UNIVERSITY OF SZEGED

FACULTY OF SCIENCE AND INFORMATICS

Chemistry MSc in English

Szeged
2015

General information

Basic information:
Responsible person for the program: **Dr. habil. István Pálinkó, PhD, DSc, associate professor**
Starting date: September 2015
Duration: 4 semesters
Mode of study: full time training
Tuition fee: yes
Location: Institute of Chemistry, Faculty of Natural Sciences and Informatics, University of Szeged, Aradi Vértanúk tere 1, Szeged
Number of students envisaged: 20

Application procedure and conditions: Inquiries are to be sent to the following email address: palinko@chem.u-szeged.hu

The expected applicants: earned BSc degree in chemistry and have decent knowledge of English

Exams and final exam: Oral and written exams at each course at the end of each semester. A final exam is to be passed after all the credits due have been earned. The final exam consists of two parts.
(1) an MSc Thesis refereed by the supervisor, a faculty member and members of the committee for the final examination,
(2) oral examination evaluated by the committee for the final examination.

Szeged, May 8, 2015

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István Pálinkó
associate professor

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 II (4 weeks)	4	0	s	AKKT	Kukovecz, Ákos

III. Elective general courses **6 credits**

The cultural history of chemistry	3	2	1	KTCs	strongly suggested

IV. Thesis **2×15 credits**

V. Industrial Training I – 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	1	SzAKT	Gajda, Tamás
Biological tools of modern chemistry	4	2	1	SzAKT	Gyurcsik, Béla
Fundamentals of pharmaceutical chemistry	5	3	1	SzAKT	Kiss, Tamás
Bioorganic chemistry	4	2	1	SzKT	Wölfling, János
Chemistry of organometallic compounds	4	2	1	SzKT	Mastalír, Ágnes
Natural organic compounds, organic syntheses	4	2	1	SzKT	Wölfling, János
Synthetic chemistry laboratory	6	6	s	KTCS	Bucsi, Imre
	31	*19*			
Material science researcher specialisation – Kónya, Zoltán					
Macromolecular systems	4	2	1	FKAT	Szabó, Tamás
Electrochemical procedures, corrosion	4	2	1	FKAT	Szűcs, Árpád
Nanocomposites	4	2	1	AKKT	Kónya, Zoltán
Interfaces and nanostructures	5	3	1	FKAT	Dékány, Imre
Heterogeneous catalysis	4	2	1	AKKT	Hernádi, Klára
Bulk and surface methods of material characterisation	4	3	1	AKKT	Kónya, Zoltán
Bulk and surface methods of material characterisation, seminar	1	1	s		
Solid-state chemistry	4	2	1	FKAT	Oszkó, Albert
	30	*17*			
Analytical chemist specialisation – Galbács, Gábor					
Analytical sensors	4	2	1	SzAKT	Galbács, Gábor
Laser- and plasma-based trace analysis	4	2	1	SzAKT	Galbács, Gábor
Modern chromatographic methods	4	2	1	SzAKT	Ilisz, István
Analytical quality assurance and quality control systems	4	2	1	SzAKT	Schrantz, Krisztina
Molecular spectroscopy	4	2	1	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	1	FKAT	Oszkó, Albert
	30	*18*			
Electives without specialisation					
Modern quantum chemistry	4	2	1	AKKT	Tasi, Gyula
Computational chemistry	4	2	1	AKKT	Tasi, Gyula
Computational chemistry seminar	3	2	s	AKKT	
Computational modeling in material and pharmaceutical research	4	2	1	FKAT	Czakó, Gábor
Nonlinear dynamics	4	2	1	FKAT	Tóth, Ágota
Physical inorganic chemistry	4	2	1	SzAKT	Jakusch, Tamás
X-ray diffractometry	4	2	1	AKKT	Sápi, András
Graphite wires and carbon nanotubes	4	2	1	AKKT	Hernádi, Klára
Chemistry of non-aqueous solutions and melts	4	2	1	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.

Final Exam

A topic (Topics discussed in the core courses)
B topic (Topics focusing on chemical intelligence)
The grades obtained for both topics count equally in the final mark of the exam

The thesis is defended in a session organized by KTCS. The grade is the mathematical average given by the supervisor, the referee and the members of the examination committee present at the session of defence.

