# MASTER OF SCIENCE IN CHEMISTRY

## Master of Science in Chemistry − Curriculum

**Outline**

| | |
|---|---|
| Natural science requirements | 11 credits |
| Compulsory core courses | 43 credits |
| Industrial training I – Project work | 5 credits |
| Elective chemistry courses | 25 credits |
| Thesis | 30 credits |
| Elective general courses – can be chemistry related as well | 6 credits |
| **Total:** | **120 credits** |

**Details**

**I. Natural science requirements** **11 credits**

**Mathematics** **7 credits**

s = seminar or practical, l = lecture

| Courses | ECTS | Hours | Type | Responsible department | Instructor |
|---|---|---|---|---|---|
| Mathematical chemistry | 4 | 2 | l | AKKT | Tasi, Gyula |
| Mathematical chemistry practical | 3 | 2 | s | | |

**Informatics** **2 credits**

| | | | | | |
|---|---|---|---|---|---|
| Chemical information retrieval | 2 | 2 | s | SzKT | Pálinkó, István |

**Physics** **2 credits**

| | | | | | |
|---|---|---|---|---|---|
| Advanced experimental physics | 2 | 2 | l | FTCs | Hopp, Béla |

**II. Compulsory core courses** **43 credits**

**Inorganic chemistry** **6 credits**

| | | | | | |
|---|---|---|---|---|---|
| Advanced inorganic chemistry | 4 | 2 | l | SzAKT | Gajda, Tamás |
| Advanced inorganic chemistry seminar | 2 | 1 | s | | |

**Physical chemistry** **11 credits**

| | | | | | |
|---|---|---|---|---|---|
| Advanced physical chemistry | 4 | 2 | l | FKAT | Tóth, Ágota |
| Advanced physical chemistry seminar | 2 | 1 | s | | |
| Advanced physical and polymer chemistry laboratory practical | 5 | 5 | s | FKAT | Peintler, Gábor |

**Organic chemistry** **8 credits**

| | | | | | |
|---|---|---|---|---|---|
| Advanced organic chemistry | 6 | 4 | l | SzKT | Pálinkó, István |
| Advanced organic chemistry seminar | 2 | 1 | s | | |

**Analytical chemistry** **7 credits**

| | | | | | |
|---|---|---|---|---|---|
| Modern instrumental analytical chemistry | 5 | 3 | l | SzAKT | Galbács, Gábor |
| Modern instrumental analytical chemistry seminar | 2 | 1 | s | | |

**Industrial chemistry** **11 credits**

| | | | | | |
|---|---|---|---|---|---|
| Unit operations | 4 | 2 | l | AKKT | Kukovecz, Ákos |
| Unit operations practical | 3 | 2 | s | | |
| Industrial training (4 weeks) | 4 | 0 | s | AKKT | Kukovecz, Ákos |

**III. Elective general courses** 6 credits

| | | | | | |
|---|---|---|---|---|---|
| The cultural history of chemistry | 3 | 2 | l | KTCs | strongly suggested |

**IV. Thesis** 2×15 credits

**V. Project work** 5 credits

**VI. Elective chemistry courses** 25 credits

## Master of Science in Chemistry – Program Plan

| **Course** | **Semester** | | | | **Type.** | **ECTS** | **Responsible Department** |
|---|---|---|---|---|---|---|---|
| | | | **1st** | | | | |
| Mathematical chemistry | 2 | | | | l | 4 | AKKT |
| Mathematical chemistry practical | 2 | | | | s | 3 | AKKT |
| Advanced experimental physics | 2 | | | | l | 2 | FTCs |
| Chemical information retrieval | 2 | | | | s | 2 | SzKT |
| Advanced physical chemistry | 2 | | | | l | 4 | FKAT |
| Advanced physical chemistry seminar | 1 | | | | s | 2 | FKAT |
| Advanced physical and polymer chemistry laboratory | 5 | | | | s | 5 | FKAT |
| Advanced inorganic chemistry | 2 | | | | l | 4 | SzAKT |
| Advanced inorganic chemistry seminar | 1 | | | | s | 2 | SzAKT |
| **Subtotal: 4 l, 5 s** | **19** | | | | | **28** | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | **2nd** | | | | |
| Advanced organic chemistry | | 4 | | | l | 6 | SzKT |
| Advanced organic chemistry seminar | | 1 | | | s | 2 | SzKT |
| Modern instrumental analytical chemistry | | 3 | | | l | 5 | SzAKT |
| Modern instrumental analytical chemistry seminar | | 1 | | | s | 2 | SzAKT |
| Unit operations | | 2 | | | l | 4 | AKKT |
| Unit operations practical | | 2 | | | s | 3 | AKKT |
| Project work | | 5 | | | s | 5 | KTCs |
| **Subtotal: 3 l, 4 s** | | **18** | | | | **27** | |
| | | | **3rd** | | | | |
| Industrial Training | | | – | | s | 4 | |
| The cultural history of chemistry | | | 2 | | l | 3 | KTCs |
| Thesis 1 | | | 15 | | s | 15 | KTCs |
| **Subtotal: 1 l, 2 s** | | | **17** | | | **22** | |
| | | | **4th** | | | | |
| Thesis 2 | | | | 15 | s | 15 | KTCs |
| **Subtotal: 1 s** | | | | **15** | | **15** | |
| **Total: 7 k, 13 g** | | | | | | **92** | |

20 credits out of the 25 credits from the elective chemistry courses will be available in semesters 3 and 4.

