorption, Surface Area and Porosity*, 2nd ed., Academic Press, London (1982).
2. G.C. Bond, *Heterogeneous Catalysis: Principles and Applications*, 2nd ed., Clarendon Press, Oxford (1987).

Supplementary Books

1. M.J. Jaycock and G.D. Parfitt, *Chemistry of Interfaces*, Ellis Harwood Ltd, Chichester, UK (1981).

CHMP-720 Advanced Solution Chemistry (Cr. 3)

Solutions: Classification; their importance in chemistry, industry and life science. **Interactions in solutions:** Concept of solute and solvent; multicomponent systems; preferential solvation. **Solvents:** Their characterization; microscopic structure of solvent and solvates; pair distribution function (PDF) and its determination using different techniques (spectroscopy and diffraction). Molecular dynamics and microscopic structure; different techniques of molecular dynamical calculations. Theories and laws related to solutions. **Macroscopic properties of solutions:** Transport properties; thermodynamics of solution; equilibria in solutions.

Recommended Books

1. C. Reichhardt, *Solvents and Solvent Effects in Organic Chemistry*, 2nd ed., VCH, Weinheim, Germany (1988).
2. J.H. Hildebrand, J.M. Prausnitz and R.L. Scott, *Regular and Related Solutions*, Van Nostrand Reinhold Company, New York (1970).
3. O. Popovych and R.P.T. Tomkins, *Nanoaqueous Solution Chemistry*, John Wiley & Sons, New York (1981).
4. D. Tabor, *Gases, Liquids and Solids*, 3rd ed., Cambridge University Press, UK (1993).

Supplementary Books

1. R.C. Reid and T.K. Sherwood, *The Properties of Gases and Liquids*, McGraw-Hill Book Company, New York (1986).
2. K. Shinoda, *Principles of Solution and Solubility*, Marcel Dekker, Inc., New York (1988).
3. H.J. Butt, G. Graf and M. Kappl, *Physics and Chemistry of Interfaces*, John Wiley-VCH, Weinheim (2003).

CHMP-721 Chemistry of Advanced Composite Materials (Cr. 3)

Introduction: Definitions and classification; natural composites; property enhancement by reinforcement and orientation; matrix interface; synthetic fibers; processing of composites. **Examples:** Metallic; ceramic and polymeric matrices; interface reactions. **Properties:** Mechanical and thermal properties of composite materials; stress relaxation and creep studies; dynamical mechanical properties, toughening mechanisms and mechanical failure in polymeric composites.

Recommended Books

1. F.L. Mathews and R.D. Rawlings, *Composite Materials: Engineering and Science*, Chapman and Hall (1994).
2. R.E. Shalin, *Polymer Matrix Composites*, Chapman and Hall (1995).

Supplementary Books

1. R.S. Scifullon, *Physical Chemistry of Inorganic Polymeric and Composite Materials*, Ellis Harwood (1992).

CHMP-722 Advanced Statistical Mechanics (Cr. 3)

Introduction: Statistical mechanics and its significance for chemical systems. Ensembles: microcanonical, canonical and grand canonical. **Probability:** Discrete states; continuously varying probabilities. **Average values:** concepts of number average and time average, fluctuations and standard deviations. **Partition functions:** Concept; different types; their determination for diatomic and polyatomic molecules. Partition functions of the systems of very large number of particles. Relationship between partition function and thermodynamic functions. **Statistical mechanical treatment:** Chemical equilibria and chemical reactions; imperfect gases; liquid state; dilute solutions: perfect crystals. Applications of Ferm-Dirac and Bose-Einstein statistics and their mutual comparison with Boltzman Maxwell statistics.

Recommended Books

1. F. Reif, *Statistical Physics (Berkeley Physics Course)*, McGraw-Hill, New York (1965).
2. N. Davidson, *Statistical Mechanics*, McGraw-Hill, New York (1962).
3. T.L. Hill, *Statistical Mechanics*, McGraw-Hill, New York (1956).
4. J.G. Aston and J.J. Fritz, *Thermodynamics and Statistical Thermodynamics*, John-Wiley, New York (1959).
5. J.M. Seddon and J.D. Gale, *Thermodynamics and Statistical Mechanics*, RSC Publishers (2001).