The grade of the degree: (Mean of the major courses + grade of A topic + grade of B topic + grade of the thesis)/4

COURSE TITLE	**Mathematical chemistry**
TYPE OF COURSE	lecture + practical
LEVEL OF COURSE	advanced [core subject]
SEMESTER	first
CREDITS	4 + 3
NAME OF THE LECTURER	Gyula Tasi, associate professor
ASSESMENT	oral and written examinations

Objectives and expected outcome

To provide a strict theoretical background to learn advanced physical chemistry, molecular spectroscopy, statistical thermodynamics, quantum chemistry, theoretical inorganic chemistry, computational chemistry and molecular modelling.

By the end of the course it is expected from students to have almost all the theoretical tools they need in studying chemistry at higher level of theory.

Course content

The most important algebraic structures for chemistry and physics. Static and dynamic symmetry of molecules. Molecular point groups of Schönflies. Molecular nuclear permutation groups with or without inversion. Molecular properties representing symmetry: equilibrium geometry, electric dipole moment, optical activity, etc. Symmetry of extended systems (crystal symmetry): space groups. Basics of matrix algebra. Special matrices and their importance in chemical physical applications. Matrix representation theory of finite groups.

The stoichiometric matrix. Algebraic and kinetic independence of chemical reactions. The role of linear algebra in the determination of mechanism of complex reaction systems. First-order and second-order scalar and vectorial differential operators (grad, div, rot, div grad).

Function, differential and integral equations. Their types, classification, and solutions. Initial and boundary value problems. The polynomial method of Sommerfeld. Parameter estimation. The (linear) least squares method: discrete and continuous case. Determination of the parameters of the Michaelis-Menten kinetic equation. Differential equations of orthogonal polynomials. Their recursive formulas and applications. Complex and real spherical harmonics. Fourier series and Fourier transformation. The Laplace transformation.

Basics of calculus of variations. Euler-Lagrange and Hamilton equations of motion. The Legendre transformation and its application in chemistry and physics. Thermodynamic potentials. The variation principle in classical and quantum mechanics. The virial theorem. The time dependent and time independent Schrödinger equation. Solution of simple problems in quantum chemistry, chemical reaction kinetics and chemical technology.

The importance of probability theory and mathematical statistics in chemistry and physics. The concept of classical probability field. Combinatorial tools. Thermodynamic probability. Classical and quantum statistics. The concept of random variables. The most important probability distributions: Bernoulli, Poisson, exponential and Gauss. The probability interpretation of the wave function in quantum mechanics. The mathematical derivation of the Heisenberg's uncertainty principle. The Central Limit Theorem and its importance in chemistry and physics.

Recommended reading

H. Margenau, G.M. Murphy, *The Mathematics of Physics and Chemistry*, D. Van Nostrand Company, Inc., 2nd edition, Princeton, 1966

C.D. Meyer, *Matrix analysis and applied linear algebra*, SIAM, 2004

J.R. Barrante, *Applied Mathematics for Physical Chemistry*, 3rd ed., Prentice-Hall, New Jersey, 1998

J.B. Dence, *Mathematical Techniques in Chemistry*, John Wiley & Sons, New York, 1975

Teaching method

Chalk-talks at the board.

COURSE TITLE	**Advanced experimental physics**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced
SEMESTER	first
CREDITS	2
NAME OF THE LECTURER	Béla Hopp, professor
ASSESMENT	oral and written examinations

Objectives and expected outcome

The main aim is to provide an overview of modern physics mainly from the aspect of applied physics. By the end of the course it is expected that the students will obtain a working knowledge of laser-physics, spectroscopy, analogue and digital electronics and their underlying principles.

Course content

Fundamentals of lasers, basic processes, resonators, population inversion, Q-switch, main parameters of lasers, relevant laser types, light-matter interactions, applications of lasers.

Fundamentals of optical spectroscopy, spectrum, spectral lines, line broadening mechanisms, basic elements (and their main parameters) of a typical spectrograph, figures of merit, optical fibres, UV-VIS spectrophotometry, laser-induced fluorescence, FT-IR, Raman and photoacoustic spectroscopies and their practical applications.

Analogue electronics, passive and active electric circuit elements (resistors, capacitors, coils, transformators), chemical current sources, basic electric circuits.

Digital electronics, Boolean-algebra, logic circuits.

Recommended readings

Orazio Svelto: "Principles of Lasers", Springer Science+Business Media, LLC 2010

Duckett, Simon: "Foundations of spectroscopy / Simon Duckett and Bruce Gilbert. – Repr. – Oxford : Oxford Univ. Press, 2002.