## Elective chemistry courses

| | | | | | |
|---|---|---|---|---|---|
| **Pharmaceutical researcher specialisation – Gajda, Tamás** | | | | | |
| Biocatalysis | 4 | 2 | l | SzAKT | Gajda, Tamás |
| Biological tools of modern chemistry | 4 | 2 | l | SzAKT | Gyurcsik, Béla |
| Fundamentals of pharmaceutical chemistry | 5 | 3 | l | SzAKT | Kiss, Tamás |
| Bioorganic chemistry | 4 | 2 | l | SzKT | Wölfling, János |
| Chemistry of organometallic compounds | 4 | 2 | l | SzKT | Mastalír, Ágnes |
| Natural organic compounds, organic syntheses | 4 | 2 | l | SzKT | Wölfling, János |
| Synthetic chemistry laboratory | 6 | 6 | s | KTCS | Bucsi, Imre |
| | *31* | *19* | | | |
| **Material science researcher specialisation – Kónya, Zoltán** | | | | | |
| Macromolecular systems | 4 | 2 | l | FKAT | Szabó, Tamás |
| Electrochemical procedures, corrosion | 4 | 2 | l | FKAT | Szűcs, Árpád |
| Nanocomposites | 4 | 2 | l | AKKT | Kónya, Zoltán |
| Interfaces and nanostructures | 5 | 3 | l | FKAT | Dékány, Imre |
| Heterogeneous catalysis | 4 | 2 | l | AKKT | Hernádi, Klára |
| Bulk and surface methods of material characterisation | 4 | 3 | l | AKKT | Kónya, Zoltán |
| Bulk and surface methods of material characterisation, seminar | 1 | 1 | s | | |
| Solid-state chemistry | 4 | 2 | l | FKAT | Oszkó, Albert |
| | *30* | *17* | | | |
| **Analytical chemist specialisation – Galbács, Gábor** | | | | | |
| Analytical sensors | 4 | 2 | l | SzAKT | Galbács, Gábor |
| Laser- and plasma-based trace analysis | 4 | 2 | l | SzAKT | Galbács, Gábor |
| Modern chromatographic methods | 4 | 2 | l | SzAKT | Ilisz, István |
| Analytical quality assurance and quality | 4 | 2 | l | SzAKT | Schrantz, Krisztina |

| | | | | | |
|---|---|---|---|---|---|
| control systems | | | | | |
| Molecular spectroscopy | 4 | 2 | l | FKAT | Berkesi, Ottó |
| Separation methods and spectroscopy laboratory | 4 | 4 | s | SzAKT | Ilisz, István |
| Chemometry | 2 | 2 | s | KTCs | Jakusch, Tamás |
| Isotope technology | 4 | 2 | l | FKAT | Oszkó, Albert |
| | *30* | *18* | | | |
| **Electives without specialisation** | | | | | |
| Modern quantum chemistry | 4 | 2 | l | AKKT | Tasi, Gyula |
| Computational chemistry | 4 | 2 | l | AKKT | Tasi, Gyula |
| Computational chemistry seminar | 3 | 2 | s | AKKT | |
| Computational modeling in material and pharmaceutical research | 4 | 2 | l | FKAT | Czakó, Gábor |
| Nonlinear dynamics | 4 | 2 | l | FKAT | Tóth, Ágota |
| Physical inorganic chemistry | 4 | 2 | l | SzAKT | Jakusch, Tamás |
| X-ray diffractometry | 4 | 2 | l | AKKT | Sápi, András |
| Graphite wires and carbon nanotubes | 4 | 2 | l | AKKT | Hernádi, Klára |
| Chemistry of non-aqueous solutions and melts | 4 | 2 | l | SzAKT | Sipos, Pál |
| | *31* | *18* | | | |

**Total: 122 credits (106 credits lectures, 16 credits seminars/laboratory practicals)**

**To fulfill the requirement of a specialisation at least 20 credits out of the listed electives must be collected.**

**<u>Course title: Analytical Quality Assurance and Quality Control Systems</u>**

**Credits: 4**

**Course description:**

Quality assurance systems. Development of the systems, elements of accreditation procedure. The goal of the quality assurance handbook and its forms. Documentation of the enquiry data, reports. Internal auditing.
Validation and documentation of analytical methods, goals of validation. Analytical parameters for validation. Evaluation of the system and method adequacy.
Definition of the quality and its role in economic competition.
Evolution of the quality assurance. Formation of the quality surveillance, phases of its development. Self-control, independent quality control and its methods, quality regulation. Quality direction and the fully comprehensive quality management.
National and international regulations of the quality assurance. Unionisation and law phasing within the EU. Formation and development of standardization, product responsibility, consumer protection.
Product and system certification, regulations for instruments, attesting and calibration.
Development of the quality direction systems. Their structure and standardised certification. Formation, development and coordinating role of ISO 9000 standard. Reviewing and interpretation of ISO 9001:2000 standard.
Formation and development of TQM. Quality awards, self-evaluation and the EFQM model.
The future of the direction systems, function orientated direction systems. Quality, environmental, information protection, workplace health protection and security direction systems.