CHMP-723 Solid State and Semiconductors (Cr. 3)

Electronic structure of solids and band theory: Band structures of metals, insulators and semiconductors. Intrinsic semi-conduction and conductivity; controlled valency semiconductors; influence of temperature; dopant content, etc. Applications of semiconductors, p-n junctions. Band structure and color of inorganic solids. **Thermoelectric (Thomson, Peltier, Seebeck) effects:** Thermocouples. Hall effect, dielectric materials; ferroelectricity; pyro-electricity; piezo-electricity – their mutual relationships and applications. **Behavior of substances in magnetic field:** Effect of temperature: Curie and Curie-Weiss laws; calculation of magnetic moments; mechanism of ferro- and antiferro-magnetic ordering; super-exchange magnetic materials. **Characterization techniques.**

Recommended Books

1. W.D. Callister, Jr., *Material Science and Engineering*, 6th ed., John Wiley, New York (2003).
2. A.R. West, *Solid State Chemistry*, 2nd ed., John Wiley, Singapore (2002).

3. R.H. Bube, *Electrons in Solids*, 3rd ed., Academic Press, San Diego (1992).

Supplementary Books

1. J.R. Christman, *Fundamentals of Solid State Physics*, John Wiley, New York (1988).
2. K. Seeger, *Semiconductor Physics*, 6th ed., Springer-Verlag, Berlin (1997).
3. R.F. Pierret and K. Harutunian, *Semiconductor Device Fundamentals*, Addison-Wesley Longman, Boston (1996).
4. R.E. Hummel, *Electronic Properties of Materials*, 3rd ed., Springer-Verlag, New York (2000).

CHMP-724 Surfactant and Colloidal Chemistry (Cr. 3)

Liquid interfaces: Surface tension; capillarity. Young's and Kehrln equations. Spreading phenomenon; work of adhesion and cohesion; adsorption from solution; Gibbs-adsorption equation. **Organized molecular assemblies:** Insoluble surface monolayers, Langmuir Blodget films, surface presence-area diagrams. **Surfactants:** micellar structures and properties; micellar catalysis; bilayers and vesicles; membranes; micro- and macroemulsions; colloidal dispersions. **Colloids:** Colloidal stability and DLVO theory. Electrokinetics-zetapotential and electrophoresis. Light scattering techniques; coagulation and flocculation.

Recommended Books

1. D.F. Evans, *The Colloidal Domain*, VCH, Weinheim (1994).
2. P.C. Hiemenzt and R. Rajagopalan, *Principles of Colloid & Surface Chemistry*, 3rd ed., Marcel Dekker, Inc., New York, Basel, Hong Kong (1997).
3. M.J. Rosen, *Surfactants & Interfacial Phenomena*, Marcel Dekker, Inc., New York (1989).
4. A.W. Adamson, *Physical Chemistry of Surfaces*, John Wiley & Sons Inc., New York (1990).

Supplementary Books

1. A.K. Arora and B.V.R. Tata, *Ordering and Phase Transitions in Charged Colloids*, VCH, Weinheim (1996).
2. A.G. Volkov, *Liquid Interfaces in Chemical, Biological and Pharmaceutical Application*, Marcel Dekker Inc., New York (2001).
3. M. Antonietti, *Colloid Chemistry*, Springer Verlag, Berlin ISBN: 3540004157.
4. G.L. Gains Jr., *Insoluble Monolayers at Liquid-Gas Interface*, John Wiley & Sons Inc., New York (1966).

CHMP-725 Nuclear and Radiation Chemistry (Cr. 3)

Fundamental: Brief history of discovery of various nuclear and sub-nuclear particles. Nuclear liquid drop model, shell model; Nuclear composition, nuclear size and density, isotope chart, classification of nuclides on the basis of composition, stability, binding energy, nuclear mass defect and binding energy, various nuclear characteristics including half-life, decay constant, decay energy. **Nuclear decay processes including:** α -decay, β -decay, positron emission, electron capture. **Nuclear kinetics:** Equations of decay and growth processes for successive and branched decay, Natural and artificial decay series and applications, transient and secular equilibria. **Radiation chemistry:** Basic types of nuclear radiations, Interaction of radiation with matter. Introduction to dosimetry; **Applications:** Medical and industrial applications of nuclear and radiation chemistry.