J. Michael Hollas: "Modern spectroscopy", Copyright#1987, 1992, 1996, 2004 by John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, England

Demtröder, Wolfgang: "Laser spectroscopy: basic concepts and instrumentation / Wolfgang Demtröder. – 3. ed. – Berlin etc.: Springer, [2003]

Grob, Bernard: „Basic electronics" / Bernard Grob, Mitchel E. Schultz. – 9. ed. – New York [etc.] : Glencoe : McGraw-Hill, [2003]

Jenkins, John: „Basic principles of electronics / J. Jenkins, W. H. Jarvis. – Oxford etc. : Pergamon P. 1966

Jenkins, John: „Basic principles of electronics. Vol. 2. Semiconductors. – Oxford - New York etc : Pergamon X, 1971

Tony R. Kuphaldt: "Lessons In Electric Circuits, Volume IV – Digital", 2000-2014, Tony R. Kuphaldt

Teaching method

PowerPoint presentation with ready-made slides and chalk-talks at the board.

COURSE TITLE	**Advanced physical chemistry**
TYPE OF COURSE	lecture + seminar + laboratory practical
LEVEL OF COURSE	advanced [core subject]
SEMESTER	first
CREDITS	4 + 2 + 5
NAME OF THE LECTURER	Ágota Tóth, professor, Gábor Peintler, associate professor
ASSESMENT	written and oral examinations; weekly experimental reports

Objectives and expected outcome
The aim of the course is to provide with an in-depth knowledge in various aspects of physical chemistry. By the end of the course, the students are expected to able to use the concepts of physical chemistry for rationalising phenomena and to apply the advanced tools of physical chemistry in solving various chemical problems.

Course content
The fundamentals of statistical thermodynamics: the canonical statistical ensemble, statistical description of state functions, the statistical description of radioactive de, Poisson distribution
Reaction kinetics. The dynamics of reactions: collision theory, transition state theory, stochastic processes.
Complex reactions: enzyme inhibitions. The kinetic description of radioactive decay series and the interpretation of the product distribution. The fundamentals of mechanistic studies.
Surface reactions: the BET isotherms, the kinetics of surface-catalysed reactions.
Photochemistry: electron-excited molecules, photochemical kinetics.
Transport processes. Fick's laws. The general equation of balance. Transportation number and its determination. Nernst-Einstein equation.
Reaction kinetics in solution: diffusion-controlled reactions, the cage effect.
Studying reactions in the gas and the liquid phases: experimental techniques.
Dynamic electrochemistry. Electrochemical potential. Butler-Volmer equation. Tafel equation.
Corrosion. The rate of corrosion. Protection against corrosion. Mixed potential.
Non-equilibrium thermodynamics.

Recommended reading
Atkins: *Physical Chemistry*
Pilling, Seakins: *Reaction kinetics*

Teaching method
Powerpoint presentation with ready-made slides and chalk-talks at the board.

COURSE TITLE	**Advanced inorganic chemistry**
TYPE OF COURSE	lecture + seminar
LEVEL OF COURSE	advanced [core subject]
SEMESTER	first
CREDITS	4 + 2
NAME OF THE LECTURER	Tamás Gajda, professor
ASSESMENT	written and oral examinations

Objectives and expected outcome

The aim of the course is to provide with advanced knowledge in various aspects of inorganic chemistry. By the end of the course, the students are expected to able to use this knowledge in rationalising various phenomena in inorganic chemistry and to apply the advanced tools of inorganic chemistry in solving various chemical problems.

Course content

Some advanced concepts. The relativistic effect. MO vs. hybridisation.
Clusters and cages. The theory of electron deficient clusters. Polyboranes. Wade's rules.The extension of the structural features of polyboranes. Cage compounds.
The electron structure of transition metal containing compounds. Crystal field theory – the one-electron case. Crystal field theory – the many-electron case. The ligand field theory.
The organometallic compounds of the transition metals. Fundamental concepts. Structural classification. Elementary organometallic reactions. Typical transformations catalysed by organometallic complexes.
Transformations of coordination compounds. Substitution reactions. Redox reactions. The self-exchange reactions – the Marcus theory.
The bioinorganic chemistry of manganese. Hydrolases. Oxido-reductases. Photsynthesis.