Literature:

J.P. Dux: *Handbook of Quality Assurance for the Analytical Laboratory*, Van Nostrand Reinhold, 1990.

**Course title: Analytical Sensors**

**Credits: 4**

**Course description:**

Definition and classification of sensors and transducers. Physical, chemical and biosensors. Functions and applications of sensors and transducers in analytical chemistry and automated measurement systems. Construction and principle of operation of relevant modern sensor types including electrochemical (e.g., potentiometric and voltammetric) and photometric (absorptive, reflective and luminescence) types, as well as sensors used for the detection/measurement of mass, temperature, pressure, liquid/gas flow, with special emphasis on semiconductor and fiber optic based sensors. Practical examples for the measurement of pH, the concentration of metal ions in solutions, noxious gases and some compounds with a diagnostic value. Sensors in portable, remotely manageable and miniaturized measurement systems.

Literature:

R.W. Cattrall: *Chemical Sensors*, Oxford Chemistry Primers Series Vol. 52, Oxford University Press, 1997.

J. Fraden: *AIP Handbook of Modern Sensors*, American Institute of Physics, 1993.

B.E. Eggins: *Chemical Sensors and Biosensors*, John Wiley & Sons, 2002.

T. Seiyama: *Chemical Sensor Technology, Vol 1.*, Elsevier, 1988.

E. Kress-Rogers: *Handbook of Biosensors and Electronic Noses* (Medicine, Food and the Environment), CRC Press, 1997.

A.J. Bard, L. Faulkner: *Electrochemical methods: Fundamentals and Applications*, John Wiley and Sons, 2000.

**<u>Course title: Biocatalysis</u>**

**Credits: 4**

**Course description:**

Introduction, basic principles and historical survey. The origin of enzymatic efficiency and (stereo)selectivity. Applications of enzyme inhibitors in medicine. Comparison of chemical and biological catalysis. Dynamic and kinetic resolvation. The possibilities of the realisation of biocatalytic reactions.
Examples for the mechanisms and practical applications of some important enzymes. Glucose-fructose transformation (xilose isomerase). Hydrolysis of lactose (lactase). Break-down of cellulose and starch (cellulase, xilanase, amilase, glucosidase). Synthesis of chiral alcohols, amines and amino acids (lipases, hydrolases, alcohol dehydrogenase, aspartase). Molecular biology (restriction enzymes). Production of acrylic amide (nitril hydratase). Production of penicillin derivatives (penicillin acylase/amidase). Production of aspartame (termolysin). Hydroxylation and epoxidation of aliphatic and aromatic compounds (cytochrome P450, dioxygenases). Application of peroxidases in the textile industry. Formation of other C−C, C−N, C−S bonds in fine chemical industry.
Modified enzymes. The evolution of enzymes. Improvement of the temperature, pH etc. resistance of enzymes, changing of regioselectivity and development of new functions by point-mutation and directed evolution. Effects achieved by the change of metal ions in the active centres of metalloenzymes (increased activity, change of the function, etc.). Introducing specificity into a non-specific enzymes and *vica versa*. Development of new enzymes by covalent coupling of proteins and simple metal complexes (Cu/Fe-containing nucleases, asymmetric synthesis by Ru/Rh-containing artificial enzymes, etc.).
Biomimetic catalysis. Catalytic properties of metal ions, some basic principles of the design of artificial enzymes.
*Artificial hydrolases*: Artificial phosphatases and nucleases. The active centres. Substrate secificity and the role of allosteric groups. The importance of oligonuclear active centres. Possible application in gene technology and gene specific chemotherapy.
*Artificial redox enzymes*: Heme and P450 models, oxygen activation by non-hem iron- and copper-complexes (*catalysts for organic reactions*). Superoxide dismutase models (*antioxidants*). $CO_2$ reduction: comparison of the enzymes and their biomimetic functional models.

Literature:

A.S. Bommarius, B.R. Riebel-Bommarius**,** *<u>Biocatalysis: fundamentals and applications</u>***,** Wiley 2004
<u>S.M Roberts</u>, <u>N.J Turner</u>, <u>A.J. Willetts</u>, *Introduction to biocatalysis using enzymes and micro-organisms*, Cambridge University Press, 1995
*Chemical Review* 2004, **104**, issue 2 (Biological Inorganic Chemistry).