Recommended Books

1. W.D. Loveland, D.J. Morrissey and G.T. Seaborg, *Modern Nuclear Chemistry*, John Wiley & Sons, New York (2006).
2. G.R. Choppin, J.O. Liljenzin, J. Rydberg and C. Ekberg, Revised Ed., *Radiochemistry and Nuclear Chemistry*, Academic Press, USA (2013).
3. H.J. Arnikar, *Essentials of Nuclear Chemistry*, New Age International publishers Ltd., Wiley Eastern Ltd., New Delhi (1995).
4. G. Friedlander and W Kennedy, *Nuclear and Radiochemistry*, John Wiley & Sons, New York (1981).
5. K.H. Lieser, *Nuclear and Radiochemistry (Fundamentals and Applications)*, John Wiley-VCH Weinheim (2001).

CHMP-726 Advanced Nuclear and Radiation Chemistry (Cr. 3)

Basic principles: Sources of nuclear radiation, radioactivity, nuclear-structure, models and stability, nuclear reactions. **Nuclear track detectors:** Kinetics and mechanism of track etching, tracers. **Nuclear waste and its management:** Nuclear hazards and benefits, transuranium elements and nuclear series, theoretical aspects of reactions, sources, absorption of radiations. **Dosimetry:** Categories, theoretical and experimental aspects, dose and dose rate. **Radiolysis:** Kinetic studies of radiolytic processes, radiolytic studies of: gaseous, aqueous and organic systems. **Applications:** Nuclear chemistry, radiobiology, analytical uses of radiation absorption.

Recommended Books

1. G. Choppin, J. Liljenzin and J. Rydberg, *Radiochemistry and Nuclear Chemistry*, 3rd ed., BH Publishers (2002).
2. K.H. Lieser, *Nuclear and Radiochemistry*, 2nd revised ed., Wiley-VCH (2001).
3. G. Friedlander and J.W. Kennedy, *Nuclear and Radiochemistry*, 3rd ed., Wiley, New York (1981).

4. W.J. Cooper, R.D. Curry and K.E. O'shea (Eds.), *Environmental Applications of Ionizing Radiations*, Wiley-IEEE (1998).

Supplementary Books

1. H.J. Arnikaar, *Essentials of Nuclear Chemistry*, 4th ed., Wiley Eastern Ltd., New Delhi (1995).
2. A. Vertes and S. Nagy, *Handbook of Nuclear Chemistry*, Springer Verlag, Berlin (2003).
3. F. Aziz and M.A.J. Rodges, *Radiation Chemistry*, VCH, Weinheim (1987).
4. J.W.T. Spinks and R.J. Woods, *An Introduction to Radiation Chemistry*, 2nd ed., John Wiley, New York (1976).
5. R.J. Woods and A.K. Pikaev, *Applied Radiation Chemistry: Radiation Processing*, Wiley-IEEE (1993).

CHMP-727 Applied Chemical Thermodynamics (Cr. 3)

Basic thermodynamics: Energy balance; entropy balance. **Thermodynamic properties interrelations:** Maxwell's equations; flow of fluids. **Power production:** The Rankine cycle, Brayton's cycle; fuel cells and batteries; internal combustion engine; compression and refrigeration. Vapor compression evaporation; vapor compression refrigeration, liquefaction of gases. **Phase equilibrium:** Non-ideal gas and liquid mixtures; chemical reaction equilibria.

Recommended Books

1. J. Winnik, *Chemical Engineering Thermodynamics*, John Wiley & Sons, Inc., New York (1997).
2. I.N. Levine, *Physical Chemistry*, McGraw Hill, New York (2002).

Supplementary Books

1. B.G. Kyle, *Chemical and Process Thermodynamics*, Printice Hall International, London (1999).
2. T. Letcher (Ed.), *Chemical Thermodynamic for Industry*, Royal Society of Chemistry, ISBN: 0854045910 (2004).