Recommended readings

D.F. Shriever, P.W. Atkins : *Inorganic Chemistry*, Oxford University Press, 2006, 2. Faigl

Teaching method

Powerpoint presentation with ready-made slides and chalk-talks at the board.

COURSE TITLE	**Chemical information retrieval**
TYPE OF COURSE	practical
LEVEL OF COURSE	advanced [core subject]
SEMESTER	first
CREDITS	2
NAME OF THE LECTURER	István Pálinkó, associate professor
ASSESMENT	written examinations

Objectives and expected outcome
Providing guidance in obtaining as much useful chemistry-related information as it is possible. By the end of the course, the students are expected to be able to use wisely the free-of-charge as well as the pay-the-fee information available through the Internet and various databases.

Course content
Classification of information sources. Printed chemical information sources in departmental libraries and the Klebelsberg (University) Library. Concepts related to the chemical literature.
General possibilities for information retrieval: concepts related to the Internet, search engines, the Wikipedia.
Databases not (directly) connected to publishers or chemical societies (Journal Citation Report, Web of Science, Scopus, Scifinder, Google Scholar, Google Books), introducing user interfaces (Publish or Perish) familiarisation through exercises with increasing complexities.
Introducing Researcher ID, Scopus ID and ORCID; personalisation and uploading possibilities.
Introducing the ruling publishers (Elsevier, Springer, Wiley), familiarisation to their databases through exercises with increasing complexities.
Introducing some of the smaller publishers (Bentham Science Publisher, Hindawi, etc.). The pirate journals and publishers.
Introducing the major chemical societies (American Chemical Society, Royal Society of Chemistry, European Chemical Society, Chinese Chemical Society) familiarisation to their journal portfolio and databases through exercises with increasing complexities.
Some smaller but important chemical societies. The Hungarian Chemical Society and its activities.
The "Open Access Initiative" – pros and cons.
Patents and patent searching possibilities.
Doctoral Schools at Hungarian universities, and major universities around the world.

Tools
Pieces of software and rights to access them.

Teaching methods
Guided as well as independent exercises in front of PCs hooked on the net.

COURSE TITLE	**Advanced organic chemistry**
TYPE OF COURSE	lecture + seminar
LEVEL OF COURSE	advanced [core subject]
SEMESTER	second
CREDITS	6 + 2
NAME OF THE LECTURER	István Pálinkó, associate professor
ASSESMENT	oral and written examinations

Objectives and expected outcome
The main aim is to provide an overview of organic chemistry mainly from the aspect of reaction mechanisms. By the end of the course it is expected that the students will obtain a working knowledge of organic chemistry as far as organic reactions and their underlying principles are concerned.

Course content
The structure of organic molecules and structural determination by instrumental and computational methods.
The conformational properties of organic compounds and their stereochemical features. The acid-base properties of organic compounds.
Reactions in organic chemistry, reaction mechanisms, chemoselectivity and stereoselectivity: nucleophilic addition to the C=O bond; conjugated additions; synthesis of C−C bonds with organometallic complexes; nucleophilic substitution reactions on the C=O bond and saturated C atom; elimination reactions; electrophilic additions; aromatic electrophilic and nucleophilic substitutions; pericyclic reactions; rearrangements; fragmentation reactions; radical reactions; polymerisation reactions.
Synthetic methods.
The synthesis of carbenes and their reactions.
Synthesis of aromatic heterocyclic compounds and their transformations.
The organic chemistry of life. Reaction mechanisms in biological chemistry. Organic compounds in Nature.

Recommended readings
J. Clayden, N. Greeves, S. Warren, P. Wothers: *Organic Chemistry*, Oxford University Press, 2012.
E.V. Anslyn, D.A. Dougherty: *Modern Physical Organic Chemistry*, University Science Books, 2006.
F.A. Carey, R.J. Sundberg: *Advanced Organic Chemistry A, B*, Plenum Press, 2004.

Teaching method
PowerPoint presentation with ready-made slides and chalk-talks at the board.

COURSE TITLE	**Unit operations**
TYPE OF COURSE	lecture + practical
LEVEL OF COURSE	advanced [core subject]
SEMESTER	second
CREDITS	4 + 3
NAME OF THE LECTURER	Ákos Kukovecz, associate professor
ASSESMENT	oral and written examinations

Objectives and expected outcome
The main aim is to provide an overview of unit operations both from the mathematical as weel as the industrial-experimental viewpoints. By the end of the course, the students are expected to perform basic engineering abilities.