**Course title: Biological Tools in Modern Chemistry**

**Credits: 4**

**Course description:**

**The overlap of the chemical and biological sciences.** The effect of molecular biology on the development of chemistry. The cell. The role of given metal ions and metalloenzymes within the organisation of living cell, and in the biochemical processes. Examples of the role of the metalloenzymes, metalloproteines, and the "free" metal ions.
**The investigation methods of molecular biology.** Historical overview. The types of microscopy and their applications. Ultracentrifuges. Electrophoresis. The determination of protein structure: theory and practice. The study of the amino acid sequence. The calculation of the secondary structure. Methods of structural characterisation. Proteins in molecular recognition.
**The basics of gene technology.** The different pathways of the enzyme or protein modifications, examples. The design of new macromolecules. The polymerase chain reaction. The design and synthesis of artificial DNA vectors. Viruses, as DNA carriers. Bacteria in DNA cloning. DNA synthesis within the cell. The analysis of DNA − sequence determination.
**The basics of proteomics.** The synthesis of proteins by chemical and biological, "in vitro" vs. "in vivo" methods. Solid phase peptide synthesis. Protein synthesis in the cell. The methods for identification and purification of proteins. HPLC, antibody-, metal ion-affinity chromatography. The application of polyacrylic amide gel electrophoreses. The solubility of proteins. Protein complexes. Denaturing – renaturing.
**Applications.** Artificial proteins, (metallo)enzymes − creation and activity. Examples of industrial, pharmacological and research applications. Future trends.

Literature:

B. Alberts, D. Bray, J. Lewis, M. Raff, K. Roberts, J.D. Watson: *The molecular biology of the cell*, Garland Publishing Inc, New York, London, 1989.

The lecture is, beside the above book based on the handbooks used in molecular biology laboratories, as well as on the scientific papers published in international journals. These new results allow for the continuous modernization of the topics.

**Course title: Bioorganic Chemistry**

**Credits: 4**

**Course description:**

**Carbohydrates.** Classification, structural features of monosaccharides. Chirality, structure in solution, mutarotation. The chemical properties of monosaccharides. Important monosaccharides, deoxy- and amino sugars. Classification, structural features of di- and polysaccharides. Fragmentation with chemical and enzymatic means. Cyclodextrins. Heteropolysaccharides. The synthesis of oligo- and polysaccharides.
**Amino-carboxylic acids, peptides, polypeptides and proteins.** The classification of amino acids, their structures, chiralities, synthesis methods, physical and chemical properties. The reactions of the their functional groups. The nomenclature of di- and polypeptides, methods of synthesis (protecting and activating groups, coupling agents). The synthesis of ring peptides. Scission of the peptide bonds by chemical and enzymatic means. The structure, structural characterization, physical and chemical properties of polypeptides and proteins. The primary, secondary, tertiary and quaternary structures of proteins.
**Nucleosides, nucleotides, nucleic acids.** Synthesis and structure of nucleosides, antiviral nucleosides. Classification and synthesis of nucleotides. Structure, biosynthesis, metabolism, physical and chemical properties of mononucleotides. Preparation methods of the internucleotide bonding. Nomenclature, synthesis and structure of oligo- and polynucleotides. Nucleotide coenzymes. The primary structures of nucleic acids. Deoxyribonucleic acids, ribonucleic acids. Their syntheses and characterization. Sequence analysis. Secondary and tertiary structures.
**Lipids.** The biosynthesis, structural features physical and chemical properties of fatty acids. Simple lipids: vaxes and fats. Complex lipids: phospho- and glycolipids.

Literature:

P. Nuhn: Naturstoffchemie, S. Hirzel Verlag, Stuttgart, Leipzig, 1997.

**<u>Course title: Bulk and Surface Methods of Material Characterisation</u>**

**Credits: 4 + 1**

**Course description:**

Structure and bonding of materials: XRD, electron diffraction, neutron scattering, XPS, UV-Vis, micro-CT, dielectric spectroscopy. The concept of equivalent networks and its correlation with the inner structure of matter.
The concept of porosity. Descriptors used for the quantitative characterization of pore systems. Adsorption methods, mercury porosimetry, SAXS.
Industrial characterization of powders and coatings: colour and thickness measurements, particle size distribution analysis.
Physical and mechanical properties: heat transfer coefficient, Young’s modulus, tensile strength, hardness.
Thermoanalytics: TG, DTA, DSC.
Common material defects and their identification in composites, alloys and welds.
The fundamentals of microscopy: definition of the image, imaging methods, image processing. Quantitative descriptors of morphology: fractal dimension, lacunarity, shape factors.
Optical microscopy, confocal microscopy. Bright field and dark field Imaging in the transmission electron microscope. Scanning electron microscopy: detectors, modes, limitations. Analytical electron microscopy: energy and wavelength dispersive spectroscopy. Scanning probe microscopy: basics and operation modes (AFM, STM, STS, MFM, chemical AFM).
Known limitations of microscopic methods: what can you expect and what not?
Sample preparation for microscopy. Recognizing typical microscopy artifacts. Combined microscopic methods: optical microscopy+AFM+Raman, IR microscopy, EM tomography.