CHMP-728 Introductory Biophysical Chemistry (Cr. 3)

Introduction: Biological molecules; proteins and polypeptides, polynucleotides, polysaccharides, fats, lipids and detergents, water, acid, base, buffer and polyelectrolytes. **Thermodynamics and interactions:** Basic principles of thermodynamics, binding of ligands to macromolecules. **Kinetics:** Basic kinetics, rapid reaction techniques, relaxation methods, hydrogen exchange, surface plasma resonance, enzyme kinetics.

Recommended Books

1. R. Chang, *Physical Chemistry for the Biosciences*, University Science Books (2005).
2. N. C. Price, R. A. Dwek, R. G. Ratcliffe and M. R. Wormald, *Principles and Problems in Physical Chemistry for Biochemists*, 3rd Ed. Oxford University Press Inc., New York (2009).
3. A. Cooper, *Biophysical Chemistry*, Royal Society of Chemistry, Thomas Graham House, UK (2004).

CHMP-729 Advanced Biophysical Chemistry (Cr. 3)

Thermodynamic aspects: Simple molecules, macromolecules, colloidal particles in solution. **Bioenergetics:** Association of biopolymers. **Lipids and biological membranes:** Membrane transport; membrane potential. **Characterization of macromolecules:** Moving-boundary sedimentation; zonal sedimentation; density gradient sedimentation; viscosity measurement; electrophoresis, isoelectric focusing. **Structure of proteins and nucleic acids:** Folding/unfolding of proteins and nucleic acids. **Enzymology:** Kinetics of enzyme catalysis; mechanisms of enzyme catalysis. **Experimental techniques:** Protein NMR, X-ray crystallography of proteins, electron microscopy of macromolecular assemblies.

Recommended Books

1. R. Cotterill, *Biophysics: An Introduction*, Wiley Publishers, New York (2002).
2. B. Nölting, *Methods in Modern Biophysics*, Springer Verlag, Berlin (2006).
3. R. Glaser, *Biophysics*, Springer Verlag, Berlin (2001).
4. R. Chang, *Physical Chemistry for the Biosciences*, University Science Books (2005).
5. G.S. Rule and T.K. Hitachens, *Fundamentals of Protein NMR Spectroscopy*, Springer Verlag, Berlin (2005).

Supplementary Books

1. L. Stryer, *Biochemistry*, Worth Publishers (2001).
2. J.P. Glusker, M. Lewis and M. Rossi, *Crystal Structure Analysis for Chemists and Biologists*, VCH Publishers, New York (1994).
3. J. Kuo, *Electron Microscopy: Methods and Protocols*, Humana Press (2007).

CHMP-730 Physical Chemistry of Environment (Cr. 3)

Environment and its resources: Resource depletion and environmental pollution; green house effect; green house gases; mechanism of reactions causing pollution; interaction of pollutants with materials; noxious emission from industrial processes; aerosol

production. **Chemistry of pollutants:** Nuclear waste and its management. Kinetic and thermodynamic aspects of atmospheric phenomena. Clean energy for future. **Experimental techniques for environmental monitoring.**

Recommended Books

1. W.W. Eckenfelder, Jr., *Industrial Water Pollution Control*, McGraw-Hill International Edition (2000).
2. J.O.M. Bockris, *Environmental Chemistry*, Plenum Press, New York (1992).

Supplementary Book

1. R.B. Martin, *Introduction to Biophysical Chemistry*, McGraw-Hill Book Company, New York.

CHMP-731 Numerical Methods and Computational Chemistry (Cr. 3)

Basic operation of computer, hardware, software. Packages useful in chemistry, experimental data manipulation and calculations. **Computer aided numerical methods:** Least square curve fitting method for linear, quadratic, cubic, exponential and logarithmic and other functions; statistical analysis. Numerical differentiation. **Numerical integration:** Rectangular, trapezoidal and parabolic methods of approximation. **Molecular modeling:** Mechanical models, model building using different force field parameters, energy calculations, geometry optimization, potential energy surfaces. Prediction of various properties.