Course content
Fundamental concepts. Korach Mór's laws. Nomograms. Operational units. Degrees of freedom, Földvári's rule. Gibbs' phase rule. Describing processes in various ways.
Balances of various kinds
Hydrodynamics. Navier-Stokes, Euler, Bernoulli, Hagen-Poiseluille, Fanning, Blake-Kozeny, Burke-Plummer and Ergun equations.
Hydrodynamical operations.
Fundamentals and classification of distillation operations. Clausius-Clapeyron, Antoine equations. Rault-Dalton law.
Fundamentals of absorption. The operation
The concept and the corresponding laws of adsorption.
The fundamentals of drying. The operation.
The fundamentals of ion exchange. Units of the process.
Extraction. Concepts and the corresponding rules and units.
Crystallisation. Fundamental laws and the corresponding operations.
Mixing and grinding. Theory and practice.
Thermal operations. Fundamental laws and operational units.
The fundamentals of reaction kinetics.
Chemical reactors, types with corresponding fundamental equations and methods of operation: well-stirred batch reactor, reactor cascades, reactors working in the flow mode, reactors for transformations catalysed by heterogeneous catalysts.

Teaching method
PowerPoint presentation with ready-made slides and chalk-talks at the board.

COURSE TITLE	**Modern instrumental analytical chemistry**
TYPE OF COURSE	lecture + seminar
LEVEL OF COURSE	advanced [core subject]
SEMESTER	second
CREDITS	6 + 2
NAME OF THE LECTURER	Gábor Galbács, associate professor
ASSESMENT	oral and written examinations

Objectives and expected outcome

To give an overview of the principles and practices of state-of-the-art instrumental methods in analytical chemistry. By the end of the course, the students are expected to be able to select the appropriate analytical methods for the solution of specific qualitative and quantitative problems.

Course content

Theoretical principles and practical aspects of sampling.
Microwave-based techniques. Techniques based on optical fibres.
The structure of modern spectrometers. The most important radioanalytical methods.
Modern methods in molecular spectroscopy (FTIR, PAS, TDLAS, CRDS, LIDAR), fundamental principles and analytical characterisation.
Modern methods in atomic spectrometry (LA, LIBS, CS-HR-AAS, ICP-MS, XRF/TXRF), fundamental principles and analytical characterisation.
Mass spectrometry in organic chemistry, its use in qualitative and quantitative analysis. Ionisation methods.
Automatic analysers working in discrete or flow modes. Their use in clinical practice.
The lab-on-a-chip concept.
Chemical sensors. Biosensors.
Modern chromatographic methods (IC, SEC, AC). Chromatographic methods based on electrophoresis (CE, CZE, MEKC, GE).
Microscopic methods (AFM, STM, SEM, TEM).
Surface analysis techniques (UPS, XPS, AES, XRF, ATR, SPR).
NMR spectroscopy and its use in structure determination.
X-ray absorption or diffraction based methods (XAS, XRD).
Mössbauer spectroscopy.

Recommended reading

http://www2.sci.u-szeged.hu/inorg/MOMA/MOMA-book%20(v1.10).html

Teaching method

PowerPoint presentation with ready-made slides.

COURSE TITLE	**Biocatalysis**
TYPE OF COURSE	Lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Tamás Gajda, professor
ASSESMENT	oral examination

Objectives and expected outcome
To give a broad overview of biocatalysts and biocatalytic reactions. By the end of the course, the students should appreciate the richness of biocatalysts and biocatalytic processes.

Course content
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 dehyidrogenase, 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 developement 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 redoxi 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.

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

Teaching method
Lecturing at the board supported by PowerPoint presentation.

COURSE TITLE	Biological tools in modern chemistry
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Béla Gyurcsik, associate professor
ASSESMENT	oral examination

Objectives and expected outcome

To give an overview on the connection of biology and chemistry. By the end of the course, the students should recognise the many possibilities of the fruitful cooperation of chemistry and biology.

Course content

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.

Recommended reading

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.

Teaching method

Lecturing at the board supported by PowerPoint presentation.

COURSE TITLE	Fundamentals of medicinal chemistry
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Tamás Kiss, professor
ASSESMENT	oral examination

Objectives and expected outcome
To give an introductory overview on medicinal chemistry. By the end of the course, the students should recognise the enormous impact of chemistry on the syntheses and studying various medications.

Course content
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.

Recommended reading
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.

Teaching method
Lecturing at the board supported by PowerPoint presentation.