Literature:

I. Pozsgai: Scanning electron microscopy and microanalysis (ELTE Eötvös Kiadó, Budapest, 1995)
I. Pozsgai: The fundamentals of analytical electron microscopy (ELTE Eötvös Kiadó, Budapest, 1996)
K. Burger: Fundamentals of quantitative analysis: Chemical and instrumnetal analysis (Semmelweis Kiadó, Budapest, 1992)

**<u>Course title: Chemometrics</u>**

**Credits: 4**

**Course description:**

Random events and chemical measurements. Statistical samples. Classification of data. Hierarchical and non-hierarchical cluster analysis. Comparison and interpretation of cluster analysis results. Treatment of outlying and missing points.
Factor analysis and principal component analysis. Data preprocessing. Principles of factor analysis. Calculation and interpretation of factors. Fundamentals of principal component analysis. Calculation and interpretation of PCA results.
Fundamentals of parameter estimation. Linear and nonlinear parameter estimation. The goodness of fit. Numeric and iterative methods of parameter estimation. Regression calculations in case of correlated variables. Principles of model set up, selection of variables. Biased parameter estimations: PCR and PLS.
Correct statistical interpretation of chemical measurements. Relationship of chemical quantities. The task of calibration. Deriving kinetic and thermochemical parameters from chemical measurements

Literature:

D.L. Massart, B.G.M. Vandeginste, *Chemometrics – A textbook*, Elsevier, Amsterdam 1990
M. Otto, *Chemometrics – Statistics and Computer Application in Analytical Chemistry*, Wiley-VCH, 1999

**<u>Course title: Computational Chemistry</u>**

**Credits: 4**

**Course description:**

A biography of the computer. Various applications of computers in chemistry: an overview. Parts of the personal computers. Operating systems: UNIX, Linux, Windows, etc. Programming personal computers at “low” (assembly), “medium” (C) and “high” levels (FORTRAN, Mathematica, Maple). Structured programming. How to write user-friendly software packages. Commercial software packages for chemical data acquisition and evaluation. Parameter estimation. Linear and non-linear regressions.

Numerical integration and derivation. Random numbers: true, pseudo and quasi. Linear congruent methods to generate pseudo-random numbers. Monte-Carlo methods. Monte-Carlo integration. Determination of van der Waals volumes and surfaces of molecules via Monte-Carlo integration. Monte-Carlo methods to integrate chemical reaction kinetic rate equations.

Molecular modelling and molecular graphics. Build-up of molecules: the Z-matrix. Transformation of molecular Z-matrix to atomic Cartesian coordinates. Molecular shape and molecular dimensions. Shape selective catalysis in chemistry and biology. Molecular modelling: molecular mechanics and quantum chemical methods. Fully variational Hartree-Fock-Roothaan-Hall *ab initio* computations on atoms and molecules. Determination of molecular structures. Symmetry of molecules: static and dynamic properties.

Numerical methods of linear algebra. An automatic procedure to determine all the symmetry elements of a molecule. Beyond point groups: framework groups. Calculation and graphical representation of molecular properties. The concept of the potential energy (hyper)surface (PES) within the Born-Oppenheimer approximation. Stationary points on the PES: local minima and saddle points.

Function minimization: the Nelder-Mead simplex method and gradient methods. Modern procedures to determine the equilibrium and transition state structures of molecules. Normal-coordinate analysis. Calculation of vibrational spectra. Reaction path following methods. Molecular similarity. Electron population analyses. Atomic charge concepts. Computational thermochemistry. Consideration of solvent effects in molecular simulations.

Literature:

M.S. Malone, *The Microprocessor, A Biography*, Springer-Verlag, New York, 1995
J. Frank, *Introduction to Computational Chemistry*, John Wiley & Sons, Chichester, 1999
A. Hinchliffe, *Modelling Molecular Structures*, John Wiley & Sons, Chichester, 2000
C. Christopher, *Essentials of Computational Chemistry*, John Wiley & Sons, Chichester, 2002
D. Cook, *Handbook of Computational Quantum Chemistry*, OUP, Oxford, 1998
G. Tasi, I. Pálinkó, J. Halász, G. Náray-Szabó, *Semiempirical Calculations on Microcomputers*, CheMicro Ltd. Budapest, 1992

**<u>Course title: Fundamentals of Medicinal Chemistry</u>**

**Credits: 4**

**Course description:**

Introduction, basic concepts.
Routes of the drug inside the organism: pharmacokinetic phase.
Original drug design and development.
Stereochemistry and drug design.
Drug solubility and its modification by pharmaceutical technological methods.
Drug action that affects the structure of cell membranes and walls.
Proteins I: Enzymes and drug design.
Proteins II.: Receptors and drug design.
Drugs that target nucleic acids.
Factors that modify the effects of drugs.
Metal compounds applied in therapy.
Diagnostic agents. Disorders in metal ion balance, Chelating therapy.
Toxicology of metals I.
Toxicology of metals II.