Recommended Books

1. K. Smith, *Calculus with Applications*, Brooks/Cole, Pacific Grove (1998).
2. R. Kumari, *Computers and Their Applications to Chemistry*, Narose Publishing House, New Delhi, India (2005).
3. R.J. Mortimer, *Mathematics for Physical Chemistry*, 3rd ed., Elsevier Academic Press (2005).

CHMP-732 Theoretical and Advanced Computational Chemistry (Cr. 3)

Introduction to computational chemistry: Basic concepts of quantum mechanics, history of development of computational chemistry and its applications, relevance of hardware and software components. **Molecular mechanics:** Force field energies and parametrization, geometry optimization and molecular modeling, potential energy surfaces. **Molecular orbital calculations:** Solution of the Schrodinger wave equation for molecular orbitals, Huckel molecular orbital theory and self consistent Hartree Fock method. Semiempirical and ab-initio molecular orbital calculations. Hybrid quantum mechanical and molecular mechanical methods. **Correlation of experimental and theoretical results:** Quantitative significance and interpretation of theoretical results. Relationship of theoretical results with spectral and molecular properties. Relationship of theoretical results to chemical reactivity indices. Interpretation and prediction of reaction mechanism using reactivity indices. **Density functional theory (DFT):** Philosophy,

early applications, Hohenberg-Kohn variational theorem. Advantages of DFT compared to MO theory.

Recommended Books

1. C.J. Cramer, *Essentials of Computational Chemistry*, John Wiley and Sons (2002).
2. F. Jensen, *Introduction to Computational Chemistry*, Wiley, Chichester (2000).

Supplementary Book

1. K.B. Lipkowitz and D.B. Boyd, *Reviews in Computational Chemistry*, VCH, New York (1991).

CHMP-733 Chemistry of Superconductors (Cr. 3)

Superconducting state: Disappearance of electrical resistance; Meissner effect. Superconducting elements: alloys; oxides and compounds. Electron-phonon interaction and Cooper pairs; isotope effect; flux quantization, energy gap, phase coherence, Josephson effects. Stability of super-conducting state; specific heat; influence of pressure; thermal conductivity. **Influence of magnetic field:** Type-I and type-II superconductors, intermediate state; interfacial energy. Critical current in type-I and type-II superconductors. Properties of superconductors. **Ceramic superconductors:** Classification of high- T_c (HTS) superconductors; chemical synthesis methods; effect of doping on structure and properties of HTS, thermal treatment of HTS. Applications of superconductivity.

Recommended Books

1. W.D. Callister, Jr., *Material Science and Engineering*, 6th ed., John Wiley, New York (2003).
2. W. Buckel, *Superconductivity*, VCH, Weinheim (1991).
3. J. Livingston, *Electronic Properties of Engineering Materials*, John Wiley, New York (1999).

Supplementary Books

1. L.D. Solymar and D. Walsh, *Electrical Properties of Materials*, 6th ed., Oxford University Press, London (1998).
2. R.E. Hummel, *Electronic Properties of Materials*, 3rd ed., Springer-Verlag, New York (2000).
3. D. Jiles, *Introduction to Magnetism and Magnetic Materials*, Nelson Thornes, Cheltenham (1998).

CHMP-734 Material Chemistry (Cr. 3)

Nanomaterials: Classification; structure and bonding; size dependent properties of mater; arrangements in 3D, 2D and 1D. Specific heats and melting points of nanocrystalline materials. **Semiconductor nanocrystals:** Spinels; quantum dots. Alloy semiconductors and their synthesis. Metal nanoparticles, double layers. Nanoparticle stability; charge transfer. **Optical properties:** Light absorption by colloids; dielectric response; size effects, electron transfer; temperature effects. **Magnetism:** Magnetic

susceptibility and permeability: diamagnetism; paramagnetism; Langevin model; quantum effects. Ferromagnetism, Curie-Weiss law. **Antiferro-magnetism:** Ferri-magnetism. Magnetic anisotropy. Magnetic domains. Hysteresis. Super-paramagnetism. Chemical and catalytic aspects of nanocrystals. **Nanotechnology:** Synthesis techniques. Applications.