COURSE TITLE	Bioorganic chemistry
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	János Wölfling, professor
ASSESMENT	oral examination

Objectives and expected outcome
To give an overview on the connection of biology and organic chemistry. By the end of the course, the students should recognise the deep relationship between compounds in biology and compounds in organic chemistry.

Course content
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. Heteropolysacharides. The synthesis of oligo- and polysacharides.
Amino-carboxylic acids, peptides, polypeptides and proteins. The classification of amino acids, their sturctures, 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. Synthess 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 sturctures 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.

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

Teaching method
Lecturing at the board supported by PowerPoint presentation.

COURSE TITLE	**Organometallic chemistry**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Ágnes Mastalir, associate professor
ASSESMENT	oral examination

Objectives and expected outcome

To give an in-depth knowledge on the synthesis, structure and synthetic applications of organometallic compounds. By the end of the course, the students should recognise the power of organometallic compounds as catalysts in selective organic syntheses.

Course content

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 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 catalyzed by chiral transition metal complexes, kinetic resolution.

Teaching method

Lecturing at the board supported by PowerPoint presentation.

COURSE TITLE	**Natural organic compounds, methods of syntheses**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	János Wölfling, professor
ASSESMENT	oral examination

Objectives and expected outcome

To give a broad knowledge on the naturally occurring organic compounds as well as on various methods in organic syntheses. By the end of the course, the students should have a working knowledge in the art of organic syntheses, partly applied on naturally occurring organic compounds.

Course content

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.

Recommended reading

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*, 2nd ed. VCH, Weinheim, New York, 1994.
W. Carruthers, I. Coldham: *Modern methods of organic synthesis*, 4th ed., Cambridge University Press, 2004.

Teaching method

Lecturing at the board supported by PowerPoint presentation.

COURSE TITLE	**Bulk and surface methods of material characterisation**
TYPE OF COURSE	lecture + seminar
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	3 + 1
NAME OF THE LECTURER	Zoltán Kónya, professor
ASSESMENT	oral and written examinations

Objectives and expected outcome
To widen the knowledge of student in the area of bulk and surface characterisation techniques by state-of-the-art instrumental methods. By the end of the course, the students should have theoretical knowledge on the use of these methods, and they also acquire hands-on experience with a couple of these methods.

Course content
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: color and thickness measurement, 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 dimention, 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 microsopy: 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.

Recommended reading
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)

Teaching method
Lecturing with the help of ready-made PowerPoint files, demonstrating some of the methods, collecting hands-on experience with some of the methods.

COURSE TITLE	**Macromoleular systems**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Tamás Szabó, assistant professor
ASSESMENT	oral examination

Objectives and expected outcome
To give an advanced overview of macromolecular systems. By the end of the course, the students should have in-depth knowledge concerning the synthesis, properties and characterisation of macromolecular systems.

Course content
Classification of macromolecules. The structural features of macomolecules and their physical properties. Synthesis methods of polymers, various types of polymerisation reactions Photopolymerisation 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. Detrmining 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.

Recommended reading
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.

Teaching method
PowerPoint presentation with ready-made slides.

COURSE TITLE	Heterogeneous catalysis
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Klára Hernádi, professor
ASSESMENT	oral examination

Objectives and expected outcome
To give an overview of heterogeneous catalysts and the major transformations promoted by them. By the end of the course, the students should have a broad perspective concerning the various types of heterogeneous catalysts, their synthesis methods, their structures and characterisation methods and their use in the lab and in industry.

Course content
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.

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

Teaching method
PowerPoint presentation with ready-made slides.

COURSE TITLE	**Interfaces and nanostructures**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Imre Dékány, professor
ASSESMENT	oral examination

Objectives and expected outcome
To give an advanced overview of interfaces and nanostructure. By the end of the course, the students should be able to appreciate the wonder world of interfaces and nanomaterials. They should be familiar to their synthesis methods, their characterisation techniques and their application possibilities.

Course content
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 andhydrophobic 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 formulatin.

Recommended reading
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).

Teaching method
PowerPoint presentation with ready-made slides.

COURSE TITLE	Chemometrics
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective – specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Tamás Jakusch, assistant professor
ASSESMENT	oral examination

Objectives and expected outcome
By the end of the course students will have an understanding of processing experimental data making use of the tools of chemometrics, in particular the acquisition of maximum relevant information from given experimental data sets and the establishment of their reliability.