Literature:

*Medicinal Chemistry: Pinciples and Practice* (Ed. F.D. King), Royal Society of Chemistry, 2002.
T. Gareth: *Medicinal Chemistry: An introduction*, Wiley, Chichester, 2004.
G.L. Patrick: An Introduction to Medicinal Chemistry, Oxford University Press, 3rd Edition, 2005.
R.B. Silverman: *The Organic Chemistry of Drug Design and Drug Action*, Elsevier Academic Press, 2nd Edition, 2004.
*Metallopharmaceuticals I and II, in Topics in Biological Inorganic Chemistry*, (Eds. M.J. Clarke, P.J. Sadler), Springer, Berlin 1999.
*Metallotherapeutic Drugs and Metal-based Diagnostic Agents* (Eds, M. Gielen, E.R.T. Tiekink), Wiley, Chichester, 2005.
*Metal Toxicology*, (Eds. R.A. Goyer, C.D. Klaassen, M.P. Waalkes), Academic Press, San Diego, 1995

**<u>Course title: Heterogeneous Catalysis</u>**

**Credits: 4**

**Course description:**

Fundamental concepts of reaction kinetics.
Principles of catalysis. Classification of catalysts and catalytic reactions. Heterogeneous catalysis.
Steps of heterogeneous catalytic processes. Types of isotherms. Kinetic description of surface reactions.
Synthesis methods of heterogeneous catalysts.
Temperature-programmed reduction and temperature-programmed reduction.
Characterisation of heterogeneous catalysts with chemical and instrumental methods.
Types of catalysts.
Catalysis by porous materials.
Photocatalysts and photocatalytic reactions.
Biomimetic catalysts.
Application of heterogeneous catalysts in fine chemical syntheses.
Industrial applications of heterogeneous catalysts.

Literature:

J.M. Thomas, W.J. Thomas: *Principles and practice of heterogeneous catalysis*, John Wiley&Sons, 2014

**Course title: Interfaces and Nanostructures**

**Credits: 4**

**Course description:**

The role of interfaces on the properties of nanostructured materials. The Kelvin equation. The optical, magnetic, semiconducting and catalytic properties of nanoparticles.
2D ordered nanostructures. Langmuir and Langmuir-Blodgett films. Self-assembling colloid systems.
Excess quantities and excess thermodynamic functions. The Gibbs adsorption equation.
The tension of curved surfaces. The Laplace and Kelvin equations. Capillary condensation and the Ostwald ripening.
Adsorption over solid/gas (S/G) interfaces. Types of isotherms. The BET specific surface and its measurement. Adsorption hysteresis and capillary condensation. Specific surface according to Harkins and Jura. The structure of porous adsorbents. The properties of active carbon and mesoporous silicas. Distribution of pore sizes.. Polányi's potential theory, characteristic curves. Application of the t-method of de Boer for the characterisation of porous adsorbents.
Instrumental methods for the characterisation of nanostructured materials (TEM, SEM, STM, AFM, SAXS, SPR, ellipsometry, QCM). Application of sensors for measuring interactions at the interface.
Interfacial adsorption (S/L) of non-electrolytes (binary liquid mixtures and dilute solutions. Types of isotherms, their measurements and their analysis. Hydrophilic and hydrophobic surfaces.
The adsorption layer as nanophase reactor.
The thermodynamic fundamentals of adsorption microcalorimetry. Determining surface potential functions. S/G and S/L interfacial microcalorimetry. The concept of adsorption heat and its defining equations.
Self-assembling of surfactants in solution and at interfaces.
Liquid/liquid (L/L) interfaces. The syntheses and properties of emulsions, nanoemulsions and microemulsions. Microemulsions as nanophase reactors.
Fundamental concepts of rheology, the rheological properties of disperse systems. Classification of the flow curves. Newtonian and structural-type viscosities. Thixotropy. The rheological behaviour of concentrated suspensions and their measuring possibilities.
Coherent systems. The gels. The structure of coherent systems, the role of gels in medicine formulation.

Literature:

D.F. Evans, H. Wennerström: *The Colloidal Domain; Where Physics, Chemistry, Biology and Technology Meet*, WileyVCH (1999).
J. Lyklema (Ed.): *Fundamentals of Interface and Colloid Science*, Elsevier, Vols. 1-5 (1991-2005).

**<u>Course title: Laser and Plasma-based Analytical Methods</u>**

**Credits: 4**

**Course description:**

Principle of operation, analytical and operational characteristics as well as primary application areas for laser and/or plasma based analytical methods are discussed. Not only laboratory based measurement systems, but also portable, miniature, remotely controllable and those that can work from a stand-off distance are covered. The following list gives an overview of the covered topics.

- Characteristics of laser lights sources
- Application possibilities of lasers in analytical chemistry
- Plasma atom/ion sources (DCP, MIP, CCP, ICP, DBD, etc.)
- Plasma diagnostics using lasers
- Modulation and high resolution laser spectroscopic methods
- Laser induced fluorescence spectroscopy (LIF)
- Laser ablation (LA) and laser induced plasma spectroscopy (LIBS/LIPS)
- Matrix-assisted laser desorption mass spectroscopy (MALDI)
- Inductively coupled plasma mass spectrometry (ICP-MS)
- Resonance ionisation spectroscopy (LEI/RIS/RIMS)
- Cavity ring-down spectroscopy (CRDS)
- Photoacoustic spektroscopy (PAS)

Application of lasers in remote measurement systems (e.g., LIDAR, LIBS, RIID)

Literature:

J.M. Hollas: *Modern spectroscopy*, John Wiley and Sons, 2004.
E.H. Piepmeier (ed.): *Analytical applications of lasers*, John Wiley and Sons, 1986.
W. Demtröder: *Laser spectroscopy: basic concepts and instrumentation*, Springer, 1996.
R. Kellner, J.M. Mermet, M. Otto, H.M. Widmer (eds.): *Analytical Chemistry* (Approved by the Federation of European Analytical Chemistry Societies, FECS), 1998.
E.H. Evans, J.J. Giglio, T.M. Castillano, J.A. Caruso: *Inductively coupled and microwave induced plasma sources for mass spectrometry*, RSC, 1995

**Course title: Macromolecular Systems**

**Credits: 4**

**Course description:**

Classification of macromolecules. The structural features of macromolecules and their physical properties. Synthesis methods of polymers, various types of polymerisation reactions. Photopolymeri-sation technologies.
Models of linear polymer chains. Solvation and dissolution of polymers. The thermodynamics of polymer solution, the Flory-Huggins theory.
Fractionation of polymers. Methods for determining molecular weight distribution. Gel chromatography.
The osmotic pressure and the thermodynamics of solvation for macromolecular solutions.
The properties of polyelectrolites – the effects of pH and the ionic strength.
The adsorption of polymers over solid surfaces.
The stabilities of colloid dispersions in polymer solutions – steric stabilisation.
Physical states of polymers. Amorphous and crystalline structures. Thermoanalytical and X-ray diffraction methods for structural characterisation.
Mechanical and rheological properties of polymers. Determining the viscosities and molecular weights of polymer solutions. The Maxwell and the Voight-Kelvin model.
Application areas of polymers. Plastics and polymer composites.
Swelling of 3D polymers, the structure of polymer gels, intelligent 3D polymers.
Polymer films and coatings. Films from solutions, dispersions and melts.

Literature:

F. Szántó: *The fundamentals of colloid chemistry*, JATE Press, 1995.
G. Bodor: *The structure of polymers*, Műszaki Könyvkiadó, Budapest, 1982.
L. Halász, M. Zrínyi: *Introduction to polymer physics*, Műszaki Kiadó, Budapest, 1989

**Course title: Modern Quantum Chemistry**

**Credits: 4**

**Course description:**

The first and second quantized forms of quantum chemistry. Bosons and fermions. Creation and annihilation operators. Assembly of coupled harmonic oscillators. Normal coordinates. Normal modes of crystal lattices. The one-electron approximation. The Fock space. Particle number and quantum mechanical operators. Evaluation of matrix elements. The Slater-Condon rules. Density matrices. Some model Hamiltonians in second quantized approach. The Hartree-Fock theory. The configuration interaction (CI) method. The multi-configuration self-consistent field (MCSCF) method. Coupled-cluster (CC) theory. Many body perturbation theory (MBPT). Atomic basis functions. Gaussian basis sets. Numerical evaluation of molecular integrals. Assessment of the accuracy of various quantum chemical methods. Computation vs. experiment. Zero-point vibrational energy (ZPVE) beyond the harmonic approximation. Limits of the Born-Oppenheimer approximation. Relativistic effects. *Ab initio* thermochemistry. Intermolecular interactions.

Literature:

A. Böhm, *Quantum Mechanics*, Springer-Verlag, 1979
P. Surján, *Second Quantised Approach to Quantum Chemistry*, Springer-Verlag, 1989
J. Avery, *Creation and Annihilation Operators*, McGraw-Hill, 1976
T. Helgaker et al., *Molecular Electronic-Structure Theory*, John Wiley & Sons, 2000
G. Tasi, R. Izsák, et al., *The Origin of Systematic Error in the Standard Enthalpies of Formation of Hydrocarbons Computed via Atomization Schemes,* ChemPhysChem 7 (2006) 1664
G. Tasi, A.G. Császár, *Hartree-Fock-limit energies and structures with a few dozen distributed Gaussian,* Chem. Phys. Lett. 438 (2007) 139

**Course title: Nanocomposites**

**Credits: 4**

**Course description:**

**Nanocomposites: past and future**
What is a nanocomposite?
Nanocomposites: past and present
Myths
Nomenclature
**Introduction to solids**
Atomic and molecular solids
Primary, secondary and tertiary structure
Effect of scale
**Properties**
Composites and nanocomposites
Surface mechanical properties
Rubbery, elasticity and viscoelasticity
Diffusion and permeability
**Features of nanocomposites**
Nanoreinforcements
Matrix materials
Role of particle size
**Synthesis of nanocomposites**
Solvent-free processing (viscosity, non-Newtonian flow, etc.)
Solvent processing, *in situ* polymerization
Thermo-kinetic processes
**Characterization of nanocomposites**
Methods for characterization
Structure characterization (texture, scales in nanocomposites, physicochemical analysis, etc.)
Physical properties (Mechanical properties, Barrier Properties etc.)
**Nanocomposites in nanotechnology**
**Nanocomposites for special applications** (high T)

Literature:

T.E. Twardowski, *Introduction to Nanocomposite Materials (Properties, Processing, Characterization)*
J. Koo, *Polymer Nanocomposites*
I. Capek, *Nanocomposite structures and dispersions*

**Course title: Natural Organic Compounds, Methods of Syntheses**

**Credits: 4**

**Course description:**

Vitamins and coenzymes. Compounds with porphyrin skeleton. The syntheses of mesoporphyrin and protoporphyrin. The metabolism of hemin. Chlorophyll and the $B_{12}$ vitamin.
Hormones of vertebrates.
Prostane derivatives and leukotrienes. Modified prostaglandin derivatives, prostaciklines, tromboxanes. The biotransformations of leukotrienes.
Pheromones. Isoprenoids. Terpenes and terpenoids. Steroids.
Phenylpropane derivatives. Flavonoids, antoxantins and antocyanins.
Polyketides. Cannabinoids, melanines.
Alkaloids. Antibiotics.