Recommended Books

1. K.J. Klabunde, *Nanoscale Materials in Chemistry*, John Wiley, New York (2001).
2. D. Jiles, *Introduction to Magnetism and Magnetic Materials*, Nelson Thornes, Cheltenham (1998).
3. C.C. Koch, *Nanostructured Materials, Processing, Properties and Potential Applications*, William Andrew Publishing, New York (2002).

Supplementary Books

1. R.D. Shull, R.D. McMichael, L.J. Swatzendruber, L.H. Bennett, *Studies of Magnetic Properties of Fine Particles and Their Relevance to Materials Science*, J.J. Pormann, D. Fiorani (Eds.), Elsevier, Amsterdam (1992).
2. M. Schwartz, *New Materials, Process, and Methods Technology*, CRC Press, New York (2006).

CHMP-735 Advanced Techniques in Physical Chemistry (Cr. 3)

Magnetic resonance spectroscopy: Introduction, different types of magnetic resonance imaging (MRI), measurement of proton density, measurement of cerebral blood flow, measurement of cerebral blood volume, measurement of fractional anisotropy, measurement of scalar couplings, measurement of dipolar couplings, measurement of “residual dipolar couplings”. **FTIR. Thermal Analysis:** TGA, TDA. **Diffraction methods:** Introduction, single crystal X-ray diffraction (XRD) of small molecules and macromolecules including natural systems; powder X-ray diffraction (XRD) of small molecules and macromolecules, measurement of lattice parameters, measurement of B-values, determination of space group, calculation of electron density map. **Electron microscopy:** Introduction, scanning electron microscopy (SEM), transmission electron microscopy (TEM), measurement of I/Q values, single particle 3-D reconstruction. **Fluorescence techniques:** Steady-state fluorescence, time-resolved fluorescence, measurement of fluorescence anisotropy.

Recommended Books

1. E.M. Haacke, R.W. Brown, M.L. Thompson and R. Venkatesan, *Magnetic Resonance Imaging: Physical Principles and Sequence Design*, John Wiley, New York (1999).
2. M.J. Duer, *Introduction to Solid-State NMR Spectroscopy*, Blackwell Publishing (2004).

3. J.P. Glusker, M. Lewis and M. Rossi, *Crystal Structure Analysis for Chemists and Biologists*, VCH Publishers, New York (1994).
4. J. Kuo, *Electron Spectroscopy: Methods and Protocols*, Humana Press (2007).
5. A. Sharma and S.G. Schulman, *Introduction to Fluorescence Spectroscopy*, Wiley Interscience (1999).

CHMP-736 Electroanalytical Methods and Techniques (Cr. 3)

Basics of the instrumentation: Controlled potential techniques; controlled current techniques. **Designing of electrochemical cells:** Fabrication of electrodes; micro and ultra-microelectrodes; chemically modified electrodes. Solvents and supporting electrolytes. **Electrocoupled methods:** Electroorganic synthesis, photo-electrochemistry, spectro-electrochemistry. **Voltammetric analysis:** Normal pulse analysis; differential pulse analysis; squarewave analysis, AC voltammetry; chronomethods; stripping analysis. **Bulk electrolysis:** Electrogravimetric analysis; electroseparation techniques; coulometric analysis. Write up of experimental instrumentation and procedure.

Recommended Books

1. P.T. Kissinger and W.R. Heineman, *Laboratory Techniques in Electroanalytical Chemistry*, 2nd revised ed., Marcel Dekker Ltd., New York (1996).
2. A.J. Bard and L.R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, 2nd ed., Wiley (2001).

Supplementary Books

1. P.M.S. Monk, *Fundamentals of Electroanalytical Chemistry (Analytical Techniques in Science)*, John Wiley & Sons (2001).
2. V.S. Bagotski, *Elementals of Electrochemistry*, 2nd ed., Wiley, New York (2005).

IV. CHMA/CHMI/CHMO/CHMP-799 Thesis and Viva Voce Exam

The student shall submit a thesis on the subject of her research work for evaluation and appear in an oral examination (viva voce exam).