Course content
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.

Recommended readings
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

Teaching methods
Lecturing at the board supported by ready-made slides.

COURSE TITLE	**Nanocomposites**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective − specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Zoltán Kónya, professor
ASSESMENT	oral and written examinations

Objectives and expected outcome
To enable students to appreciate nanodimension and manipulations on the nanoscale. Providing in-depth knowledge about various nanocomposites.

Course content
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 (highT)

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

Teaching methods
Powerpoint presentations, also accessible on a dedicated website.

COURSE TITLE	**Analytical quality assurance and quality control systems**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective − specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Krisztina Schrantz, assistant professor
ASSESMENT	oral examination

Objectives and expected outcome

− To provide an overview of quality assurance systems, focusing on the quality assurance in different analytical laboratories.

− To give a short insight in the ways of quality regulations in the EU.

By the end of the course it is expected from students to able to theoretically organise the quality assurance of an analytical laboratory, to validate an analytical method and to have an overview of quality assurance systems.

Course content

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.

Recommended reading

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

Teaching method

Lecturing at the board supported by self-made power point slides.

COURSE TITLE	**Analytical sensors**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective − specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Gábor Galbács, associate professor
ASSESMENT	oral examination

Objectives and expected outcome
To provide an overview of the basics of modern sensor technology and its application possibilities in analytical chemistry.

Course content
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.

Recommended reading
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.

Teaching method
Lecturing at the board supported by multimedia presentations and demonstrations.

COURSE TITLE	**Laser- and plasma-based analytical methods**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective − specialisation subject]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Gábor Galbács, associate professor
ASSESMENT	oral examination

Objectives and expected outcome
To provide an overview of advanced instrumental analytical methods that use laser light and/or plasma atom and ion sources.

Course content
Principle of operation, analytical and operational characteristics as well as primary appliation 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)

Recommended reading
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.

Teaching method
Lecturing at the board supported by multimedia presentations and demonstrations.

COURSE TITLE	**Separation techniques and spectroscopy laboratory**
TYPE OF COURSE	practical
LEVEL OF COURSE	advanced [elective − specialisation subject]
SEMESTER	second to fourth
CREDITS	4
NAME OF THE LECTURER	István Ílisz, associate professor
ASSESMENT	oral examination

Objectives and expected outcome
To provide practical knowledge in the field of different separation techniques and spectroscopy.
By the end of the course it is expected from students to be able to handle analytical instruments.

Course content
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.

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

Teaching method
Lecturing at the board supported by multimedia presentations and demonstrations.

COURSE TITLE	**Modern Quantum Chemistry**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Gyula Tasi, associate professor
PREREQUISITES	Mathematical Chemistry
ASSESMENT	oral and written examinations

Objectives and expected outcome
A working knowledge of advanced quantum chemistry is very important for theoreticians in chemistry. By the end of the course it is expected from students to know the fundamental elements of advanced quantum chemistry.

Course content
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.

Recommended readings
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

Teaching methods
Chalk-talks at the board.

COURSE TITLE	**Nonlinear dynamics**
TYPE OF COURSE	lecture
LEVEL OF COURSE	advanced [elective]
SEMESTER	second to fourth
CREDITS	2
NAME OF THE LECTURER	Ágota Tóth, professor
ASSESMENT	2 problem-solving take-home exams

Objectives and expected outcome

To provide an introduction to nonlinear dynamics through chemical, physical, and biological examples.

To show how mathematical tools can be applied in the field of nonlinear dynamics and to understand the foundations of the phenomena observed in these systems.

By the end of the course the students should be able to apply linear stability analysis on simple examples and understand the evolution of spatiotemporal pattern formation.

Course content

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.

Recommended readings

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.

Teaching methods

Lecturing using self-made presentations and occasionally chalk at the blackboard.

COURSE TITLE	**Computational Chemistry**
TYPE OF COURSE	lecture and practical
LEVEL OF COURSE	advanced [elective]
SEMESTER	second to fourth
CREDITS	2+2
NAME OF THE LECTURER	Gyula Tasi, associate professorreader
PREREQUISITES	Mathematical Chemistry
ASSESMENT	oral and written examinations

Objectives and expected outcome
Nowadays, computers are in the chemical labs everywhere and they are as important as other experimental equipment. By the end of the course it is expected from students to know how the computers can provide them with help in chemical labs.

Course content
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 modeling: 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.