Methods for the preparation of C−C bonds.
Methods for the preparation of C−heteroatom bonds.
Synthesis strategies.
Retrosynthetic analysis, concepts disconnection and synthon.
Synthons of carbon chains and carbocycles.
Reactions with organometallic compounds and stabilised carbanions.
Reduction and oxidation reactions.
Construction and removal of protecting groups.
Microwave-assisted syntheses.
Methods of green chemistry and catalysis in organic syntheses.

Literature:

P. Nuhn: *Naturstoffchemie*, S. Hirzel Verlag, Stuttgart, Leipzig, 1997.
R.M. Mackie, D.M. Smith, R.A. Aitken: *Guidebook to Organic Synthesis*, Longman Scientific, 1990.
E.J. Corey, X-M. Cheng: *The logic of chemical synthesis*, J.Wiley and Sons, New York, 1989.
J. Fuhrhop. G. Penzlin: *Organic synthesis*, 2$^{nd}$ ed. VCH, Weinheim, New York, 1994.
W. Carruthers, I. Coldham: *Modern methods of organic synthesis*, 4$^{th}$ ed., Cambridge University Press, 2004.

**Course title: Nonlinear Dynamics**

**Credits: 4**

**Course description:**

Applied experimental and mathematical methods. Thermodynamic basis of nonlinear dynamics.
Bistability and hysteresis: iodate-arseneous reaction, enzyme-catalysed reaction of the oxidation of NADH, combustion and thermal explosions, thermal stability of haystacks.
Linear stability analysis. Saddle-points, stable and unstable foci and nodes. Hopf bifurcation, saddle-node bifurcation.
Oscillatory reactions and the conditions for oscillations. The Poincaré-Bendixson theorem. Cross-shaped diagrams, design of chemical oscillators. The families of inorganic chemical oscillators.
The Belousov-Zhabothinsky reaction: FKN mechanism and the Oregonator model. Excitability.
Deterministic chaos. Complex (mixed-mode) oscillations, Farey arithmetics, devil's staircase. Routes to chaos: period doubling, intermittancy. Characterisation of chaos: Poincaré section, Lyapunov exponent, next-return map. Logistic map.
Spatiotemporal patterns: fronts and waves. Target patterns, spirals.
Standing steady patterns: Turing structures. Chemical examples. Biological morphogenesis.

Literature:

S. K. Scott, *Oscillations, Waves, and Chaos in Chemical Kinetics*, Oxford University Press, 1994.
I.R. Epstein, J.A. Pojman, *An Introduction to Nonlinear Chemical Dynamics*, Oxford University Press, 1998

**Course title: Organometallic Chemistry**

**Credits: 4**

**Course description:**

Classification and nomenclature of organometallic compounds.
Preparation, structural properties, chemical reactions and practical applications of organometallic compounds of
− ionic character (organometallics with alkali and alkali earth metals),
− polar character (organozinc and organocopper compounds),
− covalent character (organoboron compounds).
Classification and nomenclature of transition metal complexes.
Formation, structural characteristics and chemical reactions of transition metal complexes
− alkyl and aryl complexes,
− metal hydrides,
− carbonyl and phosphine complexes,
− alkene and alkyne complexes,
− allyl complexes,
− diene complexes.
Transformations of transition metal complexes,
− oxidative addition and reductive elimination,
− insertion and β-elimination,
− nucleophilic and electrophilic addition.

Applications of transition metal complexes in the syntheses of organic intermediates and fine chemicals. The general principles of homogeneous catalysis. Applications of transition metal complexes as homogeneous catalysts in organic syntheses. Enantioselective reactions catalysed by chiral transition metal complexes, kinetic resolution.

**<u>Course title: Separation Techniques</u>**

**Credits: 4**

**Course description:**

Instrumental analysis based on different methods of separation and spectroscopic techniques.
Sample preparation connecting to spectroscopy and chromatography.
Instrumental analysis of spectroscopy. Atomic absorption spectroscopy. ICP-atomic emission spectroscopy. Automatic analysis with flow injection and UV-Vis detection. Infrared spectroscopy. Molecular luminescence spectrometry.
Chromatography. Gas chromatography. High performance liquid chromatography. Ion chromatography. Gel electrophoresis. Gas and liquid chromatography combined with mass selective detection.

Literature:

G.D. Christian, J.E. O'Reilly: *Instrumental Analysis*
G.W. Ewing: *Instrumental methods of chemical analysis*