Recommended readings
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

Teaching method
Lecturing at the board and software presentations on personal computers.

Az oktatók idegennyelv-tudását, idegen nyelvi előadóképességét és oktatási gyakorlatát bizonyító adatok, információk (nyelvvizsga szint, külföldi, adott nyelvterületi oktatási gyakorlat, hosszabb idejű, aktív, igazolt hallgatói tapasztalat; az adott idegen nyelven tartott konferencia előadások stb.) megadása:

az idegen nyelvű képzésben résztvevő **oktató** neve	**tud. fok. /cím** (PhD/ CSc/ DSc/ akad.)	**munkakör** (ts. / adj./ e/f doc./ e/f tan./ tud. mts./ egyéb)	**részvétel az ismeretátadásban**		**előadóképes idegennyelv-tudás bizonyítéka(i)**[1]
			tantárgy előadója **I / N**	gyak. fogl.-t tart **I / N**	
Berkesi Ottó	PhD	e. doc.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, vendégkutató Nagy-Britanniában: 2 év
Bucsi Imre	PhD	e. doc.	N	I	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, vendégkutató az USA-ban: összesen 4 év
Czakó Gábor	PhD	e. adj.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, vendégkutató az USA-ban: összesen 3 év
Dékány Imre	Akad.	e. tan.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Gajda Tamás	DSc	e. tan.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Galbács Gábor	DSc	e. doc	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, vendégkutató az USA-ban: 2 év
Gyurcsik Béla	PhD	e. doc	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Hernádi Klára	DSc	e. tan.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, vendégkutató az USA-ban: 1,5 év
Hopp Béla	DSc	e. tan.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul

[1] *előadóképes idegennyelv-tudás* bizonyítéka lehet:
- *anyanyelvként bírt nyelvtudás* **vagy**
- *felsőfokú nyelvvizsga, – csak gyakorlatot vezető oktatóknál elegendő középfokú* – **vagy**
- legalább féléves, vagy rendszeres (felkéréses, meghívásos) külföldi, *adott nyelvterületi oktatási,* **vagy**
- *legalább **1** éves aktív***,** dokumentált *hallgatói tapasztalat*; **vagy**
- legalább **6**, az adott idegen nyelven tartott konferencia előadás

Ilisz István	PhD	e. doc.	I	I	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Jakusch Tamás	PhD	e. adj.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, vendégkutató az USA-ban: 2 év
Kiss Tamás	DSc	e. tan.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Kónya Zoltán	DSc	e. tan.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, vendégkutató az USA-ban: 2 év
Kukovecz Ákos	PhD	e. doc.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Mastalír Ágnes	DSc	e. doc.	I	I	felsőfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, részvétel az angol nyelvű gyógyszerészképzésben, vendég-kutató Nagy-Britanniában: 1 év
Oszkó Albert	PhD	e. adj.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Pálinkó István	DSc	e. doc.	I	N	felsőfokú angol nyelvvizsga, százötvennél több angol nyelvű konferenciaelőadás, 8 félév előadás az angol nyelvű gyógyszerészkép-zésben, vendégkutató Nagy-Britan-niá-ban és az USA-ban: összesen 3 év
Peintler Gábor	PhD	e. doc.	N	I	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, előadói részvétel az angol nyelvű gyógyszerészképzésben, vendégkutató az USA-ban: 2 év
Sápi András	PhD	e. adj.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, vendégkutató az USA-ban: 2 év
Schrantz Krisztina	PhD	e. adj.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Sipos Pál	DSc	e. tan.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, előadói részvétel az angol nyelvű gyógyszerészképzésben, vendégkutató Ausztráliában: 8 év

Szabó Tamás	PhD	e. adj.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Szűcs Árpád	PhD	e. doc.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, részvétel az angol nyelvű gyógyszerészképzésben, vendégkutató az USA-ban: 1,5 év
Tasi Gyula	PhD	e. doc.	I	I	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul
Tóth Ágota	DSc	e. tan.	I	N	felsőfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul, az USA-ban szerzett PhD
Wölfling János	DSc	e. tan.	I	N	középfokú angol nyelvvizsga, nagyszámú konferenciaelőadás angolul

Kizárólag idegen nyelven folyó képzés esetén a MAB *véleményezési lehetőségeit mérlegelve* egyedi döntést hoz arról, hogy az oktatók személyi-szakmai adatainak megadása az adott nyelven elegendő-e.